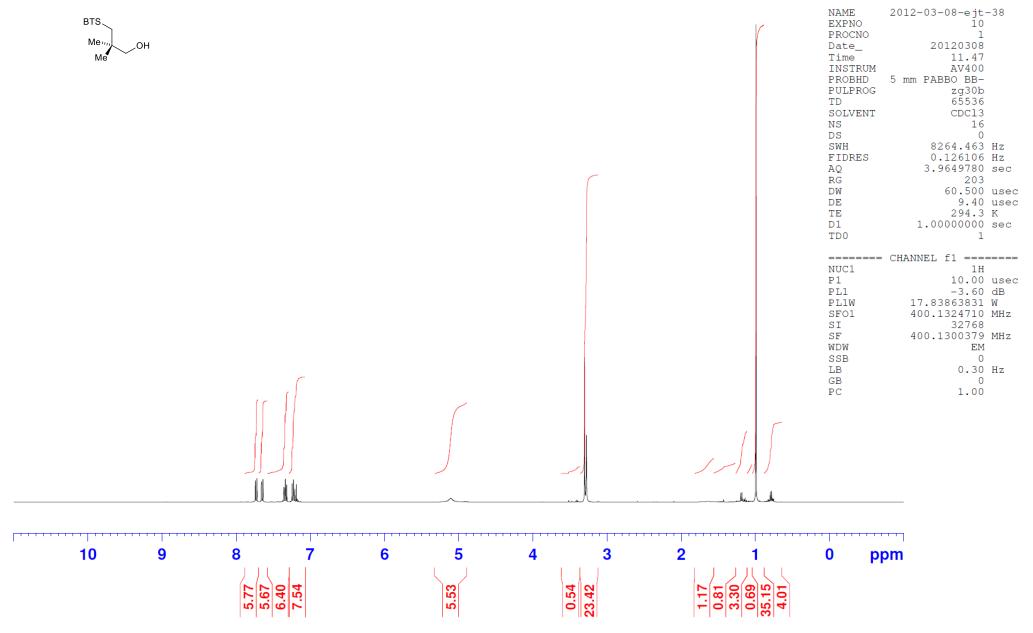


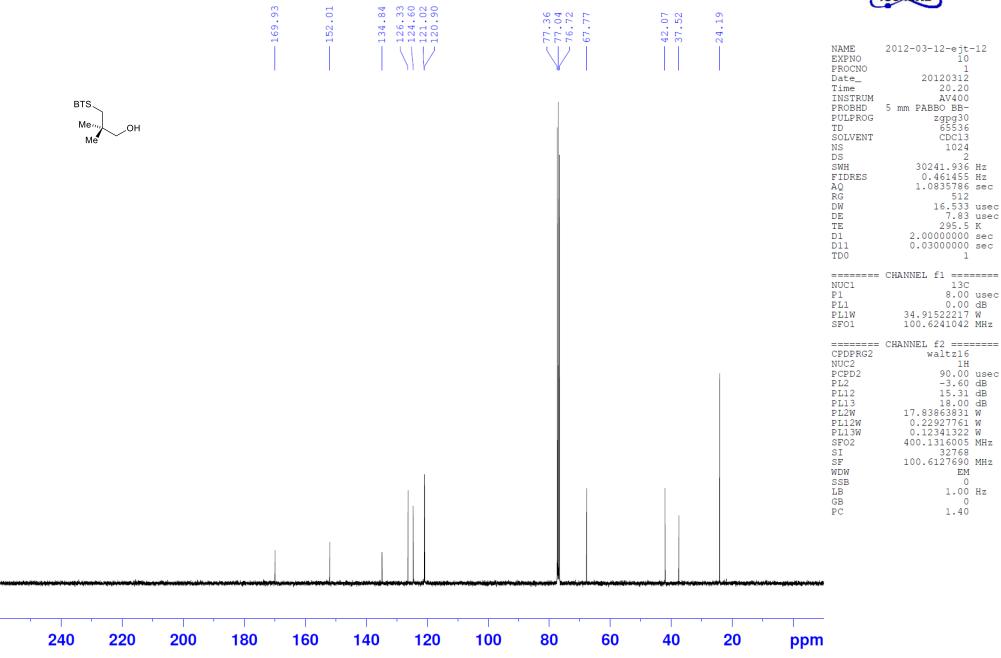
## ejt cry alcohol mPROTON CDCl3 {e:\bruk400data\2012\Mar} ejt 38





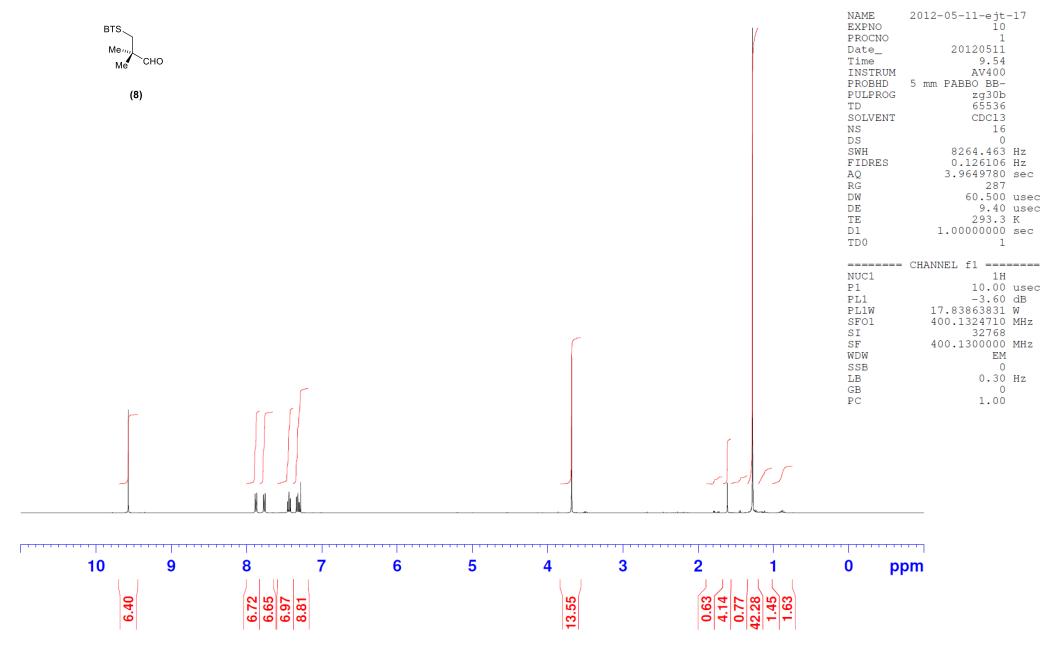






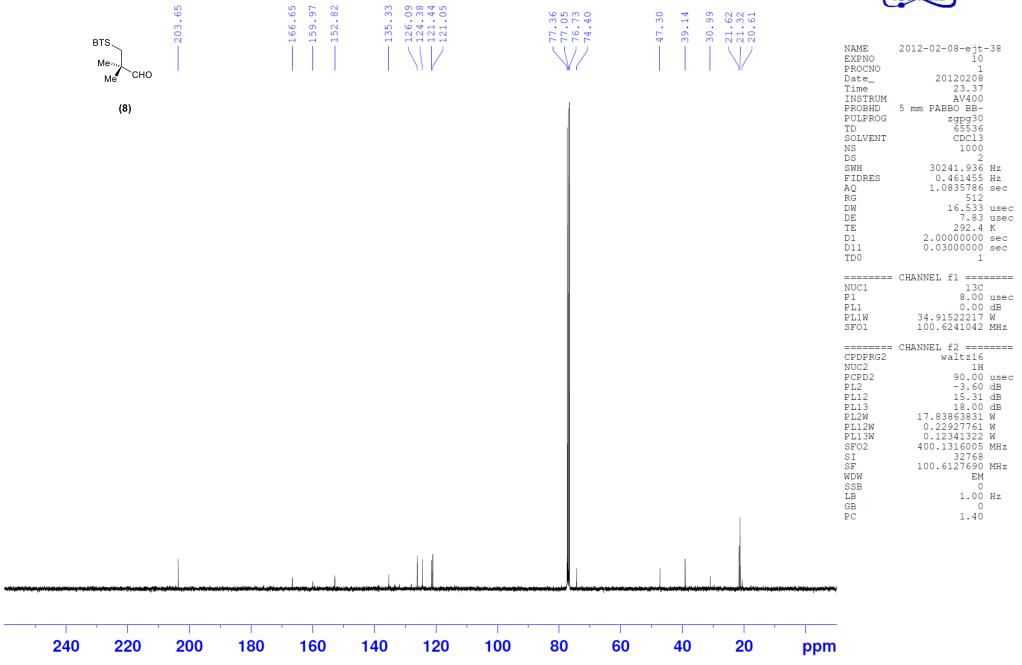
# ejt cry swern mPROTON CDCl3 {e:\bruk400data\2012\May} ejt 17





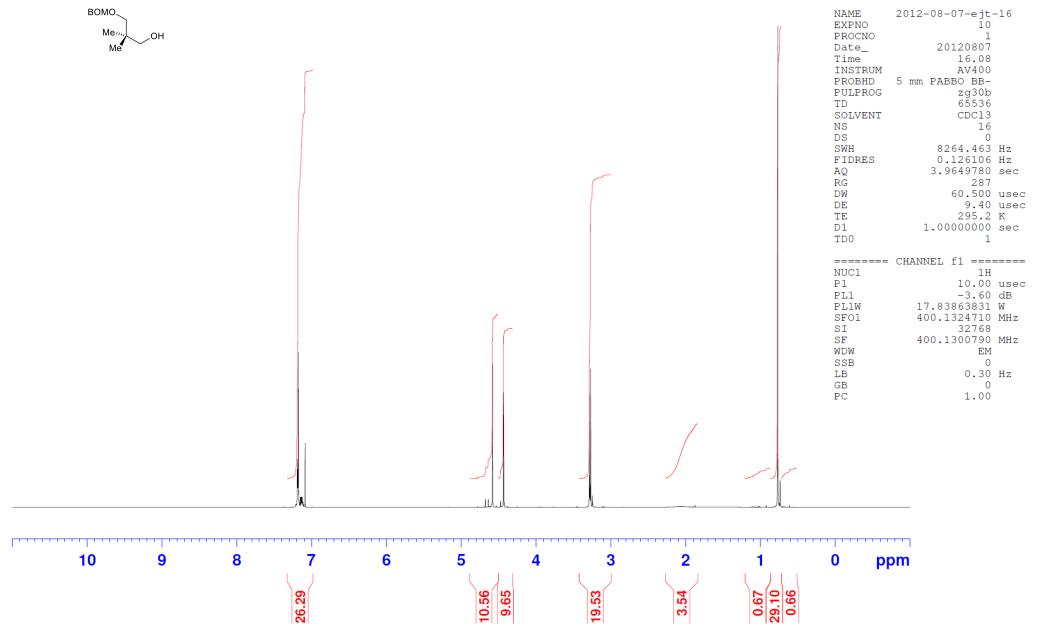
# ejt cry ald mCARBONnight CDCl3 {e:\bruk400data\2012\Feb} ejt 38

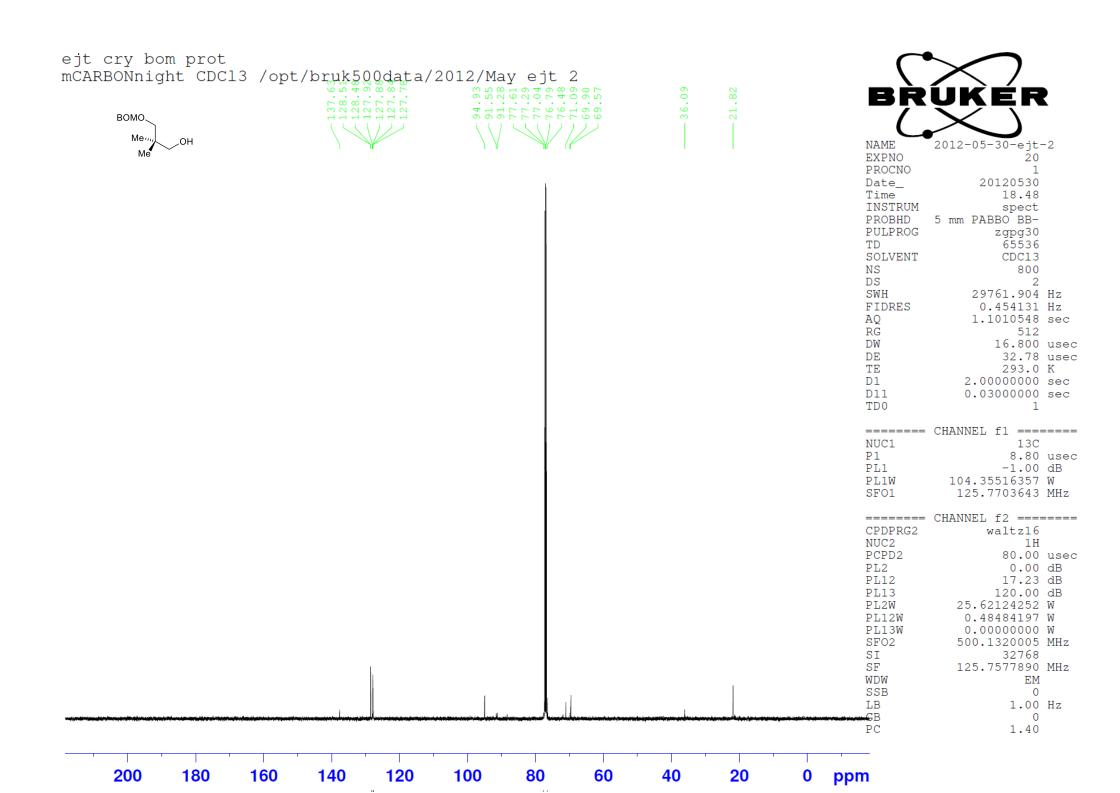




# ejt cry bom oh mPROTON CDCl3 {e:\bruk400data\2012\Aug} ejt 16

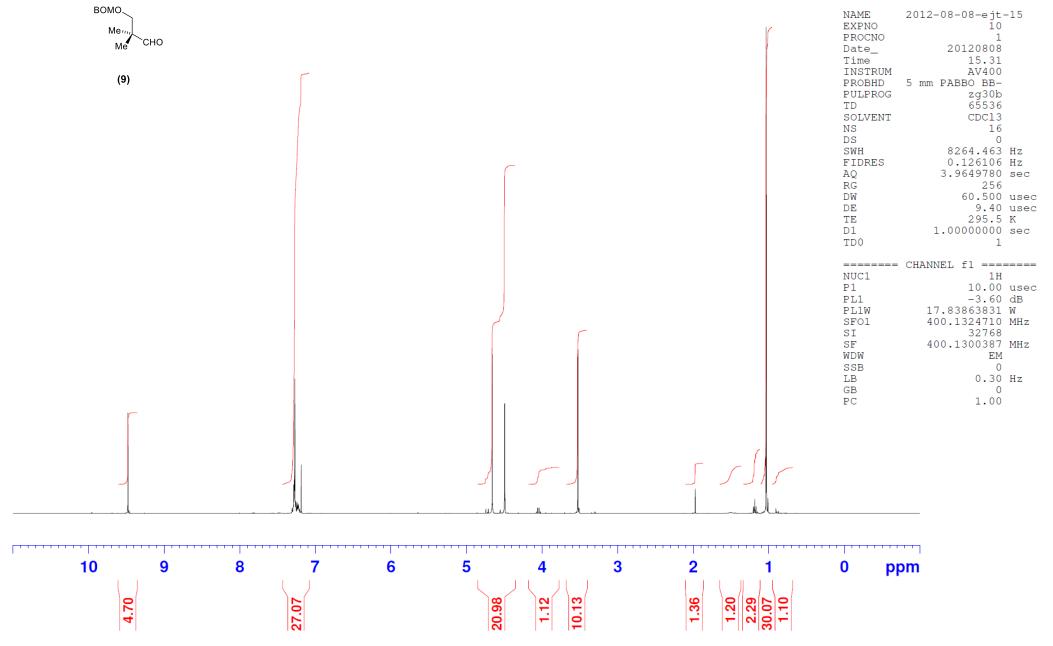






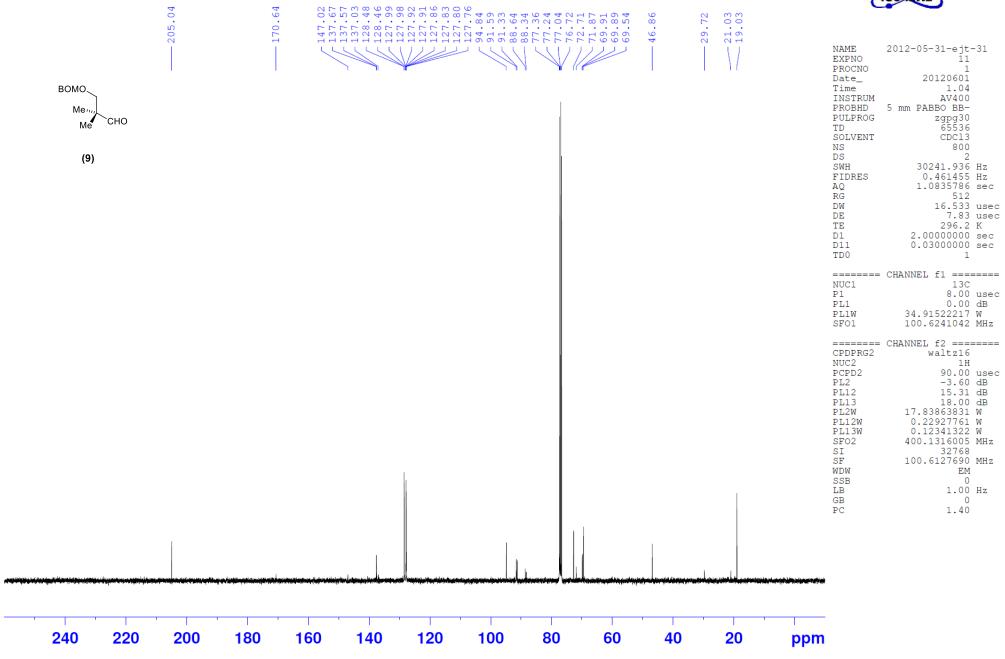
# ejt cry bom ald mPROTON CDCl3 {e:\bruk400data\2012\Aug} ejt 15





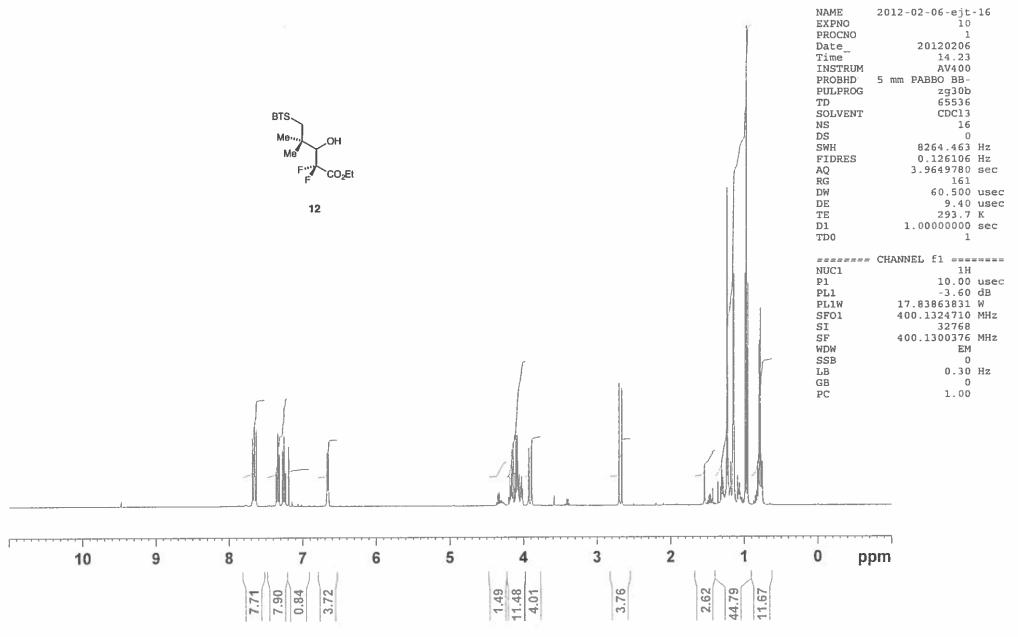
# ejt cry swern mCARBONnight CDCl3 {e:\bruk400data\2012\May} ejt 31





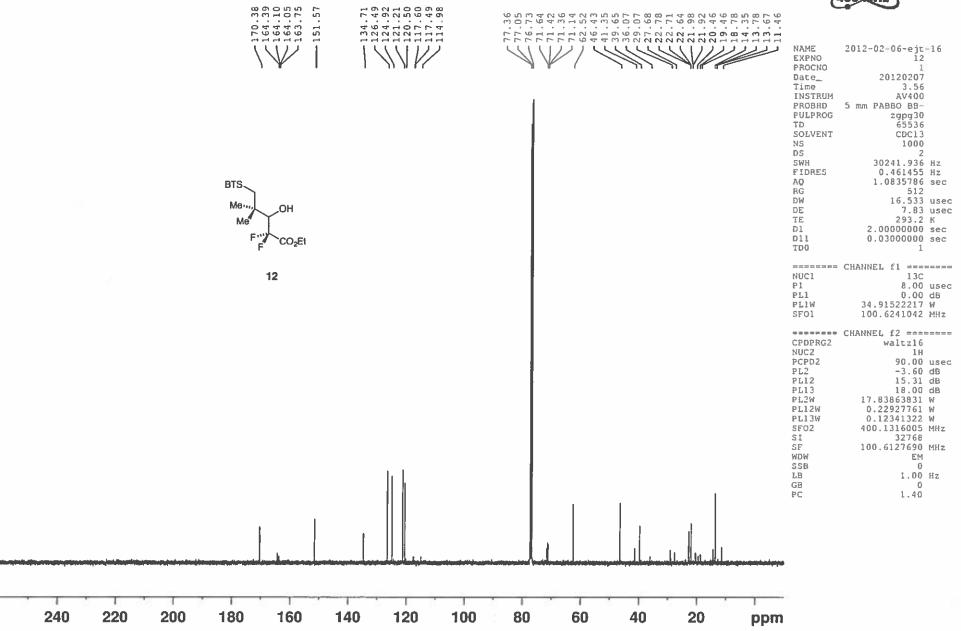
ejt cry 7-9 mPROTON CDCI3 {e:\bruk400data\2012\Feb} ejt 16



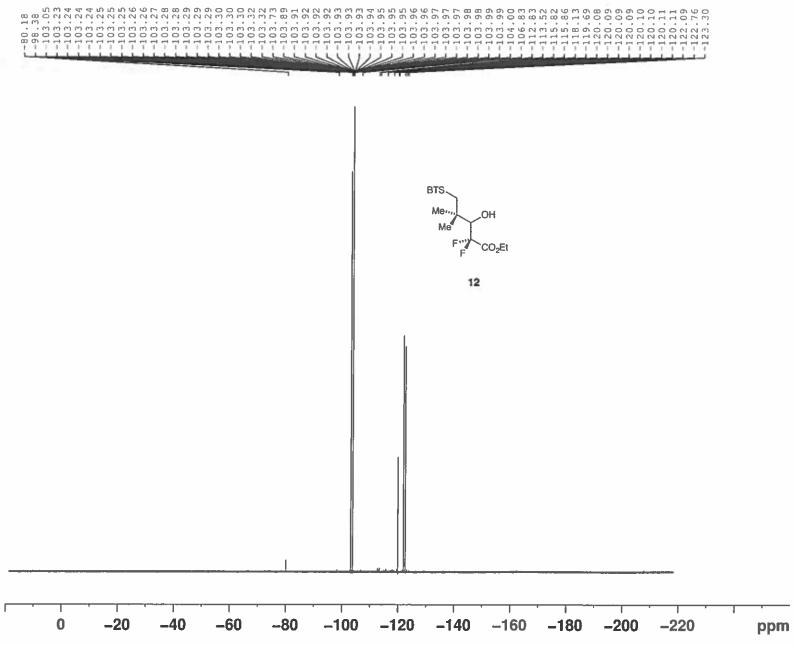


ejt cry 7–9 mCARBONnight CDCl3 {e:\bruk400data\2012\Feb} ejt 16





ejt cry 7–9 mF19CPD CDCl3 {e:\bruk400data\2012\Feb} ejt 16





| NAME<br>EXPNO<br>PROCNO<br>Date_<br>Time<br>INSTRUM<br>PROBHD<br>PULPROG<br>TD<br>SOLVENT<br>NS | 2012-02-07-ejt-<br>10<br>10<br>20120207<br>9.30<br>AV400<br>5 mm PABBO BB-<br>zgig<br>131072<br>CDC13 | -16             |
|-------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|-----------------|
| DS<br>SWH<br>FIDRES<br>AQ<br>RG                                                                 | 89285.711<br>0.681196<br>0.7340532<br>4100                                                            | Hz<br>Hz<br>sec |
| DW<br>DE<br>TE<br>D1                                                                            | 5.600<br>7.51<br>292.9<br>1.0000000                                                                   | usec<br>K       |
| TD0<br>NUC1                                                                                     | CHANNEL fl 19F                                                                                        |                 |
| P1<br>PL1<br>PL1W<br>SFO1                                                                       | 10.70<br>-5.00<br>27.00716019<br>376.4607164                                                          | dB<br>W         |
| CPDPRG2<br>NUC2<br>PCPD2                                                                        | CHANNEL f2 ====<br>waltz16<br>1H<br>90.00                                                             |                 |
| PL2<br>PL12<br>PL2W<br>PL12W<br>SF02                                                            | -3.60<br>15.31<br>17.83863831<br>0.22927761                                                           |                 |
| SI<br>SF<br>WDW<br>SSB                                                                          | 262144<br>376.4983660<br>EM<br>0                                                                      |                 |
| LB<br>GB<br>PC                                                                                  | 0.30<br>0<br>2.00                                                                                     | Hz              |
|                                                                                                 |                                                                                                       |                 |

05/07/2012 12:44:14

| Acquisition Time (se                                                          | ec) 3.1719                                                                                                  |                       | Commen                                                | t                                                          | ejt cry ti                                       | ps mPR                  | OTONnigh                                              | CDCl3 /opt                                                                       | /bruk500da                                                                             | ta/2012/J                                   | un ejt 10                                                    | Date                                                             |                                                                           | 21                    | 0 Jun 2012                                                   | 03:46:24                                                                |                                                  |
|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------|-----------------------|-------------------------------------------------------|------------------------------------------------------------|--------------------------------------------------|-------------------------|-------------------------------------------------------|----------------------------------------------------------------------------------|----------------------------------------------------------------------------------------|---------------------------------------------|--------------------------------------------------------------|------------------------------------------------------------------|---------------------------------------------------------------------------|-----------------------|--------------------------------------------------------------|-------------------------------------------------------------------------|--------------------------------------------------|
| Date Stamp                                                                    | 20 Jun 2012                                                                                                 | 03:46:24              |                                                       |                                                            |                                                  |                         |                                                       |                                                                                  |                                                                                        |                                             |                                                              |                                                                  |                                                                           |                       |                                                              |                                                                         |                                                  |
| ile Name                                                                      | \\ss7a.ds.ma                                                                                                | n.ac.uk\v             | ol5\vol3\user                                         | s\snmrdata\                                                | bruk500data                                      | \bruk500                | )data\2012\                                           | Jun\data\ejt\                                                                    | nmr\2012-0                                                                             | 6-19-ejt-1                                  | 0\10\pdata\1                                                 | \1r                                                              |                                                                           |                       |                                                              |                                                                         |                                                  |
| requency (MHz)                                                                | 500.13                                                                                                      |                       | Nucleus                                               |                                                            | 1H                                               |                         | Nu                                                    | mber of Tra                                                                      | ansients                                                                               | 16                                          |                                                              | Origin                                                           |                                                                           | S                     | pect                                                         |                                                                         |                                                  |
| Original Points Cou                                                           | nt 32768                                                                                                    |                       | Owner                                                 |                                                            | vnmr1                                            |                         | Po                                                    | ints Count                                                                       |                                                                                        | 32768                                       |                                                              | Pulse S                                                          | equence                                                                   | 20                    | g <b>30</b> b                                                |                                                                         |                                                  |
| Receiver Gain                                                                 | 203.00                                                                                                      |                       | SW(cyclie                                             | al) (Hz)                                                   | 10330.5                                          | 8                       | So                                                    | lvent                                                                            |                                                                                        | CHLORO                                      | FORM-d                                                       | Spectru                                                          | ım Offset (H                                                              | z) 31                 | 079.9768                                                     |                                                                         |                                                  |
| Spectrum Type                                                                 | STANDARD                                                                                                    |                       | Sweep W                                               | idth (Hz)                                                  | 10330.2                                          | 26                      | Te                                                    | mperature (                                                                      | (degree C)                                                                             | 20.001                                      |                                                              |                                                                  |                                                                           |                       |                                                              |                                                                         |                                                  |
| 1.0 12012-06-19-ej                                                            | 7.37<br>7.37<br>7.37                                                                                        | PticalS               | ВОМО                                                  | )                                                          | ΕΙ                                               |                         | 4.77                                                  | 4.35                                                                             |                                                                                        |                                             |                                                              |                                                                  | -2.18                                                                     |                       |                                                              | .06                                                                     |                                                  |
| 0.1<br>0.1<br>0.2<br>0.5<br>0.7<br>0.7                                        | 7.5 7.0                                                                                                     | 116461                | 6.5                                                   | 6.0                                                        | 5.5                                              | 5.0                     |                                                       | 4 4 602                                                                          | 4.0                                                                                    | 3.41                                        | 3.0                                                          | 2.5                                                              | 5.09                                                                      | <del></del>           | 1.5                                                          |                                                                         | 0.5                                              |
| 8.0<br>8.0<br>7.40<br>7.73                                                    |                                                                                                             |                       |                                                       |                                                            |                                                  |                         | 4                                                     | 5<br>chemical Sh                                                                 | 4.0<br>ift (ppm)                                                                       | 3.5                                         | 3.0                                                          |                                                                  | 2.0                                                                       | <del>)</del>          | 1.5                                                          | 1.00                                                                    |                                                  |
| 8.0<br>8.7<br>7.39                                                            | (Hz) Height                                                                                                 | No.                   | (ppm)                                                 | (Hz)                                                       | Height                                           | No.                     | (ppm)                                                 | 5<br>chemical Sh                                                                 | 4.0 ift (ppm)                                                                          | 3.5                                         | 3.0<br>(ppm)                                                 | (Hz)                                                             | 2.0                                                                       | No.                   | 1.5 (ppm)                                                    | 1.0 (Hz)                                                                | Height                                           |
| 8.0<br>8.0<br>8.7<br>7.39                                                     | (Hz) Height 501.0 0.0255                                                                                    | No.<br>12             | (ppm)<br>1.26                                         | (Hz)<br>630.2                                              | Height 0.0225                                    | No. 23                  | (ppm)<br>1.37                                         | 5<br>Chemical Sh<br>(Hz)<br>686.0                                                | 4.0<br>ift (ppm)<br>Height                                                             | 3.5<br>No.                                  | 3.0<br>(ppm)<br>3.97                                         | (Hz)                                                             | 2.0<br>Height 0.0410                                                      | No. 45                | 1.5 (ppm)<br>4.59                                            | 1.0<br>(Hz)<br>2297.3                                                   | Height 0.0249                                    |
| 8.0<br>No. (ppm)<br>1 1.00 5<br>2 1.06 5                                      | (Hz) Height<br>501.0 0.0255<br>531.9 0.2281                                                                 | No. 12 13             | (ppm)<br>1.26<br>1.27                                 | (Hz)<br>630.2<br>634.0                                     | Height 0.0225 0.0282                             | No. 23 24               | (ppm)<br>1.37<br>1.38                                 | 5<br>chemical Sh<br>(Hz)<br>686.0<br>690.1                                       | 4.0<br>ift (ppm)<br>Height<br>0.0604<br>0.4235                                         | 3.5<br>No. 34<br>35                         | 3.0 (ppm) 3.97 4.02                                          | (Hz)<br>1987.4<br>2008.6                                         | 2.0<br>Height<br>0.0410<br>0.0394                                         | No. 45 46             | 1.5 (ppm)<br>4.59<br>4.61                                    | 1.0<br>(Hz)<br>2297.3<br>2304.0                                         | Height 0.0249 0.3359                             |
| 8.0<br>No. (ppm) 6<br>1 1.00 5<br>2 1.06 5<br>3 1.07 5                        | (Hz) Height<br>501.0 0.0255<br>531.9 0.2281<br>533.7 0.0986                                                 | No.<br>12<br>13<br>14 | (ppm)<br>1.26<br>1.27<br>1.29                         | (Hz)<br>630.2<br>634.0<br>644.1                            | Height 0.0225 0.0282 0.0230                      | No. 23 24 25            | (ppm)<br>1.37<br>1.38<br>1.63                         | 5.<br>hernical Sh<br>(Hz)<br>686.0<br>690.1<br>815.6                             | 4.0 ift (ppm)  Height 0.0604 0.4235 0.0229                                             | 3.5<br>No. 34<br>35<br>36                   | 3.0 (ppm) 3.97 4.02 4.02                                     | (Hz)<br>1987.4<br>2008.6<br>2012.3                               | 2.0<br>Height<br>0.0410<br>0.0394<br>0.0387                               | No. 45 46 47          | 1.5 (ppm)<br>4.59<br>4.61<br>4.62                            | 1.0<br>(Hz)<br>2297.3<br>2304.0<br>2309.9                               | Height 0.0249 0.3359 0.3286                      |
| 8.0<br>No. (ppm) 6<br>1 1.00 5<br>2 1.06 5<br>3 1.07 5<br>4 1.09 5            | (Hz) Height<br>501.0 0.0255<br>531.9 0.2281<br>533.7 0.0986<br>544.5 0.4125                                 | No. 12 13 14 15       | (ppm)<br>1.26<br>1.27<br>1.29<br>1.30                 | (Hz)<br>630.2<br>634.0<br>644.1<br>651.0                   | Height 0.0225 0.0282 0.0230 0.0371               | No.   23   24   25   26 | (ppm)<br>1.37<br>1.38<br>1.63<br>2.06                 | 5.<br>Chemical Sh<br>(Hz)<br>686.0<br>690.1<br>815.6<br>1028.1                   | 4.0 ift (ppm)  Height 0.0604 0.4235 0.0229 0.0322                                      | 3.5<br>No. 34<br>35<br>36<br>37             | 3.0 (ppm)<br>3.97<br>4.02<br>4.02<br>4.33                    | (Hz)<br>1987.4<br>2008.6<br>2012.3<br>2163.7                     | 2.0<br>Height<br>0.0410<br>0.0394<br>0.0387<br>0.0224                     | No. 45 46 47 48       | 1.5 (ppm)<br>4.59<br>4.61<br>4.62<br>4.64                    | 1.0<br>(Hz)<br>2297.3<br>2304.0<br>2309.9<br>2321.6                     | Height 0.0249 0.3359 0.3286 0.0757               |
| 0.1 8.0 8.0 8.0 8.0 9.5 1.09 5 5 1.09 5 5                                     | (Hz) Height<br>501.0 0.0255<br>531.9 0.2281<br>533.7 0.0986<br>544.5 0.4125<br>546.7 0.4379                 | No. 12 13 14 15 16    | (ppm)<br>1.26<br>1.27<br>1.29<br>1.30<br>1.32         | (Hz)<br>630.2<br>634.0<br>644.1<br>651.0<br>658.3          | Height 0.0225 0.0282 0.0230 0.0371 0.0293        | No. 23 24 25 26 27      | (ppm)<br>1.37<br>1.38<br>1.63<br>2.06<br>2.18         | 5.5chemical Sh<br>(Hz)<br>686.0<br>690.1<br>815.6<br>1028.1<br>1091.4            | 4.0 ift (ppm)  Height 0.0604 0.4235 0.0229 0.0322 0.7925                               | 3.5<br>No. 34<br>35<br>36<br>37<br>38       | 3.0 (ppm) 3.97 4.02 4.02 4.33 4.33                           | (Hz)<br>1987.4<br>2008.6<br>2012.3<br>2163.7<br>2167.8           | 2.0<br>Height<br>0.0410<br>0.0394<br>0.0387<br>0.0224<br>0.0898           | No. 45 46 47 48 49    | 1.5 (ppm)<br>4.59<br>4.61<br>4.62<br>4.64<br>4.74            | 1.0<br>(Hz)<br>2297.3<br>2304.0<br>2309.9<br>2321.6<br>2372.4           | Height 0.0249 0.3359 0.3286 0.0757 0.1213        |
| 0.1 8.0 8.0 8.0 8.0 5 1.00 5 5 1.09 5 6 1.11 5                                | (Hz) Height<br>501.0 0.0255<br>531.9 0.2281<br>533.7 0.0986<br>544.5 0.4125<br>546.7 0.4379<br>557.4 0.0224 | No. 12 13 14 15 16 17 | (ppm)<br>1.26<br>1.27<br>1.29<br>1.30<br>1.32<br>1.33 | (Hz)<br>630.2<br>634.0<br>644.1<br>651.0<br>658.3<br>665.2 | Height 0.0225 0.0282 0.0230 0.0371 0.0293 0.0251 | No. 23 24 25 26 27 28   | (ppm)<br>1.37<br>1.38<br>1.63<br>2.06<br>2.18<br>3.40 | 5.5 chemical Sh<br>(Hz)<br>686.0<br>690.1<br>815.6<br>1028.1<br>1091.4<br>1698.0 | 4.0<br>ift (ppm)<br>Height<br>0.0604<br>0.4235<br>0.0229<br>0.0322<br>0.7925<br>0.1140 | 3.5<br>No. 34<br>35<br>36<br>37<br>38<br>39 | 3.0<br>(ppm)<br>3.97<br>4.02<br>4.02<br>4.33<br>4.33<br>4.34 | (Hz)<br>1987.4<br>2008.6<br>2012.3<br>2163.7<br>2167.8<br>2170.6 | 2.0<br>Height<br>0.0410<br>0.0394<br>0.0387<br>0.0224<br>0.0898<br>0.0238 | No. 45 46 47 48 49 50 | 1.5<br>(ppm)<br>4.59<br>4.61<br>4.62<br>4.64<br>4.74<br>4.75 | 1.0<br>(Hz)<br>2297.3<br>2304.0<br>2309.9<br>2321.6<br>2372.4<br>2376.1 | Height 0.0249 0.3359 0.3286 0.0757 0.1213 0.0240 |
| 8.0  No. (ppm) 1 1.00 5 2 1.06 5 3 1.07 5 4 1.09 5 5 1.09 5 6 1.11 5 7 1.20 5 | (Hz) Height<br>501.0 0.0255<br>531.9 0.2281<br>533.7 0.0986<br>544.5 0.4125<br>546.7 0.4379                 | No. 12 13 14 15 16    | (ppm)<br>1.26<br>1.27<br>1.29<br>1.30<br>1.32         | (Hz)<br>630.2<br>634.0<br>644.1<br>651.0<br>658.3          | Height 0.0225 0.0282 0.0230 0.0371 0.0293        | No. 23 24 25 26 27      | (ppm)<br>1.37<br>1.38<br>1.63<br>2.06<br>2.18         | 5.5chemical Sh<br>(Hz)<br>686.0<br>690.1<br>815.6<br>1028.1<br>1091.4            | 4.0 ift (ppm)  Height 0.0604 0.4235 0.0229 0.0322 0.7925                               | 3.5<br>No. 34<br>35<br>36<br>37<br>38       | 3.0 (ppm) 3.97 4.02 4.02 4.33 4.33                           | (Hz)<br>1987.4<br>2008.6<br>2012.3<br>2163.7<br>2167.8           | 2.0<br>Height<br>0.0410<br>0.0394<br>0.0387<br>0.0224<br>0.0898           | No. 45 46 47 48 49    | 1.5 (ppm)<br>4.59<br>4.61<br>4.62<br>4.64<br>4.74            | 1.0<br>(Hz)<br>2297.3<br>2304.0<br>2309.9<br>2321.6<br>2372.4           | Height 0.0249 0.3359 0.3286 0.0757               |

3.84

3.93

3.97

1920.3

1964.7

1983.6

31

32

33

42

43

44

0.1186

0.0215

0.0433

4.37

4.38

4.58

2186.0

2189.2

2292.3

53

54

55

0.0262

0.0866

0.0859

4.78

7.27

7.30

0.1141

0.6329

0.0243

2391.0

3635.9

3650.1

1.22

1.24

1.25

10

11

609.7

618.6

627.1

0.5571

0.0300

0.0214

1.35

1.36

1.37

21

22

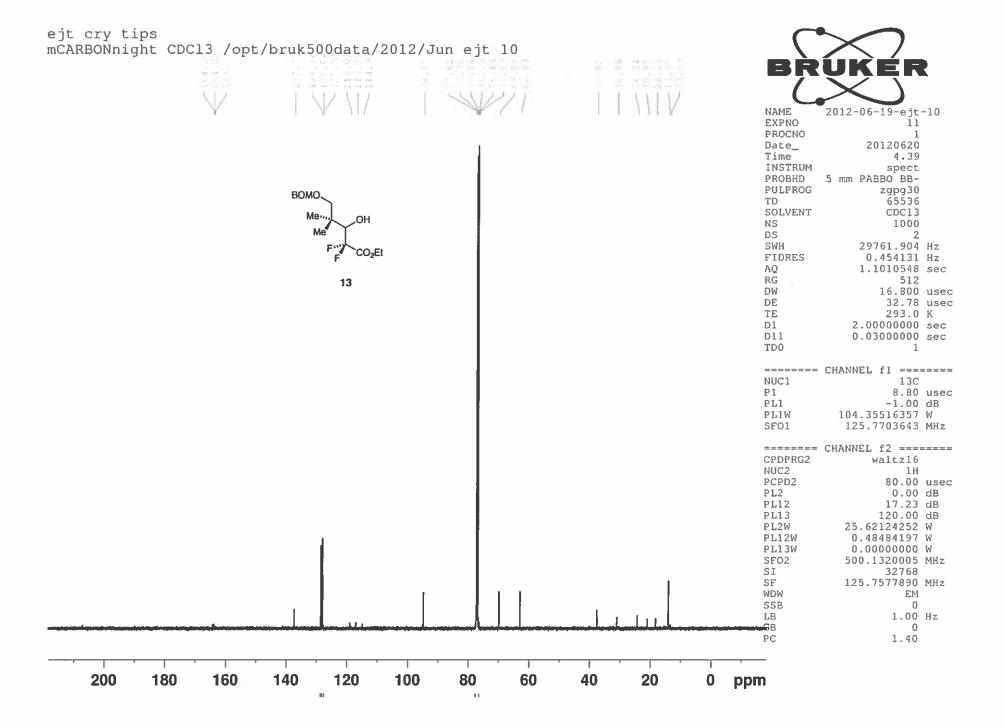
675.9

679.4

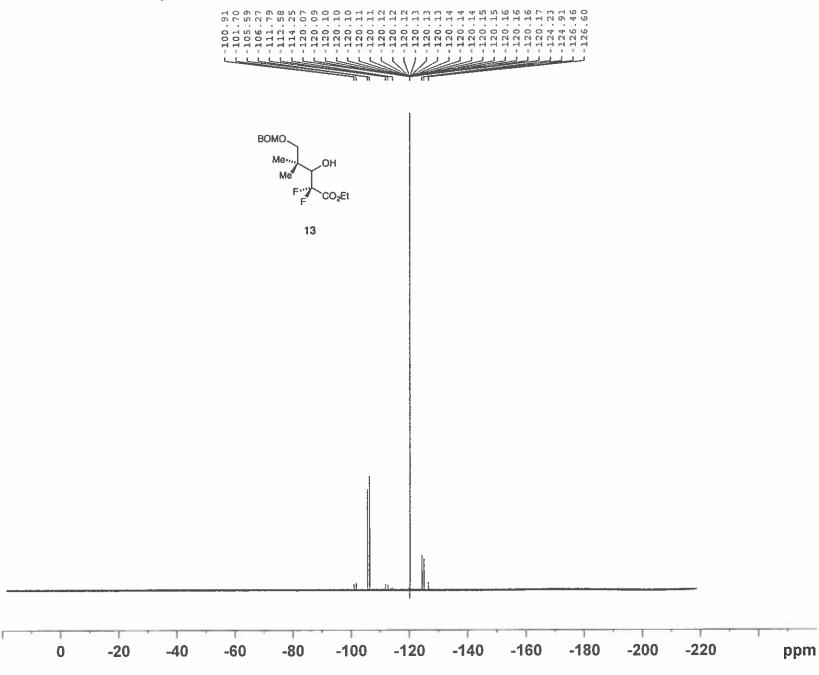
683.2

0.4465

0.0452



ejt cry zinc 2-6 mF19CPD CDCl3 {e:\bruk400data\2012\Jun} ejt 39





| NAME<br>EXPNO<br>PROCNO<br>Date<br>Time<br>INSTRUM | 2012-06-11-ejt<br>11<br>1<br>20120611<br>12.34<br>AV400                | -39                                                         |
|----------------------------------------------------|------------------------------------------------------------------------|-------------------------------------------------------------|
| PROBHD PULPROG TD SOLVENT NS                       | 5 mm PABBO BB-<br>2gig<br>131072<br>CDC13<br>16                        |                                                             |
| SWH<br>FIDRES<br>AQ<br>RG<br>DW                    | 89285.711<br>0.681196<br>0.7340532<br>4100<br>5.600                    | sec                                                         |
| DE<br>TE<br>D1<br>D11<br>TD0                       | 7.51<br>293.7<br>1.00000000<br>0.03000000                              | usec<br>K<br>sec                                            |
|                                                    |                                                                        |                                                             |
| NUC1<br>P1<br>PL1<br>PL1W<br>SF01                  | CHANNEL fl ====<br>19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164 | usec<br>dB<br>W                                             |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1                  | 19F<br>10.70<br>-5.00<br>27.00716019                                   | usec<br>dB<br>W<br>MHZ<br>usec<br>dB<br>dB<br>W<br>W<br>MHZ |

| TOWNSHIP I THE COLL                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 3.9649                                                                          |                      | Comment                                       |                                                        | ejl cry z                                 | inc produc                   | t mPRO                                               | ONnight CE                                                                   | OCI3 (e:\br                                                                 | uk400data          | \2012\Sep}                                    | ejt 37                                                 |                                           |                                    |                                           |                                              |                                    |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------|----------------------|-----------------------------------------------|--------------------------------------------------------|-------------------------------------------|------------------------------|------------------------------------------------------|------------------------------------------------------------------------------|-----------------------------------------------------------------------------|--------------------|-----------------------------------------------|--------------------------------------------------------|-------------------------------------------|------------------------------------|-------------------------------------------|----------------------------------------------|------------------------------------|
| ate                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 25 Sep 2012 08                                                                  | 3:06:40              |                                               |                                                        |                                           |                              |                                                      | te Stamp                                                                     |                                                                             |                    | 012 08:06:                                    |                                                        |                                           |                                    |                                           |                                              |                                    |
| ile Name                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | \\ss7a.ds.man.a                                                                 |                      | 15\vol3\user:                                 | s\snmrdala\bi                                          | ruk400data\                               | \2012\Sep                    | \data\ejt\r                                          | mr\2012-09-                                                                  | -24-ejt-37\                                                                 | 21\pdata\1         | \1r                                           | Freque                                                 | ncy (MHz)                                 | 4                                  | 00.13                                     |                                              |                                    |
| lucleus                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 1H                                                                              | i                    |                                               | f Transients                                           |                                           |                              |                                                      | igin                                                                         |                                                                             | AV400              |                                               | Origina                                                | l Points Co                               | unt 3                              | 2768                                      |                                              |                                    |
| wner                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Administrator                                                                   |                      | Points Co                                     | unt                                                    | 32768                                     |                              | Pu                                                   | lse Sequend                                                                  | ce                                                                          | zg30b              |                                               | Receiv                                                 | er Gain                                   | 9                                  | 0.50                                      |                                              |                                    |
| W(cyclical) (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 8264.46                                                                         |                      | Solvent                                       |                                                        | CHLOR                                     | OFORM-                       | d Sp                                                 | ectrum Offs                                                                  | et (Hz)                                                                     | 2464.927           | 72                                            | Spectro                                                | ım Type                                   | S                                  | TANDARD                                   |                                              |                                    |
| weep Width (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 8264.21                                                                         |                      | Temperat                                      | ure (degree                                            | C) 21.100                                 |                              |                                                      |                                                                              |                                                                             |                    |                                               |                                                        |                                           |                                    |                                           |                                              |                                    |
| 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 7.021.001.1 <b>4,669</b> (i                                                     | icalSc               | TBDPSC<br>Me                                  | )                                                      | a a                                       |                              |                                                      |                                                                              |                                                                             |                    |                                               |                                                        |                                           |                                    | 1.10                                      |                                              |                                    |
| 0.4 =                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                 |                      |                                               |                                                        |                                           |                              |                                                      |                                                                              |                                                                             |                    |                                               |                                                        |                                           |                                    | 1                                         |                                              |                                    |
| 0.3 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 7.44<br>-7.42<br>-7.38<br>-7.27                                                 |                      |                                               |                                                        |                                           |                              |                                                      | 4.38<br>-4.13<br>-4.07                                                       | -3.87                                                                       | 3.39               |                                               |                                                        |                                           | 1,41 1.39                          | 1.19                                      | 111111111                                    |                                    |
| 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 7.44<br>5.27<br>0.2<br>0.2<br>0.2                                               |                      | 6.5                                           | 6.0                                                    | 5.5                                       | 5.0                          | 4.5                                                  | 4.0<br>Chemical Sh                                                           | 3.ift (ppm)                                                                 | 5                  | 3.0                                           | 2.5                                                    | 2.0                                       | 1.5                                | 1.0                                       | 0.5                                          | 0                                  |
| 0.3<br>0.2<br>0.2<br>0.2<br>0.2<br>0.2<br>0.2<br>0.2<br>0.2<br>0.2<br>0.2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                 | No.                  | (ppm)                                         | (Hz)                                                   | 5.5<br>Height                             | No.                          | 4.5<br>(ppm)                                         | 4.0<br>Chemical Sh                                                           | 3.ift (ppm)                                                                 | 5 No.              | (ppm)                                         | (Hz)                                                   | Height                                    | 1.5<br>No.                         | 1.0 (ppm)                                 | (Hz)                                         | Height                             |
| 0.3<br>0.2<br>9.7<br>9.7<br>9.7<br>9.0<br>(Hz                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | z) Height<br>3.7 0.0991                                                         | No.<br>9             | (ppm)<br>3.42                                 | (Hz)                                                   | Height<br>0.0266                          | No.                          | 4.5<br>(ppm)<br>7.38                                 | 4.0<br>Chemical Sh<br>(Hz)<br>2954.1                                         | 3.ift (ppm) Height 0.0268                                                   | No. 25             | (ppm)<br>7.46                                 | (Hz)<br>2984.4                                         | Height 0.0597                             | 1.5<br>No.<br>33                   | 1.0 (ppm) 7.73                            | (Hz)<br>3092.1                               | Height 0.0258                      |
| 0.3<br>0.2<br>0.2<br>0.1<br>92.2<br>0.1<br>8.0<br>0. (ppm) (Hz<br>1 1.01 404<br>2 1.01 406                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | z) Height<br>3.7 0.0991<br>5.0 0.1034                                           | No.<br>9             | (ppm)<br>3.42<br>3.87                         | (Hz)<br>1367.4<br>1549.3                               | Height 0.0266 0.0257                      | No.   17   18                | 4.5<br>(ppm)<br>7.38<br>7.40                         | 4.0<br>Chemical Sh<br>(Hz)<br>2954.1<br>2960.4                               | 3.<br>ift (ppm)<br>Height<br>0.0268<br>0.0893                               | No. 25 26          | (ppm)<br>7.46<br>7.47                         | (Hz)<br>2984.4<br>2988.6                               | Height 0.0597 0.0512                      | 1.5<br>No.<br>33<br>34             | 1.0 (ppm) 7.73 7.73                       | (Hz)<br>3092.1<br>3094.3                     | Height 0.0258 0.0699               |
| 0.3 0.2 4 52.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 62.7 4 | z) Height<br>3.7 0.0991<br>5.0 0.1034<br>9.0 1.0000                             | No.<br>9<br>10       | (ppm)<br>3.42<br>3.87<br>3.90                 | (Hz)<br>1367.4<br>1549.3<br>1559.4                     | Height 0.0266 0.0257 0.0233               | No.   17   18   19           | 4.5<br>(ppm)<br>7.38<br>7.40<br>7.42                 | 4.0<br>Chemical Sh<br>(Hz)<br>2954.1<br>2960.4<br>2967.7                     | 3.<br>ift (ppm)<br>Height<br>0.0268<br>0.0893<br>0.1354                     | 5 No. 25 26 27     | (ppm)<br>7.46<br>7.47<br>7.49                 | (Hz)<br>2984.4<br>2988.6<br>2995.2                     | Height 0.0597 0.0512 0.0433               | 1.5<br>No.<br>33<br>34<br>35       | 1.0 (ppm) 7.73 7.73 7.74                  | (Hz)<br>3092.1<br>3094.3<br>3095.6           | Height 0.0258 0.0699 0.0802        |
| 0.3<br>0.2<br>9.2<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | z) Height<br>3.7 0.0991<br>6.0 0.1034<br>9.0 1.0000                             | No.<br>9             | (ppm)<br>3.42<br>3.87<br>3.90<br>4.07         | (Hz)<br>1367.4<br>1549.3<br>1559.4<br>1629.2           | Height 0.0266 0.0257 0.0233 0.0093        | No.   17   18   19   20      | 4.5<br>(ppm)<br>7.38<br>7.40<br>7.42<br>7.42         | 4.0<br>Chemical Sh<br>(Hz)<br>2954.1<br>2960.4<br>2967.7<br>2969.2           | 3.<br>ift (ppm)<br>Height<br>0.0268<br>0.0893<br>0.1354<br>0.1038           | 5 No. 25 26 27 28  | (ppm)<br>7.46<br>7.47<br>7.49<br>7.68         | (Hz)<br>2984.4<br>2988.6<br>2995.2<br>3074.4           | Height 0.0597 0.0512 0.0433 0.0505        | 1.5<br>No.<br>33<br>34<br>35<br>36 | 1.0 (ppm)<br>7.73<br>7.73<br>7.74<br>7.75 | (Hz)<br>3092.1<br>3094.3<br>3095.6<br>3101.9 | Height 0.0258 0.0699 0.0802 0.0759 |
| 0.3<br>0.2<br>9.2<br>0.1<br>0.1<br>0.1<br>0.2<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | z) Height<br>1.7 0.0991<br>1.0 0.1034<br>1.0000<br>1.9 0.1219                   | No.<br>9<br>10       | (ppm)<br>3.42<br>3.87<br>3.90<br>4.07<br>4.13 | (Hz)<br>1367.4<br>1549.3<br>1559.4<br>1629.2<br>1653.7 | Height 0.0266 0.0257 0.0233 0.0093 0.0094 | No.   17   18   19   20   21 | 4.5<br>(ppm)<br>7.38<br>7.40<br>7.42<br>7.42<br>7.43 | 4.0<br>Chemical Sh<br>(Hz)<br>2954.1<br>2960.4<br>2967.7<br>2969.2<br>2971.0 | 3.<br>ift (ppm)<br>Height<br>0.0268<br>0.0893<br>0.1354<br>0.1038<br>0.0623 | No. 25 26 27 28 29 | (ppm)<br>7.46<br>7.47<br>7.49<br>7.68<br>7.70 | (Hz)<br>2984.4<br>2988.6<br>2995.2<br>3074.4<br>3081.2 | Height 0.0597 0.0512 0.0433 0.0505 0.0732 | 1.5<br>No.<br>33<br>34<br>35       | 1.0 (ppm) 7.73 7.73 7.74                  | (Hz)<br>3092.1<br>3094.3<br>3095.6           | Height 0.0258 0.0699 0.0802        |
| 0.3<br>0.2<br>92.2<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1<br>0.1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | z) Height<br>3.7 0.0991<br>3.0 0.1034<br>9.0 1.0000<br>1.9 0.1219<br>1.3 0.0775 | No.<br>9<br>10<br>11 | (ppm)<br>3.42<br>3.87<br>3.90<br>4.07         | (Hz)<br>1367.4<br>1549.3<br>1559.4<br>1629.2           | Height 0.0266 0.0257 0.0233 0.0093        | No.   17   18   19   20      | 4.5<br>(ppm)<br>7.38<br>7.40<br>7.42<br>7.42         | 4.0<br>Chemical Sh<br>(Hz)<br>2954.1<br>2960.4<br>2967.7<br>2969.2           | 3.<br>ift (ppm)<br>Height<br>0.0268<br>0.0893<br>0.1354<br>0.1038           | 5 No. 25 26 27 28  | (ppm)<br>7.46<br>7.47<br>7.49<br>7.68         | (Hz)<br>2984.4<br>2988.6<br>2995.2<br>3074.4           | Height 0.0597 0.0512 0.0433 0.0505        | 1.5<br>No.<br>33<br>34<br>35<br>36 | 1.0 (ppm)<br>7.73<br>7.73<br>7.74<br>7.75 | (Hz)<br>3092.1<br>3094.3<br>3095.6<br>3101.9 | Height 0.0258 0.0699 0.0802 0.0759 |

7.46

24

2983.3

3.39

1357.3

16

0.0242

7.27

2908.9

0.0286

32

0.0587

7.72

0.0400

|                                                                      |                                                                          |                                                              | 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                                                             |                       |                                                      |                                                          |                                                 |                    |                                                         |                                                             |                                           |                                   |                                                         |                                                             | 11/2012 13:                               |
|----------------------------------------------------------------------|--------------------------------------------------------------------------|--------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------|-----------------------|------------------------------------------------------|----------------------------------------------------------|-------------------------------------------------|--------------------|---------------------------------------------------------|-------------------------------------------------------------|-------------------------------------------|-----------------------------------|---------------------------------------------------------|-------------------------------------------------------------|-------------------------------------------|
| cquisition                                                           | n Time (sec)                                                             |                                                              | Comment                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                             |                       |                                                      | 30Nnight CDC                                             | 13 {e:\bru                                      | k400data           | 1\2012\Sep} e                                           | 1 37                                                        |                                           |                                   |                                                         |                                                             |                                           |
| Date                                                                 |                                                                          | 25 Sep 2012 08:04                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                             | p 2012 08:0           |                                                      |                                                          |                                                 |                    |                                                         |                                                             |                                           |                                   |                                                         |                                                             |                                           |
| ile Name                                                             |                                                                          |                                                              | vol5\vol3\users\snmrd                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | ata\bruk400dat                                                              | a\2012\Sep            | \data\ejt\n                                          | mr\2012-09-24                                            | -ejt-37\20                                      |                    | \1r                                                     |                                                             | ency (MHz)                                |                                   | 100.61                                                  |                                                             |                                           |
| lucleus                                                              |                                                                          | 13C                                                          | Number of Trans                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | sients 1000                                                                 |                       | 0                                                    | rigin                                                    |                                                 | AV400              |                                                         |                                                             | al Points C                               | ount                              | 32768                                                   |                                                             |                                           |
| wner                                                                 |                                                                          | Administrator                                                | Points Count                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 32768                                                                       |                       |                                                      | ulse Sequence                                            |                                                 | zgpg30             |                                                         |                                                             | ver Gain                                  |                                   | 512.00                                                  |                                                             |                                           |
| W(cyclica                                                            | al) (Hz)                                                                 | 30241.94                                                     | Solvent                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                             | DROFORM-              | d S                                                  | pectrum Offse                                            | et (Hz)                                         | 11328.5            | 381                                                     | Specti                                                      | rum Type                                  |                                   | STANDAR                                                 | lD                                                          |                                           |
| weep Wid                                                             | dth (Hz)                                                                 | 30241.01                                                     | Temperature (de                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | gree C) 21.60                                                               | 0                     |                                                      |                                                          |                                                 |                    |                                                         |                                                             |                                           |                                   |                                                         |                                                             |                                           |
| 0.9 0.8 0.7 0.6 0.7 0.6 0.3 majarajarajarajarajarajarajarajarajaraja | 12-0 <del>9-24-cj</del> t-37                                             | 164.36<br>164.06<br>163.73<br>158.97                         | Cca   135.68   136.77   136.63   136.77   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61   129.61 |                                                                             |                       | e                                                    | OH<br>CO₂Et                                              | 77.32.77.00                                     |                    |                                                         |                                                             |                                           | - 38.04                           | -29.67<br>-26.76<br>-26.52                              | $\frac{-20.16}{-18.98} -19.11$ $-13.92$                     |                                           |
| 1                                                                    | 176 168                                                                  | 160 152                                                      | 144 136 12                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 28 120                                                                      | 112                   | 104                                                  | 96 88                                                    | 71111111111111111111111111111111111111          | 72                 | 64                                                      | 56 4                                                        | 48 40                                     | 3                                 | 24                                                      | 16                                                          | 8                                         |
|                                                                      |                                                                          |                                                              | 144 136 12                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 28 120                                                                      | 112 1                 | 104 S                                                | hemical Shift                                            |                                                 | 72                 | 64<br>(ppm)                                             | 56 4                                                        | 48 40                                     | No.                               | 2 24 (ppm)                                              | 16 (Hz)                                                     | 8<br>Height                               |
| lo. (pp                                                              | pm) (Hz)                                                                 | ) Height N                                                   | 144 136 12<br>(ppm) (Hz                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 28 120<br>) Height                                                          | 112<br>No.            | 104                                                  | Chemical Shift<br>(Hz)                                   | (ppm)                                           |                    | (ppm)                                                   |                                                             |                                           |                                   |                                                         |                                                             |                                           |
| lo. (pp                                                              | pm) (Hz)                                                                 | ) Height 1 0.0093                                            | 144 136 12<br>(ppm) (Hz<br>26.52 2668                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 28 120<br>) Height<br>.4 0.6070                                             | 112 1                 | (ppm)                                                | (Hz) 7747.2                                              | (ppm)<br>Height                                 | No.                | (ppm)                                                   | (Hz)                                                        | Height                                    | No.                               | (ppm)                                                   | (Hz)                                                        | Height                                    |
| lo. (pp<br>1 5.7<br>2 6.5                                            | pm) (Hz)<br>.74 577.<br>.56 660.                                         | ) Height N<br>1 0.0093<br>2 0.0119                           | 144 136 12<br>(ppm) (Hz<br>26.52 2668<br>26.76 2692                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | ) Height<br>.4 0.6070<br>.4 0.6829                                          | No. 19                | (ppm)<br>77.00                                       | (Hz) 7747.2 7767.5                                       | (ppm) Height 1.0000                             | No. 28             | (ppm)<br>127.84<br>129.61                               | (Hz)<br>12862.0                                             | Height<br>0.5090                          | No.                               | (ppm)<br>135.68                                         | (Hz)<br>13651.0                                             | Height 0.3960                             |
| lo. (pp<br>1 5.7<br>2 6.5<br>3 6.7                                   | pm) (Hz)<br>.74 577.<br>.56 660.<br>.79 683.                             | Height 1 0.0093 2 0.0119 2 0.0090                            | 144 136 12<br>(ppm) (Hz<br>26.52 2668<br>26.76 2692<br>29.67 2985                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 28 120 ) Height 1.4 0.6070 1.4 0.6829 1.0 0.0095                            | No. 19 20 21          | (ppm)<br>77.00<br>77.20<br>77.32                     | (Hz) 7747.2 7767.5 7779.5                                | (ppm) Height 1.0000 0.0691                      | No. 28 29          | (ppm)<br>127.84<br>129.61                               | (Hz)<br>12862.0<br>13040.1                                  | Height 0.5090 0.4893                      | No.<br>37<br>38                   | (ppm)<br>135.68<br>158.97                               | (Hz)<br>13651.0<br>15994.3                                  | Height 0.3960 0.0089                      |
| lo. (pp<br>1 5.7<br>2 6.5<br>3 6.7<br>4 13.                          | pm) (Hz)<br>.74 577.<br>.56 660.<br>.79 683.<br>3.92 1400.               | Height 1 0.0093 2 0.0119 2 0.0090 3 0.2237                   | 144 136 12<br>(ppm) (Hz<br>26.52 2668<br>26.76 2692<br>29.67 2985<br>38.04 3827                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | ) Height .4 0.6070 .4 0.6829 .0 0.0095 .6 0.1250                            | No. 19 20 21 22       | (ppm)<br>77.00<br>77.32<br>114.42                    | (Hz)<br>7747.2<br>7767.5<br>7779.5                       | (ppm) Height 1.0000 0.0691 0.8987 0.0121        | No. 28 29 30 31    | (ppm)<br>127.84<br>129.61<br>129.98<br>130.01           | (Hz)<br>12862.0<br>13040.1<br>13077.9<br>13080.7            | Height 0.5090 0.4893 0.2343               | No.<br>37<br>38<br>39             | (ppm)<br>135.68<br>158.97<br>163.73<br>164.02           | (Hz)<br>13651.0<br>15994.3<br>16473.3<br>16502.8            | Height 0.3960 0.0089 0.0166               |
| lo. (pp<br>1 5.7<br>2 6.5<br>3 6.7<br>4 13.<br>5 18.                 | pm) (Hz)<br>.74 577.<br>.56 660.<br>.79 683.<br>.92 1400.<br>.8.98 1909. | Height 1 0.0093 2 0.0119 2 0.0090 3 0.2237 8 0.1580          | 144 136 12<br>(ppm) (Hz<br>26.52 2668<br>26.76 2692<br>29.67 2985<br>38.04 3827<br>62.77 6315                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 28 120 ) Height .4 0.6070 .4 0.6829 .0 0.0095 .6 0.1250 .7 0.1868           | No. 19 20 21 22 23    | (ppm)<br>77.00<br>77.20<br>77.32<br>114.42<br>116.95 | (Hz)<br>7747.2<br>7767.5<br>7779.5<br>11511.7            | (ppm) Height 1.0000 0.0691 0.8987 0.0121 0.0172 | No. 28 29 30 31 32 | (ppm)<br>127.84<br>129.61<br>129.98<br>130.01<br>132.09 | (Hz)<br>12862.0<br>13040.1<br>13077.9<br>13080.7<br>13290.2 | Height 0.5090 0.4893 0.2343 0.2185 0.1047 | No.<br>37<br>38<br>39<br>40<br>41 | (ppm)<br>135.68<br>158.97<br>163.73<br>164.02<br>164.06 | (Hz)<br>13651.0<br>15994.3<br>16473.3<br>16502.8<br>16506.5 | Height 0.3960 0.0089 0.0166 0.0220 0.0221 |
| o. (pp<br>1 5.7<br>2 6.5<br>3 6.7<br>4 13.<br>5 18.<br>6 19.         | pm) (Hz)<br>.74 577.<br>.56 660.<br>.79 683.<br>.92 1400.<br>.8.98 1909. | Height 1 0.0093 2 0.0119 2 0.0090 3 0.2237 8 0.1580 7 0.2472 | 144 136 12<br>(ppm) (Hz<br>26.52 2668<br>26.76 2692<br>29.67 2985<br>38.04 3827<br>62.77 6315<br>73.31 7376                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 28 120 ) Height .4 0.6070 .4 0.6829 .0 0.0095 .6 0.1250 .7 0.1868 .2 0.0789 | No. 19 20 21 22 23 24 | (ppm)<br>77.00<br>77.32<br>114.42                    | (Hz)<br>7747.2<br>7767.5<br>7779.5<br>11511.7<br>11766.5 | (ppm) Height 1.0000 0.0691 0.8987 0.0121        | No. 28 29 30 31    | (ppm)<br>127.84<br>129.61<br>129.98<br>130.01<br>132.09 | (Hz)<br>12862.0<br>13040.1<br>13077.9<br>13080.7            | Height 0.5090 0.4893 0.2343 0.2185        | No.<br>37<br>38<br>39<br>40       | (ppm)<br>135.68<br>158.97<br>163.73<br>164.02           | (Hz)<br>13651.0<br>15994.3<br>16473.3<br>16502.8            | Height 0.3960 0.0089 0.0166 0.0220        |

0.4990

12860.1

135.63

13646.4

0.4880

0.0754

7739.8

0.0903

23.80

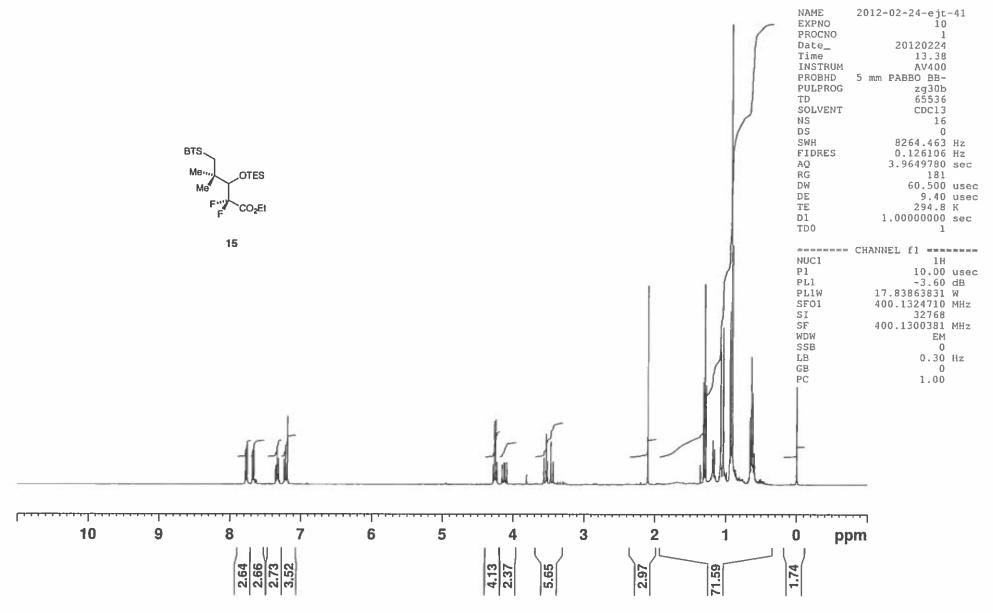
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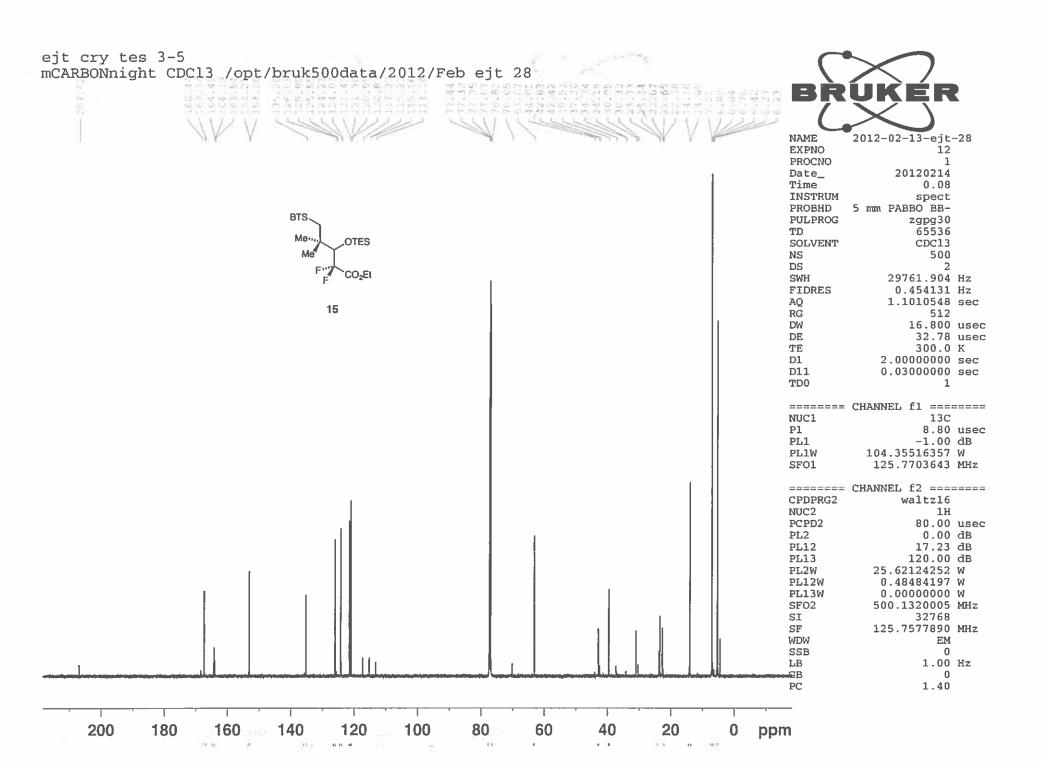
76.93

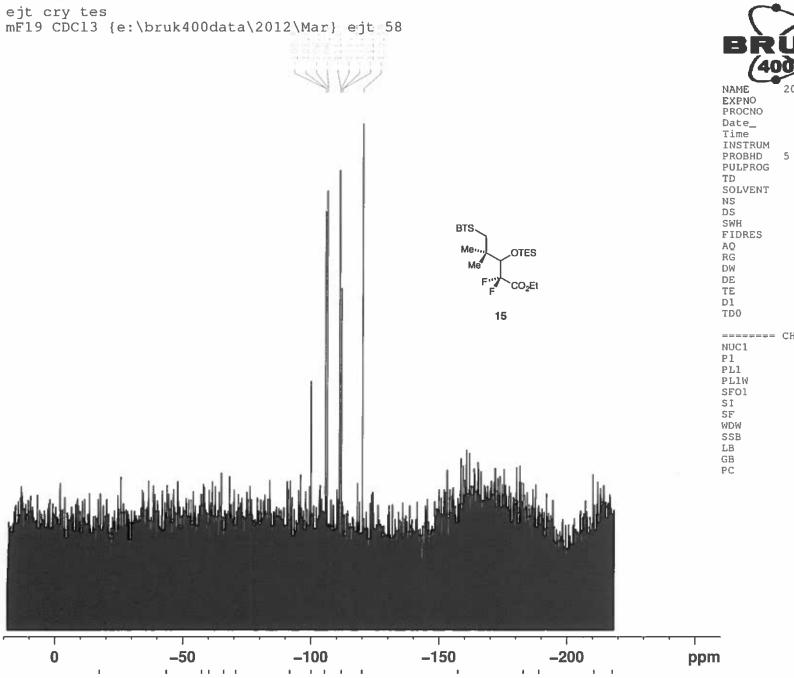
18

27











| NAME    | 2012-03-21-ejt | -58  |
|---------|----------------|------|
| EXPNO   | 10             |      |
| PROCNO  | 1              |      |
| Date_   | 20120321       |      |
| Time    | 15.43          |      |
| INSTRUM | AV400          |      |
| PROBHD  | 5 mm PABBO BB- |      |
| PULPROG | żg             |      |
| TD      | 131072         |      |
| SOLVENT | CDC13          |      |
| NS      | 16             |      |
| DS      | 4              |      |
| SWH     | 89285.711      | Hz   |
| FIDRES  | 0.681196       | Hz   |
| AQ      | 0.7340532      | sec  |
| RG      | 4100           |      |
| DW      | 5.600          | usec |
| DE      | 11.01          | usec |
| TE      | 295.1          | K    |
| D1      | 1.00000000     | sec  |
| TD0     | 1              |      |
|         |                |      |

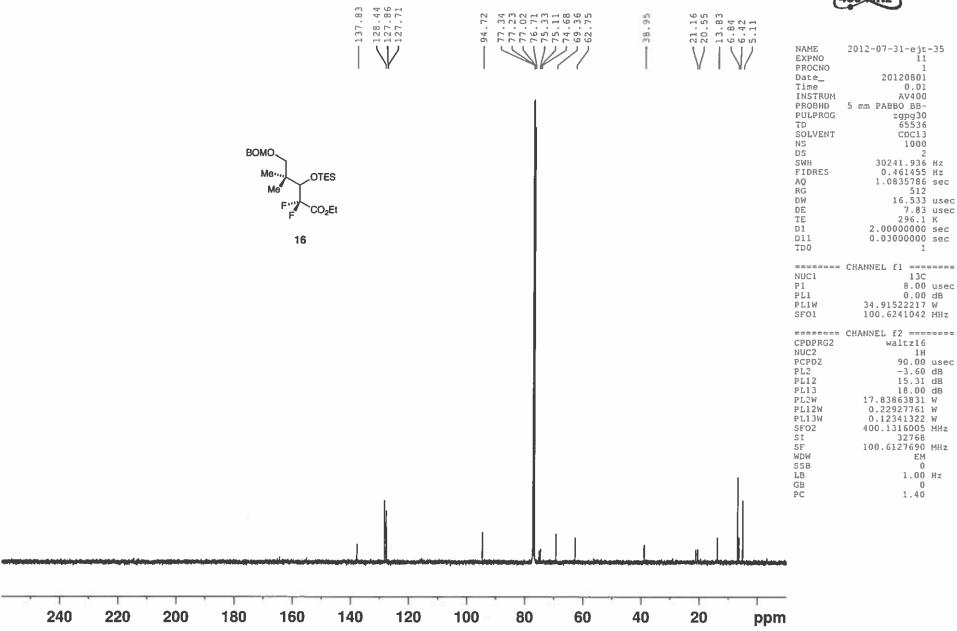
| ======= | CHANNEL f1 ==== |      |
|---------|-----------------|------|
| NUC1    | 19F             |      |
| P1      | 10.70           | usec |
| PL1     | -5.00           | dB   |
| PL1W    | 27.00716019     | W    |
| SF01    | 376.4607164     | MHz  |
| SI      | 262144          |      |
| SF      | 376.4983660     | MHz  |
| WDW     | EM              |      |
| SSB     | 0               |      |
| LB      | 0.30            | Hz   |
| GB      | 0               |      |
| PC      | 2.00            |      |

|                                                                                     |                         |                                       |                                       |                             |                        |                             |                                  | 29/11/2012 16:44:47                                    |
|-------------------------------------------------------------------------------------|-------------------------|---------------------------------------|---------------------------------------|-----------------------------|------------------------|-----------------------------|----------------------------------|--------------------------------------------------------|
| Acquisition Time (sec)                                                              | 3.1719                  | Comment                               | ejt cry tes prot mPROT                | ON CDCl3 /opt/bruk500da     | ta/2012/Jul ejt 10     | Date                        | 31 Jul 2012 11:08:00             |                                                        |
| Date Stamp                                                                          | 31 Jul 2012 11:08:00    | File Name                             | \\ss7a.ds.man.ac.uk\vc                | ol5\vol3\users\snmrdata\bru | k500data\bruk500data\2 | 2012\Juf\data\ejt\nmr\2012- | 07-31-ejt-10\10\pdata\1          | 1r                                                     |
| Frequency (MHz)                                                                     | 500.13                  | Nucleus                               | 1H                                    | Number of Transients        | 16                     | Origin                      | spect                            |                                                        |
| Original Points Count                                                               | 32768                   | Owner                                 | vnmr1                                 | Points Count                | 32768                  | Pulse Sequence              | zg30b                            |                                                        |
| Receiver Gain                                                                       | 90.50                   | SW(cyclical) (Hz)                     | 10330.58                              | Solvent                     | CHLOROFORM-d           | Spectrum Offset (Hz)        | 3080.2925                        |                                                        |
| Spectrum Type                                                                       | STANDARD                | Sweep Width (Hz)                      | 10330.26                              | Temperature (degree C)      | 27.000                 |                             |                                  |                                                        |
| Normalized Intensity  7.37  7.37  7.37  7.36  Normalized Intensity  6.0  7.37  7.37 | 0.010.001.11.46PticalSc | BOMO Me OTES Me CO <sub>2</sub> Et 16 | 0.5<br>0.4.76<br>4.75<br>4.72<br>4.72 |                             | 3.45                   | 2.5 2.0                     | -1.58<br>-1.38<br>-1.35<br>-1.03 | 0.69 0.69 0.69 0.65 0.65 0.65 0.65 0.65 0.65 0.65 0.65 |
|                                                                                     |                         |                                       |                                       | Chemical Shift (ppm)        |                        |                             |                                  |                                                        |

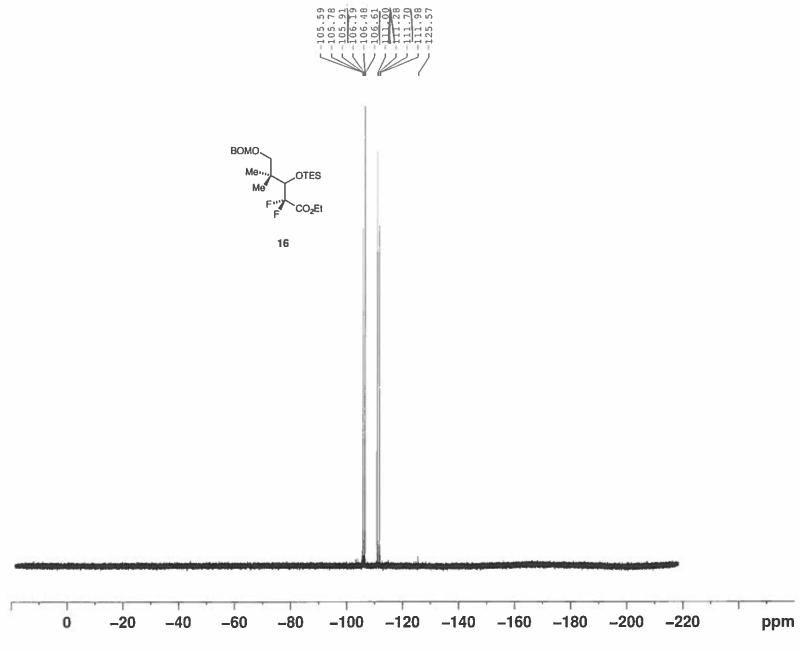
| Ala. | (     | (1.1-) | 11-1-64 | Ma  | />    | 71.1-1 | 11-1-64 | N1= | (     | (1.1-1 | 1 letelet | Ma  | (     | 46.1-3 | I Intolet | Ma  | (     | 71.1-3 | I totalet |
|------|-------|--------|---------|-----|-------|--------|---------|-----|-------|--------|-----------|-----|-------|--------|-----------|-----|-------|--------|-----------|
| No.  | (ppm) | (Hz)   | Height  | No. | (ppm) | (Hz)   | Height  | No. | (ppm) | Hz)    | Height    | No. | (ppm) | (Hz)   | Height    | No. | (ppm) | (Hz)   | Height    |
| 1    | 0.52  | 259.2  | 0.0866  | 10  | 0.69  | 347.1  | 0.0698  | 19  | 1.35  | 676.2  | 0.1536    | 28  | 4.29  | 2146.6 | 0.0634    | 37  | 4.75  | 2373.3 | 0.1291    |
| 2    | 0.53  | 267.0  | 0.0938  | 11  | 0.92  | 461.9  | 0.0986  | 20  | 1.36  | 679.7  | 0.0425    | 29  | 4.31  | 2153.9 | 0.0958    | 38  | 4.76  | 2379.9 | 0.0568    |
| 3    | 0.64  | 319.4  | 0.0536  | 12  | 0.94  | 469.7  | 0.1950  | 21  | 1.37  | 683.5  | 0.3057    | 30  | 4.32  | 2161.1 | 0.0920    | 39  | 7.27  | 3635.9 | 0.3093    |
| 4    | 0.65  | 323.8  | 0.0573  | 13  | 0.96  | 477.6  | 0.1019  | 22  | 1.38  | 690.4  | 0.1533    | 31  | 4.56  | 2278.4 | 0.0522    | 40  | 7.35  | 3675.0 | 0.0455    |
| 5    | 0.65  | 327.6  | 0.1427  | 14  | 0.96  | 479.5  | 0.0617  | 23  | 1.58  | 789.4  | 0.0789    | 32  | 4.58  | 2290.1 | 0.1087    | 41  | 7.36  | 3678.8 | 0.4257    |
| 6    | 0.66  | 331.7  | 0.1452  | 15  | 0.97  | 484.9  | 0.3933  | 24  | 3.30  | 1652.3 | 0.0458    | 33  | 4.62  | 2311.8 | 0.1047    | 42  | 7.36  | 3681.7 | 0.1335    |
| 7    | 0.67  | 335.4  | 0.1599  | 16  | 0.99  | 492.8  | 1.0000  | 25  | 3.32  | 1661.4 | 0.0594    | 34  | 4.65  | 2323.5 | 0.0587    | 43  | 7.37  | 3684.5 | 0.1228    |
| 8    | 0.68  | 339.5  | 0.1533  | 17  | 1.00  | 500.6  | 0.3154  | 26  | 3.43  | 1716.3 | 0.0788    | 35  | 4.72  | 2358.5 | 0.0520    |     |       |        |           |
| 9    | 0.69  | 343.6  | 0.0687  | 18  | 1.03  | 515.1  | 0.2534  | 27  | 3.45  | 1725.4 | 0.0613    | 36  | 4.73  | 2365.1 | 0.1230    |     |       |        |           |

## ejt cry tes prot mCARBONnight CDCl3 {e:\bruk400data\2012\Jul} ejt 35





# ejt cry tes prot mF19CPD CDCl3 {e:\bruk400data\2012\Jul} ejt 35

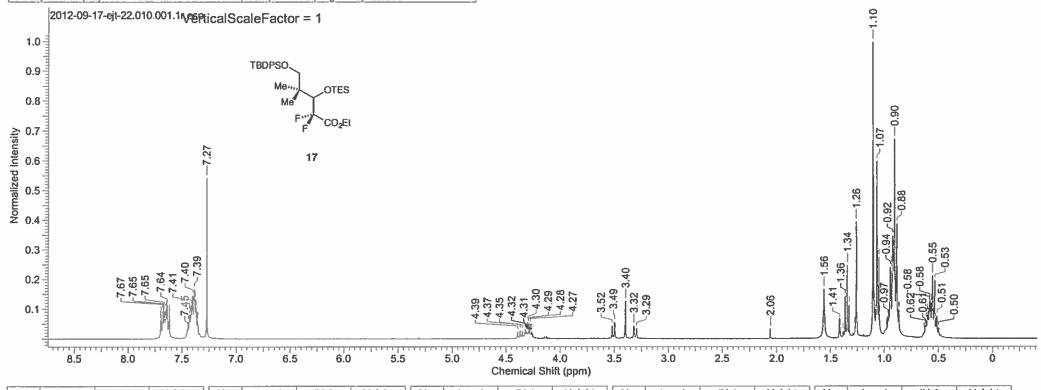




| NAME<br>EXPNO<br>PROCNO<br>Date_<br>Time<br>INSTRUM<br>PROBHD<br>PULPROG<br>TD<br>SOLVENT<br>NS<br>DS | 2012-07-31-e jt-<br>10<br>20120731<br>11.44<br>AV400<br>5 mm PABBO BB-<br>zgig<br>131072<br>CDC13<br>16<br>4   | -35             |
|-------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|-----------------|
| SWH<br>FIDRES<br>AQ<br>RG<br>DW<br>DE<br>TE<br>D1<br>D11<br>TD0                                       | 89285.711<br>0.681196<br>0.7340532<br>4100<br>5.600<br>7.51<br>295.6<br>1.00000000<br>0.03000000               |                 |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1                                                                     | CHANNEL f1 ====<br>19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164                                         | usec<br>dB<br>W |
| CPDPRG2<br>NUC2<br>PCPD2<br>PL12<br>PL12W<br>PL12W<br>SFO2<br>SI<br>SF WDW<br>SSB<br>LB<br>GB<br>PC   | CHANNEL f2 waltz16 1H 90.00 -3.60 15.31 17.83863831 0.22927761 400.1316005 262144 376.4983660 EM 0 0.30 0 2.00 | usec<br>dB      |

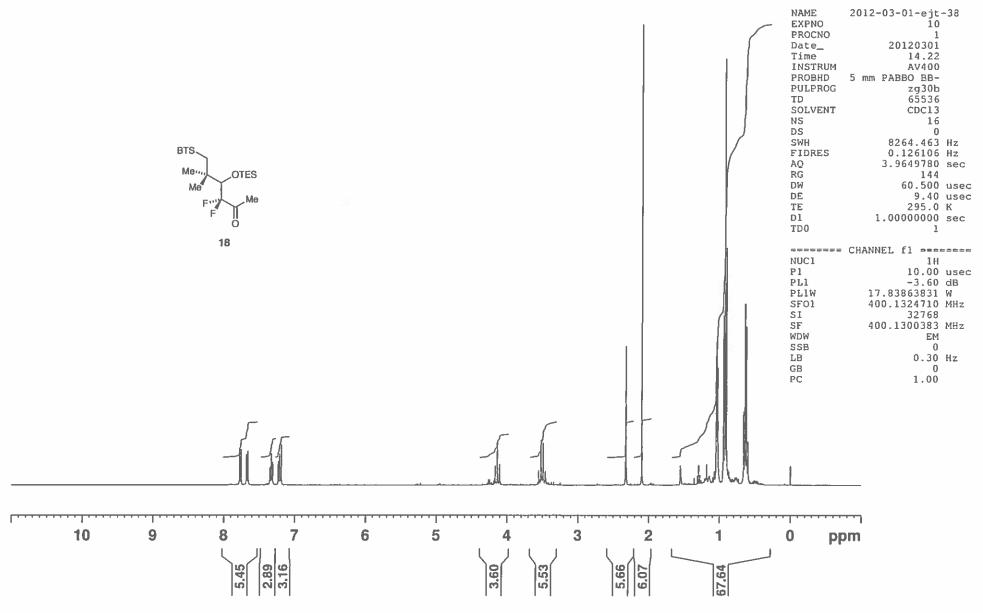
30/11/2012 14:32:02

| Acquisition Time (sec) | 3.9649                 | Comment                     | ejt cry tes protection m | PROTON CDCl3 (e:\bruk4      | 100data\2012\Sep} ejt 22 |                       |          |
|------------------------|------------------------|-----------------------------|--------------------------|-----------------------------|--------------------------|-----------------------|----------|
| Date                   | 17 Sep 2012 15:04:48   |                             |                          | Date Stamp                  | 17 Sep 2012 15:04:48     |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\vc | ol5\vol3\users\snmrdata\bru | k400data\2012\Sep\data   | \ejt\nmr\2012-09-17-ejt-22\ | \10\pdata\1\1r           | Frequency (MHz)       | 400.13   |
| Nucleus                | 1H                     | Number of Transients        | 16                       | Origin                      | AV400                    | Original Points Count | 32768    |
| Owner                  | Administrator          | Points Count                | 32768                    | Pulse Sequence              | zg30b                    | Receiver Gain         | 287.00   |
| SW(cyclical) (Hz)      | 8264.46                | Solvent                     | CHLOROFORM-d             | Spectrum Offset (Hz)        | 2464.6750                | Spectrum Type         | STANDARD |
| Sweep Width (Hz)       | 8264.21                | Temperature (degree C)      | 22.200                   |                             |                          |                       |          |



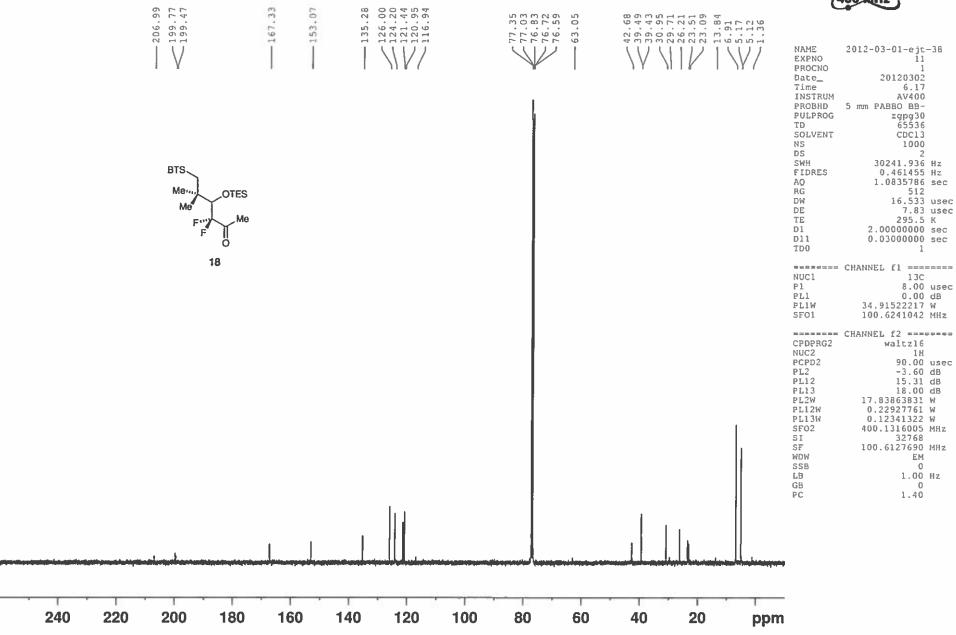
| N | lo. | (ppm) | (Hz)  | Height | No. | (ppm) | (Hz)   | Height |
|---|-----|-------|-------|--------|-----|-------|-------|--------|-----|-------|-------|--------|-----|-------|-------|--------|-----|-------|--------|--------|
|   | 1   | 0.50  | 198.9 | 0.0365 | 12  | 0.61  | 244.1 | 0.0597 | 23  | 0.94  | 377.0 | 0.2404 | 34  | 1.26  | 503.4 | 0.3944 | 45  | 3.29  | 1318.0 | 0.0350 |
|   | 2   | 0.51  | 205.2 | 0.0761 | 13  | 0.61  | 245.8 | 0.0438 | 24  | 0.95  | 378.3 | 0.2398 | 35  | 1.27  | 508.1 | 0.0415 | 46  | 3.32  | 1327.8 | 0.0429 |
|   | 3   | 0.53  | 213.1 | 0.1953 | 14  | 0.62  | 247.9 | 0.0422 | 25  | 0.96  | 383.8 | 0.0689 | 36  | 1.33  | 530.6 | 0.1129 | 47  | 3.40  | 1359.1 | 0.1272 |
|   | 4   | 0.54  | 217.3 | 0.0733 | 15  | 0.63  | 251.6 | 0.0247 | 26  | 0.97  | 386.3 | 0.0770 | 37  | 1.34  | 537.7 | 0.2470 | 48  | 3.49  | 1398.5 | 0.0558 |
|   | 5   | 0.55  | 220.9 | 0.2121 | 16  | 0.86  | 345.7 | 0.0959 | 27  | 0.97  | 389.4 | 0.0415 | 38  | 1.36  | 544.7 | 0.1441 | 49  | 3.52  | 1408.3 | 0.0440 |
|   | 6   | 0.56  | 225.2 | 0.1204 | 17  | 0.88  | 353.0 | 0.3885 | 28  | 0.98  | 391.6 | 0.0350 | 39  | 1.38  | 552.0 | 0.0236 | 50  | 4.26  | 1704.4 | 0.0213 |
| 1 | 7   | 0.58  | 230.2 | 0.1316 | 18  | 0.90  | 360.9 | 0.6733 | 29  | 1.05  | 419.6 | 0.2737 | 40  | 1.41  | 564.4 | 0.0379 | 51  | 4.27  | 1709.4 | 0.0484 |
|   | 8   | 0.58  | 233.0 | 0.1224 | 19  | 0.91  | 362.4 | 0.5130 | 30  | 1.07  | 426.7 | 0.5991 | 41  | 1.41  | 565.9 | 0.0633 | 52  | 4.28  | 1711.7 | 0.0527 |
|   | 9   | 0.59  | 236.0 | 0.0720 | 20  | 0.92  | 366.7 | 0.3024 | 31  | 1.08  | 432.5 | 0.0672 | 42  | 1.42  | 567.4 | 0.0394 | 53  | 4.29  | 1716.5 | 0.0498 |
| 1 | 10  | 0.60  | 238.3 | 0.0895 | 21  | 0.92  | 368.7 | 0.3475 | 32  | 1.09  | 434.5 | 0.0747 | 43  | 1.56  | 624.4 | 0.1664 | 54  | 4.30  | 1718.8 | 0.0555 |
| 1 | l1  | 0.60  | 240.5 | 0.0780 | 22  | 0.93  | 370.4 | 0.2798 | 33  | 1.10  | 440.8 | 1.0000 | 44  | 2.06  | 822.9 | 0.0340 | 55  | 4.31  | 1723.6 | 0.0223 |



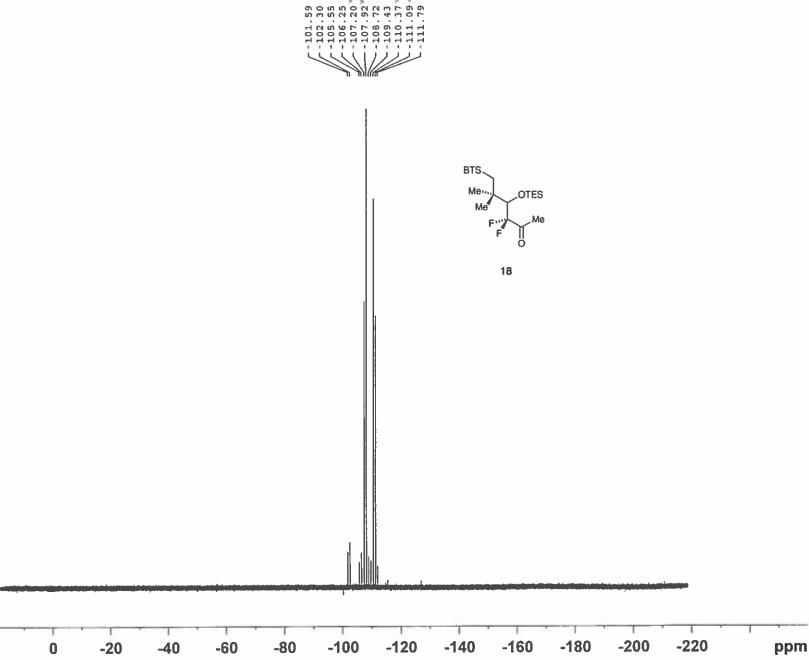


## me ketone mCARBONnight CDCl3 {e:\bruk400data\2012\Mar} ejt 38





## me ketone mF19CPD CDCl3 {e:\bruk400data\2012\Mar} ejt 38

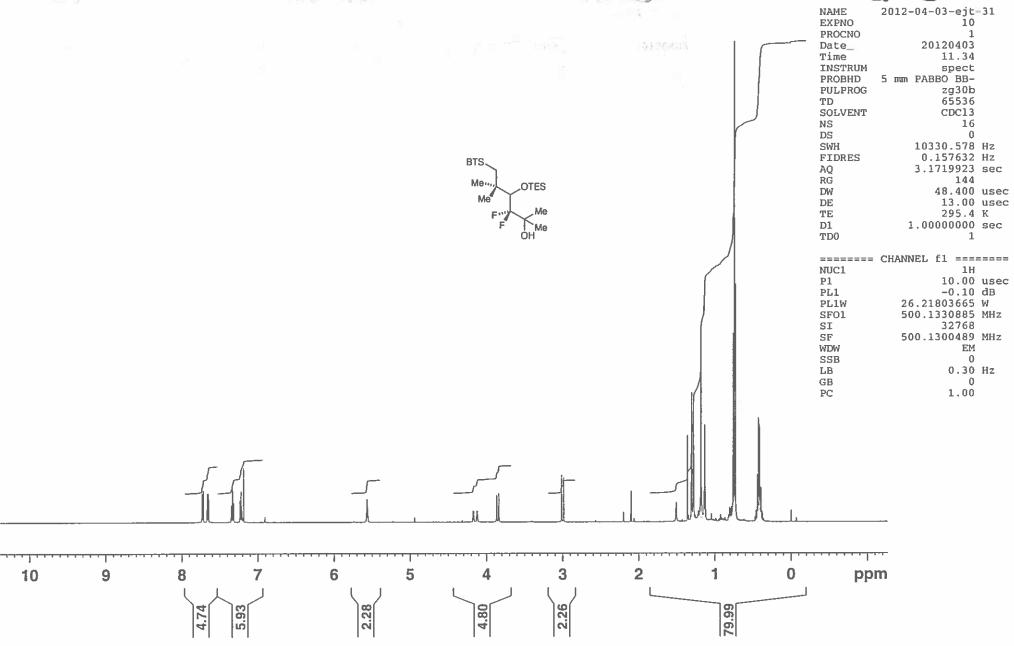


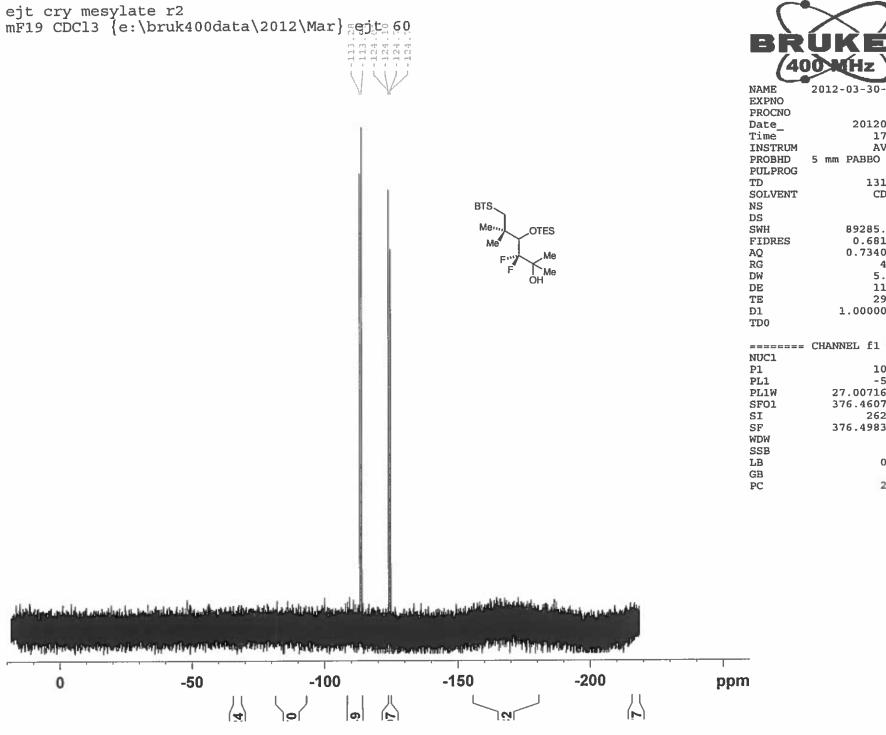


| NAME                                                                                                                                | 2012-03-01-ejt-                                                                                                                                                                          | -38                                                         |
|-------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------|
| EXPNO                                                                                                                               | 12                                                                                                                                                                                       |                                                             |
| PROCNO                                                                                                                              | 1                                                                                                                                                                                        |                                                             |
| Date                                                                                                                                | 20120301                                                                                                                                                                                 |                                                             |
| Time                                                                                                                                | 14.23                                                                                                                                                                                    |                                                             |
| INSTRUM                                                                                                                             | AV400                                                                                                                                                                                    |                                                             |
| PROBHD                                                                                                                              | 5 mm PABBO BB-                                                                                                                                                                           |                                                             |
| PULPROG                                                                                                                             | zgig                                                                                                                                                                                     |                                                             |
| TD                                                                                                                                  | 131072                                                                                                                                                                                   |                                                             |
| SOLVENT                                                                                                                             | CDC13                                                                                                                                                                                    |                                                             |
| NS                                                                                                                                  | 16                                                                                                                                                                                       |                                                             |
| DS                                                                                                                                  | 4                                                                                                                                                                                        |                                                             |
| SWH                                                                                                                                 | 89285.711                                                                                                                                                                                | Hz                                                          |
| FIDRES                                                                                                                              |                                                                                                                                                                                          | Hz                                                          |
| AO                                                                                                                                  | 0.7340532                                                                                                                                                                                | sec                                                         |
| RG                                                                                                                                  | 4100                                                                                                                                                                                     |                                                             |
| DW                                                                                                                                  | 5,600                                                                                                                                                                                    | usec                                                        |
| DE                                                                                                                                  | 7.51                                                                                                                                                                                     |                                                             |
| TE                                                                                                                                  | 295.1                                                                                                                                                                                    |                                                             |
| Di                                                                                                                                  | 1.00000000                                                                                                                                                                               |                                                             |
| D11                                                                                                                                 | 0.03000000                                                                                                                                                                               |                                                             |
| TDO                                                                                                                                 | 1                                                                                                                                                                                        |                                                             |
|                                                                                                                                     | -                                                                                                                                                                                        |                                                             |
|                                                                                                                                     |                                                                                                                                                                                          |                                                             |
| *****                                                                                                                               | CHANNEL f1 ====                                                                                                                                                                          | ====                                                        |
|                                                                                                                                     | CHANNEL f1 ====                                                                                                                                                                          |                                                             |
| NUC1<br>P1                                                                                                                          | 19F                                                                                                                                                                                      |                                                             |
| NUC1                                                                                                                                |                                                                                                                                                                                          | usec                                                        |
| NUC1<br>P1<br>PL1                                                                                                                   | 19F<br>10.70<br>-5.00                                                                                                                                                                    | usec<br>dB                                                  |
| NUC1<br>P1                                                                                                                          | 19F<br>10.70                                                                                                                                                                             | usec<br>dB<br>W                                             |
| NUC1<br>P1<br>PL1<br>PL1W                                                                                                           | 19F<br>10.70<br>-5.00<br>27.00716019                                                                                                                                                     | usec<br>dB<br>W                                             |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1                                                                                                   | 19F<br>10.70<br>-5.00<br>27.00716019                                                                                                                                                     | usec<br>dB<br>W<br>MHz                                      |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1                                                                                                   | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164                                                                                                                                      | usec<br>dB<br>W<br>MHz                                      |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1                                                                                                   | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2                                                                                                                        | usec<br>dB<br>W<br>MHz                                      |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2                                                                                        | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2 ====<br>waltz16                                                                                                        | usec<br>dB<br>W<br>MHz                                      |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2<br>NUC2                                                                                | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2 ====<br>waltz16<br>1H                                                                                                  | usec<br>dB<br>W<br>MHz                                      |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2<br>NUC2<br>PCPD2                                                                       | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2                                                                                                                        | usec<br>dB<br>W<br>MHz<br>usec<br>dB                        |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2<br>NUC2<br>PCPD2<br>PL2                                                                | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2 ====<br>waltz16<br>1H<br>90.00<br>-3.60                                                                                | usec<br>dB<br>W<br>MHZ<br>usec<br>dB<br>dB                  |
| NUC1<br>P1<br>PL1<br>PL1W<br>SF01<br>CPDPRG2<br>NUC2<br>PCPD2<br>PL2<br>PL12                                                        | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2 ====<br>waltz16<br>1H<br>90.00<br>-3.60<br>15.31                                                                       | usec<br>dB<br>W<br>MHz<br>usec<br>dB<br>dB                  |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2<br>NUC2<br>PCPD2<br>PL2<br>PL12<br>PL12<br>PL2W                                        | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2 ====<br>waltz16<br>1H<br>90.00<br>-3.60<br>15.31<br>17.83863831<br>0.22927761                                          | usec<br>dB<br>W<br>MHz<br>usec<br>dB<br>dB                  |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2<br>NUC2<br>PCPD2<br>PL2<br>PL12<br>PL12<br>PL12W<br>PL12W                              | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2<br>waltz16<br>1H<br>90.00<br>-3.60<br>15.31<br>17.83863831<br>0.22927761                                               | usec<br>dB<br>W<br>MHz<br>usec<br>dB<br>dB<br>W             |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2<br>NUC2<br>PCPD2<br>PL2<br>PL12<br>PL12<br>PL12W<br>PL12W<br>SFO2                      | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2 ====<br>waltz16<br>1H<br>90.00<br>-3.60<br>15.31<br>17.83863831<br>0.22927761<br>400.1316005                           | usec<br>dB<br>W<br>MHZ<br>usec<br>dB<br>dB<br>W<br>W<br>MHZ |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2<br>NUC2<br>PCPD2<br>PL2<br>PL12<br>PL12W<br>PL12W<br>PL12W<br>SFO2<br>SI               | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2 ====<br>waltz16<br>1H<br>90.00<br>-3.60<br>15.31<br>17.83863831<br>0.22927761<br>400.1316005<br>262144                 | usec<br>dB<br>W<br>MHZ<br>usec<br>dB<br>dB<br>W<br>W<br>MHZ |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2<br>NUC2<br>PCPD2<br>PL12<br>PL12W<br>PL12W<br>PL12W<br>SFO2<br>SI<br>SF                | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2 ====<br>waltz16<br>1H<br>90.00<br>-3.60<br>15.31<br>17.83863831<br>0.22927761<br>400.1316005<br>262144<br>376.4983660  | usec<br>dB<br>W<br>MHZ<br>usec<br>dB<br>dB<br>W<br>W<br>MHZ |
| NUC1<br>P1<br>PL1<br>PL1W<br>SF01<br>=======<br>CPDPRG2<br>NUC2<br>PCPD2<br>PL2<br>PL12<br>PL12<br>PL12W<br>SF02<br>SI<br>SF<br>WDW | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2<br>waltz16<br>1H<br>90.00<br>-3.60<br>15.31<br>17.83863831<br>0.22927761<br>400.1316005<br>262144<br>376.4983660<br>EM | usec<br>dB<br>W<br>MHZ<br>usec<br>dB<br>dB<br>W<br>W<br>MHZ |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1<br>CPDPRG2<br>NUC2<br>PCPD2<br>PL12<br>PL12<br>PL12W<br>PL12W<br>SFO2<br>SI<br>SFO2<br>SSF        | 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164<br>CHANNEL f2<br>waltz16<br>1H<br>90.00<br>-3.60<br>15.31<br>17.83863831<br>0.22927761<br>400.1316005<br>262144<br>376.4983660<br>EM | usec<br>dB<br>W<br>MHZ<br>usec<br>dB<br>dB<br>W<br>W<br>MHZ |
| NUC1 P1 PL1 PL1 PL1W SFO1  CCPDPRG2 NUC2 PCPD2 PL2 PL12 PL12W PL112W SFO2 SI SF WDW SSB LB                                          | 19F 10.70 -5.00 27.00716019 376.4607164  CHANNEL f2 waltz16 1H 90.00 -3.60 15.31 17.83863831 0.22927761 400.1316005 262144 376.4983660 EM 0 0.30                                         | usec<br>dB<br>W<br>MHZ<br>usec<br>dB<br>dB<br>W<br>W<br>MHZ |









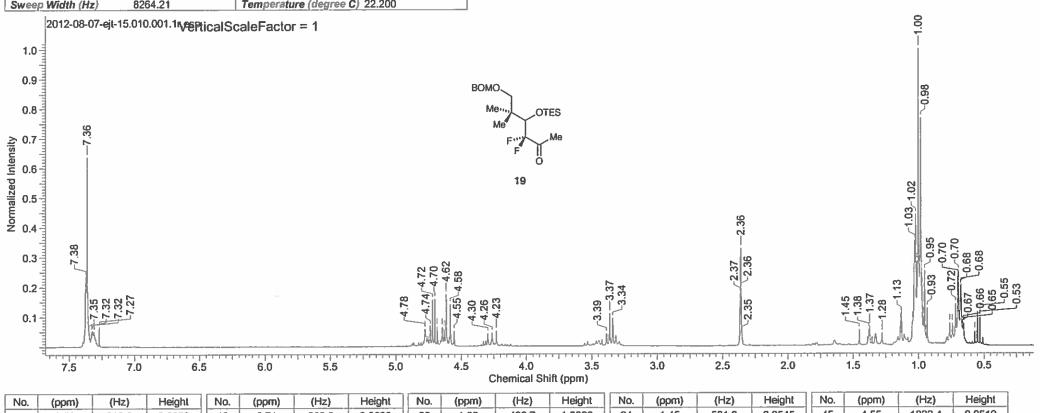


|         | ,  |      |         |       |      |
|---------|----|------|---------|-------|------|
| NAME    | 21 | 012- | -03-30- | -ejt∙ | -60  |
| EXPNO   |    |      |         | 10    |      |
| PROCNO  |    |      |         | 1     |      |
| Date_   |    |      | 20120   | 0330  |      |
| Time _  |    |      | 17      | 7.57  |      |
| INSTRUM |    |      | A)      | 7400  |      |
| PROBHD  | 5  | mm   | PABBO   | BB-   |      |
| PULPROG |    |      |         | zg    |      |
| TD      |    |      | 133     | L072  |      |
| SOLVENT |    |      | CI      | Cl3   |      |
| NS      |    |      |         | 16    |      |
| DS      |    |      |         | 4     |      |
| SWH     |    |      | 89285   | 711   | Hz   |
| FIDRES  |    |      | 0.681   | 1196  | Hz   |
| AQ      |    |      | 0.7340  | )532  | sec  |
| RG      |    |      | 4       | 1100  |      |
| DW      |    |      | 5.      | 600   | used |
| DE      |    |      | 11      | L.01  | used |
| TE      |    |      | 29      | 95.1  | K    |
| D1      |    | 3    | L.00000 | 0000  | sec  |
| TD0     |    |      |         | 1     |      |
|         |    |      |         |       |      |

| ======= | CHANNEL fl ====== |
|---------|-------------------|
| NUCl    | 19F               |
| P1      | 10.70 used        |
| PL1     | -5.00 dB          |
| PL1W    | 27.00716019 W     |
| SF01    | 376.4607164 MHz   |
| SI      | 262144            |
| SF      | 376.4983660 MHz   |
| WDW     | EM                |
| SSB     | 0                 |
| LB      | 0.30 Hz           |
| GB      | 0                 |
| PC      | 2.00              |
|         |                   |

29/11/2012 17:03:06

| Acquisition Time (sec) | 3.9649                | Comment                     | ejt cry meli mPROTO   | N CDCI3 (e:\bruk400data\2    | 2012\Aug} ejt 15 | Date                  | 07 Aug 2012 16:04:32 |
|------------------------|-----------------------|-----------------------------|-----------------------|------------------------------|------------------|-----------------------|----------------------|
| Date Stamp             | 07 Aug 2012 16:04:32  | 2                           |                       |                              |                  |                       |                      |
| File Name              | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bri | uk400data\2012\Aug\da | sta\ejt\nmr\2012-08-07-ejt-1 | 5\10\pdata\1\1r  | Frequency (MHz)       | 400.13               |
| Nucleus                | 1H                    | Number of Transients        | 16                    | Origin                       | AV400            | Original Points Count | 32768                |
| Owner                  | Administrator         | Points Count                | 32768                 | Pulse Sequence               | zg30b            | Receiver Gain         | 57.00                |
| SW(cyclical) (Hz)      | 8264.46               | Solvent                     | CHLOROFORM-d          | Spectrum Offset (Hz)         | 2464.9272        | Spectrum Type         | STANDARD             |
| Sween Width (Hz)       | 8264 21               | Temperature (degree C       | 1 22 200              |                              |                  |                       |                      |



| No. | (ppm) | (Hz)  | Height | No. | (ppm) | (Hz)  | Height | No. | (ppm) | Hz)   | Height | No. | (ppm) | (HZ)   | Height | NO. | (ppm) | (HZ)   | Height |
|-----|-------|-------|--------|-----|-------|-------|--------|-----|-------|-------|--------|-----|-------|--------|--------|-----|-------|--------|--------|
| 1   | 0.53  | 212.0 | 0.0952 | 12  | 0.71  | 282.9 | 0.0629 | 23  | 1.00  | 400.7 | 1.0000 | 34  | 1.45  | 581.3  | 0.0545 | 45  | 4.55  | 1822.4 | 0.0519 |
| 2   | 0.55  | 220.1 | 0.1146 | 13  | 0.72  | 287.2 | 0.1403 | 24  | 1.01  | 404.7 | 0.2829 | 35  | 2.35  | 941.7  | 0.0446 | 46  | 4.58  | 1834.0 | 0.1428 |
| 3   | 0.57  | 228.2 | 0.0492 | 14  | 0.74  | 296.8 | 0.0743 | 25  | 1.02  | 408.8 | 0.4415 | 36  | 2.36  | 943.5  | 0.1913 | 47  | 4.62  | 1846.9 | 0.1761 |
| 4   | 0.65  | 262.0 | 0.0748 | 15  | 0.76  | 304.9 | 0.0762 | 26  | 1.03  | 410.5 | 0.2809 | 37  | 2.36  | 945.2  | 0.3289 | 48  | 4.63  | 1853.2 | 0.0599 |
| 5   | 0.66  | 264.3 | 0.0802 | 16  | 0.93  | 373.5 | 0.1267 | 27  | 1.03  | 412.1 | 0.3534 | 38  | 2.37  | 946.7  | 0.1756 | 49  | 4.65  | 1858.7 | 0.0647 |
| 6   | 0.67  | 266.8 | 0.0663 | 17  | 0.94  | 377.2 | 0.0432 | 28  | 1.04  | 417.9 | 0.0848 | 39  | 3.34  | 1337.2 | 0.0945 | 50  | 4.69  | 1874.6 | 0.0660 |
| 7   | 0.68  | 270.3 | 0.2067 | 18  | 0.95  | 381.3 | 0.2509 | 29  | 1.13  | 451.9 | 0.0942 | 40  | 3.37  | 1346.5 | 0.1099 | 51  | 4.70  | 1881.2 | 0.1598 |
| 8   | 0.68  | 272.1 | 0.2004 | 19  | 0.96  | 385.1 | 0.0987 | 30  | 1.13  | 453.4 | 0.1088 | 41  | 3.39  | 1355.8 | 0.0427 | 52  | 4.72  | 1888.5 | 0.1570 |
| 9   | 0.69  | 275.1 | 0.0892 | 20  | 0.97  | 389.4 | 0.1997 | 31  | 1.28  | 511.2 | 0.0430 | 42  | 4.23  | 1692.8 | 0.0518 | 53  | 4.74  | 1895.1 | 0.0676 |
| 10  | 0.70  | 278.6 | 0.2478 | 21  | 0.98  | 392.9 | 0.7667 | 32  | 1.37  | 549.0 | 0.0650 | 43  | 4.26  | 1706.1 | 0.0454 | 54  | 4.74  | 1896.8 | 0.0426 |
| 11  | 0.70  | 279.6 | 0.2340 | 22  | 0.99  | 396.9 | 0.2736 | 33  | 1.38  | 552.0 | 0.0558 | 44  | 4.30  | 1719.0 | 0.0431 | 55  | 4.78  | 1910.7 | 0.0575 |

30/11/2012 10:40:20

|                                                                    |        |                                        |          |              |              |                   |                  |          |              |              |           |            |          |              |                  |            | 30/        | 11/2012 10:40 |
|--------------------------------------------------------------------|--------|----------------------------------------|----------|--------------|--------------|-------------------|------------------|----------|--------------|--------------|-----------|------------|----------|--------------|------------------|------------|------------|---------------|
| Acquisition Time                                                   |        | 0835                                   |          | Commen       | 1            | ejt cry n         | neli mC/         | ARBONnig | ht CDCI3 (e: | \bruk400dat  | a\2012\A  | ug) ejt 15 | Date     |              | 0                | 8 Aug 2012 | 2 01:51:12 |               |
| Date Stamp                                                         |        | Aug 2012 0                             |          |              |              |                   |                  |          |              |              |           |            |          |              |                  |            |            |               |
| File Name                                                          | l/s    | s7a.ds.man.                            | ac.uk\vc | l5\vol3\user | s\snmrdata\t | ruk400data        | 2012VA           |          | nmr\2012-08  | -07-ejt-15\2 | 2\pdata\1 | \1г        | Freque   | ncy (MHz)    |                  | 00.61      |            |               |
| Nucleus                                                            | 13     | C                                      |          | Number o     | of Transient | s 1000            |                  | 0        | rigin        |              | AV400     |            | Origina  | il Points Co |                  | 2768       |            |               |
| Owner                                                              | Ac     | Iministrator                           |          | Points Co    | ount         | 32768             |                  | P        | ulse Seguen  | ıce          | zgpg30    |            | Receiv   | er Gain      | 5                | 12.00      |            |               |
| SW(cyclical) (Hz)                                                  | 30     | 241.94                                 |          | Solvent      |              | CHLOF             | OFOR             | VI-d S   | pectrum Off  | set (Hz)     | 11330.3   | 838        | Spectro  | ım Type      | S                | STANDARD   | )          |               |
| Sweep Width (Hz)                                                   | 30     | 241.01                                 |          | Temperat     | ure (degree  | <b>C</b> ) 23.100 |                  |          |              |              |           |            |          |              |                  |            |            |               |
| 1.0<br>0.9<br>0.8<br>0.7<br>0.6<br>0.5<br>0.5<br>0.4<br>0.3<br>0.2 | 199.11 | 2.001.1r <sub>v</sub> e <sub>p</sub> p |          |              |              | 140               | 05 127.68 127.84 | 150      | . ]          | 00 90        | 15.77     |            | -62.69   |              | 05-1/-38.9138.84 | -29.6      | 20.94      | 0-5.04 -6.84  |
| No. (ppm)                                                          | (Hz)   | Height                                 | No.      | (ppm)        | (Hz)         | Height            | No.              | (ppm)    | (Hz)         | Height       | No.       | (ppm)      | (Hz)     | Height       | No.              | (ppm)      | (Hz)       | Height        |
| 1 5.04                                                             | 506.9  | 0.5443                                 | 11       | 13.78        | 1386.5       | 0.0286            | 21               | 69.31    | 6973.8       | 0.0433       | 31        | 77.00      | 7747.2   | 1.0000       | 41               | 127.84     | 12862.0    | 0.4885        |
| 2 5.40                                                             | 542.9  | 0.1020                                 | 12       | 20.94        | 2107.3       | 0.1033            | 22               | 69.37    | 6979.3       | 0.2156       | 32        | 77.31      | 7778.6   | 0.9035       | 42               | 127.93     | 12871.2    | 0.0317        |
| 3 5.47                                                             | 550.3  | 0.0425                                 | 13       | 21.12        | 2124.8       | 0.0187            | 23               | 69.45    | 6987.6       | 0.0507       | 33        | 90.76      | 9131.5   | 0.0177       | 43               | 128.40     | 12918.3    | 0.5878        |
| 4 6.26                                                             | 629.7  | 0.0241                                 | 14       | 21.60        | 2172.8       | 0.1212            | 24               | 69.79    | 7021.8       | 0.0204       | 34        | 94.50      | 9508.1   | 0.2119       | 44               | 137.72     | 13856.9    | 0.1744        |
| 5 6.38                                                             | 641.7  | 0.0241                                 | 15       | 26.00        | 2615.8       | 0.1999            | 25               | 74.17    | 7462.0       | 0.1225       | 35        | 94.68      | 9525.6   | 0.0300       | 45               | 137.80     | 13864.2    | 0.0260        |
| 6 6.74                                                             | 678.6  | 0.1336                                 | 16       | 29.68        | 2985.9       | 0.1999            | 26               | 74.54    | 7499.8       | 0.0398       | 36        | 94.71      | 9529.3   | 0.0407       | 46               | 199.11     | 20033.0    | 0.0260        |
|                                                                    |        | -                                      | 17       | 38.84        | 3907.9       | 0.1899            | 27               | 74.63    | 7509.1       | 0.0360       | 37        | 117.14     | 11785.8  | 0.0240       | 47               | 199.41     | 20063.4    | 0.0447        |
|                                                                    | 681.4  | 0.1883                                 |          | ž            |              |                   |                  |          |              | 1            | 38        | 119.71     | 12044.3  | 0.0240       | 48               | 199.72     | 20093.9    | 0.0240        |
| 8 6.80                                                             | 684.1  | 0.1352                                 | 18       | 38.91        | 3915.3       | 0.0243            | 28               | 74.78    | 7523.8       | 0.0857       | 7 —       |            | 1        |              | 40               | 155.12     | 20093.9    | 0.0240        |
| 9 6.84                                                             | 687.8  | 0.7244                                 | 19       | 39.72        | 3996.5       | 0.0196            | 29               | 75.02    | 7547.8       | 0.0449       | 39        | 127.68     | 12846.3  | 0.2237       |                  |            |            |               |
|                                                                    | 7000   | 1 0 4000 1                             | . ~~     |              |              | 0.0000            | - 20             | . 70.00  | 77440        | . 0.0700     | 11 40 1   | 477 07     | : 400004 | 0.7060       |                  |            |            |               |

30

0.0302

76.68

7714.9

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10

6.98

702.6

0.1890

20

62.69

6307.4

127.82

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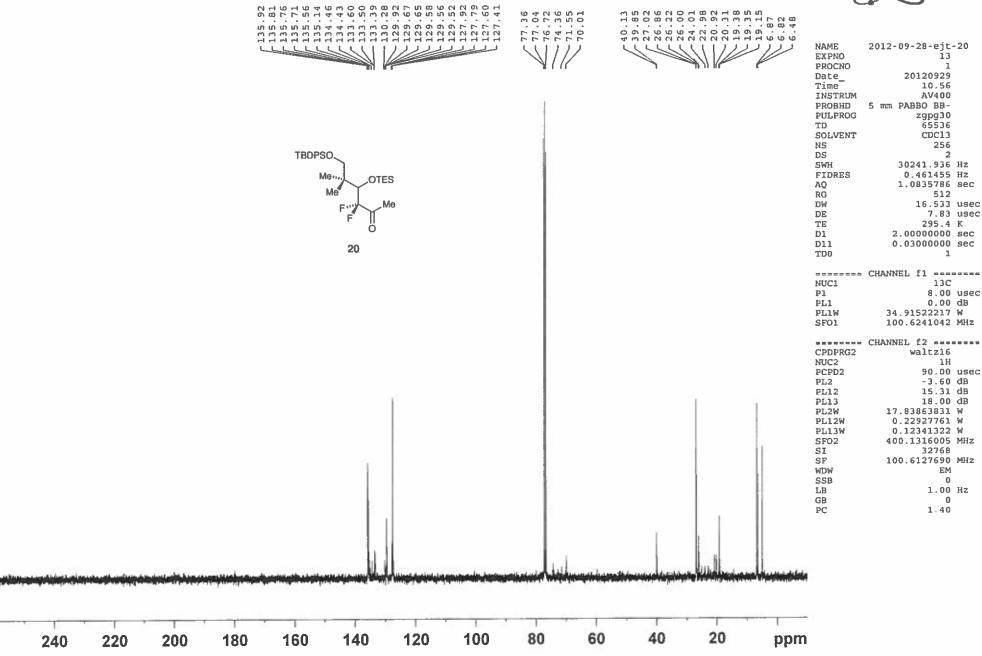
12860.1

29/11/2012 13:22:34

|                                                       |                                                                              | _ <del>.</del>                                                               |                                                                |                             |                                                               |                                                                              |                                                                |                             |                                                               |                                                                                                                                     |                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                     |                                                                |                                                            |                                                                              |                                                                                     |                                                                |
|-------------------------------------------------------|------------------------------------------------------------------------------|------------------------------------------------------------------------------|----------------------------------------------------------------|-----------------------------|---------------------------------------------------------------|------------------------------------------------------------------------------|----------------------------------------------------------------|-----------------------------|---------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|----------------------------------------------------------------|------------------------------------------------------------|------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|----------------------------------------------------------------|
|                                                       | sition Time                                                                  |                                                                              |                                                                | ł                           | Comment                                                       |                                                                              | ejt cry m                                                      | neli 3 mP                   | ROTON C                                                       | DCI3 /opt/bruk500                                                                                                                   | data/2012/O                                              | t ejt 34                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Date                                                                                |                                                                | 19                                                         | Oct 2012 1                                                                   | 11:33:36                                                                            |                                                                |
|                                                       | Stamp                                                                        |                                                                              | Oct 2012 11:                                                   |                             |                                                               |                                                                              |                                                                |                             |                                                               |                                                                                                                                     |                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                     |                                                                |                                                            |                                                                              |                                                                                     |                                                                |
| ile Na                                                |                                                                              |                                                                              |                                                                | c.uk\vol                    |                                                               | \snmrdata\b                                                                  |                                                                | \bruk500                    |                                                               | Oct\data\ejt\nmr\2                                                                                                                  |                                                          | -34\10\pdata\                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                                                     |                                                                |                                                            |                                                                              |                                                                                     |                                                                |
|                                                       | ency (MHz)                                                                   |                                                                              | 0.13                                                           |                             | Nucleus                                                       |                                                                              | <u>1H</u>                                                      |                             |                                                               | mber of Transien                                                                                                                    |                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Origin                                                                              |                                                                |                                                            | ect                                                                          |                                                                                     |                                                                |
|                                                       | al Points C                                                                  |                                                                              | 768                                                            |                             | Owner                                                         |                                                                              | vnmr1                                                          |                             |                                                               | ints Count                                                                                                                          | 32768                                                    | 0.700                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Pulse Se                                                                            |                                                                |                                                            | 30b                                                                          |                                                                                     |                                                                |
|                                                       | ver Gain                                                                     |                                                                              | 0.80                                                           |                             | SW(cyclic                                                     |                                                                              | 10330.5                                                        |                             |                                                               | lvent                                                                                                                               |                                                          | OFORM-d                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Spectrui                                                                            | m Offset (Ha                                                   | z) 30                                                      | 80.2925                                                                      |                                                                                     |                                                                |
| pectr                                                 | rum Type                                                                     |                                                                              | FANDARD                                                        |                             | Sweep Win                                                     |                                                                              | 10330.2                                                        | (6                          | lei                                                           | mperature (degre                                                                                                                    | (C) 27.000                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                     |                                                                |                                                            |                                                                              |                                                                                     | 3                                                              |
| 1.0 - 0.9 - 0.8 - 0.7 - 0.6 - 0.5 - 0.4 - 0.4 -       | ]                                                                            | o ojeonio (C                                                                 | 0.001.1 <b>ı√eşp</b> ti                                        | caisc                       | aleraciói                                                     | -1                                                                           |                                                                |                             | TBDPS<br>A                                                    | OTES Me F O  20                                                                                                                     |                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                     |                                                                |                                                            | -1.12                                                                        |                                                                                     |                                                                |
| 0.5 -<br>0.4 -<br>0.3 -<br>0.2 -                      | 1                                                                            | 7.68                                                                         | 7.44                                                           | L7.39                       | 7                                                             |                                                                              |                                                                |                             |                                                               | 4.35                                                                                                                                | 3.52<br>-3.48<br>-3.42                                   | 13.34<br>13.34<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>13.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44<br>14.44 | 2.34                                                                                |                                                                | 1.57                                                       |                                                                              | 0.50                                                                                | 0.55                                                           |
| 0.3                                                   | 8.5                                                                          | 7.68                                                                         | 7.44                                                           | 7.39                        | 6.5                                                           | 6.0                                                                          | 5.5                                                            | ;                           |                                                               | 4.5 4.0<br>Chemical Shift (pp                                                                                                       |                                                          | 3.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 2.5                                                                                 | 2.0                                                            | 1.5                                                        | 0.1.15                                                                       | 0.59                                                                                | 0.55                                                           |
| 0.3 -<br>0.2 -<br>0.1 -                               | 8.5<br>(ppm)                                                                 | (Hz)                                                                         | Height                                                         | No.                         | (ppm)                                                         | (Hz)                                                                         | Height                                                         | No.                         | (ppm)                                                         | 4.5 4.0 Chemical Shift (pp                                                                                                          | n)<br>ght No.                                            | (ppm)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 2.5 (Hz)                                                                            | Height                                                         | 1.5                                                        | 0.1 (bbu)                                                                    | 0.5<br>65.0<br>0.5<br>0.5<br>(Hz)                                                   | Height                                                         |
| 0.3 -<br>0.2 -<br>0.1 -                               | 8.5<br>(ppm)                                                                 | (Hz)<br>267.7                                                                | Height 0.0431                                                  | No.                         | (ppm)<br>0.63                                                 | (Hz)<br>314.0                                                                | Height 0.0186                                                  | No.<br>23                   | (ppm)<br>0.94                                                 | 4.5 4.0<br>Chemical Shift (pp<br>(Hz) He<br>469.1 0.3                                                                               | n)<br>ght No.<br>353 34                                  | (ppm)<br>1.03                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 2.5 (Hz) 517.0                                                                      | Height 0.0402                                                  | 1.5<br>No.<br>45                                           | 1.0 (ppm)<br>1.16                                                            | 09:0<br>09:0<br>0.5<br>(Hz)<br>581.4                                                | Height 0.0182                                                  |
| 0.3 -<br>0.2 -<br>0.1 -                               | 8.5<br>(ppm)<br>0.54<br>0.54                                                 | (Hz)<br>267.7<br>268.9                                                       | Height 0.0431 0.0464                                           | No.<br>12<br>13             | (ppm)<br>0.63<br>0.63                                         | (Hz)<br>314.0<br>317.2                                                       | Height 0.0186 0.0284                                           | No. 23 24                   | (ppm)<br>0.94<br>0.96                                         | 4.5 4.0<br>Chemical Shift (pp<br>(Hz) He<br>469.1 0.3<br>478.9 0.0                                                                  | n) ght No. 353 34 683 35                                 | (ppm)<br>1.03<br>1.04                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 2.5 (Hz) 517.0 518.6                                                                | Height 0.0402 0.0352                                           | 1.5<br>No.<br>45<br>46                                     | 1.0 (ppm)<br>1.16<br>1.17                                                    | 09:0<br>09:0<br>0.5<br>(Hz)<br>581.4<br>584.8                                       | Height 0.0182 0.0152                                           |
| 0.3 -<br>0.2 -<br>0.1 -<br>1   2   3                  | 8.5<br>(ppm)<br>0.54<br>0.54<br>0.55                                         | (Hz)<br>267.7<br>268.9<br>276.8                                              | Height 0.0431 0.0464 0.1038                                    | No.<br>12<br>13<br>14       | (ppm)<br>0.63<br>0.63<br>0.65                                 | (Hz)<br>314.0<br>317.2<br>325.0                                              | Height 0.0186 0.0284 0.0140                                    | No. 23 24 25                | (ppm)<br>0.94<br>0.96<br>0.96                                 | 4.5 4.0<br>Chemical Shift (pp<br>(Hz) He<br>469.1 0.3<br>478.9 0.0<br>481.4 0.0                                                     | m) ght No. 353 34 383 35 315 36                          | (ppm)<br>1.03<br>1.04<br>1.04                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 2.5 (Hz) 517.0 518.6 522.4                                                          | Height 0.0402 0.0352 0.0359                                    | 1.5<br>No.<br>45<br>46<br>47                               | 1.0<br>(ppm)<br>1.16<br>1.17<br>1.28                                         | 0.5<br>0.5<br>0.5<br>0.5<br>0.5<br>0.5<br>0.5                                       | Height 0.0182 0.0152 0.1818                                    |
| 0.3 - 0.2 - 0.1 - 0.1 - 1   2   3   4                 | 8.5<br>(ppm)<br>0.54<br>0.54                                                 | (Hz)<br>267.7<br>268.9                                                       | Height 0.0431 0.0464                                           | No.<br>12<br>13<br>14<br>15 | (ppm)<br>0.63<br>0.63<br>0.65<br>0.67                         | (Hz)<br>314.0<br>317.2<br>325.0<br>336.7                                     | Height 0.0186 0.0284 0.0140 0.0190                             | No. 23 24 25 26             | (ppm)<br>0.94<br>0.96<br>0.96<br>0.97                         | 4.5 4.0<br>Chemical Shift (pp<br>(Hz) He<br>469.1 0.3<br>478.9 0.0<br>481.4 0.0<br>486.8 0.0                                        | ght No. 353 34 683 35 36 15 36 37                        | (ppm)<br>1.03<br>1.04<br>1.04<br>1.06                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 2.5<br>(Hz)<br>517.0<br>518.6<br>522.4<br>531.2                                     | Height 0.0402 0.0352 0.0359 0.1567                             | 1.5<br>No.<br>45<br>46<br>47<br>48                         | 1.0<br>(ppm)<br>1.16<br>1.17<br>1.28<br>1.34                                 | 0.5<br>(Hz)<br>581.4<br>584.8<br>639.0<br>671.2                                     | Height 0.0182 0.0152 0.1818 0.0200                             |
| 0.3 - 0.2 - 0.1 - 0.1 - 1 2 3 4                       | 8.5<br>(ppm)<br>0.54<br>0.54<br>0.55                                         | (Hz)<br>267.7<br>268.9<br>276.8                                              | Height 0.0431 0.0464 0.1038                                    | No.<br>12<br>13<br>14<br>15 | (ppm)<br>0.63<br>0.63<br>0.65                                 | (Hz)<br>314.0<br>317.2<br>325.0<br>336.7<br>344.9                            | Height 0.0186 0.0284 0.0140                                    | No. 23 24 25 26 27          | (ppm)<br>0.94<br>0.96<br>0.96<br>0.97<br>0.98                 | 4.5 4.0<br>Chemical Shift (pp<br>(Hz) He<br>469.1 0.3<br>478.9 0.0<br>481.4 0.0<br>486.8 0.0<br>491.5 0.0                           | m) ght No. 353 34 683 35 615 36 106 37 607 38            | (ppm)<br>1.03<br>1.04<br>1.04<br>1.06<br>1.07                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 2.5<br>(Hz)<br>517.0<br>518.6<br>522.4<br>531.2<br>534.1                            | Height 0.0402 0.0352 0.0359 0.1567 0.0731                      | 1.5<br>No.<br>45<br>46<br>47<br>48<br>49                   | 1.0<br>(ppm)<br>1.16<br>1.17<br>1.28<br>1.34<br>1.36                         | 0.5<br>(Hz)<br>581.4<br>584.8<br>639.0<br>671.2<br>678.5                            | Height 0.0182 0.0152 0.1818 0.0200 0.0397                      |
| 0.3 - 0.2 - 0.1 - 0.1 - 1 2 3 4 5 5                   | 8.5<br>(ppm)<br>0.54<br>0.54<br>0.55<br>0.56                                 | (Hz)<br>267.7<br>268.9<br>276.8<br>282.5                                     | Height 0.0431 0.0464 0.1038 0.0932                             | No.<br>12<br>13<br>14<br>15 | (ppm)<br>0.63<br>0.63<br>0.65<br>0.67                         | (Hz)<br>314.0<br>317.2<br>325.0<br>336.7                                     | Height 0.0186 0.0284 0.0140 0.0190                             | No. 23 24 25 26 27 28       | (ppm)<br>0.94<br>0.96<br>0.96<br>0.97                         | 4.5 4.0<br>Chemical Shift (pp<br>(Hz) He<br>469.1 0.3<br>478.9 0.0<br>481.4 0.0<br>486.8 0.0<br>491.5 0.0                           | ght No. 353 34 683 35 36 15 36 37                        | (ppm)<br>1.03<br>1.04<br>1.04<br>1.06                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 2.5<br>(Hz)<br>517.0<br>518.6<br>522.4<br>531.2                                     | Height 0.0402 0.0352 0.0359 0.1567                             | 1.5<br>No.<br>45<br>46<br>47<br>48                         | 1.0<br>(ppm)<br>1.16<br>1.17<br>1.28<br>1.34                                 | 0.5<br>(Hz)<br>581.4<br>584.8<br>639.0<br>671.2                                     | Height 0.0182 0.0152 0.1818 0.0200                             |
| 0.3-<br>0.2-<br>0.1-<br>0.1-<br>2<br>3<br>4<br>5<br>6 | 8.5<br>(ppm)<br>0.54<br>0.54<br>0.55<br>0.56<br>0.57                         | (Hz)<br>267.7<br>268.9<br>276.8<br>282.5<br>284.7                            | Height 0.0431 0.0464 0.1038 0.0932 0.1130                      | No.<br>12<br>13<br>14<br>15 | (ppm)<br>0.63<br>0.63<br>0.65<br>0.67<br>0.69                 | (Hz)<br>314.0<br>317.2<br>325.0<br>336.7<br>344.9                            | Height 0.0186 0.0284 0.0140 0.0190 0.0219                      | No. 23 24 25 26 27          | (ppm)<br>0.94<br>0.96<br>0.96<br>0.97<br>0.98                 | 4.5 4.0<br>Chemical Shift (pp<br>(Hz) He<br>469.1 0.3<br>478.9 0.0<br>481.4 0.0<br>486.8 0.0<br>491.5 0.0                           | m)  ght No. 353 34 383 35 363 36 360 37 3607 38 414 39   | (ppm)<br>1.03<br>1.04<br>1.04<br>1.06<br>1.07                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 2.5<br>(Hz)<br>517.0<br>518.6<br>522.4<br>531.2<br>534.1                            | Height 0.0402 0.0352 0.0359 0.1567 0.0731                      | 1.5<br>No.<br>45<br>46<br>47<br>48<br>49                   | 1.0<br>(ppm)<br>1.16<br>1.17<br>1.28<br>1.34<br>1.36                         | 0.5<br>(Hz)<br>581.4<br>584.8<br>639.0<br>671.2<br>678.5<br>685.7<br>719.8          | Height 0.0182 0.0152 0.1818 0.0200 0.0397                      |
| 0.3-<br>0.2-<br>0.1-<br>1<br>2<br>3<br>4<br>5<br>6    | 8.5<br>(ppm)<br>0.54<br>0.54<br>0.55<br>0.56<br>0.57<br>0.58                 | (Hz)<br>267.7<br>268.9<br>276.8<br>282.5<br>284.7<br>290.4                   | Height 0.0431 0.0464 0.1038 0.0932 0.1130 0.0931               | No. 12 13 14 15 16 17       | (ppm)<br>0.63<br>0.63<br>0.65<br>0.67<br>0.69                 | (Hz)<br>314.0<br>317.2<br>325.0<br>336.7<br>344.9<br>352.8                   | Height 0.0186 0.0284 0.0140 0.0190 0.0219 0.0133               | No. 23 24 25 26 27 28       | (ppm)<br>0.94<br>0.96<br>0.96<br>0.97<br>0.98                 | 4.5 4.0<br>Chemical Shift (pp<br>(Hz) He<br>469.1 0.3<br>478.9 0.0<br>481.4 0.0<br>486.8 0.0<br>491.5 0.0<br>494.7 0.0              | m)  ght No. 353 34 683 35 615 36 607 38 614 39 647 40    | (ppm)<br>1.03<br>1.04<br>1.04<br>1.06<br>1.07                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 2.5<br>(Hz)<br>517.0<br>518.6<br>522.4<br>531.2<br>534.1<br>536.9                   | Height 0.0402 0.0352 0.0359 0.1567 0.0731 0.0888               | 1.5<br>No.<br>45<br>46<br>47<br>48<br>49<br>50             | 1.0<br>(ppm)<br>1.16<br>1.17<br>1.28<br>1.34<br>1.36<br>1.37                 | 0.5<br>(Hz)<br>581.4<br>584.8<br>639.0<br>671.2<br>678.5<br>685.7<br>719.8<br>784.1 | Height 0.0182 0.0152 0.1818 0.0200 0.0397 0.0202               |
| 0.3                                                   | 8.5<br>(ppm)<br>0.54<br>0.54<br>0.55<br>0.56<br>0.57<br>0.58<br>0.59         | (Hz)<br>267.7<br>268.9<br>276.8<br>282.5<br>284.7<br>290.4<br>294.5          | Height 0.0431 0.0464 0.1038 0.0932 0.1130 0.0931 0.0897        | No. 12 13 14 15 16 17 18    | (ppm)<br>0.63<br>0.63<br>0.65<br>0.67<br>0.69<br>0.71         | (Hz)<br>314.0<br>317.2<br>325.0<br>336.7<br>344.9<br>352.8<br>430.3          | Height 0.0186 0.0284 0.0140 0.0190 0.0219 0.0133 0.0132        | No. 23 24 25 26 27 28 29    | (ppm)<br>0.94<br>0.96<br>0.96<br>0.97<br>0.98<br>0.99         | 4.5 4.0<br>Chemical Shift (pp<br>(Hz) He<br>469.1 0.3<br>478.9 0.0<br>481.4 0.0<br>486.8 0.0<br>491.5 0.0<br>494.7 0.0<br>499.4 0.0 | ght No. 353 34 683 35 3615 36 37 38 114 39 347 40 289 41 | (ppm)<br>1.03<br>1.04<br>1.04<br>1.06<br>1.07<br>1.07                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 2.5<br>(Hz)<br>517.0<br>518.6<br>522.4<br>531.2<br>534.1<br>536.9<br>537.8          | Height 0.0402 0.0352 0.0359 0.1567 0.0731 0.0888 0.0738        | 1.5<br>No.<br>45<br>46<br>47<br>48<br>49<br>50<br>51       | 1.0<br>(ppm)<br>1.16<br>1.17<br>1.28<br>1.34<br>1.36<br>1.37                 | 0.5<br>(Hz)<br>581.4<br>584.8<br>639.0<br>671.2<br>678.5<br>685.7<br>719.8          | Height 0.0182 0.0152 0.1818 0.0200 0.0397 0.0202 0.0216        |
| 0.3 - 0.2 - 0.1 - 1 2 3 4 5 6 7 8                     | 8.5<br>(ppm)<br>0.54<br>0.54<br>0.55<br>0.56<br>0.57<br>0.58<br>0.59<br>0.60 | (Hz)<br>267.7<br>268.9<br>276.8<br>282.5<br>284.7<br>290.4<br>294.5<br>298.6 | Height 0.0431 0.0464 0.1038 0.0932 0.1130 0.0931 0.0897 0.0594 | No. 12 13 14 15 16 17 18 19 | (ppm)<br>0.63<br>0.63<br>0.65<br>0.67<br>0.69<br>0.71<br>0.86 | (Hz)<br>314.0<br>317.2<br>325.0<br>336.7<br>344.9<br>352.8<br>430.3<br>441.1 | Height 0.0186 0.0284 0.0140 0.0190 0.0219 0.0133 0.0132 0.0372 | No. 23 24 25 26 27 28 29 30 | (ppm)<br>0.94<br>0.96<br>0.96<br>0.97<br>0.98<br>0.99<br>1.00 | 4.5 4.0 Chemical Shift (pp (Hz) He 469.1 0.3 478.9 0.0 481.4 0.0 491.5 0.0 494.7 0.0 499.4 0.0 504.7 0.0                            | ght No. 353 34 355 363 35 365 360 37 38 39 41 40 330 42  | (ppm)<br>1.03<br>1.04<br>1.04<br>1.06<br>1.07<br>1.07<br>1.08<br>1.09                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 2.5<br>(Hz)<br>517.0<br>518.6<br>522.4<br>531.2<br>534.1<br>536.9<br>537.8<br>542.9 | Height 0.0402 0.0352 0.0359 0.1567 0.0731 0.0888 0.0738 0.3437 | 1.5<br>No.<br>45<br>46<br>47<br>48<br>49<br>50<br>51<br>52 | 1.0<br>(ppm)<br>1.16<br>1.17<br>1.28<br>1.34<br>1.36<br>1.37<br>1.44<br>1.57 | 0.5<br>(Hz)<br>581.4<br>584.8<br>639.0<br>671.2<br>678.5<br>685.7<br>719.8<br>784.1 | Height 0.0182 0.0152 0.1818 0.0200 0.0397 0.0202 0.0216 0.0186 |

ejt cry meli mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} ejt 20





30/11/2012 11:35:13

|                                                                                                          | •                                      |         | _           |             |            |           |                  |                       |                   |                      |              |               |              |       |              | 30/                       | 11/2012 11:35:13 |
|----------------------------------------------------------------------------------------------------------|----------------------------------------|---------|-------------|-------------|------------|-----------|------------------|-----------------------|-------------------|----------------------|--------------|---------------|--------------|-------|--------------|---------------------------|------------------|
| Acquisition Time (sec)                                                                                   | 3.1719                                 | 10      | Comment     |             | ejt cry w  | ittig mPl | ROTON CI         | OCI3 /opt/bru         | ık500data/2       | 012/Aug              | ejt 15       | Date          |              | 06    | Aug 2012     | 11:08:00                  |                  |
| Date Stamp                                                                                               | 06 Aug 2012 11                         |         |             |             |            |           |                  |                       |                   |                      |              |               |              |       |              |                           |                  |
| File Name                                                                                                | \\ss7a.ds.man.a                        |         | \vol3\users | \snmrdata\t | ruk500data | bruk500   | )data\2012\      | Aug\data\ejt\         | .nmr\2012-0       | 8-06-ejt-            | 15\10\pdata\ | .1\1 <u>r</u> |              |       |              |                           |                  |
| Frequency (MHz)                                                                                          | 500.13                                 | ٨       | Vucleus     |             | 1H         |           | Nu               | mber of Tra           | nsients           | 16                   |              | Origin        |              | sp    | ect          |                           |                  |
| Original Points Count                                                                                    | 32768                                  | C       | Owner       |             | vnmr1      |           | Po               | ints Count            |                   | 32768                |              | Pulse S       | equence      | zg    | 3 <b>0</b> b |                           |                  |
| Receiver Gain                                                                                            | 90.50                                  | S       | SW(cyclica  | ıl) (Hz)    | 10330.5    | 8         | So               | vent                  |                   | CHLORO               | FORM-d       | Spectru       | m Offset (Ha | z) 30 | 80.2925      |                           |                  |
| Spectrum Type                                                                                            | STANDARD                               | S       | Sweep Wid   | fth (Hz)    | 10330.2    | 6         | Te               | nperature (           | degree C)         | 19.310               |              |               |              |       |              |                           |                  |
| 2012-08-06-ejt-1                                                                                         | 5.010.001.1 <b>ւ<sub>/ՔБРէ</sub></b> ј | calScal | leFactor    | = 1         |            |           |                  |                       |                   |                      |              |               |              |       |              | 0.98                      |                  |
| 0.9                                                                                                      |                                        |         |             | ВОМО        | _          |           |                  |                       |                   |                      |              |               |              |       |              |                           |                  |
| 0.8                                                                                                      |                                        |         |             | Me<br>N     | OTE        | S         |                  |                       |                   |                      |              |               |              |       |              |                           |                  |
| 0.7-9e-7-36                                                                                              |                                        |         |             |             | F          | /le       |                  |                       |                   |                      |              |               |              |       |              | :                         |                  |
| Normalized Intensity 0.0 0.0 0.4 0.0 0.4 0.0 0.4 0.0 0.4 0.0 0.4 0.3 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 |                                        |         |             |             | 21         |           |                  |                       |                   |                      |              |               |              |       |              | _                         |                  |
| 0.5 mg                                                                                                   |                                        |         |             |             |            |           |                  |                       |                   |                      |              |               | 191          |       |              | 1.01                      |                  |
| 2 0.4                                                                                                    |                                        |         |             |             |            |           |                  |                       |                   |                      |              |               |              |       | 9            | 2                         | T)               |
| 0.3                                                                                                      | 77.1-                                  |         |             |             |            | 4.75      | 583              |                       |                   |                      |              |               |              |       | 4            | 0.69                      | 0.67             |
| 0.2                                                                                                      | !                                      |         |             |             | 5.40       | -         | 4.65<br>4.56.4.6 | 22                    | 4                 | 32.42                |              |               |              |       | 1.44         | 96.071                    | 0.65             |
|                                                                                                          |                                        |         |             |             | 5 5        | 7.4       | 4114             | 4.07<br>-4.05<br>4.02 | ઌૄ૽               | 9.33<br>9.33<br>9.30 |              |               |              | 1.59  | .27          | o o                       | o<br>            |
| 0.1 4                                                                                                    |                                        |         |             |             |            |           |                  | 4                     |                   |                      |              |               | Į.           | 1     | Ī            | $\mathbb{N}_{\mathbb{N}}$ |                  |
| 1,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,                                                                  | <u> </u>                               |         |             |             |            | 11111     |                  |                       |                   |                      | 3.0          | 2.5           | 2.0          | 1.    |              | 1.0                       | 0.5              |
| 7.5                                                                                                      | 7.0                                    | 6.5     | 6.0         | 5.          | o :        | i.0       | 4.5              | 4.0<br>Chemical Sh    | 3.5<br>aift (ppm) |                      | 3.0          | 2.5           | 2.0          |       |              |                           | 0.5              |
| No. (ppm) (Hz                                                                                            | z) Height                              | No.     | (ppm)       | (Hz)        | Height     | No.       | (ppm)            | (Hz)                  | Height            | No.                  | (ррт)        | (Hz)          | Height       | No.   | (ppm)        | (Hz)                      | Height           |
| 1 0.65 327                                                                                               | .6 0.0833                              | 10      | 0.96        | 481.7       | 0.0726     | 19        | 3.30             | 1649.5                | 0.0662            | 28                   | 4.63         | 2314.0        | 0.1497       | 37    | 7.31         | 3654.5                    | 0.0471           |
| 2 0.66 330                                                                                               | .7 0.0898                              | 11      | 0.98        | 487.7       | 0.9220     | 20        | 3.32             | 1658.6                | 0.0885            | 29                   | 4.65         | 2325.7        | 0.0829       | 38    | 7.31         | 3657.7                    | 0.0381           |
| 3 0.67 335                                                                                               | .8 0.2117                              | 12      | 0.99        | 495.3       | 1.0000     | 21        | 3.42             | 1709.4                | 0.1050            | 30                   | 4.73         | 2365.7        | 0.0640       | 39    | 7.32         | 3659.6                    | 0.0439           |
| 4 0.68 338                                                                                               | .6 0.2200                              | 13      | 1.01        | 503.5       | 0.4271     | 22        | 3.44             | 1718.5                | 0.0793            | 31                   | 4.74         | 2372.4        | 0.1916       | 40    | 7.32         | 3663.1                    | 0.0375           |
| 5 0.69 344                                                                                               |                                        | 14      | 1.03        | 517.4       | 0.3013     | 23        | 4.02             | 2012.3                | 0.0466            | 32                   | 4.75         | 2377.7        | 0.1894       | 41    | 7.35         | 3676.0                    | 0.0414           |
| 6 0.69 346                                                                                               |                                        | 15      | 1.27        | 632.7       | 0.0427     | 24        | 4.05             | 2023.1                | 0.0813            | 33                   | 4.77         | 2384.3        | 0.0667       | 42    | 7.36         | 3681.0                    | 0.6262           |
| 7 0.70 352                                                                                               |                                        | 16      | 1.44        | 722.6       | 0.1420     | 25        | 4.07             | 2033.8                | 0.0442            | 34                   | 5.15         | 2575.1        | 0.0948       | 43    | 7.37         | 3684.5                    | 0.2032           |
| 8 0.71 354                                                                                               |                                        | 17      | 1.59        | 794.5       | 0.0578     | 26        | 4.56             | 2281.3                | 0.0744            | 35                   | 5.40         | 2701.8        | 0.0979       | 44    | 7.37         | 3686.1                    | 0.2121           |
| 9 0.95 474                                                                                               | .8 0.0435                              | 18      | 1.91        | 956.8       | 0.3996     | 27        | 4.58             | 2292.9                | 0.1522            | 36                   | 7.27         | 3635.9        | 0.2110       |       |              |                           |                  |

30/11/2012 11:46:40

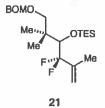
|                                                              |              |               | <del>.</del>                  |                    |              |            | ****      |                     |                   |                  |           |              |             |              |                                        |            |                                                | 11/2012 11:       | 46:40    |
|--------------------------------------------------------------|--------------|---------------|-------------------------------|--------------------|--------------|------------|-----------|---------------------|-------------------|------------------|-----------|--------------|-------------|--------------|----------------------------------------|------------|------------------------------------------------|-------------------|----------|
| Acquisition Time (                                           |              | 010           | 4.00.04                       | Commen             | £            | ejt cry v  | vittig m( | ARBONIII            | ght CDCI3 /d      | pvbruk500d       | lata/2012 | /Aug ejt 23  | Date        |              |                                        | 06 Aug 201 | 2 14:26:24                                     |                   |          |
| Date Stamp File Name                                         |              | Aug 2012 1    |                               | IE)vol2)vicos      | eleamedatali | auk600data | hauk50    | 34345\2012\         | Aug\data\ejt\     | nm42012 0        | 9 06 dt 1 | 22\10\ndata\ | 1116        |              |                                        |            |                                                |                   |          |
| Frequency (MHz)                                              |              | 5.76          | ac.ukwo                       | Nucleus            | Sistinualau  | 13C        | טוטאטוט   |                     | umber of Ti       |                  | 1000      | corropoalar  | Origin      |              |                                        | spect      |                                                |                   |          |
| Original Points Co                                           |              |               |                               | Owner              |              | vnmr1      |           |                     | oints Count       |                  | 32768     |              |             | Sequence     |                                        | zgpg30     |                                                |                   |          |
| Receiver Gain                                                |              | 2.00          |                               | SW(cyclic          | onli /H=1    | 29761.9    | 20        |                     | olvent            |                  |           | OFORM-d      | -           | rum Offset ( |                                        | 12570.2578 |                                                |                   |          |
| Spectrum Type                                                |              | ANDARD        |                               | Sweep W            |              | 29761.     |           |                     | emperature        | (degree C)       |           | OFORIVI-U    | Speca       | rum Onsec    | 112)                                   | 12370.2370 | <u>,                                      </u> |                   |          |
| 2012-08-06                                                   |              |               | RcalSc                        |                    |              | 20101.     |           |                     | 77.00             | 100g.00 0)       | 10.000    |              |             |              |                                        |            |                                                |                   |          |
| Normalized Intensity 0.40 0.00 0.00 0.10 0.10 0.10 0.10 0.10 | t 140.59<br> | 128.40 127.84 | ~123.22<br>~121.26<br>~119.29 | 116.22<br>(-116.08 | BOMC<br>Me   | )          | S<br>Ne   |                     | 75.02             |                  |           |              | -38.81      | -30.29       | 21 14                                  |            |                                                |                   |          |
| 0                                                            |              |               |                               | L                  |              |            |           | والمراجعة والمراجعة | JU                |                  |           |              |             |              | ······································ |            |                                                | <b>VALUE - 10</b> | -        |
| <del>1,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,</del>             | 136          | 128           | 120                           | 0 112              | 2 104        | 96         | 88        |                     | 72<br>Chemical SI | 64<br>hift (ppm) | 56        | 48           | <del></del> | 32           | 24                                     | 16         | <del>1111111111111</del><br>8                  | 0                 | -8<br>8- |
| No. (ppm)                                                    | (Hz)         | Height        | No.                           | (ppm)              | (Hz)         | Height     | No.       | (ppm)               | (Hz)              | Height           | No.       | (ppm)        | (Hz)        | Height       | No.                                    | (ppm)      | (Hz)                                           | Height            | ]        |
| 1 5.04                                                       | 633.4        | 0.2561        | 8                             | 21.14              | 2657.9       | 0.0346     | 15        | 76.75               | 9651.6            | 0.9667           | 22        | 116.22       | 14616.1     | 0.0151       | 29                                     | 127.99     | 16095.7                                        | 0.0101            |          |
| 2 6.41                                                       | 806.0        | 0.0136        | 9                             | 30.29              | 3808.7       | 0.0208     | 16        | 76.86               | 9666.1            | 0.0343           | 23        | 119.29       | 15002.1     | 0.0117       | 30                                     | 128.40     | 16147.4                                        | 0.1971            |          |
| 3 6.76                                                       | 849.6        | 0.0164        | 10                            | 38.81              | 4880.5       | 0.0501     | 17        | 77.00               | 9683.3            | 1.0000           | 24        | 121.26       | 15249.2     | 0.0223       | 31                                     | 137.87     | 17338.2                                        | 0.0763            | ]        |
| 4 6.95                                                       | 874.1        | 0.3625        | 11                            | 69.25              | 8708.8       | 0.1144     | 18        | 77.25               | 9715.1            | 0.9716           | 25        | 123.22       | 15496.2     | 0.0117       | 32                                     | 140.40     | 17657.0                                        | 0.0125            | 1        |
|                                                              | 2395.5       | 0.0298        | 12                            | 75.02              | 9434.5       | 0.0423     | 19        | 94.74               | 11914.0           | 0.0742           | 26        | 127.66       | 16054.8     | 0.1289       | 33                                     | 140.59     | 17680.6                                        | 0.0279            | 1        |
|                                                              | 2398.2       | 0.0512        | 13                            | 76.41              | 9609.8       | 0.0225     | 20        | 116.08              | 14598.0           | 0.0146           | 27        | 127.74       | 16064.8     | 0.0119       | 34                                     | 140.78     | 17704.2                                        | 0.0156            | 1        |
|                                                              | 2590.7       | 0.0517        | 14                            | 76,64              | 9637.9       | 0.0394     | 21        | 116.15              | 14607.0           | 0.0313           | 28        | 127.84       | 16076.6     | 0.2612       |                                        | ,          |                                                | 1                 | J        |
| - T 40.00                                                    | 2000.6       | 0.0011        |                               | 1 41,47            | 00000        | 0.0007     |           | 7 10.10             | 1 1 1 0 0 1 1 0   | , 5,5510         |           | 1-1-1-1      |             | 0.2012       |                                        |            |                                                |                   |          |

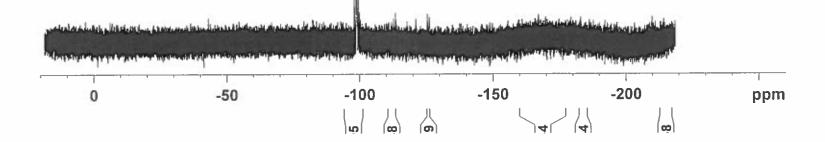
ejt cry wittig
mF19 CDCl3 {e:\bruk400data\2012\Aug} ejt 14



| NAME    | 2012-08-07-ejt | -14  |
|---------|----------------|------|
| EXPNO   | 10             |      |
| PROCNO  | 1              |      |
| Date    | 20120807       |      |
| Time    | 15.57          |      |
| INSTRUM | AV400          |      |
| PROBHD  | 5 mm PABBO BB- |      |
| PULPROG | 29             |      |
| TD      | 131072         |      |
| SOLVENT | CDC13          |      |
| NS      | 16             |      |
| DS      | 4              |      |
| SWH     | 89285.711      | Hz   |
| FIDRES  | 0.681196       | Hz   |
| AQ      | 0.7340532      | sec  |
| RG      | 4100           |      |
| DW      | 5.600          | usec |
| DE      | 11.01          | usec |
| TE      | 295.2          | K    |
| D1      | 1.00000000     | sec  |
| TD0     | 1              |      |

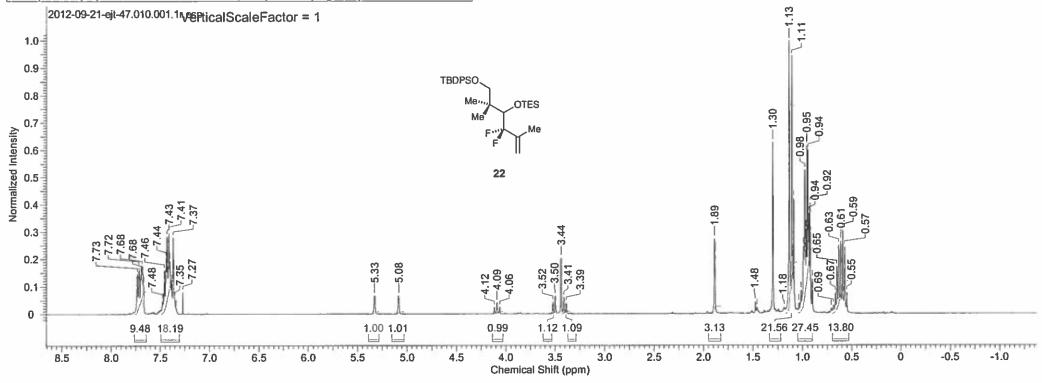
| CHANNEL fl ==== | ====                                                                             |
|-----------------|----------------------------------------------------------------------------------|
| 19F             |                                                                                  |
| 10.70           | usec                                                                             |
| -5.00           | dB                                                                               |
| 27.00716019     | W                                                                                |
| 376.4607164     | MHz                                                                              |
| 262144          |                                                                                  |
| 376.4983660     | MHz                                                                              |
| EM              |                                                                                  |
| 0               |                                                                                  |
| 0.30            | Hz                                                                               |
| 0               |                                                                                  |
| 2.00            |                                                                                  |
|                 | 10.70<br>-5.00<br>27.00716019<br>376.4607164<br>262144<br>376.4983660<br>EM<br>0 |





23/11/2012 15:30:05

| Acquisition Time (sec) | 3.9649                | Comment                      | ejt cry wittig mPROTO | Nnight CDCl3 (e:\bruk400c | data\2012\Sep} ejt 47 | Date                  | 23 Sep 2012 05:48:00 |
|------------------------|-----------------------|------------------------------|-----------------------|---------------------------|-----------------------|-----------------------|----------------------|
| Date Stamp             | 23 Sep 2012 05:48:00  | )                            |                       |                           |                       |                       |                      |
| File Name              | \\ss7a.ds.man.ac.uk\w | ol5\vol3\users\srimrdata\bru | Frequency (MHz)       | 400.13                    |                       |                       |                      |
| Nucleus                | 1H                    | Number of Transients         | 16                    | Origin                    | AV400                 | Original Points Count | 32768                |
| Owner                  | Administrator         | Points Count                 | 32768                 | Pulse Sequence            | zg30b                 | Receiver Gain         | 40.30                |
| SW(cyclical) (Hz)      | 8264.46               | Solvent                      | CHLOROFORM-d          | Spectrum Offset (Hz)      | 2464.9272             | Spectrum Type         | STANDARD             |
| Sweep Width (Hz)       | 8264.21               | Temperature (degree C        | 21.200                |                           |                       |                       |                      |



| No. | (ppm)            | Value               | Absolute Value | Non-Negative Value |
|-----|------------------|---------------------|----------------|--------------------|
| 1   | 5311 0.69        | 3.7977647           | 1.79901200e+8  | 13.79776478        |
| 2   | 3997 1.04        | 7.4501934           | 3.57907424e+8  | 27.45019341        |
| 3   | 0554 1.17        | 1.5567245           | 2.81065856e+8  | 21.55672455        |
| 4   | 3255 1.94        | 3. <b>1294</b> 6820 | 4.08033520e+7  | 3.12946820         |
| 5   | 3494 3.43        | 1.09304404          | 1.42515790e+7  | 1.09304404         |
| 6   | <b>1723</b> 3.56 | 1.11904001          | 1.45905260e+7  | 1.11904001         |

| l | No. | (ppm)              | Value               | Absolute Value | Non-Negative Value |
|---|-----|--------------------|---------------------|----------------|--------------------|
| 1 | 7   | 0295 4.13          | 0.98917204          | 1.28972510e+7  | 0.98917204         |
| Ì | 8   | 0290 5.15          | 1 <b>.011</b> 08396 | 1.31829480e+7  | 1.01108396         |
|   | 9   | 2830 5.38          | 1.00019169          | 1.30409290e+7  | 1.00019169         |
| 1 | 10  | 3067 <b>7.4</b> 9  | 8.18846893          | 2.37149088e+8  | 18.18846893        |
| 1 | 11  | 54 <b>26 7.7</b> 6 | 9.48153591          | 1.23624344e+8  | 9.48153591         |
| 1 |     |                    |                     |                |                    |

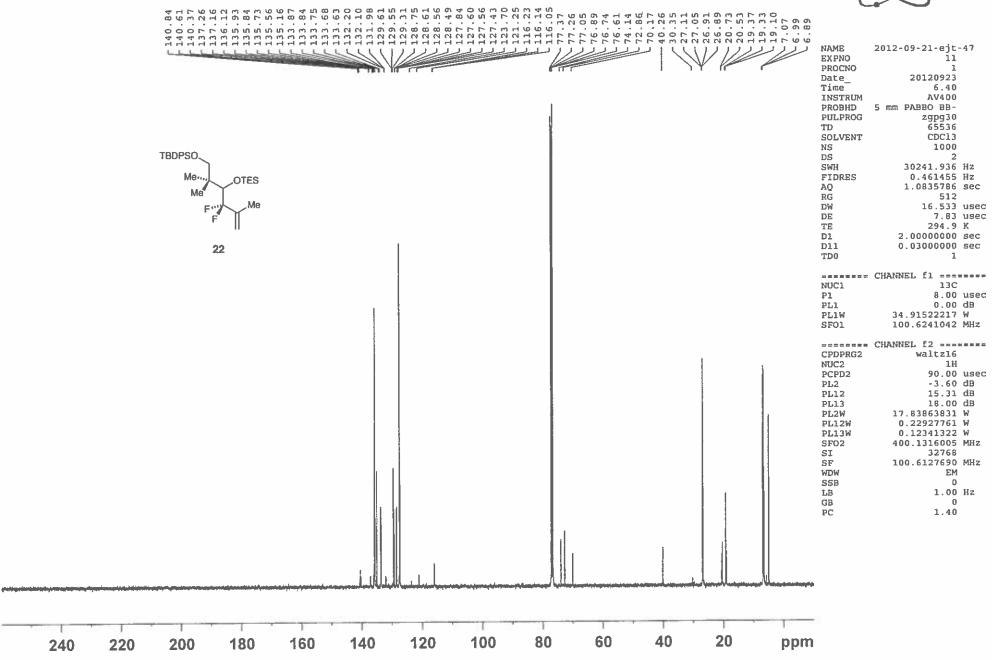
| į | No. | (ppm) | (Hz)  | Height | П  |
|---|-----|-------|-------|--------|----|
| İ | 1   | 0.55  | 220.6 | 0.0768 | П  |
| İ | 2   | 0.57  | 228.4 | 0.2431 | П  |
| i | 3   | 0.59  | 236.5 | 0.3054 | li |

| No. | (ppm) | (Hz)  | Height | No. | (ppm) | (Hz)  | Height |
|-----|-------|-------|--------|-----|-------|-------|--------|
| 4   | 0.61  | 244.6 | 0.2646 | 7   | 0.67  | 267.0 | 0.0752 |
| 5   | 0.63  | 252.7 | 0.2509 | 8   | 0.69  | 274.6 | 0.0313 |
| 6   | 0.65  | 259.7 | 0.1726 | 9   | 0.71  | 283.7 | 0.0202 |

|   | No. | (ppm) | (Hz)  | Height |
|---|-----|-------|-------|--------|
| ٦ | 10  | 0.90  | 360.9 | 0.1269 |
| ٦ | 11  | 0.92  | 369.7 | 0.4047 |
|   | 12  | 0.94  | 374.2 | 0.3671 |

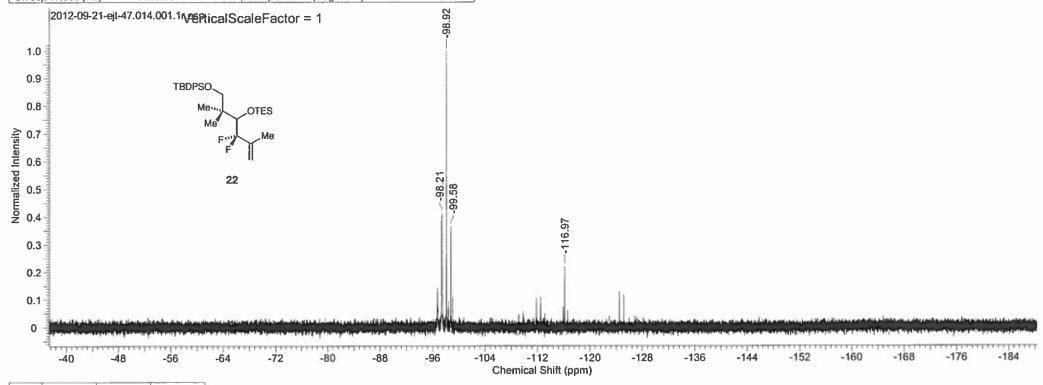
| No.    | (ppm) | (Hz)  | Height |
|--------|-------|-------|--------|
| 13     | 0.94  | 377.8 | 0.6009 |
| 14     | 0.95  | 382.0 | 0.6156 |
| <br>15 | 0.96  | 385.8 | 0.3093 |





24/09/2012 09:56:17

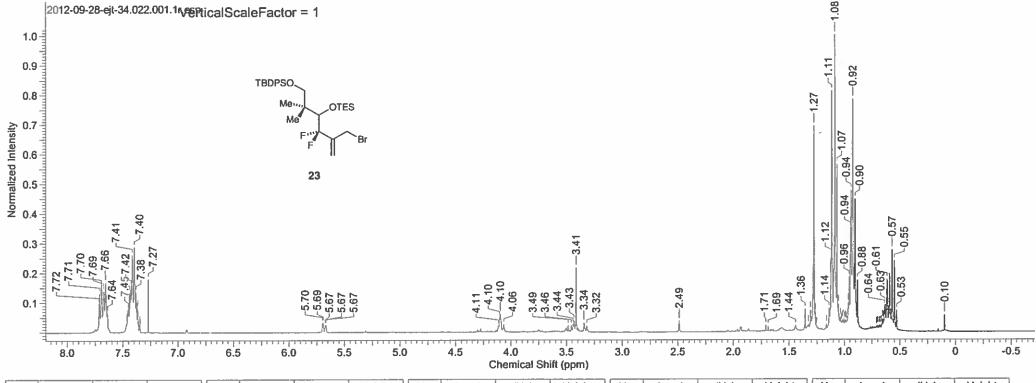
| Acquisition Time (sec) | 0.7340                 | Comment                     | ejt cry wittig mF19CPD | CDCl3 (e:\bruk400data\20 | 012\Sep} ejt 47 | Date                  | 21 Sep 2012 17:08:32 |
|------------------------|------------------------|-----------------------------|------------------------|--------------------------|-----------------|-----------------------|----------------------|
| Date Stamp             | 21 Sep 2012 17:08:32   |                             |                        |                          |                 |                       | <u> </u>             |
| File Name              | \\ss7a.ds.man.ac.uk\vc | ol5\vol3\users\snmrdata\bru | k400data\2012\Sep\data | Frequency (MHz)          | 376.50          |                       |                      |
| Nucleus                | 19F                    | Number of Transients        | 16                     | Origin                   | AV400           | Original Points Count | 65536                |
| Owner                  | Administrator          | Points Count                | 262144                 | Pulse Sequence           | zgig            | Receiver Gain         | 4100.00              |
| SW(cyclical) (Hz)      | 89285.71               | Solvent                     | CHLOROFORM-d           | Spectrum Offset (Hz)     | -37649.5977     | Spectrum Type         | STANDARD             |
| Sweep Width (Hz)       | 89285.37               | Temperature (degree C)      | 21.300                 |                          |                 |                       |                      |



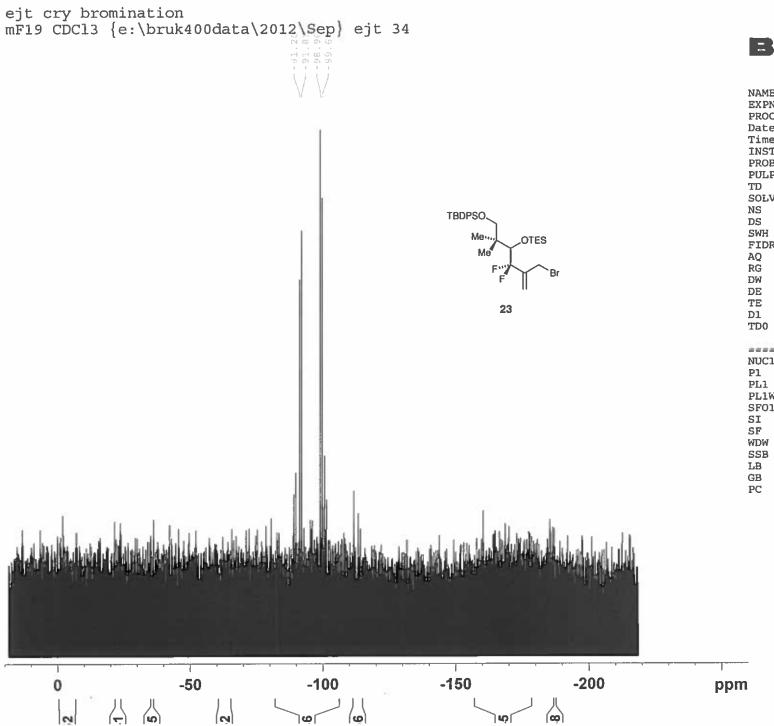
|   | No. | (ppm)   | (Hz)     | Height |
|---|-----|---------|----------|--------|
|   | 1   | -116.97 | -44039.7 | 0.2203 |
|   | 2   | -99.58  | -37493.1 | 0.3652 |
|   | 3   | -98.92  | -37241.4 | 1.0000 |
| İ | 4   | -98.21  | -36974.7 | 0.4116 |

30/11/2012 16:12:31

| Acquisition Time (sec) | 3.9649                 | Comment                     | ejt cry bromination mPf | ROTONnight CDCl3 (e:\bri   | .k400data\2012\Sep} ejt | 34                    |          |
|------------------------|------------------------|-----------------------------|-------------------------|----------------------------|-------------------------|-----------------------|----------|
| Date                   | 29 Sep 2012 06:41:20   |                             |                         | Date Stamp                 | 29 Sep 2012 06:41:20    |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\vo | 15\vol3\users\snmrdata\brul | 400data\2012\Sep\data   | ejt\nmr\2012-09-28-ejt-34\ | 22\pdata\1\1r           | Frequency (MHz)       | 400.13   |
| Nucleus                | 1H                     | Number of Transients        |                         | Origin                     |                         | Original Points Count | 32768    |
| Оwпег                  | Administrator          | Points Count                | 32768                   | Pulse Sequence             | zg30b                   | Receiver Gain         | 90.50    |
| SW(cyclical) (Hz)      | 8264.46                | Solvent                     | CHLOROFORM-d            | Spectrum Offset (Hz)       | 2464.9272               | Spectrum Type         | STANDARD |
| Sweep Width (Hz)       | 8264.21                | Temperature (degree C)      | 21.900                  |                            |                         |                       |          |



| No. | (ppm) | (Hz)  | Height | No. | (ppm) | (Hz)  | Height | No. | (ppm) | (H2)  | Height | No. | (ppm) | (Hz)  | Height | No. | (ppm) | (HZ)   | Height |
|-----|-------|-------|--------|-----|-------|-------|--------|-----|-------|-------|--------|-----|-------|-------|--------|-----|-------|--------|--------|
| 1   | 0.10  | 39.3  | 0.0569 | 12  | 0.64  | 255.4 | 0.0854 | 23  | 0.92  | 369.2 | 0.7846 | 34  | 1.02  | 410.0 | 0.0333 | 45  | 1.25  | 500.8  | 0.0197 |
| 2   | 0.53  | 211.5 | 0.0728 | 13  | 0.65  | 258.7 | 0.0423 | 24  | 0.94  | 374.7 | 0.4768 | 35  | 1.04  | 414.6 | 0.0491 | 46  | 1.26  | 505.6  | 0.0664 |
| 3   | 0.55  | 219.6 | 0.2398 | 14  | 0.66  | 262.7 | 0.0431 | 25  | 0.94  | 377.2 | 0.3485 | 36  | 1.05  | 421.1 | 0.0929 | 47  | 1.27  | 510.2  | 0.6938 |
| 4   | 0.57  | 227.4 | 0.2773 | 15  | 0.67  | 266.3 | 0.0256 | 26  | 0.96  | 382.8 | 0.1848 | 37  | 1.07  | 426.4 | 0.5648 | 48  | 1.31  | 522.3  | 0.0724 |
| 5   | 0.58  | 232.0 | 0.0477 | 16  | 0.67  | 270.1 | 0.0215 | 27  | 0.96  | 386.1 | 0.0974 | 38  | 1.07  | 430.0 | 0.1603 | 49  | 1.33  | 530.8  | 0.0254 |
| 6   | 0.59  | 235.8 | 0.1562 | 17  | 0.68  | 273.3 | 0.0229 | 28  | 0.98  | 391.6 | 0.0344 | 39  | 1.08  | 433.5 | 1.0000 | 50  | 1.36  | 542.4  | 0.0765 |
| 7   | 0.59  | 236.8 | 0.1676 | 18  | 0.69  | 277.4 | 0.0206 | 29  | 0.99  | 394.1 | 0.0378 | 40  | 1.09  | 436.8 | 0.2914 | 51  | 1.44  | 577.0  | 0.0218 |
| 8   | 0.60  | 240.0 | 0.0879 | 19  | 0.70  | 281.4 | 0.0220 | 30  | 0.99  | 396.4 | 0.0415 | 41  | 1.11  | 444.8 | 0.8124 | 52  | 1.69  | 675.4  | 0.0202 |
| 9   | 0.61  | 244.8 | 0.1781 | 20  | 0.71  | 284.9 | 0.0185 | 31  | 1.00  | 398.7 | 0.0372 | 42  | 1,12  | 447.9 | 0.2577 | 53  | 1.71  | 683.2  | 0.0231 |
| 10  | 0.62  | 247.9 | 0.1145 | 21  | 0.88  | 352.3 | 0.1744 | 32  | 1.01  | 402.2 | 0.0435 | 43  | 1.14  | 455.2 | 0.0789 | 54  | 2.49  | 995.7  | 0.0366 |
| 11  | 0.63  | 252.7 | 0.0927 | 22  | 0.90  | 360.9 | 0.4475 | 33  | 1.02  | 407.3 | 0.0412 | 44  | 1.16  | 465.0 | 0.0262 | 55  | 3.32  | 1328.1 | 0.0218 |



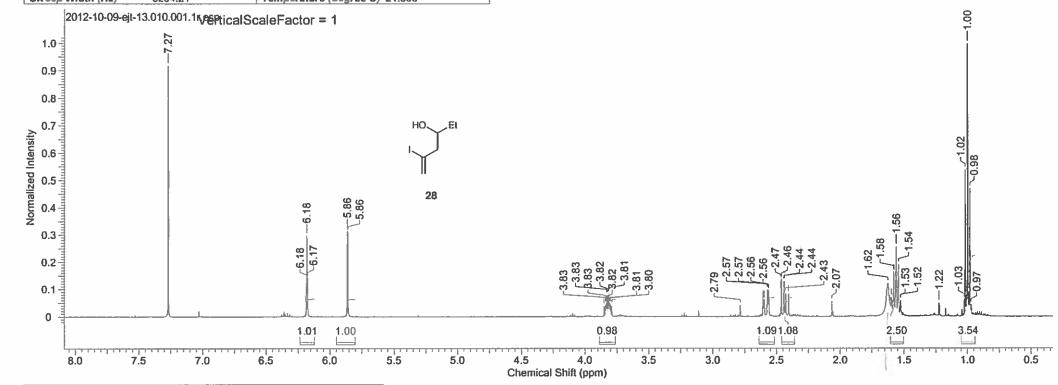


| NAME<br>EXPNO | 20 | 012- | -09-28         | ejt.<br>20 | -34 |
|---------------|----|------|----------------|------------|-----|
| PROCNO        |    |      |                | 1          |     |
| Date          |    |      | 2012           | 0928       |     |
| Time          |    |      | 1.             | 3.29       |     |
| INSTRUM       |    |      | A <sup>1</sup> | V400       |     |
| PROBHD        | 5  | mm   | PABBO          | BB-        |     |
| PULPROG       |    |      |                | zg         |     |
| TD            |    |      | 13:            | 1072       |     |
| SOLVENT       |    |      | Cl             | DC13       |     |
| NS            |    |      |                | 16         |     |
| DS            |    |      |                | 4          |     |
| SWH           |    |      | 89285          | .711       | Hz  |
| FIDRES        |    |      | 0.683          | 1196       | Hz  |
| AQ            |    |      | 0.734          | 3532       | sec |
| RG            |    |      | 4              | 4100       |     |
| ÐW            |    |      | _              | .600       |     |
| ĐE            |    |      |                | 1.01       |     |
| TE            |    |      |                | 95.2       |     |
| D1            |    | 1    | L.0000         | 0000       | sec |
| TDO           |    |      |                | 1          |     |
|               |    |      |                |            |     |

|      | CHANNEL | f1   |      | ===== |
|------|---------|------|------|-------|
| NUCL |         |      | 19F  |       |
| P1   |         | 10   | 3.70 | usec  |
| PL1  |         | - 5  | 00.6 | đВ    |
| PL1W | 27.00   | 716  | 019  | W     |
| SF01 | 376.4   | 1607 | 7164 | MHz   |
| SI   |         | 262  | 2144 |       |
| SF   | 376.4   | 1983 | 3660 | MHz   |
| WDW  |         |      | EM   |       |
| SSB  |         |      | 0    |       |
| LB   |         | (    | 0.30 | Hz    |
| GB   |         |      | 0    |       |
| PC   |         | - 2  | 00.5 |       |
|      |         |      |      |       |

20/11/2012 17:35:28

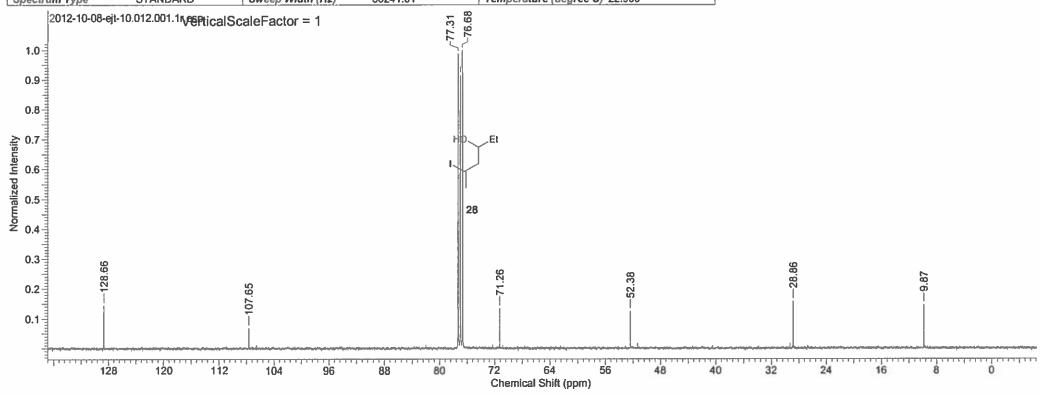
| Acquisition Time (sec) | 3.9649                | Comment                     | ejt cry vinyl iodide mPF | ROTON CDCI3 (e:\bruk400    | )data\2012\Oct} ejt 13 | Date                  | 09 Oct 2012 12:46:08 |
|------------------------|-----------------------|-----------------------------|--------------------------|----------------------------|------------------------|-----------------------|----------------------|
| Date Stamp             | 09 Oct 2012 12:46:08  |                             |                          |                            |                        |                       |                      |
| File Name              | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bru | k400data\2012\Oct\data   | \ejt\nmr\2012-10-09-ejt-13 | \10\pdata\1\1r         | Frequency (MHz)       | 400.13               |
| Nucleus                | 1H                    | Number of Transients        | 16                       | Origin                     | AV400                  | Original Points Count | 32768                |
| Owner                  | Administrator         | Points Count                | 32768                    | Pulse Sequence             | zg30b                  | Receiver Gain         | 322.00               |
| SW(cyclical) (Hz)      | 8264.46               | Solvent                     | CHLOROFORM-d             | Spectrum Offset (Hz)       | 2464.9272              | Spectrum Type         | STANDARD             |
| Sweep Width (Hz)       | 8264.21               | Temperature (degree C)      | 21.300                   |                            |                        |                       |                      |



| No. | (ppm)              | Value      | Absolute Value | Non-Negative Value |
|-----|--------------------|------------|----------------|--------------------|
| 1   | 9398 1.04          | 3.54017091 | 1.01245312e+8  | 3.54017091         |
| 2   | 5041 1.60          | 2.49626207 | 7.13905760e+7  | 2.49626207         |
| 3   | 8854 <b>2.</b> 48  | 1.07680511 | 3.07955380e+7  | 1.07680511         |
| 4   | 5 <b>185 2.</b> 63 | 1.09013748 | 3.11768320e+7  | 1.09013748         |
| 5   | 7612 3.88          | 0.97696531 | 2.79402220e+7  | 0.97696531         |
| 6   | 3027 5.94          | 1.00033140 | 2.86084700e+7  | 1.00033140         |
| 7   | 1198 6.23          | 1.00761056 | 2.88166460e+7  | 1.00761056         |

20/11/2012 17:36:58

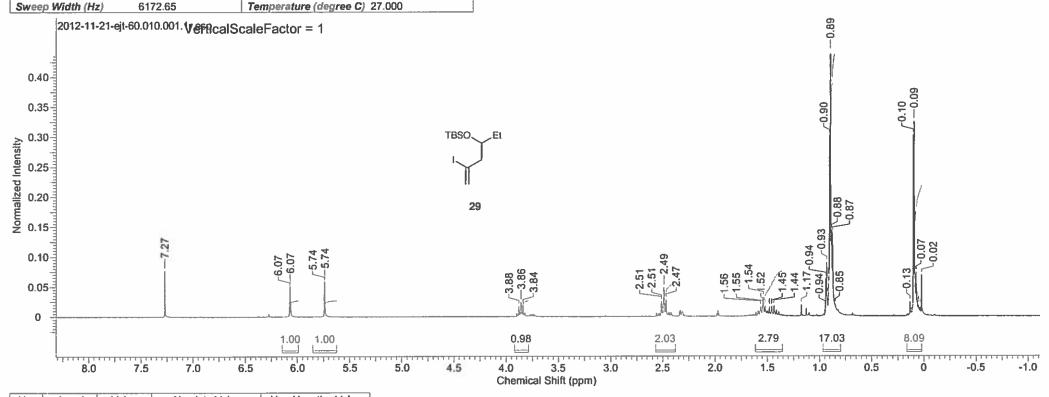
| Acquisition Time (sec) | 1.0835               | Comment           | ejt cry iodide 10 mCAR | BONnight CDCl3 {e:\bruk4                                                                                      | 00data\2012\Oct} ejt 10 | Date                 | 08 Oct 2012 19:35:44 |  |
|------------------------|----------------------|-------------------|------------------------|---------------------------------------------------------------------------------------------------------------|-------------------------|----------------------|----------------------|--|
| Date Stamp             | 08 Oct 2012 19:35:44 | File Name         | \\ss7a.ds.man.ac.uk\vo | Nss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Oct\data\ejt\nmr\2012-10-08-ejt-10\12\pdata\1\1r |                         |                      |                      |  |
| Frequency (MHz)        | 100.61               | Nucleus           | 13C                    | Number of Transients                                                                                          | 800                     | Origin               | AV400                |  |
| Original Points Count  | 32768                | Owner             | Administrator          | Points Count                                                                                                  | 32768                   | Pulse Sequence       | zgpg30               |  |
| Receiver Gain          | 512.00               | SW(cyclical) (Hz) | 30241.94               | Solvent                                                                                                       | CHLOROFORM-d            | Spectrum Offset (Hz) | 11332.2295           |  |
| Spectrum Type          | STANDARD             | Sween Width (Hz)  | 30241 01               | Temperature (degree C                                                                                         | 22 900                  |                      |                      |  |



| No. | (ppm)  | (Hz)    | Height |
|-----|--------|---------|--------|
| 1   | 9.87   | 993.3   | 0.1460 |
| 2   | 28.86  | 2903.7  | 0.1572 |
| 3   | 52.38  | 5270.1  | 0.1243 |
| 4   | 71.26  | 7169.4  | 0.1335 |
| 5   | 76.68  | 7714.9  | 1.0000 |
| 6   | 77.00  | 7747.2  | 0.9152 |
| 7   | 77.31  | 7778.6  | 0.9874 |
| 8   | 107.65 | 10830.6 | 0.0683 |
| 9   | 128.66 | 12945.0 | 0.1445 |

21/11/2012 11:54:23

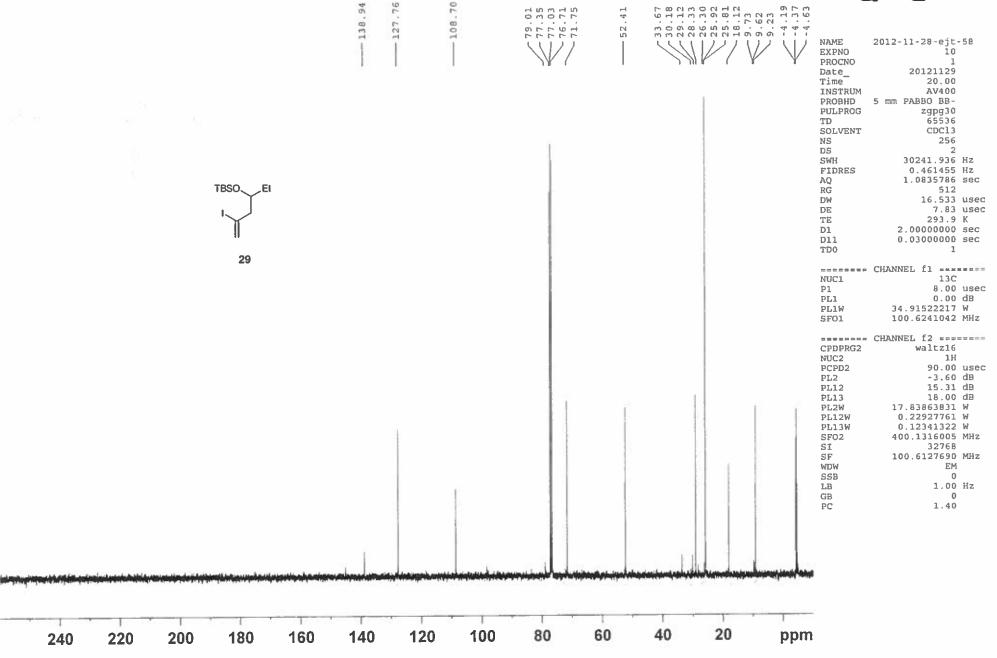
| Acquisition Time (sec) | 5.3084                | Comment                                                                                                        | ejt cry vinyl mPROTO | N CDCl3 (E:\bruk300data\ | 2012\Nov} ejt 60 | Date                  | 21 Nov 2012 10:22:56 |
|------------------------|-----------------------|----------------------------------------------------------------------------------------------------------------|----------------------|--------------------------|------------------|-----------------------|----------------------|
| Date Stamp             | 21 Nov 2012 10:22:56  |                                                                                                                |                      |                          |                  |                       |                      |
| File Name              | \\ss7a.ds.man.ac.uk\v | \\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk300data\2012\Nov\data\ejt\nmr\2012-11-21-ejt-60\10\pdata\1\1r |                      |                          |                  | Frequency (MHz)       | 299.95               |
| Nucleus                | 1H                    | Number of Transients                                                                                           | 16                   | Origin                   | DPX300           | Original Points Count | 32768                |
| Owner                  | Administrator         | Points Count                                                                                                   | 32768                | Pulse Sequence           | zg30             | Receiver Gain         | 456.10               |
| SW(cyclical) (Hz)      | 6172.84               | Solvent                                                                                                        | CHLOROFORM-d         | Spectrum Offset (Hz)     | 1848.6169        | Spectrum Type         | STANDARD             |
| D 145 144 (14 )        | 0470.05               | T                                                                                                              | 1 07 000             |                          |                  |                       |                      |



| No. | (ppm)     | Value               | Absolute Value | Non-Negative Value |
|-----|-----------|---------------------|----------------|--------------------|
| 1   | 223 0.16  | 8 <b>.08682</b> 060 | 4.68993120e+8  | 8.08682060         |
| 2   | 7955 0.96 | 7.0270633           | 9.87480256e+8  | 17.02706337        |
| 3   | 3579 1.61 | 2. <b>785492</b> 66 | 1.61543936e+8  | 2.78549266         |
| 4   | 3810 2.56 | 2. <b>03447</b> 366 | 1.17988776e+8  | 2.03447366         |
| 5   | 7869 3.91 | 0.98051947          | 5.68649760e+7  | 0.98051947         |
| 6   | 5223 5.84 | 0.99646074          | 5.77894880e+7  | 0.99646074         |
| 7   | 9894 6.14 | 0.99959248          | 5.79711120e+7  | 0.99959248         |

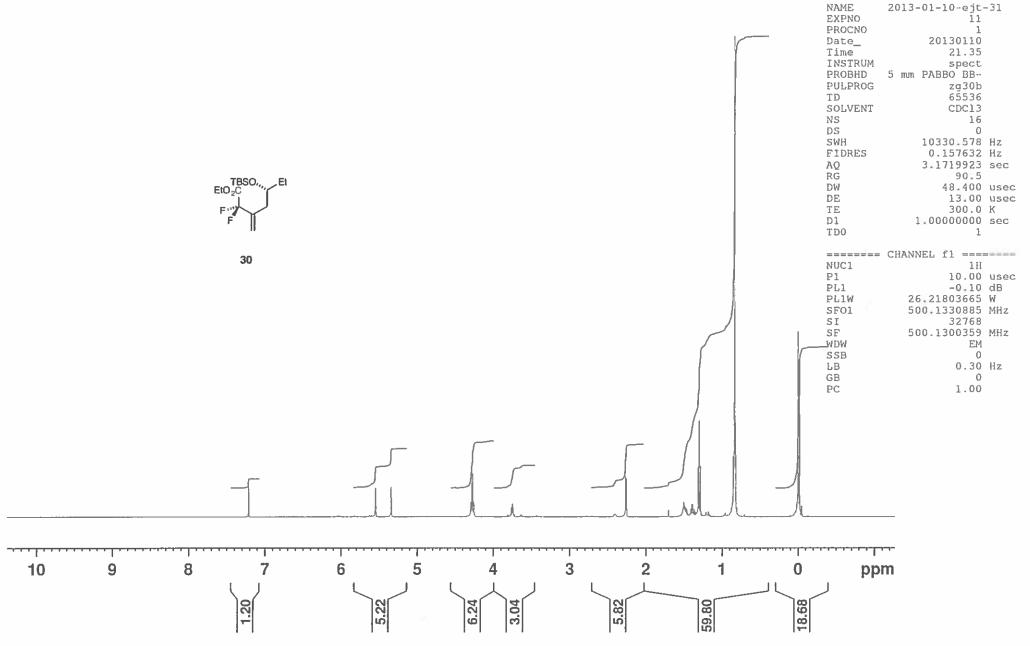
## EJT-PRM46 TBS vinyl iodide data mCARBONnight CDCl3 {e:\bruk400data\2012\Nov} ejt 58





# EJT-PRM48c f4-5 8mg full data mPROTONnight CDCl3 /opt/bruk500data/2013/Jan ejt 31





20

ppm

40

120

200

180

160

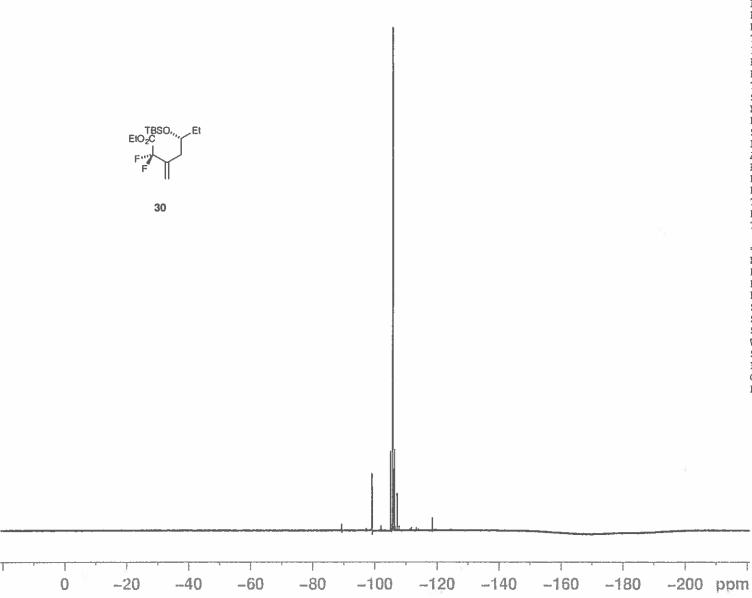
140

100

80

60

EJT-PRM48c f4-5 8mg m19F CDCl3 /opt/bruk500data/2013/Jan ejt 29



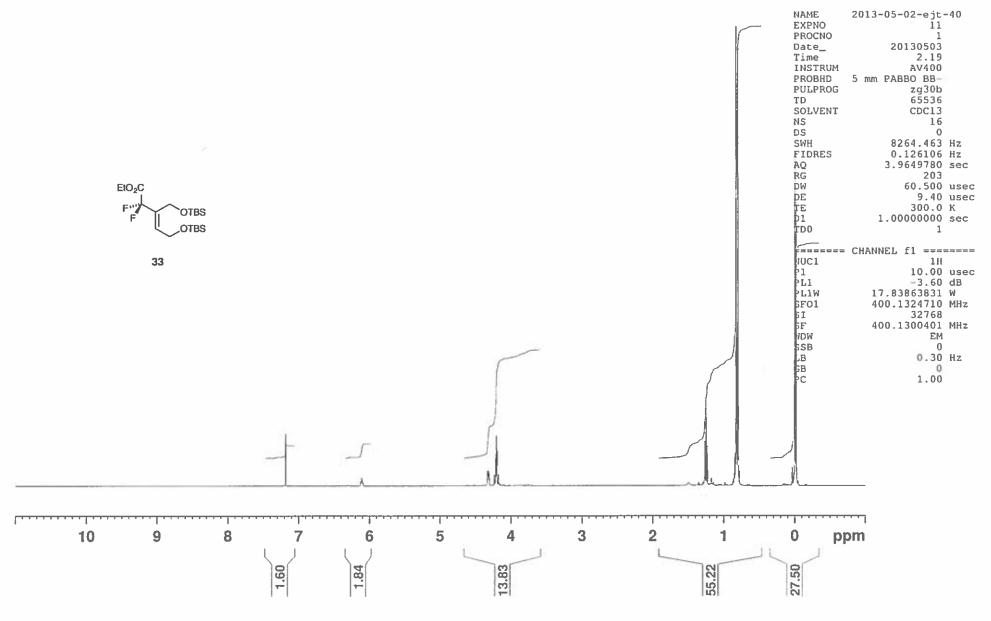


| NAME    | 2013-01-10-ejt- | -29  |
|---------|-----------------|------|
| EXPNO   | 12              |      |
| PROCNO  | 1               |      |
| Date_   | 20130110        |      |
| Time    | 17.38           |      |
| INSTRUM | spect           |      |
| PROBHD  | 5 mm PABBO BB-  |      |
| PULPROG | zgflgn          |      |
| TD      | 131072          |      |
| SOLVENT | CDC13           |      |
| NS      | 16              |      |
| DS      | 4               |      |
| SWH     | 113636.367      | Hz   |
| FIDRES  | 0.866977        | Hz   |
| AQ      | 0.5767668       | sec  |
| RG      | 203             |      |
| DW      | 4.400           | usec |
| DE      | 6.50            | used |
| TE      | 300.0           | K    |
| D1      | 1.00000000      | sec  |
| TD0     | 1               |      |
|         |                 |      |

| ======= | CHANNEL fl ==== |     |
|---------|-----------------|-----|
| NUC1    | 19F             |     |
| P1      | 17.50           | use |
| PL1     | -2.90           | dB  |
| PLIW    | 48.97788239     | W   |
| SF01    | 470.5453180     | MHz |
| SI      | 65536           |     |
| SF      | 470.5923770     | MHz |
| WDW     | EM              |     |
| SSB     | 0               |     |
| LB      | 0.30            | Ηz  |
| GB      | 0               |     |
| PC      | 1.00            |     |
|         |                 |     |

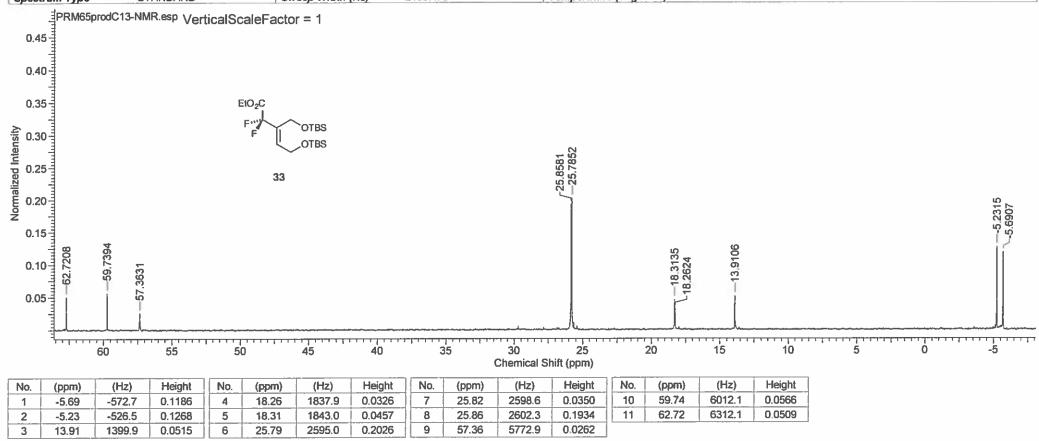
## EJT-PRM65 Product data mPROTONnight CDCl3 {e:\bruk400data\2013\May} ejt 40





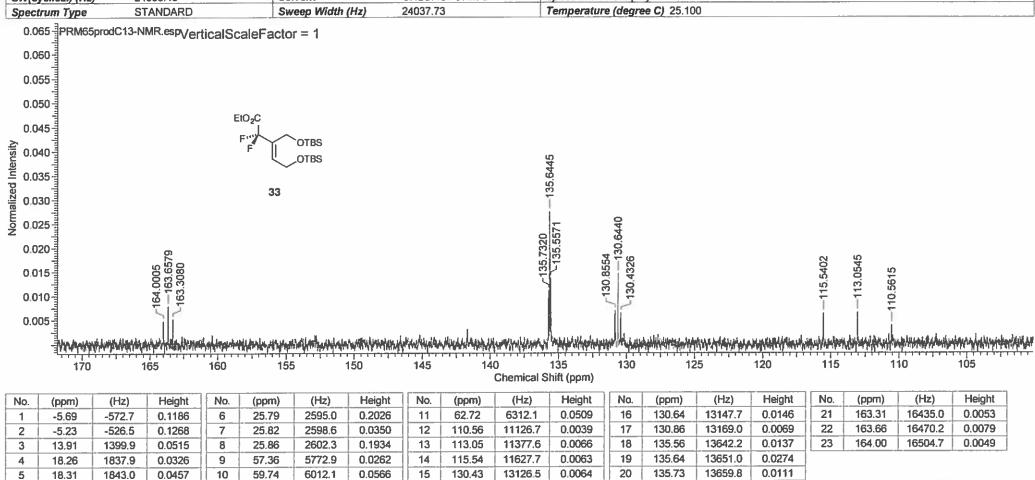
12/06/2013 18:27:58

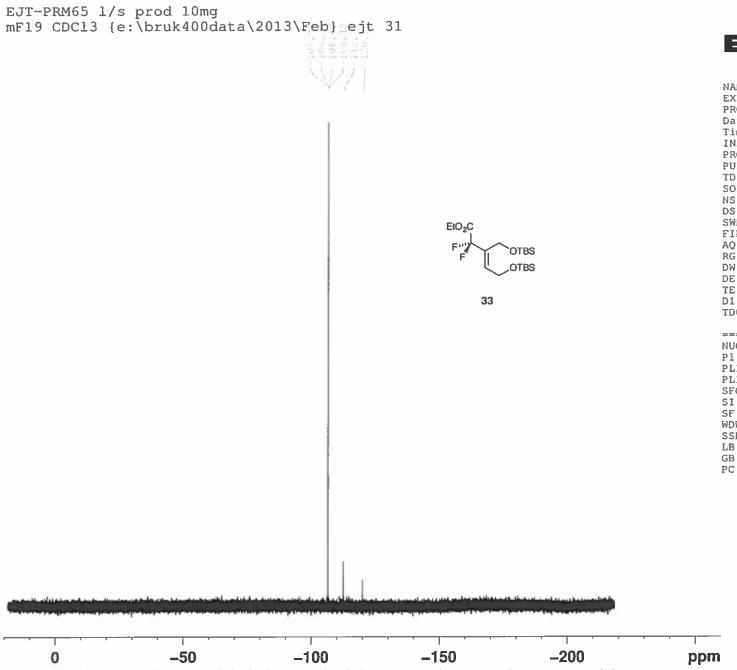
| Acquisition Time (sec) | 1.3631                     | Comment               | P. Mears EJT-PRM 65 Prod data 0513-008 mCARBON CDCl3 {E:\bruk400service_data\2013\May} Administrator 24 |                       |                                                   |
|------------------------|----------------------------|-----------------------|---------------------------------------------------------------------------------------------------------|-----------------------|---------------------------------------------------|
| Date                   | 10 May 2013 09:34:08       | Date Stamp            | 10 May 2013 09:34:08                                                                                    |                       |                                                   |
| File Name              | \\ss7a.ds.man.ac.uk\vol5\V | OL3\USERS\SNMRDATA\BF | RUK400SERVICE_DATA\201                                                                                  | 3WAYDATA\ADMINISTRA   | TOR\NMR\2013-05-09-ADMINISTRATOR-24\12\PDATA\1\1R |
| Frequency (MHz)        | 100.64                     | Nucleus               | 13C                                                                                                     | Number of Transients  | 10240                                             |
| Origin                 | AV400_S                    | Original Points Count | 32768                                                                                                   | Owner                 | Administrator                                     |
| Points Count           | 32768                      | Pulse Sequence        | zgpg30                                                                                                  | Receiver Gain         | 2050.00                                           |
| SW(cyclical) (Hz)      | 24038.46                   | Solvent               | CHLOROFORM-d                                                                                            | Spectrum Offset (Hz)  | 10063.3350                                        |
| Spectrum Type          | STANDARD                   | Sweep Width (Hz)      | 24037.73                                                                                                | Temperature (degree C | 25.100                                            |



12/06/2013 18:28:32

| Acquisition Time (sec) | 1.3631                      | Comment               | P. Mears EJT-PRM 65 Prod data 0513-008 mCARBON CDCl3 {E:\bruk400service_data\2013\May} Administrator 24 |                       |                                                  |
|------------------------|-----------------------------|-----------------------|---------------------------------------------------------------------------------------------------------|-----------------------|--------------------------------------------------|
| Date                   | 10 May 2013 09:34:08        | Date Stamp            | 10 May 2013 09:34:08                                                                                    |                       |                                                  |
| File Name              | \\ss7a.ds.man.ac.uk\vol5\VO | L3\USERS\SNMRDATA\BF  | RUK400SERVICE_DATA\201                                                                                  | 3\MAY\DATA\ADMINISTRA | TORWMR\2013-05-09-ADMINISTRATOR-24\12\PDATA\1\1R |
| Frequency (MHz)        | 100.64                      | Nucleus               | 13C                                                                                                     | Number of Transients  | 10240                                            |
| Origin                 | AV400_S                     | Original Points Count | 32768                                                                                                   | Owner                 | Administrator                                    |
| Points Count           | 32768                       | Pulse Sequence        | zgpg30                                                                                                  | Receiver Gain         | 2050.00                                          |
| SW(cyclical) (Hz)      | 24038.46                    | Solvent               | CHLOROFORM-d                                                                                            | Spectrum Offset (Hz)  | 10063.3350                                       |
| Spectrum Type          | STANDARD                    | Sweep Width (Hz)      | 24037.73                                                                                                | Temperature (degree C | 25.100                                           |





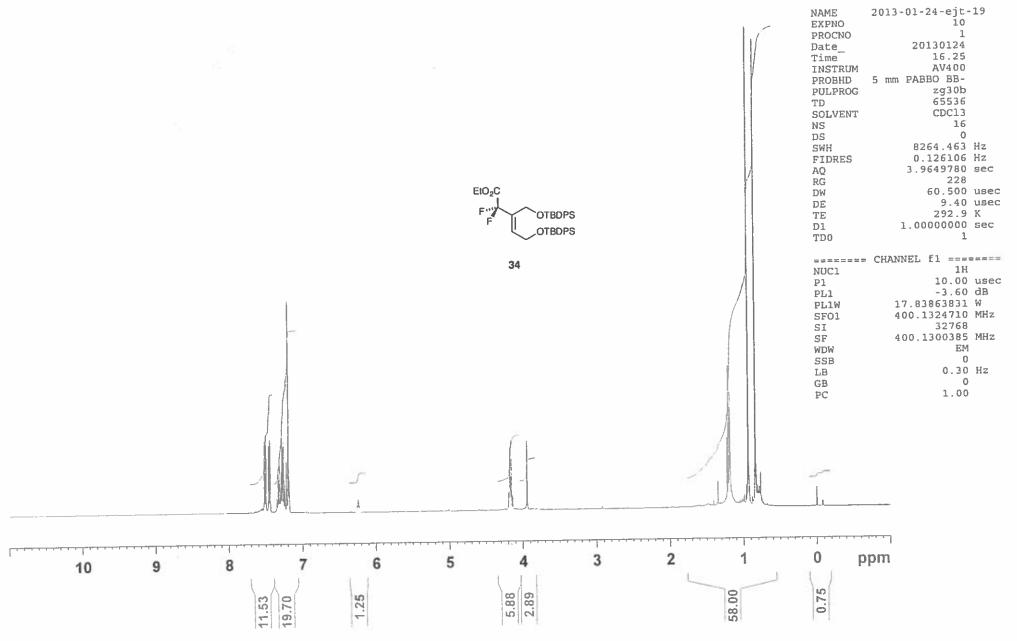


| NAME    | 2013-02-14-ejt- | -31  |
|---------|-----------------|------|
| EXPNO   | 12              |      |
| PROCNO  | 1               |      |
| Date_   | 20130214        |      |
| Time    | 12.58           |      |
| INSTRUM | AV400           |      |
| PROBHD  | 5 mm PABBO BB-  |      |
| PULPROG | zq              |      |
| TD      | 131072          |      |
| SOLVENT | CDC13           |      |
| NS      | 16              |      |
| DS      | 4               |      |
| SWH     | 89285.711       | Hz   |
| FIDRES  | 0.681196        | Hz   |
| AQ      | 0.7340532       | sec  |
| RG      | 4100            |      |
| DW      | 5.600           | usec |
| DE      | 11.01           | usec |
| TE      | 292.9           | K    |
| D1      | 1.00000000      | sec  |
| TD0     | 1               |      |
|         |                 |      |

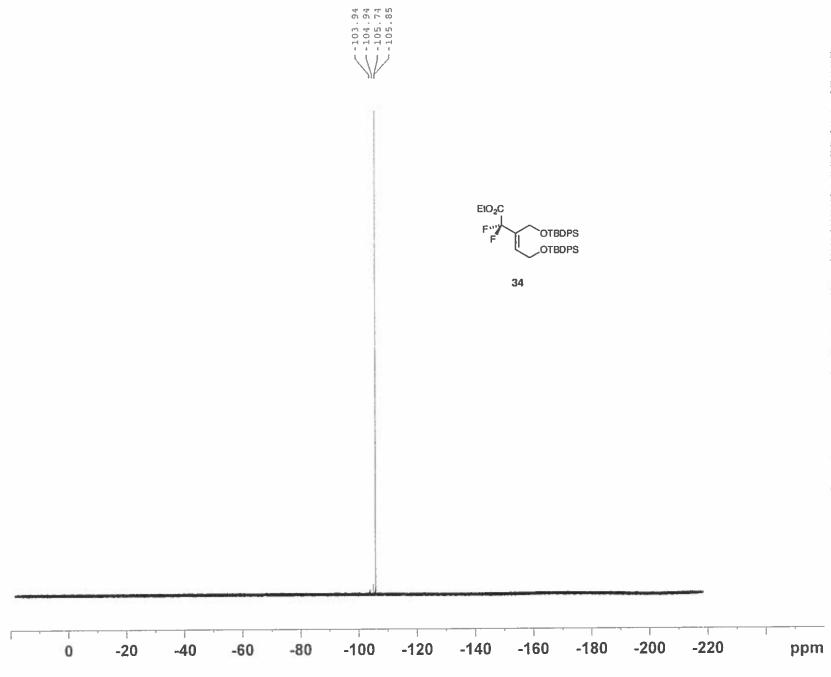
|      | CHANNEL fl ==== | 2222 |
|------|-----------------|------|
| NUC1 | 19F             |      |
| P1   | 10.70           | used |
| PL1  | -5.00           | dB   |
| PL1W | 27.00716019     | W    |
| SFO1 | 376.4607164     | MHz  |
| SI   | 262144          |      |
| SF   | 376.4983660     | MHz  |
| WDW  | EM              |      |
| SSB  | 0               |      |
| LB   | 0.30            | Hz   |
| GB   | 0               |      |
| PC   | 2.00            |      |

EJT-PRM58 f1-30 4mg mPROTON CDCl3 {e:\bruk400data\2013\Jan} ejt 19





# EJT-PRM58 f1-30 4mg mF19CPD CDCl3 {e:\bruk400data\2013\Jan} ejt 19

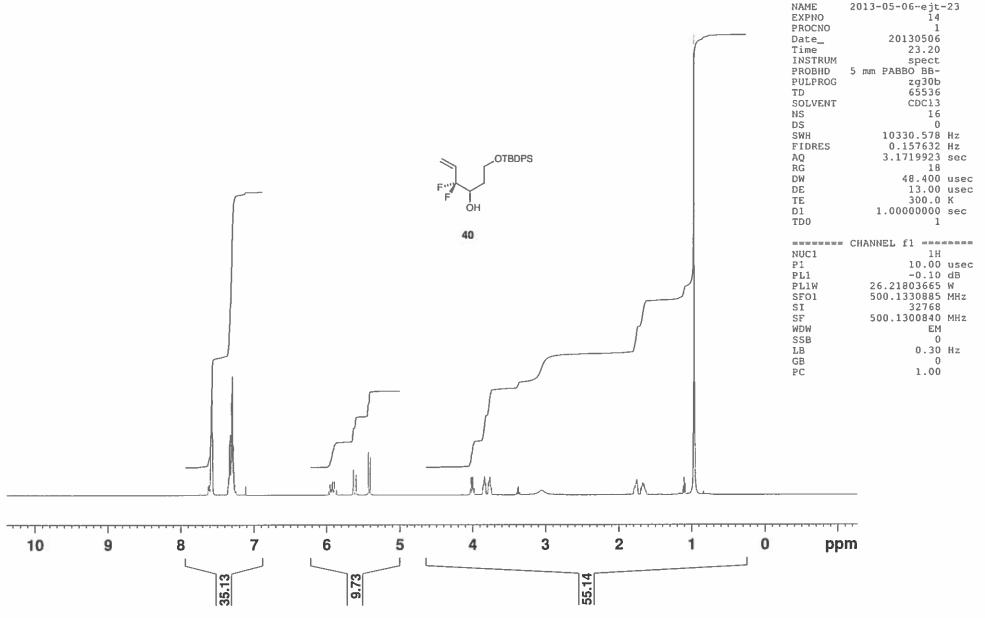




| NAME    | 2013-01-24-ejt- | 19    |
|---------|-----------------|-------|
| EXPNO   | 12              |       |
| PROCNO  | 1               |       |
| Date    | 20130124        |       |
| Time    | 16.28           |       |
| INSTRUM | AV400           |       |
| PROBHD  | 5 mm PABBO BB-  |       |
| PULPROG | zgig            |       |
| TD      | 131072          |       |
| SOLVENT | CDC13           |       |
| NS      | 16              |       |
| DS      | 4               |       |
| SWH     | 89285.711       | Hz    |
| FIDRES  | 0.681196        | Hz    |
| AQ      | 0.7340532       | sec   |
| RG      | 4100            |       |
| DW      | 5.600           | usec  |
| DE      |                 | usec  |
| TE      | 293.0           | K     |
| D1      | 1.00000000      | sec   |
| D11     | 0.03000000      |       |
| TDO     | 1               |       |
|         |                 |       |
|         | CHANNEL fl ==== |       |
| NUCl    | 19F             |       |
| P1      | 10.70           | usec  |
| PLI     | -5.00           | ďΒ    |
| PL1W    | 27.00716019     | W     |
| SF01    | 376.4607164     | MHZ   |
|         | 4. 9100         |       |
|         | CHANNEL f2      |       |
| CPDPRG2 | waltz16         |       |
| NUC2    | 1H              |       |
| PCPD2   | 90.00           |       |
| PL2     | -3.60           |       |
| PL12    |                 | dB    |
| PL2W    | 17.83963831     | W     |
| PL12W   |                 | W     |
| SFO2    | 400.1316005     | MHZ   |
| SI      | 262144          |       |
| SF      | 376.4983660     | MHZ   |
| WDW     | EM              |       |
| SSB     | 0               | 11.00 |
| LB      | 0.30            | HZ    |
| GB      | 0               |       |
| PC      | 2.00            |       |
|         |                 |       |
|         |                 |       |

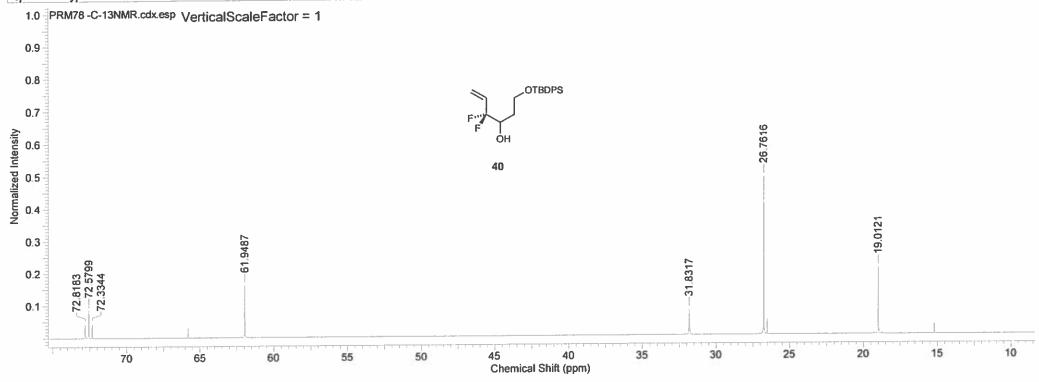
EJT-PRM78 Prod data mPROTONnight CDCl3 /opt/oldbruk500data.11vii11/2013/May ejt 23





23/05/2014 17:17:55

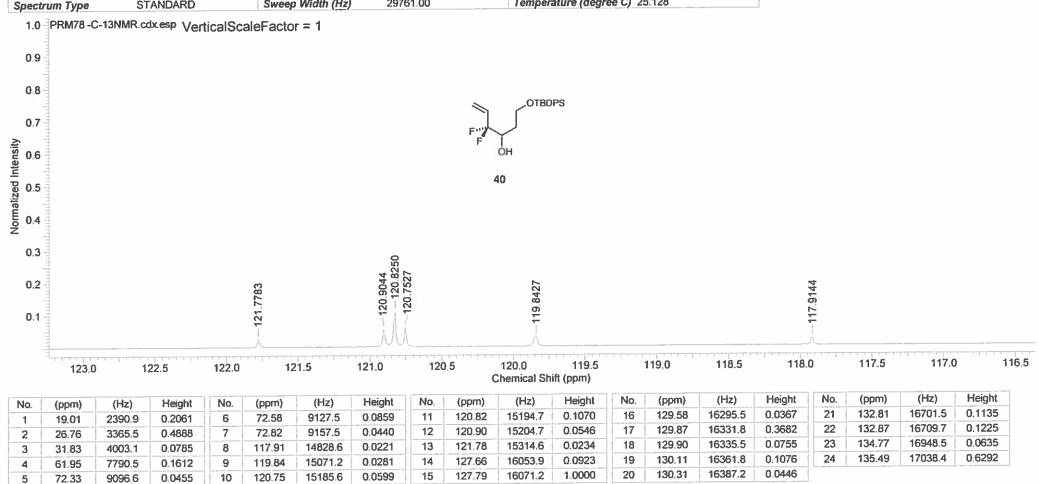
| Acquisition Time (sec) | 1.1010                   | Comment             | EJT-PRM78 Prod data m | CARBONnight CDCl3 /opt/ | oldbruk500data.11vii11/20 | 013/May ejt 23       |            |
|------------------------|--------------------------|---------------------|-----------------------|-------------------------|---------------------------|----------------------|------------|
| Date                   | 06 May 2013 22:20:00     | Date Stamp          | 06 May 2013 22:20:00  |                         |                           |                      |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | SIVOL3IUSERSISNMRDA | TA\BRUK500DATA\BRUK50 | ODATA\2013\MAY\DATA\E   | JT\NMR\2013-05-06-EJ      |                      |            |
| Frequency (MHz)        | 125.76                   | Nucleus             | 13C                   | Number of Transients    | 3000                      | Origin               | spect      |
| Original Points Count  | 32768                    | Owner               | vnmr1                 | Points Count            | 32768                     | Pulse Sequence       | zgpg30     |
| Receiver Gain          | 512.00                   | SW(cyclical) (Hz)   | 29761.90              | Solvent                 | CHLOROFORM-d              | Spectrum Offset (Hz) | 12562.9922 |
| Spactrum Tune          | STANDARD                 | Sweep Width (Hz)    | 29761.00              | Temperature (degree C   | 25.128                    |                      |            |



| No. | (ppm) | (Hz)   | Height |
|-----|-------|--------|--------|
| 1   | 19.01 | 2390.9 | 0.2061 |
| 2   | 26.76 | 3365.5 | 0.4888 |
| 3   | 31.83 | 4003.1 | 0.0785 |
| 4   | 61.95 | 7790.5 | 0.1612 |
| 5   | 72.33 | 9096.6 | 0.0455 |
| 6   | 72.58 | 9127.5 | 0.0859 |
| 7   | 72.82 | 9157.5 | 0.0440 |

23/05/2014 17:23:24

| Acquisition Time (sec) | 1.1010                   | Comment           | EJT-PRM78 Prod data m | CARBONnight CDCl3 /opt/ | oldbruk500data.11vii11/20 | 13/May ejt 23        |            |
|------------------------|--------------------------|-------------------|-----------------------|-------------------------|---------------------------|----------------------|------------|
| Date                   | 06 May 2013 22:20:00     | Date Stamp        | 06 May 2013 22:20:00  |                         |                           |                      |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | VOL3\USERS\SNMRDA | TA\BRUK500DATA\BRUK50 | ODATA\2013\MAY\DATA\E   | JT\NMR\2013-05-06-EJT     | -23\10\PDATA\1\1R    |            |
| Frequency (MHz)        | 125.76                   | Nucleus           | 13C                   | Number of Transients    | 3000                      | Origin               | spect      |
| Original Points Count  | 32768                    | Owner             | vnmr1                 | Points Count            | 32768                     | Pulse Sequence       | zgpg30     |
| Receiver Gain          | 512.00                   | SW(cyclical) (Hz) | 29761.90              | Solvent                 | CHLOROFORM-d              | Spectrum Offset (Hz) | 12562.9922 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)  | 29761.00              | Temperature (degree C   | 25.128                    |                      |            |

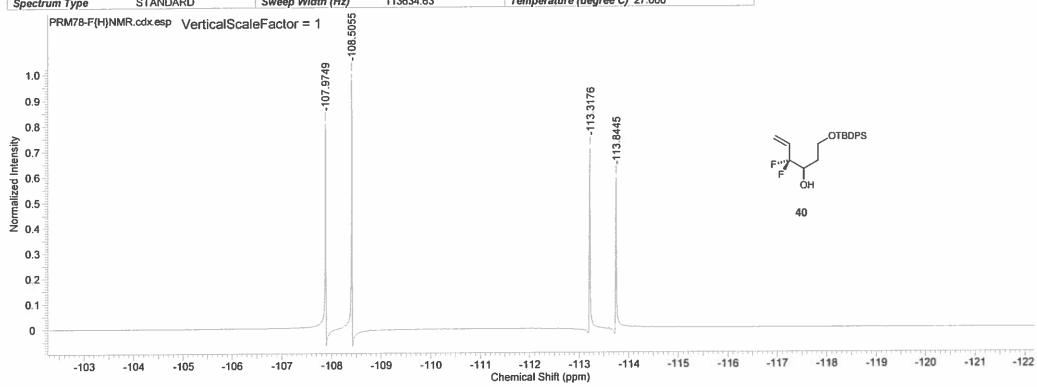


23/05/2014 17:53:06

| Acquisition Tim               | e (sec) 1. | .1010        |           | Comr     | nent          |        |       |            |                    | night CDCl3       | /opt/old | bruk500data | .11vii11/201 | 3/May ejt | 23        |         |                    |                                       |
|-------------------------------|------------|--------------|-----------|----------|---------------|--------|-------|------------|--------------------|-------------------|----------|-------------|--------------|-----------|-----------|---------|--------------------|---------------------------------------|
| ate                           | 0(         | 6 May 2013 2 | 2:20:00   | Date     | Stamp         |        |       | 3 22:20:00 |                    |                   |          |             |              |           |           |         |                    |                                       |
| ile Name                      | W:         | ss7a.ds.man. | ac.uk\vol | 5\VOL3\U | SERS\SNMF     |        |       | \TA\BRUK   | (500DATA\2         | D13VMAY\DA        |          |             | -05-06-EJT-: | 23\10\PD/ | ATA\1\1R  |         | major og overgeten |                                       |
| requency (MH:                 | 2) 12      | 25.76        | 10.45     | Nucle    | us            | 130    |       |            | Numbe              | r of Transie      |          | 3000        |              | Origin    |           |         | pect               |                                       |
| riginal Points                |            | 2768         |           | Owne     | r             | vnm    | r1    |            | Points             | Count             | 3        | 32768       |              |           | Sequence  |         | pg30               |                                       |
| Receiver Gain                 |            | 12.00        |           | SW(c     | yclical) (Hz) | 297    | 61.90 |            | Solven             | t                 | C        | CHLOROFO    | RM-d         | Spectri   | um Offset | (Hz) 12 | 2562.9922          |                                       |
| pectrum Type                  |            | TANDARD      |           |          | p Width (Hz)  | 297    | 61.00 |            | Tempe              | rature (degr      | ee C) 2  | 5.128       |              | }         |           |         |                    |                                       |
| 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0 | C-13NMR.c  | odx.esp Veri | ticalSca  | aleFacto | or = 1        |        | •     | F F F      | ОТВО<br>ОН<br>40   |                   | 6        |             |              | 3         |           |         |                    |                                       |
| 0.2 response                  |            |              |           |          | 134.7712      |        |       | 132.8068   |                    | 130 3078          | 130.1056 | 129.5784    |              | -127,6573 |           |         |                    | · · · · · · · · · · · · · · · · · · · |
| 139                           | 138        | 137          | 1:        | 36       | 135           | 134    | 133   |            | 132<br>Chemical Sh | 131<br>nift (ppm) | 130      | 129         | 12           | 28        | 127       | 126     | 125                | 124                                   |
| lo. (ppm)                     | (Hz)       | Height       | No.       | (ppm)    | (Hz)          | Height | No.   | (ppm)      | (Hz)               | Height            | No.      | (ppm)       | (Hz)         | Height    | No.       | (ppm)   | (Hz)               | Height                                |
| 1 19.01                       | 2390.9     | 0.2061       | 6         | 72.58    | 9127.5        | 0.0859 | 11    | 120.82     | 15194.7            | 0.1070            | 16       | 129.58      | 16295.5      | 0.0367    | 21        | 132.81  | 16701.5            | 0.1135                                |
| 2 26.76                       | 3365.5     | 0.4888       | 7         | 72.82    | 9157.5        | 0.0440 | 12    | 120.90     | 15204.7            | 0.0546            | 17       | 129.87      | 16331.8      | 0.3682    | 22        | 132.87  | 16709.7            | 0.1225                                |
|                               | 4003.1     | 0.0785       | 8         | 117.91   | 14828.6       | 0.0221 | 13    | 121.78     | 15314.6            | 0.0234            | 18       | 129.90      | 16335.5      | 0.0755    | 23        | 134.77  | 16948.5            | 0.0635                                |
| 3 31.83                       | 100001     | 9,0100       |           |          |               | 0.0281 | 14    | 127.66     | 16053.9            | 0.0923            | 19       | 130.11      | 16361.8      | 0.1076    | 24        | 135.49  | 17038.4            | 0.6292                                |
| 3 31.83<br>4 61.95            | 7790.5     | 0.1612       | 9         | 119.84   | 15071.2       | U.UZBT | 19    | 127.00     | 10000.0            | 0.0323            | 1.0      | 130.11      | 10001.0      | 0,1010    |           |         | 11000.             |                                       |

23/05/2014 18:08:10

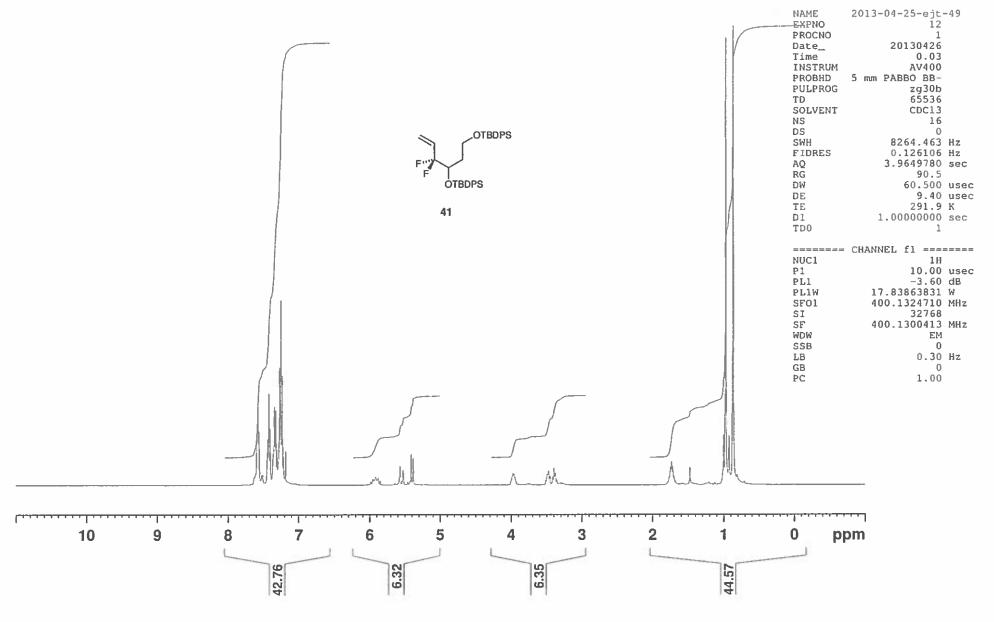
| Acquisition Time (sec) | 0.5767                   | Comment           | EJT-PRM78 Prod data m | 19FCPD CDCl3 /opt/oldbru | ık500data.11vii11/2013/M | ay ejt 23            |             |
|------------------------|--------------------------|-------------------|-----------------------|--------------------------|--------------------------|----------------------|-------------|
| Date                   | 06 May 2013 22:24:16     | Date Stamp        | 06 May 2013 22:24:16  |                          |                          |                      |             |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | VOL3\USERS\SNMRDA | TA\BRUK500DATA\BRUK5  | 00DATA\2013\MAY\DATA\    | EJT\NMR\2013-05-06-EJ    | T-23\12\PDATA\1\1R   |             |
| Frequency (MHz)        | 470.59                   | Nucleus           | 19F                   | Number of Transients     | 16                       | Origin               | spect       |
| Original Points Count  | 65536                    | Owner             | vnmr1                 | Points Count             | 65536                    | Pulse Sequence       | zgfhigqn    |
| Receiver Gain          | 287.00                   | SW(cyclical) (Hz) | 113636.37             | Solvent                  | CHLOROFORM-d             | Spectrum Offset (Hz) | -47059.0234 |
| Spectrum Type          | STANDARD                 | Sween Width (Hz)  | 113634.63             | Temperature (degree C    | 27.000                   |                      |             |



| No. | (ppm)   | (Hz)     | Height |
|-----|---------|----------|--------|
| 1   | -113.84 | -53574.4 | 0.5903 |
| 2   | -113.32 | -53326.4 | 0.7057 |
| 3   | -108.51 | -51061.9 | 1.0000 |
| 4   | -107.97 | -50812.2 | 0.8064 |

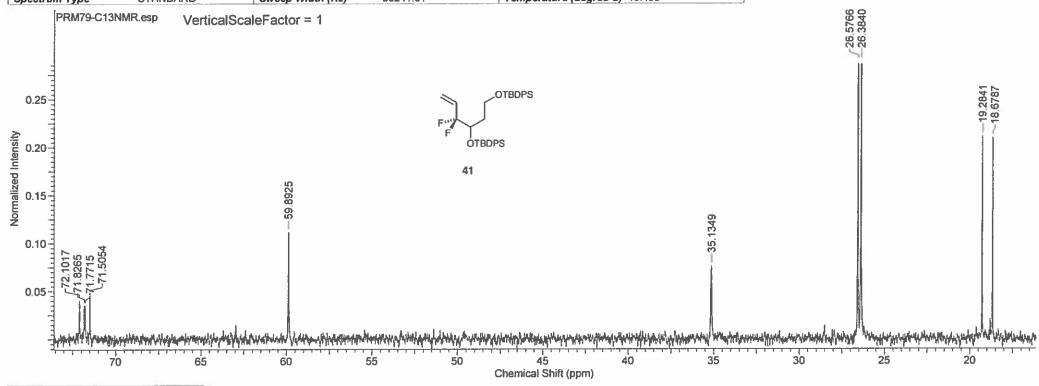
## EJT-PRM77/79 Prod data mPROTONnight CDCl3 {e:\bruk400data\2013\Apr} ejt 49





12/06/2013 11:53:18

| Acquisition Time (sec)                                                                                                   | 1.0835               | Comment           | EJT-PRM77/79 Prod dat | EJT-PRM77/79 Prod data mCARBONnight CDCl3 {e:\bruk400data\2013\Apr} ejt 49 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                      |            |  |  |  |
|--------------------------------------------------------------------------------------------------------------------------|----------------------|-------------------|-----------------------|----------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------|------------|--|--|--|
| Date                                                                                                                     | 25 Apr 2013 23:47:28 | Date Stamp        | 25 Apr 2013 23:47:28  |                                                                            | AND STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE STATE OF THE S |                      |            |  |  |  |
| File Name \\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2013\APR\DATA\EJT\NMR\2013-04-25-EJT-49\10\PDATA\1\1R |                      |                   |                       |                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                      |            |  |  |  |
| Frequency (MHz)                                                                                                          | 100.61               | Nucleus           | 13C                   | Number of Transients                                                       | 600                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Origin               | AV400      |  |  |  |
| Original Points Count                                                                                                    | 32768                | Owner             | Administrator         | Points Count                                                               | 32768                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Pulse Sequence       | zgpg30     |  |  |  |
| Receiver Gain                                                                                                            | 512.00               | SW(cyclical) (Hz) | 30241.94              | Solvent                                                                    | CHLOROFORM-d                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Spectrum Offset (Hz) | 11297.1592 |  |  |  |
| Spectrum Type                                                                                                            | STANDARD             | Sween Width (Hz)  | 30241 01              | Temperature (degree C                                                      | 19.400                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                      |            |  |  |  |



| No. | (ppm) | (Hz)   | Height |
|-----|-------|--------|--------|
| 1   | 18.68 | 1879.3 | 0.2102 |
| 2   | 19.28 | 1940.2 | 0.2114 |
| 3   | 26.38 | 2654.6 | 0.5291 |
| 4   | 26.58 | 2673.9 | 0.5033 |
| 5   | 35.13 | 3535.0 | 0.0761 |
| 6   | 59.89 | 6026.0 | 0.1114 |
| 7   | 71.51 | 7194.4 | 0.0453 |
| 8   | 71.77 | 7221.1 | 0.0348 |
| 9   | 71.83 | 7226.7 | 0.0355 |
| 10  | 72.10 | 7254.3 | 0.0405 |

| Acquisition Time (sec)                              | 1.0835                                      | Comment                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | EJT-PRM77/79 Prod dat                                    | a mCARBONnight CDCl3 (e                                                        | e:\bruk400data\2013\Ap                            | or} ejt 49                                                          |                                                |                      |
|-----------------------------------------------------|---------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------|--------------------------------------------------------------------------------|---------------------------------------------------|---------------------------------------------------------------------|------------------------------------------------|----------------------|
| Date                                                | 25 Apr 2013 23:47:28                        | Date Stamp                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 25 Apr 2013 23:47:28                                     |                                                                                |                                                   |                                                                     |                                                |                      |
| File Name                                           | \\ss7a.ds.man.ac.uk\vol5                    | NVOL3/USERS/SNMRDA                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | TA\BRUK400DATA\2013\A                                    |                                                                                |                                                   |                                                                     |                                                |                      |
| Frequency (MHz)                                     | 100.61                                      | Nucleus                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 13C                                                      | Number of Transients                                                           | 600                                               | <u>Origin</u>                                                       | AV400                                          |                      |
| Original Points Count                               | 32768                                       | Owner                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Administrator                                            | Points Count                                                                   | 32768                                             | Pulse Sequence                                                      | zgpg30                                         |                      |
| Receiver Gain                                       | 512.00                                      | SW(cyclical) (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 30241.94                                                 | Solvent                                                                        | CHLOROFORM-d                                      | Spectrum Offset (H.                                                 | z) 11297.1592                                  |                      |
| Spectrum Type                                       | STANDARD                                    | Sweep Width (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 30241.01                                                 | Temperature (degree C)                                                         | 19.400                                            |                                                                     |                                                |                      |
| 0.15 - 0.10 - 0.05 - 0.05                           | A September 135,5965                        | 133,216 all and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second and a second a second and cond and ——————————————————————————————————————                   | 127.2124                                                                       | OTBOPS<br>F OTBOPS                                |                                                                     | -120.3236 $-120.4153$                          |                      |
| 137 136                                             | 135 134                                     | 133 132 131                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                          | 28 127 126<br>Chemical Shift (ppm)                                             | 125 124                                           | 123 122 121                                                         | 120 119                                        | 118                  |
| 137 136                                             |                                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                          | Chemical Shift (ppm)                                                           |                                                   |                                                                     |                                                | 118                  |
| 137 136                                             | ) Height No.                                | (ppm) (Hz) H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Height No. (ppm)                                         | Chemical Shift (ppm)  (Hz) Height I                                            | 125 124  No. (ppm) (H                             | z) Height No.                                                       |                                                |                      |
| 137 136 lo. (ppm) (Hz) 1 18.68 1879.                | ) Height No. 3 0.2102 7                     | (ppm) (Hz) F<br>71.51 7194.4 0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | Height No. (ppm)<br>1.0453 13 120.51                     | Chemical Shift (ppm)  (Hz) Height 12124.5 0.0424                               | No. (ppm) (H                                      | z) Height No.<br>22.5 0.1720 25                                     | (ppm) (Hz)                                     | Height               |
| 137 136  No. (ppm) (Hz) 1 18.68 1879. 2 19.28 1940. | Height No. 3 0.2102 7 .2 0.2114 8           | (ppm) (Hz) H<br>71.51 7194.4 0<br>71.77 7221.1 0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Height No. (ppm)<br>1.0453 13 120.51<br>1.0348 14 127.16 | Chemical Shift (ppm)  (Hz) Height 12124.5 0.0424 12793.7 0.4051                | No. (ppm) (H:                                     | z) Height No.<br>22.5 0.1720 25<br>51.2 0.0625 26                   | (ppm) (Hz)<br>133.34 13415.7                   | Height 0.1369        |
| 137 136<br>No. (ppm) (Hz)<br>1 18.68 1879.          | Height No. 3 0.2102 7 2 0.2114 8 6 0.5291 9 | (ppm) (Hz) H<br>71.51 7194.4 0<br>71.77 7221.1 0<br>71.83 7226.7 0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | Height No. (ppm)<br>1.0453 13 120.51                     | Chemical Shift (ppm)  (Hz) Height 12124.5 0.0424 12793.7 0.4051 12799.2 0.7568 | No. (ppm) (H:<br>19 129.43 1302<br>20 129.72 1305 | z) Height No.<br>22.5 0.1720 25<br>51.2 0.0625 26<br>77.0 0.0402 27 | (ppm) (Hz)<br>133.34 13415.7<br>135.08 13591.1 | Height 0.1369 0.4275 |

24

133.32

13413.9

0.1326

0.1114

12

120.42

0.0735

12115,3

18

129,31

13010.5

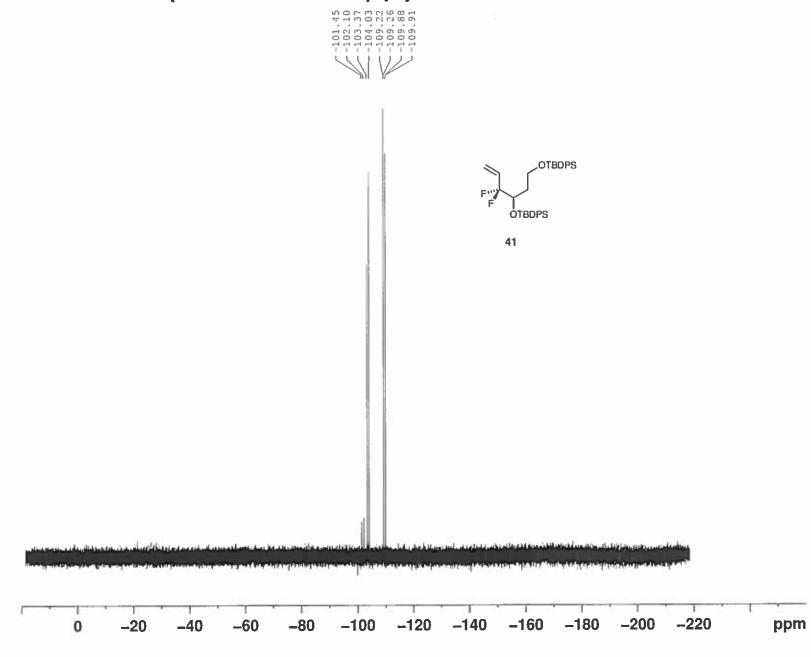
0.1777

6026.0

59.89

6

# EJT-PRM77 f5-11 86mg mF19CPD CDCl3 {e:\bruk400data\2013\Apr} ejt 56

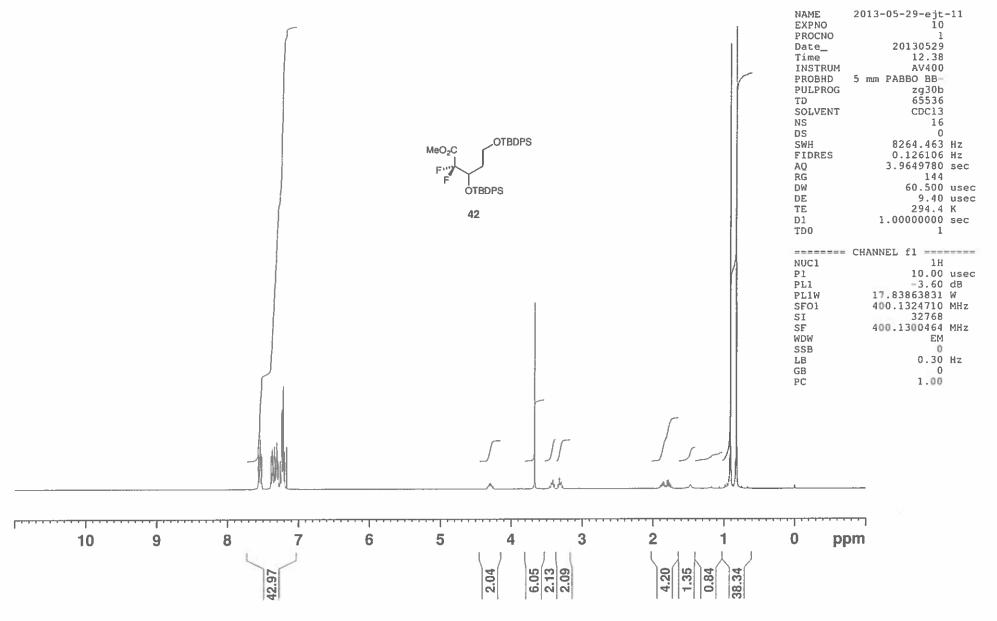




| NAME<br>EXPNO<br>PROCNO<br>Date_<br>Time<br>INSTRUM<br>PROBHD<br>PULPROG | 2013-04-24-ejt-<br>11<br>1<br>20130424<br>18.18<br>AV400<br>5 mm PABBO BB-<br>29ig<br>131072 | 56                       |
|--------------------------------------------------------------------------|----------------------------------------------------------------------------------------------|--------------------------|
| SOLVENT<br>NS<br>DS                                                      | CDC13<br>16<br>4                                                                             |                          |
| SWH<br>FIDRES<br>AQ<br>RG                                                | 89285.711<br>0.681196<br>0.7340532<br>4100                                                   | Hz<br>Hz<br>sec          |
| DW<br>DE<br>TE<br>D1                                                     | 5.600<br>7.51<br>293.3<br>1.00000000                                                         | used<br>used<br>K<br>sec |
| D11<br>TD0                                                               | 0.03000000                                                                                   | sec                      |
| NUC1<br>P1                                                               | CHANNEL fl ====<br>19F<br>10.70                                                              |                          |
| PL1<br>PL1W<br>SFO1                                                      | -5.00<br>27.00716019<br>376.4607164                                                          |                          |
| CPDPRG2<br>HUC2                                                          | CHANNEL f2 ====<br>waltz16<br>1H                                                             | -                        |
| PCPD2<br>PL2<br>PL12<br>PL2W                                             |                                                                                              | used<br>dB<br>dB<br>W    |
| PL12W<br>SFO2<br>SI                                                      | 0.22927761<br>400.1316005<br>262144                                                          | W<br>MHz                 |
| SF<br>WDW<br>SSB                                                         | 376.4983660<br>EM<br>0                                                                       | MHz                      |
| LB<br>GB<br>PC                                                           | 0.30<br>0<br>2.00                                                                            | Hz                       |
|                                                                          |                                                                                              |                          |

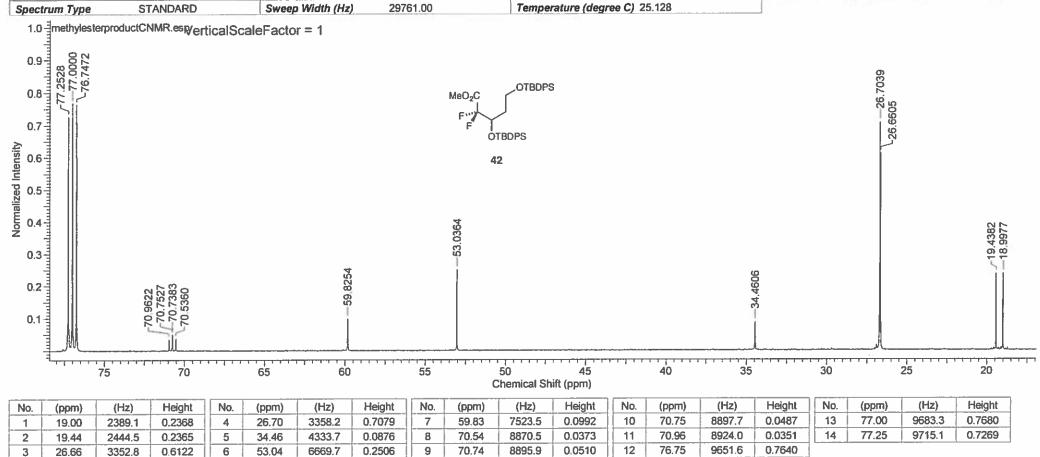
## EJT-PRM89 f10-24 20mg mPROTON CDCI3 {e:\bruk400data\2013\May} ejt 11



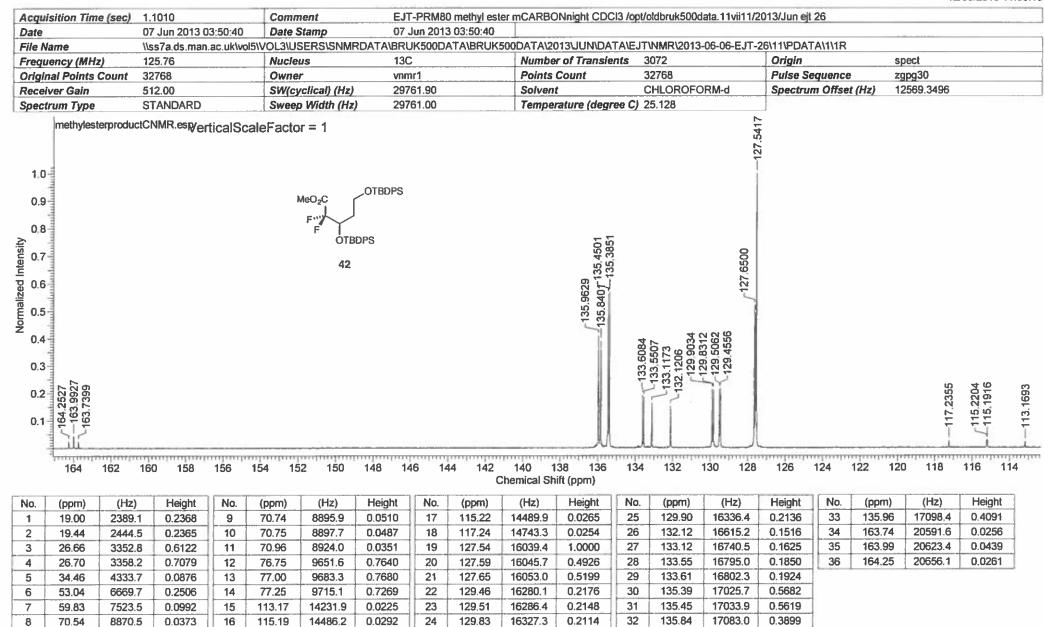


12/06/2013 11:05:49

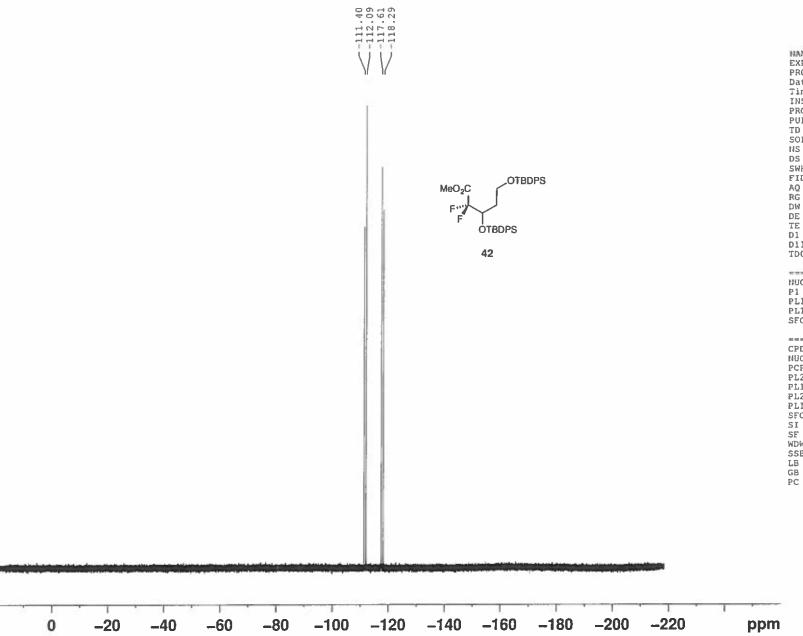
| Acquisition Time (sec) | 1.1010                     | Comment            | EJT-PRM80 methyl ester | r mCARBONnight CDCl3 /o | pt/oldbruk500data.11vii11           | /2013/Jun ejt 26     |            |
|------------------------|----------------------------|--------------------|------------------------|-------------------------|-------------------------------------|----------------------|------------|
| Date                   | 07 Jun 2013 03:50:40       | Date Stamp         | 07 Jun 2013 03:50:40   |                         | CONTRACTOR CONTRACTOR CONTRACTOR CO |                      |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5\\ | VOL3\USERS\SNMRDAT | ABRUK500DATABRUK50     | ODATA\2013\JUN\DATA\E   | JTWMR\2013-06-06-EJT                | -26\11\PDATA\1\1R    |            |
| Frequency (MHz)        | 125.76                     | Nucleus            | 13C                    | Number of Transients    | 3072                                | Origin               | spect      |
| Original Points Count  | 32768                      | Owner              | vnmr1                  | Points Count            | 32768                               | Pulse Sequence       | zgpg30     |
| Receiver Gain          | 512.00                     | SW(cyclical) (Hz)  | 29761.90               | Solvent                 | CHLOROFORM-d                        | Spectrum Offset (Hz) | 12569.3496 |
| Spectrum Type          | STANDARD                   | Sweep Width (Hz)   | 29761.00               | Temperature (degree C   | 25.128                              |                      |            |



12/06/2013 11:06:19



# EJT-PRM89 f10-24 20mg mF19CPD CDCl3 {e:\bruk400data\2013\May} ejt 11

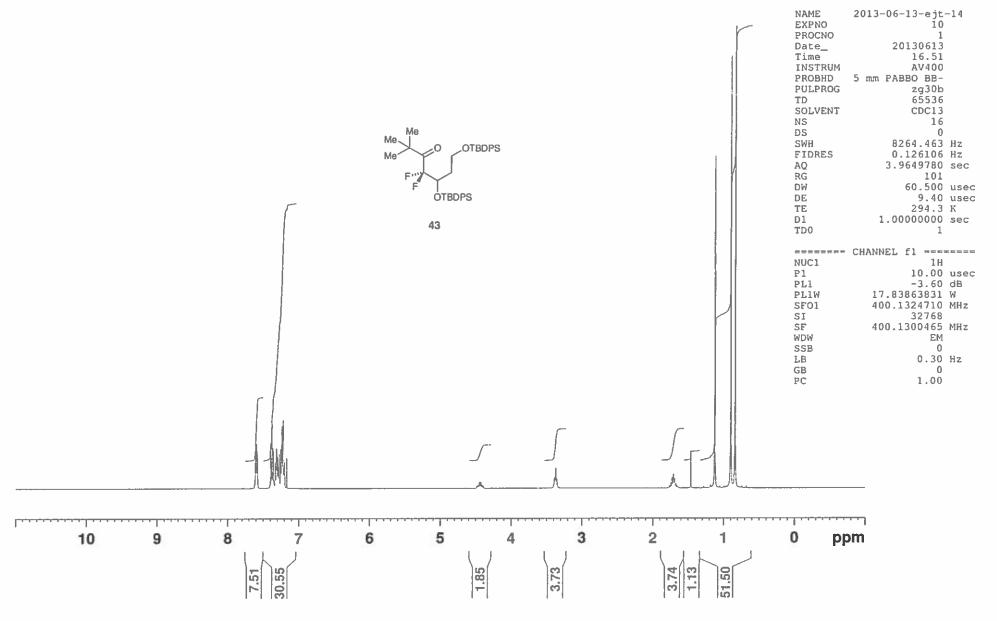




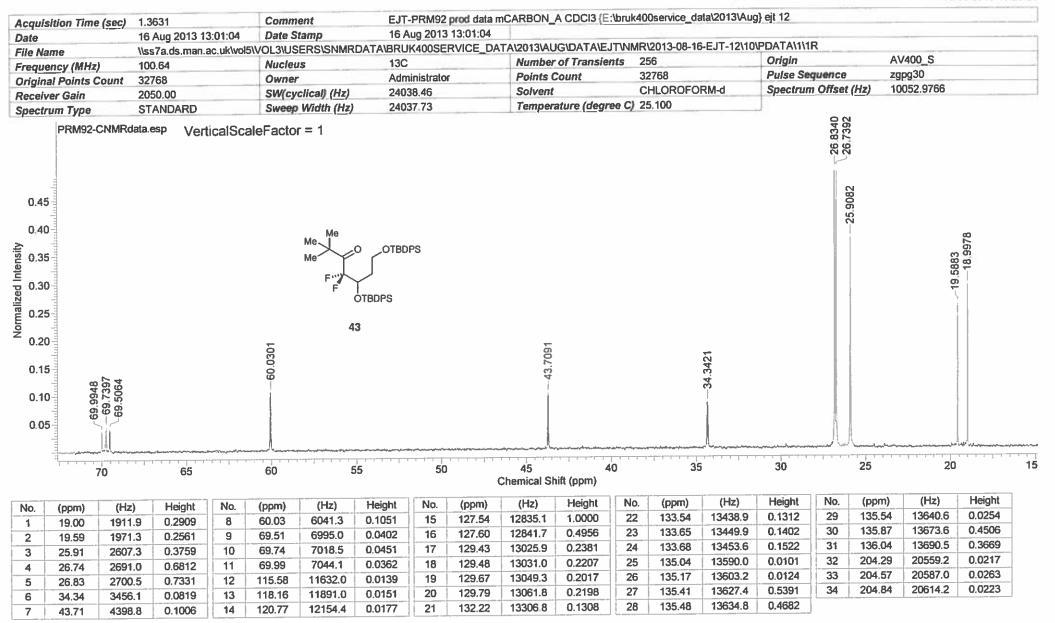
| NAME EXPNO PROCNO Date_ Time INSTRUM PROBHD PULPROG TD SOLVENT INS DS | 2013-05-29-ejt-<br>11<br>20130529<br>12.39<br>AV400<br>5 mm PABBO BB-<br>2gig<br>131072<br>CDC13<br>16 | -11                             |
|-----------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|---------------------------------|
| SWH<br>FIDRES<br>AQ<br>RG<br>DW                                       | 89285.711<br>0.681196<br>0.7340532<br>4100<br>5.600                                                    | Hz<br>Hz<br>sec                 |
| DE<br>TE<br>D1<br>D11<br>TD0                                          | 7.51<br>294.6<br>1.0000000<br>0.03000000                                                               | usec<br>usec<br>K<br>sec<br>sec |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFO1                                     | CHANNEL f1 ====<br>19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164                                 | usec<br>dB                      |
| CPDPRG2 NUC2 PCPD2 PL12 PL12 PL12W SFO2 SI SF WDW SSB LB GB           | 15.31<br>17.83863831<br>0.22927761<br>400.1316005<br>262144<br>376.4983660<br>EM<br>0                  |                                 |
| PC                                                                    | 2.00                                                                                                   |                                 |

# EJT-PRM92 prod fracs 40mg mPROTON CDCI3 {e:\bruk400data\2013\Jun} ejt 14





16/08/2013 13:28:26

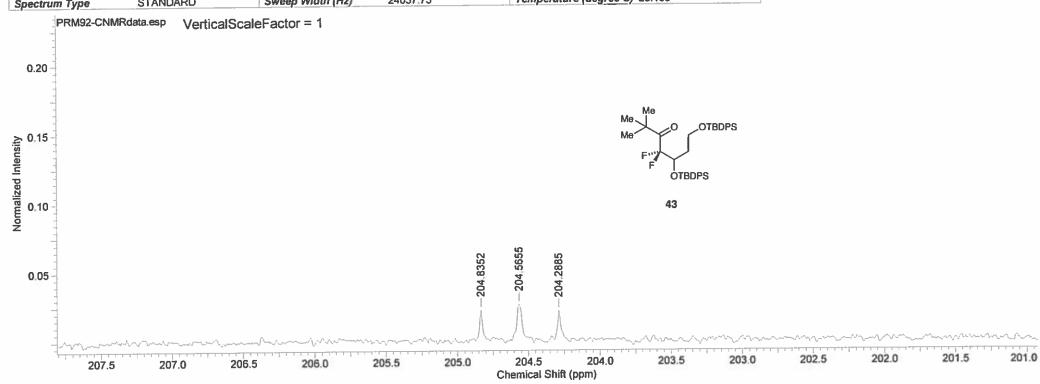


16/08/2013 13:27:53

| cquisition Time (se                                 | 1.3631                                                |                   | Comme                     | int                               | EJT-F                       | PRM92 pro    | od data mo                | CARBON A                                                                                                        | CDCI3 (E:                                | \bruk400        | Oservice_da               | ata\2013\Aug               | } ejt 12                                     |              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                            | 1100000              |
|-----------------------------------------------------|-------------------------------------------------------|-------------------|---------------------------|-----------------------------------|-----------------------------|--------------|---------------------------|-----------------------------------------------------------------------------------------------------------------|------------------------------------------|-----------------|---------------------------|----------------------------|----------------------------------------------|--------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------|----------------------|
| ate                                                 | 16 Aug 2013                                           | 13:01:04          | Date Sta                  | amp                               | 16 Au                       | ig 2013 13   | 1:01:04                   |                                                                                                                 |                                          |                 |                           | F IT 401451                | DDATALCIA                                    | _            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                            |                      |
| le Name                                             | \\ss7a.ds.ma                                          | n.ac.uk\vol5      | SIVOL3IUSE                | ERSISNMRE                         | DATAIBRUK                   | 400SERV      | ICE_DAT                   | A\2013\AU                                                                                                       | G\DATA\EJ                                | TWMRV           | 2013-08-16                | 5-EJT-12\10\               | PDATA\1\1                                    | R            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 4400.0                     |                      |
| requency (MHz)                                      | 100.64                                                |                   | Nucleus                   |                                   | 13C                         |              |                           | Number                                                                                                          | of Transien                              | nts 25          | 6                         |                            | Origin                                       |              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | /400_S                     |                      |
| riginal Points Coun                                 | 32768                                                 |                   | Owner                     |                                   | Admii                       | nistrator    |                           | Points C                                                                                                        | ount                                     |                 | 768                       |                            | Pulse Sec                                    |              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | pg30                       |                      |
| eceiver Gain                                        | 2050.00                                               |                   | SW(cyc                    | lical) (Hz)                       | 24038                       |              |                           | Solvent                                                                                                         |                                          |                 | HLOROFO                   | RM-d                       | Spectrum                                     | Offset (     | Hz) 10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 052.9766                   |                      |
| pectrum Type                                        | STANDARD                                              |                   | Sweep                     | Width (Hz)                        | 24037                       | 7.73         |                           | Tempera                                                                                                         | ture (degre                              | ee C) 25        | 5.100                     |                            | J                                            |              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                            |                      |
| 0.15<br>0.10                                        | 136.0363<br>1135.5416                                 | 135.0387 135.0387 | 133,6828 electric         | 132.2249                          | 129.7902                    | 129,433      |                           | for a now and a not a not a not a not a not a not a not a not a not a not a not a not a not a not a not a not a | h ha ha do marche de si de parache de si | Me Me Me Fi     | OTBDF                     | -120.7732                  | ~. 257 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ | -118.1563    | a contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of the contract of | -115.5831                  | standing in          |
| 138                                                 | 137 136                                               |                   |                           | <del>minamina ina</del>           | 131 130                     | 129          |                           | 127 126<br>hemical Sh                                                                                           |                                          | 124             |                           | 22 121                     | 120 1                                        | 19 11        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                            | 115 114              |
| 138                                                 | 137 136                                               | 411111111111111   | 34 133                    | <del>minnimin</del>               | 131 130                     | 129          |                           |                                                                                                                 |                                          | 124<br>No.      | (ppm)                     | 22 121<br>(Hz)             | 120 1<br>Height                              | 19 11<br>No. | (ppm)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | (Hz)                       | Height               |
| 138<br>o. (ppm)                                     | 137 136<br>Hz) Height                                 | 135 1             | 34 133 (ppm)              | 132                               | 131 130                     | 129<br>No.   | С                         | hemical Sh                                                                                                      | ift (ppm)                                |                 |                           | (Hz)<br>13627.4            | 120 1  Height  0.5391                        | No. 21       | (ppm)<br>204.29                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | (Hz)<br>20559.2            | Height 0.0217        |
| 0. (ppm) 0<br>1 115.58 11                           | 137 136<br>Hz) Height<br>532.0 0.0139                 | 135 1<br>No. 6    | (ppm)<br>129.43           | 132<br>(Hz)                       | 131 130<br>Height           | 129<br>No.   | (ppm)                     | hemical Sh<br>(Hz)                                                                                              | ift (ppm)<br>Height                      | No.             | (ppm)                     | (Hz)<br>13627.4<br>13634.8 | 120 1  Height 0.5391 0.4682                  | No. 21 22    | (ppm)<br>204.29<br>204.57                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | (Hz)<br>20559.2<br>20587.0 | Height 0.0217 0.0263 |
| o. (ppm) 0<br>1 115.58 11<br>2 118.16 11            | 137 136<br>Hz) Height<br>532.0 0.0139<br>391.0 0.0151 | 135 1<br>No. 6    | (ppm)<br>129.43<br>129.48 | 132<br>(Hz)<br>13025.9<br>13031.0 | Height 0.2381 0.2207        | No. 11 12    | (ppm)<br>133.54<br>133.65 | (Hz)<br>13438.9                                                                                                 | ift (ppm) Height 0.1312                  | No.             | (ppm)<br>135.41           | (Hz)<br>13627.4            | 120 1  Height  0.5391                        | No. 21       | (ppm)<br>204.29                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | (Hz)<br>20559.2            | Height 0.0217        |
| 138  lo. (ppm) (1 115.58 11 2 118.16 11 3 120.77 12 | 137 136<br>Hz) Height<br>532.0 0.0139                 | 135 1<br>No. 6    | (ppm)<br>129.43           | 132<br>(Hz)<br>13025.9            | 131 130<br>Height<br>0.2381 | No. 11 12 13 | (ppm)  <br>133.54         | (Hz)<br>13438.9<br>13449.9                                                                                      | Height 0.1312 0.1402                     | No.<br>16<br>17 | (ppm)<br>135.41<br>135.48 | (Hz)<br>13627.4<br>13634.8 | 120 1  Height 0.5391 0.4682                  | No. 21 22    | (ppm)<br>204.29<br>204.57                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | (Hz)<br>20559.2<br>20587.0 | Height 0.0217 0.0263 |

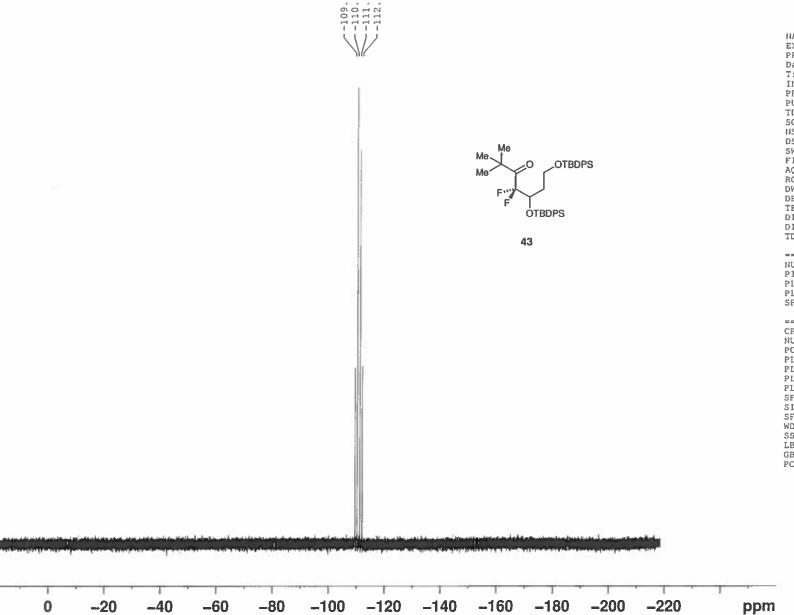
16/08/2013 13:27:10

| Acquisition Time (sec) | 1.3631                    | Comment             | EJT-PRM92 prod data mC | CARBON_A CDC13 (E:\bru | k400service_data\2013\Aug | } ejt 12             |            |
|------------------------|---------------------------|---------------------|------------------------|------------------------|---------------------------|----------------------|------------|
| Data                   | 16 Aug 2013 13:01:04      | Date Stamp          | 16 Aug 2013 13:01:04   |                        |                           |                      |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5\ | VOL3\USERS\SNMRDATA | NBRUK400SERVICE_DATA   |                        | MR\2013-08-16-EJT-12\10\  | PDATA\1\1R           | 11100 0    |
| Frequency (MHz)        | 100.64                    | Nucleus             | 13C                    | Number of Transients   | 256                       | Origin               | AV400_S    |
| Original Points Count  | 32768                     | Owner               | Administrator          | Points Count           | 32768                     | Pulse Sequence       | zgpg30     |
| Receiver Gain          | 2050.00                   | SW(cyclical) (Hz)   | 24038.46               | Solvent                | CHLOROFORM-d              | Spectrum Offset (Hz) | 10052.9766 |
| Spectrum Type          | STANDARD                  | Sweep Width (Hz)    | 24037.73               | Temperature (degree C  | ) 25.100                  |                      |            |



| No. | (ppm)  | (Hz)    | Height |
|-----|--------|---------|--------|
| 1   | 204.29 | 20559.2 | 0.0217 |
| 2   | 204.57 | 20587.0 | 0.0263 |
| 3   | 204.84 | 20614.2 | 0.0223 |

# EJT-PRM92 prod fracs 40mg mF19CPD CDCl3 {e:\bruk400data\2013\Jun} ejt 14

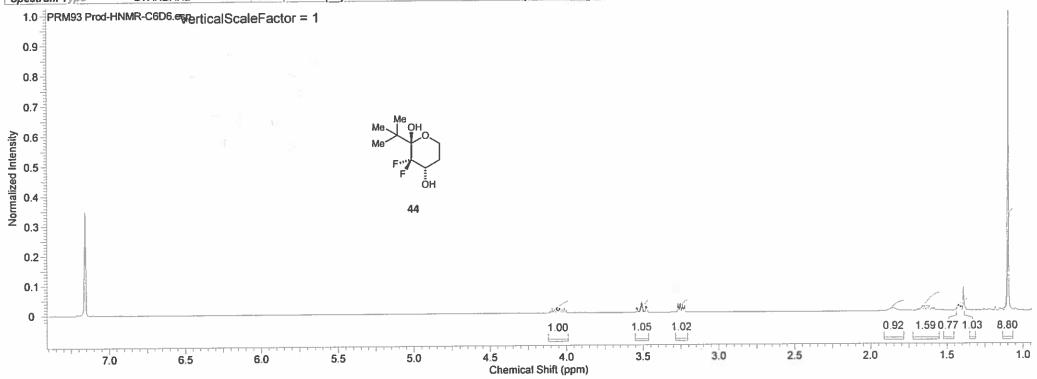




| NAME<br>EXPNO<br>PROCNO<br>Date_<br>Time<br>INSTRUM<br>PROBHD<br>PULPROG<br>TD<br>SOLVENT<br>HS | 2013-06-13-ejt-<br>11<br>20130613<br>16.53<br>AV400<br>5 mm PABBO BB-<br>2gig<br>131072<br>CDC13      | -14             |
|-------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|-----------------|
| DS<br>SWH<br>FIDRES<br>AQ<br>RG<br>DW<br>DE<br>TE<br>D1<br>D1<br>TD0                            | 4<br>89285.711<br>0.681196<br>0.7340532<br>4100<br>5.600<br>7.51<br>294.5<br>1.00000000<br>0.03000000 | used<br>K       |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFOI                                                               | CHANNEL fl =====<br>19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164                               | used<br>dB<br>W |
| CPDPRG2<br>NUC2<br>PCPD2<br>PL2<br>PL12<br>PL12W<br>PL12W<br>SFO2<br>SI<br>SF<br>WDW            | 17.83863831                                                                                           | usec            |
| SSB<br>LB<br>GB<br>PC                                                                           | 0<br>0.30<br>0                                                                                        | Hz              |

17/09/2013 11:11:49

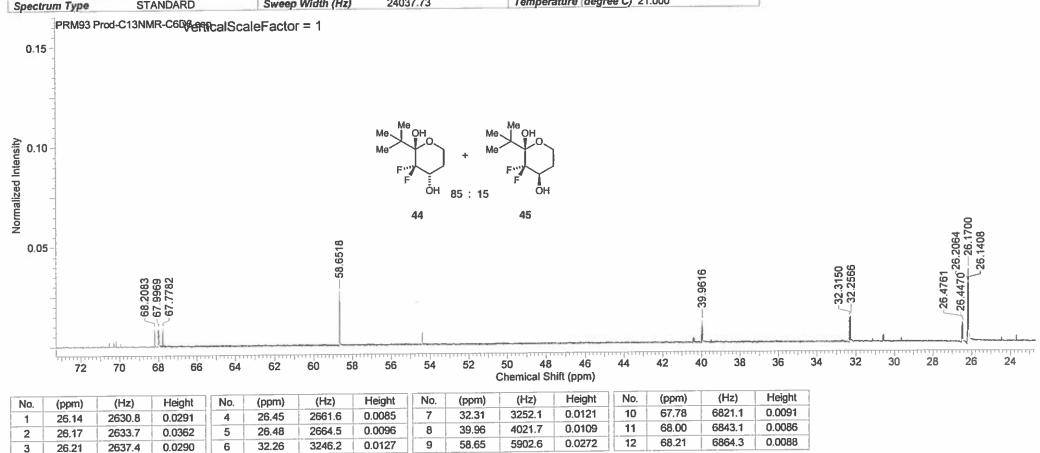
| Acquisition Time (sec) | 3.9846                    | Comment                   | EJT-PRM93 Product data    | C-13 mPROTON C6D6 {        | E:\bruk400service_data\20   | 13\Sep} Administrator 4 |           |
|------------------------|---------------------------|---------------------------|---------------------------|----------------------------|-----------------------------|-------------------------|-----------|
| Date                   | 16 Sep 2013 13:05:20      | Date Stamp                | 16 Sep 2013 13:05:20      |                            |                             |                         |           |
| File Name              | \\ss7a.ds.man.ac.uk\vol5\ | vol3\users\snmrdata\bruk4 | 00service_data\2013\Sep\d | ata\Administrator\nmr\2013 | 1-09-16-Administrator-4\10\ | īd                      |           |
| Frequency (MHz)        | 400.23                    | Nucleus                   | 1H                        | Number of Transients       | 16                          | Origin                  | AV400_S   |
| Original Points Count  | 32768                     | Owner                     | Administrator             | Points Count               | 32768                       | Pulse Sequence          | zg30      |
| Receiver Gain          | 181.00                    | SW(cyclical) (Hz)         | 8223.68                   | Solvent                    | BENZENE-d6                  | Spectrum Offset (Hz)    | 2424.5730 |
| Spectrum Type          | STANDARD                  | Sweep Width (Hz)          | 8223.43                   | Temperature (degree C      | 21.000                      |                         |           |



| No. | (ppm)     | Value      | Absolute Value | Non-Negative Value |
|-----|-----------|------------|----------------|--------------------|
| 1   | 0663 1.13 | 8.79730225 | 3.25690757e+10 | 8.79730225         |
| _2  | 3673 1.40 | 1.02738047 | 3.80353306e+9  | 1.02738047         |
| 3   | 1051 1.47 | 0.77102357 | 2.85445734e+9  | 0.77102357         |
| 4   | 5520 1.72 | 1.59436548 | 5.90260582e+9  | 1.59436548         |
| 5   | 7838 1.91 | 0.91760439 | 3.39712384e+9  | 0.91760439         |
| 6   | 2054 3.28 | 1.02023995 | 3.77709773e+9  | 1.02023995         |
| 7   | 4649 3.55 | 1.04753137 | 3.87813530e+9  | 1.04753137         |
| 8   | 9897 4.11 | 0.99798036 | 3.69468902e+9  | 0.99798036         |
|     |           |            |                |                    |

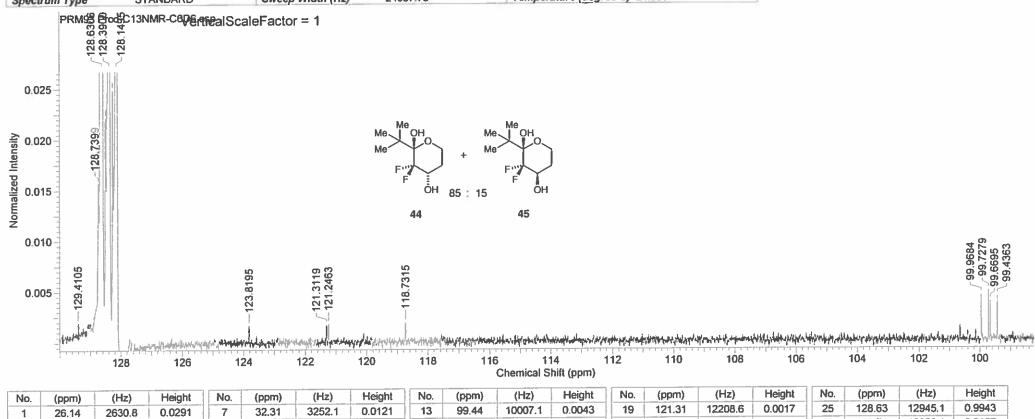
17/09/2013 19:18:31

| Acquisition Time (sec) | 1.3631                   | Comment                   | EJT-PRM93 Product dat      | a C-13 mCARBON C6D6 (E      | :\bruk400service_data   | (2013\Sep) Administrator 4 |            |
|------------------------|--------------------------|---------------------------|----------------------------|-----------------------------|-------------------------|----------------------------|------------|
| Date                   | 16 Sep 2013 13:56:32     | Date Stamp                | 16 Sep 2013 13:56:32       |                             |                         |                            |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | /vol3/users/snmrdata/bruk | 400service_data\2013\Sep\d | ata\Administrator\nmr\2013- | 09-16-Administrator-4\1 | 3\fid                      |            |
| Frequency (MHz)        | 100.64                   | Nucleus                   | 13C                        | Number of Transients        | 12000                   | Origin                     | AV400_S    |
| Original Points Count  | 32768                    | Owner                     | Administrator              | Points Count                | 32768                   | Pulse Sequence             | zgpg30     |
| Receiver Gain          | 2050.00                  | SW(cyclical) (Hz)         | 24038.46                   | Solvent                     | BENZENE-d6              | Spectrum Offset (Hz)       | 10119.6650 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)          | 24037.73                   | Temperature (degree C       | 21.000                  |                            |            |



17/09/2013 19:19:15

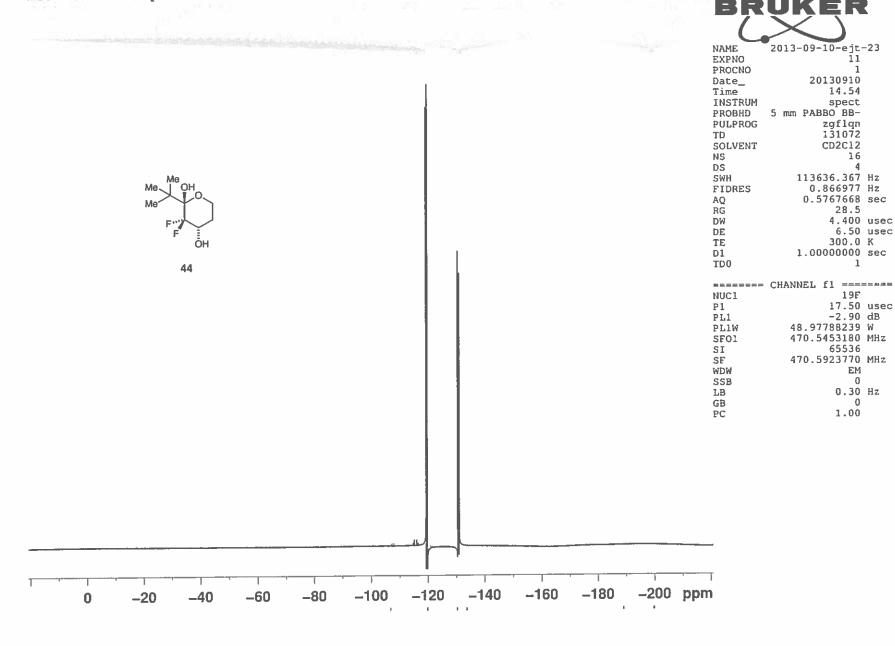
| Acquisition Time (sec) | 1.3631                   | Comment                   | EJT-PRM93 Product dat      | a C-13 mCARBON C6D6 {E      | E:\bruk400service_data | \2013\Sep} Administrator 4 |            |
|------------------------|--------------------------|---------------------------|----------------------------|-----------------------------|------------------------|----------------------------|------------|
| Date                   | 16 Sep 2013 13:56:32     | Date Stamp                | 16 Sep 2013 13:56:32       |                             |                        |                            |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | \vol3\users\snmrdata\bruk | 400service_data\2013\Sep\d | ata\Administrator\nmr\2013- | 09-16-Administrator-4\ | 13\fid                     |            |
| Frequency (MHz)        | 100.64                   | Nucleus                   | 13C                        | Number of Transients        | 12000                  | Origin                     | AV400_S    |
| Original Points Count  | 32768                    | Owner                     | Administrator              | Points Count                | 32768                  | Pulse Sequence             | zgpg30     |
| Receiver Gain          | 2050.00                  | SW(cyclical) (Hz)         | 24038.46                   | Solvent                     | BENZENE-d6             | Spectrum Offset (Hz)       | 10119.6650 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)          | 24037.73                   | Temperature (degree C       | 21.000                 |                            |            |



| (ppm) | (Hz)                                               | Height                                                                       | No.                                                                                                                                                                                                                         | (ppm)                                                                                                                                                                                                                                                                           | (Hz)                                                                                                                                                                                                                                                                                                                                                  | Height                                                                                                                                                                                                                                                                                                                                                                                                                           | No.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | (ppm)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Height                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | No.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | (ppm)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Height                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | No.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           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|-------|----------------------------------------------------|------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------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|       | 2630.8                                             | 0.0291                                                                       | 7                                                                                                                                                                                                                           | 32.31                                                                                                                                                                                                                                                                           | 3252.1                                                                                                                                                                                                                                                                                                                                                | 0.0121                                                                                                                                                                                                                                                                                                                                                                                                                           | 13                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 99.44                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 10007.1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 0.0043                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 19                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 121.31                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 12208.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.0017                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 25                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|       |                                                    | 0.0362                                                                       | 8                                                                                                                                                                                                                           | 39.96                                                                                                                                                                                                                                                                           | 4021.7                                                                                                                                                                                                                                                                                                                                                | 0.0109                                                                                                                                                                                                                                                                                                                                                                                                                           | 14                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 99.67                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 10030.5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 0.0039                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 20                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 123.82                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 12460.9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.0016                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 26                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|       |                                                    | 0.0290                                                                       | 9                                                                                                                                                                                                                           | 58.65                                                                                                                                                                                                                                                                           | 5902.6                                                                                                                                                                                                                                                                                                                                                | 0.0272                                                                                                                                                                                                                                                                                                                                                                                                                           | 15                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 99.73                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 10036.4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 0.0049                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 21                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 128.15                                                                                                                                                                                                                                                                                                                                                                                                                                                                            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                                                                                                                                                                                                                                                                           | 0.9836                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 27                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|       |                                                    |                                                                              | 10                                                                                                                                                                                                                          | 67.78                                                                                                                                                                                                                                                                           | 6821.1                                                                                                                                                                                                                                                                                                                                                | 0.0091                                                                                                                                                                                                                                                                                                                                                                                                                           | 16                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 99.97                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 10060.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 0.0045                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 22                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 128.27                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 12909.2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.0249                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
|       |                                                    |                                                                              |                                                                                                                                                                                                                             |                                                                                                                                                                                                                                                                                 | 6843.1                                                                                                                                                                                                                                                                                                                                                | 0.0086                                                                                                                                                                                                                                                                                                                                                                                                                           | 17                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 118.73                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 11948.9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 0.0019                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 23                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 128.39                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 12920.9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 1.0000                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| 32.26 | 3246.2                                             | 0.0127                                                                       | 12                                                                                                                                                                                                                          | 68.21                                                                                                                                                                                                                                                                           | 6864.3                                                                                                                                                                                                                                                                                                                                                | 0.0088                                                                                                                                                                                                                                                                                                                                                                                                                           | 18                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 121.25                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 12202.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 0.0018                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 24                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 128.51                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 12932.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.0222                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| _     | (ppm)<br>26.14<br>26.17<br>26.21<br>26.45<br>26.48 | 26.14 2630.8<br>26.17 2633.7<br>26.21 2637.4<br>26.45 2661.6<br>26.48 2664.5 | 26.14         2630.8         0.0291           26.17         2633.7         0.0362           26.21         2637.4         0.0290           26.45         2661.6         0.0085           26.48         2664.5         0.0096 | 26.14         2630.8         0.0291         7           26.17         2633.7         0.0362         8           26.21         2637.4         0.0290         9           26.45         2661.6         0.0085         10           26.48         2664.5         0.0096         11 | 26.14         2630.8         0.0291         7         32.31           26.17         2633.7         0.0362         8         39.96           26.21         2637.4         0.0290         9         58.65           26.45         2661.6         0.0085         10         67.78           26.48         2664.5         0.0096         11         68.00 | 26.14         2630.8         0.0291         7         32.31         3252.1           26.17         2633.7         0.0362         8         39.96         4021.7           26.21         2637.4         0.0290         9         58.65         5902.6           26.45         2661.6         0.0085         10         67.78         6821.1           26.48         2664.5         0.0096         11         68.00         6843.1 | 26.14         2630.8         0.0291         7         32.31         3252.1         0.0121           26.17         2633.7         0.0362         8         39.96         4021.7         0.0109           26.21         2637.4         0.0290         9         58.65         5902.6         0.0272           26.45         2661.6         0.0085         10         67.78         6821.1         0.0091           26.48         2664.5         0.0096         11         68.00         6843.1         0.0086 | 26.14         2630.8         0.0291         7         32.31         3252.1         0.0121         13           26.17         2633.7         0.0362         8         39.96         4021.7         0.0109         14           26.21         2637.4         0.0290         9         58.65         5902.6         0.0272         15           26.45         2661.6         0.0085         10         67.78         6821.1         0.0091         16           26.48         2664.5         0.0096         11         68.00         6843.1         0.0086         17 | 26.14         2630.8         0.0291         7         32.31         3252.1         0.0121         13         99.44           26.17         2633.7         0.0362         8         39.96         4021.7         0.0109         14         99.67           26.21         2637.4         0.0290         9         58.65         5902.6         0.0272         15         99.73           26.45         2661.6         0.0085         10         67.78         6821.1         0.0091         16         99.97           26.48         2664.5         0.0096         11         68.00         6843.1         0.0086         17         118.73 | 26.14         2630.8         0.0291         7         32.31         3252.1         0.0121         13         99.44         10007.1           26.17         2633.7         0.0362         8         39.96         4021.7         0.0109         14         99.67         10030.5           26.21         2637.4         0.0290         9         58.65         5902.6         0.0272         15         99.73         10036.4           26.45         2661.6         0.0085         10         67.78         6821.1         0.0091         16         99.97         10060.6           26.48         2664.5         0.0096         11         68.00         6843.1         0.0086         17         118.73         11948.9 | 26.14         2630.8         0.0291         7         32.31         3252.1         0.0121         13         99.44         10007.1         0.0043           26.17         2633.7         0.0362         8         39.96         4021.7         0.0109         14         99.67         10030.5         0.0039           26.21         2637.4         0.0290         9         58.65         5902.6         0.0272         15         99.73         10036.4         0.0049           26.45         2661.6         0.0085         10         67.78         6821.1         0.0091         16         99.97         10060.6         0.0045           26.48         2664.5         0.0096         11         68.00         6843.1         0.0086         17         118.73         11948.9         0.0019 | 26.14         2630.8         0.0291         7         32.31         3252.1         0.0121         13         99.44         10007.1         0.0043         19           26.17         2633.7         0.0362         8         39.96         4021.7         0.0109         14         99.67         10030.5         0.0039         20           26.21         2637.4         0.0290         9         58.65         5902.6         0.0272         15         99.73         10036.4         0.0049         21           26.45         2661.6         0.0085         10         67.78         6821.1         0.0091         16         99.97         10060.6         0.0045         22           26.48         2664.5         0.0096         11         68.00         6843.1         0.0086         17         118.73         11948.9         0.0019         23 | 26.14         2630.8         0.0291         7         32.31         3252.1         0.0121         13         99.44         10007.1         0.0043         19         121.31           26.17         2633.7         0.0362         8         39.96         4021.7         0.0109         14         99.67         10030.5         0.0039         20         123.82           26.21         2637.4         0.0290         9         58.65         5902.6         0.0272         15         99.73         10036.4         0.0049         21         128.15           26.45         2661.6         0.0085         10         67.78         6821.1         0.0091         16         99.97         10060.6         0.0045         22         128.27           26.48         2664.5         0.0096         11         68.00         6843.1         0.0086         17         118.73         119.78.9         0.0019         24         428.51 | 26.14         2630.8         0.0291         7         32.31         3252.1         0.0121         13         99.44         10007.1         0.0043         19         121.31         12208.6           26.17         2633.7         0.0362         8         39.96         4021.7         0.0109         14         99.67         10030.5         0.0039         20         123.82         12460.9           26.21         2637.4         0.0290         9         58.65         5902.6         0.0272         15         99.73         10036.4         0.0049         21         128.15         12896.7           26.45         2661.6         0.0085         10         67.78         6821.1         0.0091         16         99.97         10060.6         0.0045         22         128.27         12909.2           26.48         2664.5         0.0096         11         68.00         6843.1         0.0086         17         118.73         118.73         118.78         0.0019         24         128.39         12920.9 | 26.14         2630.8         0.0291         7         32.31         3252.1         0.0121         13         99.44         10007.1         0.0043         19         121.31         12208.6         0.0017           26.17         2633.7         0.0362         8         39.96         4021.7         0.0109         14         99.67         10030.5         0.0039         20         123.82         12460.9         0.0016           26.21         2637.4         0.0290         9         58.65         5902.6         0.0272         15         99.73         10036.4         0.0049         21         128.15         12896.7         0.9836           26.45         2661.6         0.0085         10         67.78         6821.1         0.0091         16         99.97         10060.6         0.0045         22         128.27         12909.2         0.0249           26.48         2664.5         0.0096         11         68.00         6843.1         0.0086         17         118.73         11948.9         0.0019         23         128.39         12920.9         0.0022 |

| No. | (ppm)  | (Hz)    | Height |
|-----|--------|---------|--------|
| 25  | 128.63 | 12945.1 | 0.9943 |
| 26  | 128.74 | 12956.1 | 0.0157 |
| 27  | 129.41 | 13023.6 | 0.0020 |

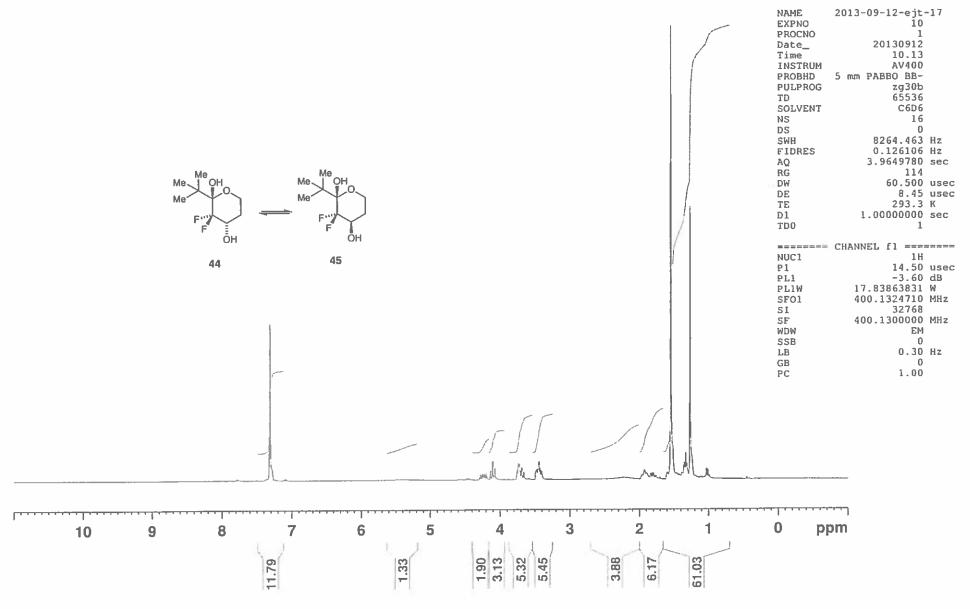
EJT-PRM93 Prod crystals CD2Cl2 m19F CD2Cl2 /opt/oldbruk500data.11vii11/2013/Sep ejt 23



EM 

## EJT-PRM93 Prod crystals in C6D6 2\*o/n mPROTON C6D6 {e:\bruk400data\2013\Sep} ejt 17

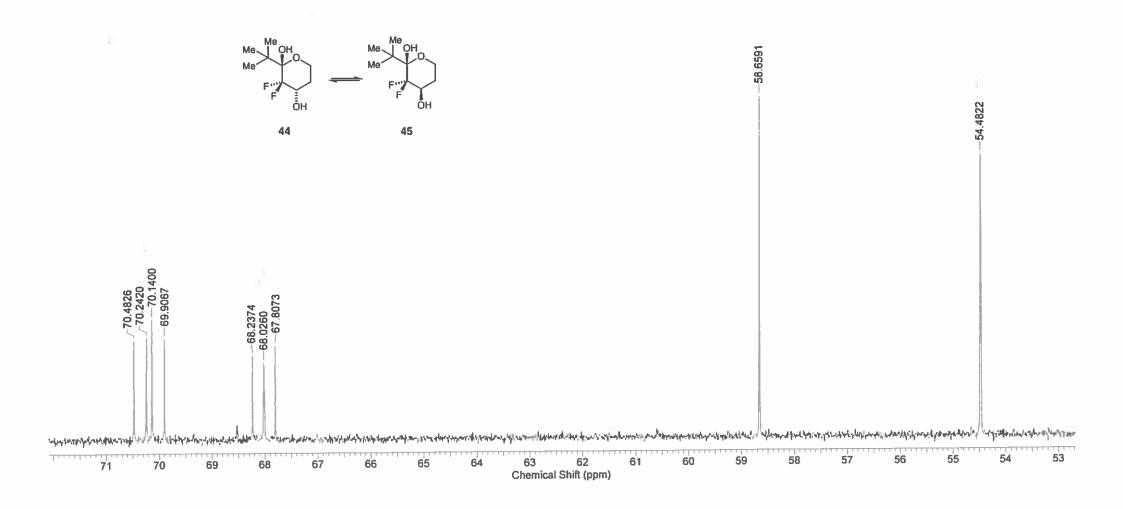




| Date   12 Sep 2013 0.60.048   Date Stamp   12 Sep 2013 0.60.048                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | quisition Time (sec)   |                        | Comment                                                                                    | EJT-PRM93 Prod cr                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | vatals mCARBON C6D      | 6 (E:\bruk40 | Oservice_data\2013  | 3\Sep) Administrator 10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                            |          |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|------------------------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------|--------------|---------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------|----------|
| New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New   New    |                        | 12 Sen 2013 06:00:48   | Date Stamp                                                                                 | 12 Sep 2013 06:00:4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 8                       |              |                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                            |          |
| 100.64   Nucleus   13C   Number of Translents   12000   Origin   Pulse Sequence   2   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   120   12   |                        | \\ss7a ds man ac.uk\vo | 15\vol3\users\snmrdata\bruk                                                                | (400service data\2013\S                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | ep\data\Administrator\n | mr\2013-09-  | 11-Administrator-10 | )\10\fid                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                            |          |
| Total   Points Count   32768                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                        |                        |                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Number of Trai          | nsients 1    | 2000                | Origin                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | AV400_S                    |          |
| Section   2050.00   SW(cyclical) (Hz)   24038.46   Solvent   BENZENE-46   Spectrum Offset (Hz)   1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                        |                        |                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Points Count            |              |                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | zgpg30                     |          |
| Pectrum Type STANDARD Sweep Width (Hz) 24037.73 Temperature (degree C) 18.900  IM93 equilibratedmixture-C13-C606(APA)icalScaleFactor = 1  When the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the standard of the 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of the standard of the standard of the standard of |                        |                        |                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                         |              |                     | Spectrum Offset (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 10119,6650                 |          |
| 178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077   178 8077    |                        |                        |                                                                                            | 24037.73                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | Temperature (d          | legree C) 1  | 8.900               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                            |          |
| 40.428<br>0.0126<br>9616<br>39.990                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | м93 equilibratedmixtur | Me Me Me F ""          | OH Me Me F"                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                         |              |                     | 26.2064                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             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| book withough with the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of | 40.0126                | 39.9616                | ولار منز کو اور در از او از مواد مود در آن و در اور در در در در در در در در در در در در در | ند المؤولة بالعالم الإنوان الإندان عود الدورية المراجع والإندان المراجع والمراجع المراجع 32.2421                 |              | 29.6179             | from no not negligible his his second since to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second to be second | stile angustrykthekrisolaw | -24.4351 |

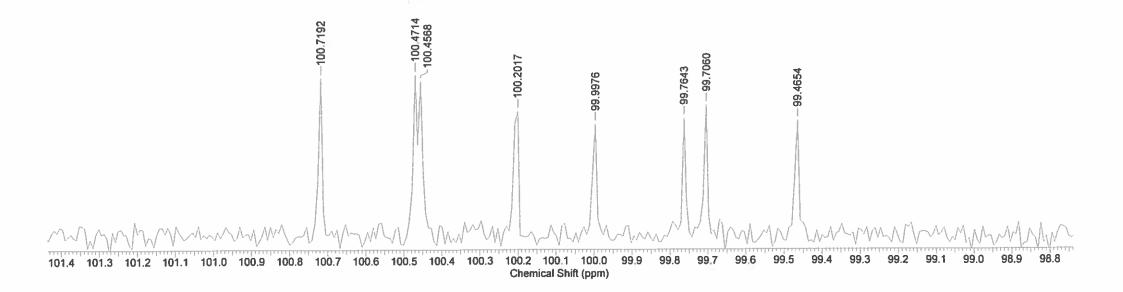
| Acquisition Time (sec) | 1.3631                   | Comment                   | EJT-PRM93 Prod crysta      | ls mCARBON C6D6 (E:\bru     | k400service_data\2013  | 3\Sep} Administrator 10 |            |
|------------------------|--------------------------|---------------------------|----------------------------|-----------------------------|------------------------|-------------------------|------------|
| Date                   | 12 Sep 2013 06:00:48     | Date Stamp                | 12 Sep 2013 06:00:48       |                             |                        |                         |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | /vol3/users/snmrdata/brul | 400service_data\2013\Sep\d | ata\Administrator\nmr\2013- | 09-11-Administrator-10 | 0\10\fid                |            |
| Frequency (MHz)        | 100.64                   | Nucleus                   | 13C                        | Number of Transients        |                        | Origin                  | AV400_S    |
| Original Points Count  | 32768                    | Owner                     | Administrator              | Points Count                | 32768                  | Pulse Sequence          | zgpg30     |
| Receiver Gain          | 2050.00                  | SW(cyclical) (Hz)         | 24038.46                   | Solvent                     | BENZENE-d6             | Spectrum Offset (Hz)    | 10119.6650 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)          | 24037.73                   | Temperature (degree C       | 18.900                 |                         |            |

PRM93 equilibratedmixture-C13-C6D6/efficalScaleFactor = 1



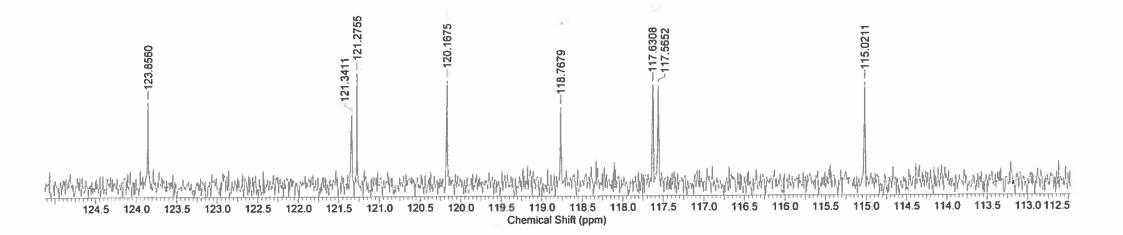
| Acquisition Time (sec) | 1.3631                   | Comment                   | EJT-PRM93 Prod crysta       | is mCARBON C6D6 (E:\bru      | k400service_data\2013\Se   | p) Administrator 10  |            |
|------------------------|--------------------------|---------------------------|-----------------------------|------------------------------|----------------------------|----------------------|------------|
| Date                   | 12 Sep 2013 06:00:48     | Date Stamp                | 12 Sep 2013 06:00:48        |                              |                            |                      |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | \vol3\users\snmrdata\bruk | <400service_data\2013\Sep\d | lata\Administrator\nmr\2013- | 09-11-Administrator-10\10\ | fid                  |            |
| Frequency (MHz)        | 100.64                   | Nucleus                   | 13C                         | Number of Transients         | 12000                      | Origin               | AV400_S    |
| Original Points Count  | 32768                    | Owner                     | Administrator               | Points Count                 | 32768                      | Pulse Sequence       | zgpg30     |
| Receiver Gain          | 2050.00                  | SW(cyclical) (Hz)         | 24038.46                    | Solvent                      | BENZENE-d6                 | Spectrum Offset (Hz) | 10119.6650 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)          | 24037.73                    | Temperature (degree C        | ) 18.900                   |                      |            |

PRM93 equilibratedmixture-C13-C6D6.esp

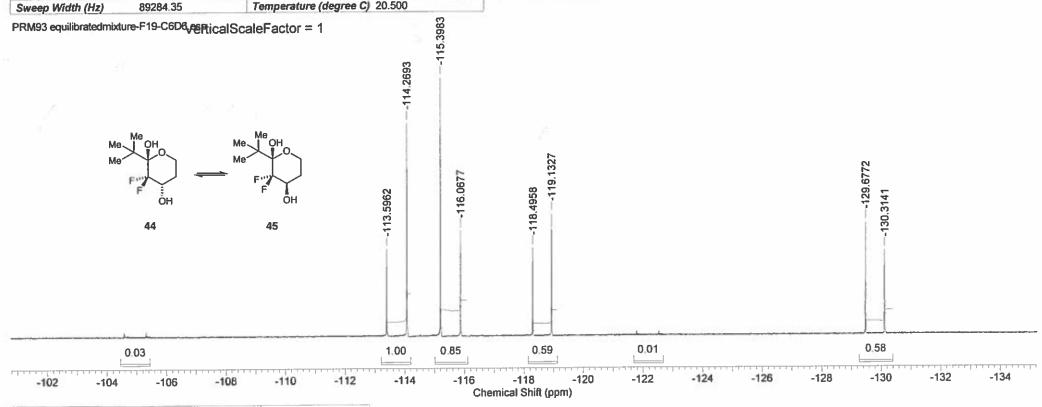


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|------------------------|--------------------------|---------------------------|-----------------------------|------------------------------|-------------------------|-----------------------|------------|
| Date                   | 12 Sep 2013 06:00:48     | Date Stamp                | 12 Sep 2013 06:00:48        |                              |                         |                       |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | \vol3\users\snmrdata\bruk | <400service_data\2013\Sep\d | lata\Administrator\nmr\2013- | 09-11-Administrator-10\ | 10\fid                |            |
| Frequency (MHz)        | 100.64                   | Nucleus                   | 13C                         | Number of Transients         | 12000                   | Origin                | AV400_S    |
| Original Points Count  | 32768                    | Owner                     | Administrator               | Points Count                 | 32768                   | Pulse Sequence        | zgpg30     |
| Receiver Gain          | 2050.00                  | SW(cyclical) (Hz)         | 24038.46                    | Solvent                      | BENZENE-d6              | Spectrum Offset (Hz)  | 10119.6650 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)          | 24037.73                    | Temperature (degree C        | 18.900                  |                       |            |

PRM93 equilibratedmixture-C13-C6D6.esp



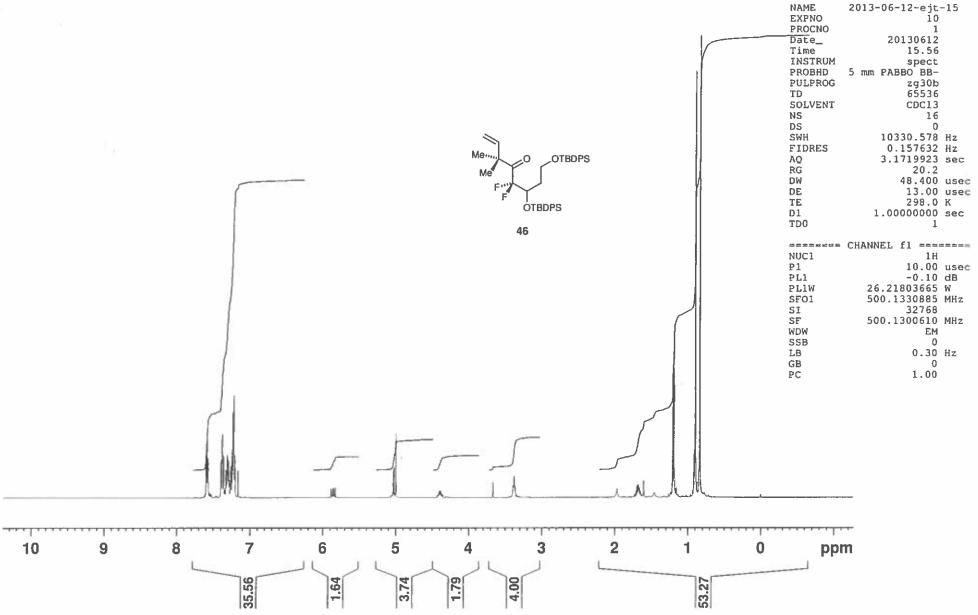
| Acquisition Time (sec) | 0.7340                 | Comment                     | EJT-PRM93 Prodicrys     | tals in C6D6 2*o/n mF19C   | PD C6D6 (e:\bruk400 | Odata\2013\Sep} ejt 17 |          |
|------------------------|------------------------|-----------------------------|-------------------------|----------------------------|---------------------|------------------------|----------|
| Date                   |                        | Date Stamp                  | 12 Sep 2013 10:14:40    |                            |                     |                        |          |
|                        | \\ss7a.ds.man.ac.uk\vo | 15\vol3\users\snmrdata\brul | <400data\2013\Sep\data\ | ejt\nmr\2013-09-12-ejt-17\ | 1Vid                | Frequency (MHz)        | 376.50   |
| Nucleus                | 19F                    | Number of Transients        | 16                      | Origin                     | AV400               | Original Points Count  | 65536    |
| Owner                  | Administrator          | Points Count                | 65536                   | Pulse Sequence             | zgig                | Receiver Gain          | 4100.00  |
| SW(cyclical) (Hz)      | 89285.71               | Solvent                     | BENZENE-d6              | Spectrum Offset (Hz)       | -37649.5977         | Spectrum Type          | STANDARD |
|                        |                        | T                           | 20 500                  |                            |                     |                        |          |



| No. | (ppm)   | Value      | Absolute Value | Non-Negative Value |
|-----|---------|------------|----------------|--------------------|
| 1   | 5932129 | 0.57895821 | 1.36767340e+7  | 0.57895821         |
| 2   | 3756121 | 0.00921777 | 2.17751453e+5  | 0.00921777         |
| 3   | 3266118 | 0.59456044 | 1.40453060e+7  | 0.59456044         |
| 4   | 3128115 | 0.84520292 | 1.99662340e+7  | 0.84520292         |
| 5   | 3975113 | 1.00384212 | 2.37137700e+7  | 1,00384212         |
| 6   | 5377104 | 0.02603587 | 6.15045438e+5  | 0.02603587         |

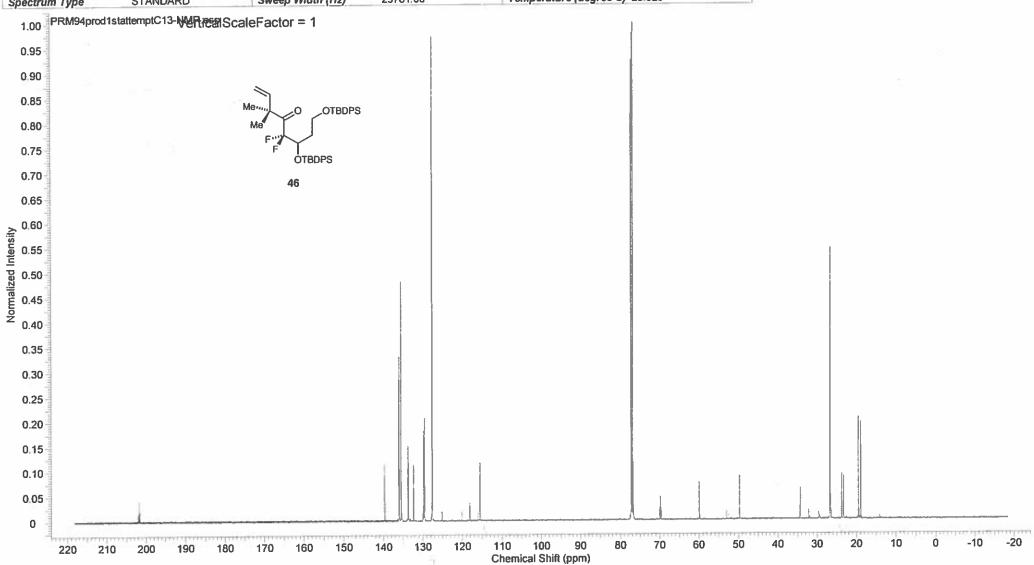
EJT-PRM94 f7-16 47mg mPROTON CDCl3 /opt/oldbruk500data.11vii11/2013/Jun ejt 15





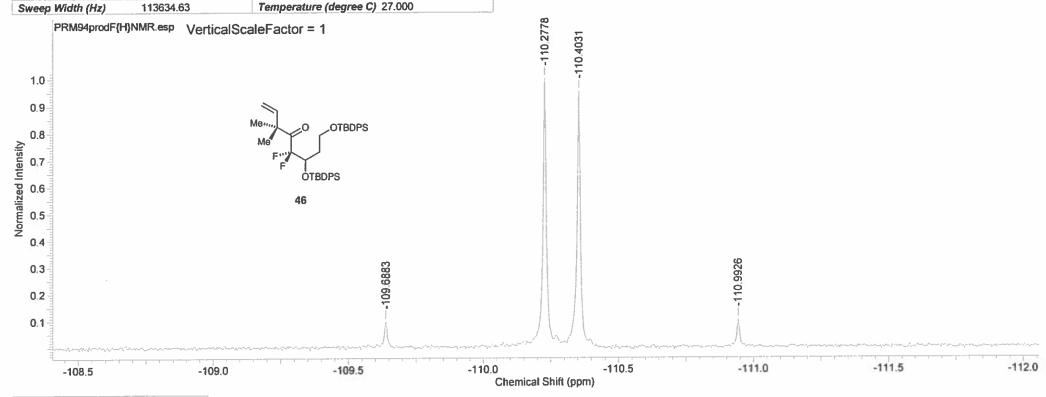
26/07/2013 11:08:37

| Acquisition Time (sec) | 1.1010                   | Comment            | EJT-PRM94 Prod data r | mCARBONnight CDCl3 /opt/ | oldbruk500data.11vii11/2 | 013/Jun ejt 15       |            |
|------------------------|--------------------------|--------------------|-----------------------|--------------------------|--------------------------|----------------------|------------|
| Date                   | 13 Jun 2013 04:54:40     | Date Stamp         | 13 Jun 2013 04:54:40  |                          |                          |                      | 10.00      |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | SVOL3/USERS/SNMRDA | TA\BRUK500DATA\BRUK5  | 00DATA\2013\JUN\DATA\E   | JT\NMR\2013-06-12-EJ     |                      |            |
| Frequency (MHz)        | 125.76                   | Nucleus            | 13C                   | Number of Transients     | 3072                     | Origin               | spect      |
| Original Points Count  | 32768                    | Owner              | vnmr1                 | Points Count             | 32768                    | Pulse Sequence       | zgpg30     |
| Receiver Gain          | 512.00                   | SW(cyclical) (Hz)  | 29761.90              | Solvent                  | CHLOROFORM-d             | Spectrum Offset (Hz) | 12571.1670 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)   | 29761.00              | Temperature (degree C    | 25.029                   |                      |            |



29/05/2014 15:09:13

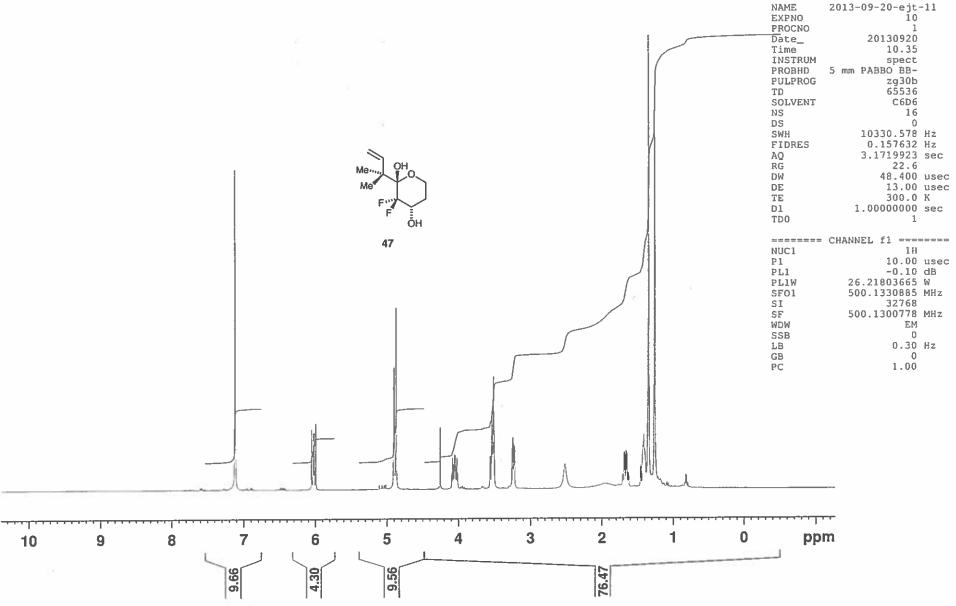
| Acquisition Time (sec) | 0.5767                  | Comment                    | ETJ-PRM94 prod fracs    | 354mg m19FCPD CDCl3        | opt/oldbruk500data.1 | 1vii11/2013/Aug ejt 1 |          |
|------------------------|-------------------------|----------------------------|-------------------------|----------------------------|----------------------|-----------------------|----------|
| Date                   | 24 Aug 2013 18:04:00    | Date Stamp                 | 24 Aug 2013 18:04:00    |                            |                      |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 500data\bruk500data\201 | 3\Aug\data\ejt\nmr\2013-08 | l-24-ejt-1\12\fid    | Frequency (MHz)       | 470.59   |
| Nucleus                | 19F                     | Number of Transients       | 16                      | Origin                     | spect                | Original Points Count | 65536    |
| Owner                  | vnmr1                   | Points Count               | 65536                   | Pulse Sequence             | zgfhigan             | Receiver Gain         | 32.00    |
| SW(cyclical) (Hz)      | 113636.37               | Solvent                    | CHLOROFORM-d            | Spectrum Offset (Hz)       | -47059.0234          | Spectrum Type         | STANDARD |
| 011/0/01/01/01         |                         |                            | . 07.000                |                            |                      |                       |          |



| No. | (ppm)   | (Hz)     | Height |
|-----|---------|----------|--------|
| 1   | -110.99 | -52232.3 | 0.1008 |
| 2   | -110.40 | -51954.8 | 0.9523 |
| 3   | -110.28 | -51895.9 | 1.0000 |
| 4   | -109.69 | -51618.5 | 0.0963 |

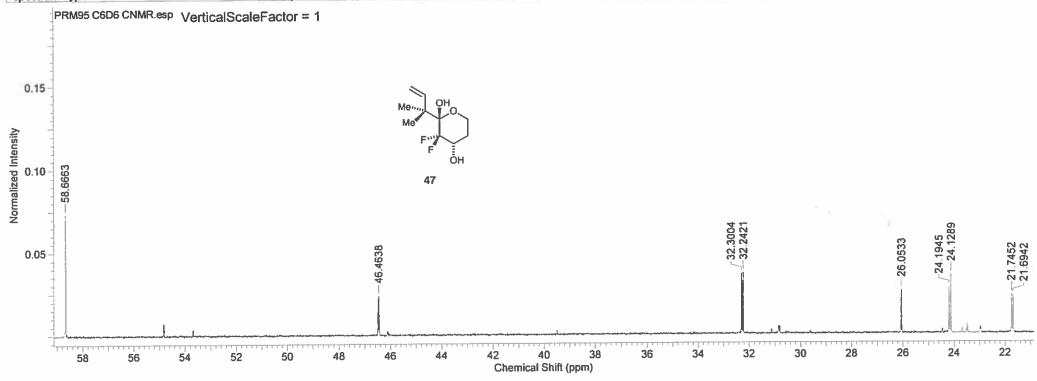
EJT-PRM95 Product data mPROTON C6D6 /opt/oldbruk500data.11vii11/2013/Sep ejt 11





23/09/2013 18:37:19

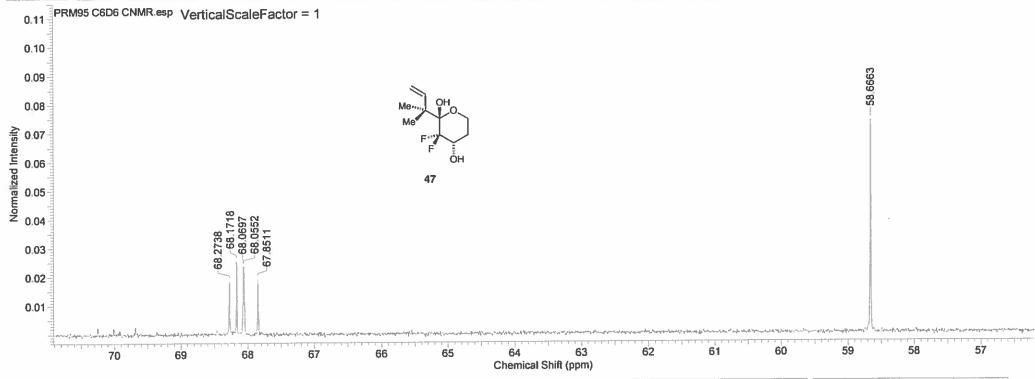
| Acquisition Time (sec) | 1.3631                   | Comment                   | P Mears 0913-081 ejt-pri    | m95 prod xtals mCARBON C     | C6D6 (E:\bruk400servic | e_data\2013\Sep} Administrator | 13         |
|------------------------|--------------------------|---------------------------|-----------------------------|------------------------------|------------------------|--------------------------------|------------|
| Date                   | 20 Sep 2013 10:46:40     | Date Stamp                | 20 Sep 2013 10:46:40        |                              |                        |                                |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | \vol3\users\snmrdata\bruk | 400service_data\2013\Sep\da | nta/Administrator\nmr\2013-0 | 9-20-Administrator-13\ | 11\fid                         |            |
| Frequency (MHz)        | 100.64                   | Nucleus                   | 13C                         | Number of Transients         | 6144                   | Origin                         | AV400_S    |
| Original Points Count  | 32768                    | Owner                     | Administrator               | Points Count                 | 32768                  | Pulse Sequence                 | zgpg30     |
| Receiver Gain          | 2050.00                  | SW(cyclical) (Hz)         | 24038.46                    | Solvent                      | BENZENE-d6             | Spectrum Offset (Hz)           | 10120.3975 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)          | 24037.73                    | Temperature (degree C        | 21.700                 |                                |            |



| No. | (ppm) | (Hz)   | Height |
|-----|-------|--------|--------|
| 1   | 21.69 | 2183.3 | 0.0226 |
| 2   | 21.75 | 2188.4 | 0.0232 |
| 3   | 24.13 | 2428.3 | 0.0351 |
| 4   | 24.19 | 2434.9 | 0.0275 |
| 5   | 26.05 | 2622.0 | 0.0258 |
| 6   | 32.24 | 3244.8 | 0.0365 |
| 7   | 32.30 | 3250.6 | 0.0363 |
| 8   | 46.46 | 4676.0 | 0.0235 |
| 9   | 58.67 | 5904.1 | 0.0736 |

23/09/2013 18:40:51

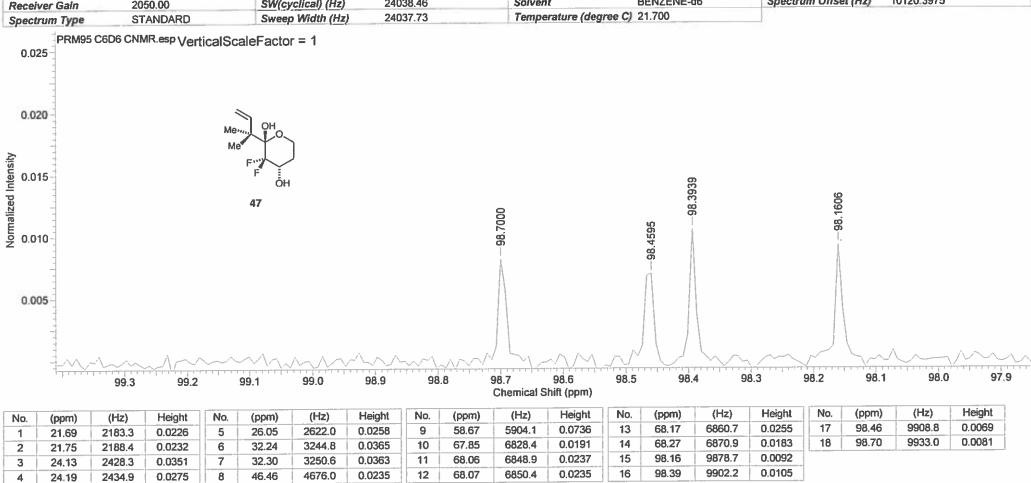
| Acquisition Time (sec) | 1.3631                   | Comment                   | P Mears 0913-081 ejt-pm     | n95 prod xtals mCARBON C    | C6D6 {E:\bruk400servic | e_data\2013\Sep} Administrator | 13         |
|------------------------|--------------------------|---------------------------|-----------------------------|-----------------------------|------------------------|--------------------------------|------------|
| Date                   | 20 Sep 2013 10:46:40     | Date Stamp                | 20 Sep 2013 10:46:40        |                             |                        |                                |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | /vol3/users/snmrdata/bruk | 400service_data\2013\Sep\da | ta\Administrator\nmr\2013-0 | 9-20-Administrator-13\ | 11\fid                         |            |
| Frequency (MHz)        | 100.64                   | Nucleus                   | 13C                         | Number of Transients        | 6144                   | Origin                         | AV400_S    |
| Original Points Count  | 32768                    | Owner                     | Administrator               | Points Count                | 32768                  | Pulse Sequence                 | zgpg30     |
| Receiver Gain          | 2050.00                  | SW(cyclical) (Hz)         | 24038.46                    | Solvent                     | BENZENE-d6             | Spectrum Offset (Hz)           | 10120.3975 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)          | 24037.73                    | Temperature (degree C       | 21.700                 |                                |            |



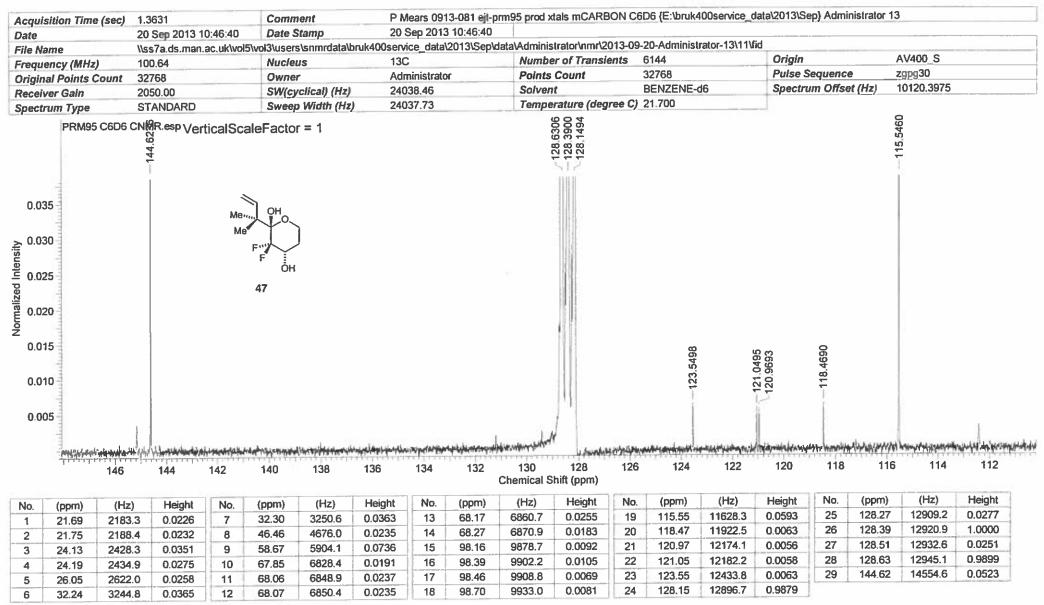
| No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)   | Height |
|-----|-------|--------|--------|-----|-------|--------|--------|-----|-------|--------|--------|-----|-------|--------|--------|-----|-------|--------|--------|
| 1   | 21.69 | 2183.3 | 0.0226 | 4   | 24.19 | 2434.9 | 0.0275 | 7   | 32.30 | 3250.6 | 0.0363 | 10  | 67.85 | 6828.4 | 0.0191 | 13  | 68.17 | 6860.7 | 0.0255 |
| 2   | 21.75 | 2188.4 | 0.0232 | 5   | 26.05 | 2622.0 | 0.0258 | 8   | 46.46 | 4676.0 | 0.0235 | 11  | 68.06 | 6848.9 | 0.0237 | 14  | 68.27 | 6870.9 | 0.0183 |
| 3   | 24.13 | 2428.3 | 0.0351 | 6   | 32.24 | 3244.B | 0.0365 | 9   | 58.67 | 5904.1 | 0.0736 | 12  | 68.07 | 6850.4 | 0.0235 |     |       |        |        |

23/09/2013 18:43:57

| Acquisition Time (sec) | 1.3631                   | Comment                   | P Mears 0913-081 ejt-pri    | n95 prod xtals mCARBON C    | C6D6 (E:\bruk400servic | e_data\2013\Sep) Administrator | 13         |
|------------------------|--------------------------|---------------------------|-----------------------------|-----------------------------|------------------------|--------------------------------|------------|
| Date                   | 20 Sep 2013 10:46:40     | Date Stamp                | 20 Sep 2013 10:46:40        |                             |                        |                                |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | \vol3\users\snmrdata\bruk | 400service_data\2013\Sep\da | ta\Administrator\nmr\2013-0 | 9-20-Administrator-13\ | 11\fid                         |            |
| Frequency (MHz)        | 100.64                   | Nucleus                   | 13C                         | Number of Transients        | 6144                   | Origin                         | AV400_S    |
| Original Points Count  | 32768                    | Owner                     | Administrator               | Points Count                | 32768                  | Pulse Sequence                 | zgpg30     |
| Receiver Gain          | 2050.00                  | SW(cyclical) (Hz)         | 24038.46                    | Solvent                     | BENZENE-d6             | Spectrum Offset (Hz)           | 10120.3975 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)          | 24037.73                    | Temperature (degree C       | 21.700                 |                                |            |

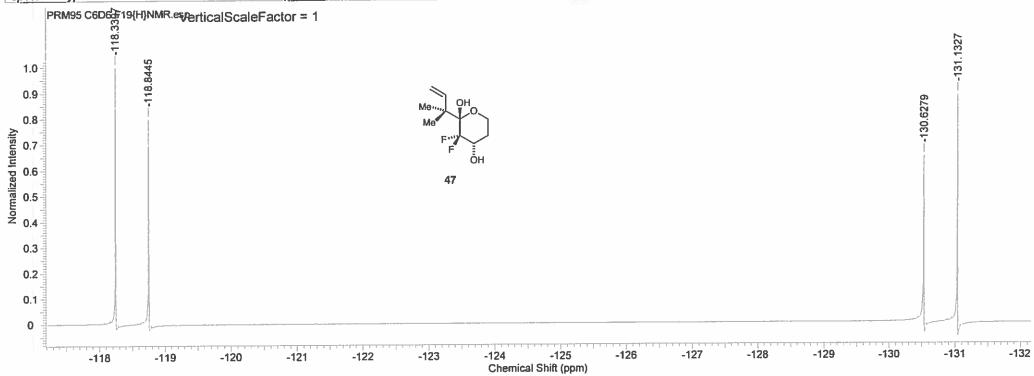


23/09/2013 18:46:37



20/09/2013 11:40:52

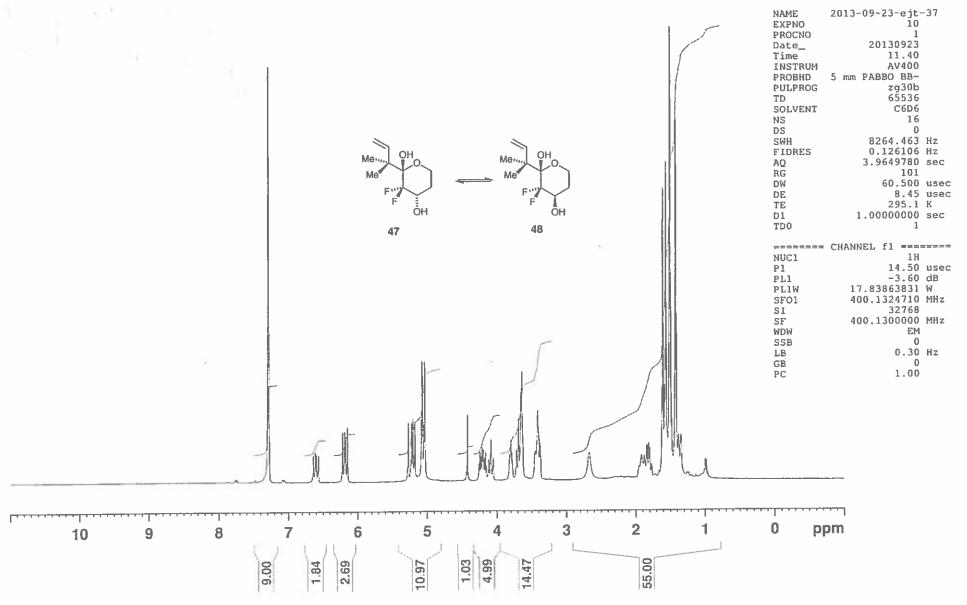
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|------------------------|---------------------------|---------------------|------------------------|------------------------|----------------------------|----------------------|-------------|
| Date                   | 20 Sep 2013 10:40:16      | Date Stamp          | 20 Sep 2013 10:40:16   |                        |                            |                      |             |
| File Name              | \\ss7a,ds.man.ac.uk\vol5\ | VOL3\USERS\SNMRDATA | NBRUK500DATA\BRUK50    | ODATA\2013\SEP\DATA\   | EJT\NMR\2013-09-20-EJT     | 11\12\PDATA\1\1R     |             |
| Frequency (MHz)        | 470.59                    | Nucleus             | 19F                    | Number of Transients   | 16                         | Origin               | spect       |
| Original Points Count  | 65536                     | Owner               | vnmr1                  | Points Count           | 65536                      | Pulse Sequence       | zgfhigan    |
| Receiver Gain          | 32.00                     | SW(cyclical) (Hz)   | 113636.37              | Solvent                | BENZENE-d6                 | Spectrum Offset (Hz) | -47059.0234 |
| Spectrum Type          | STANDARD                  | Sweep Width (Hz)    | 113634.63              | Temperature (degree C  | 27.000                     | j                    |             |



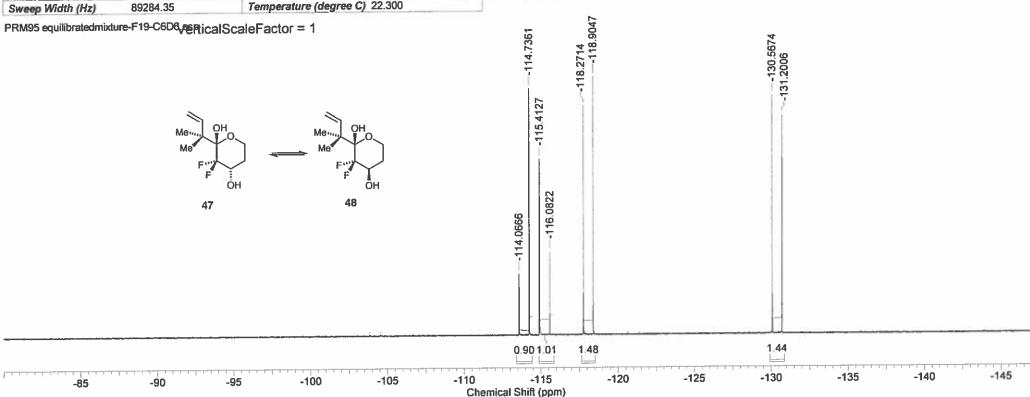
| 1 | No. | (ppm)   | (Hz)     | Height |
|---|-----|---------|----------|--------|
|   | 1   | -131.13 | -61710.1 | 0.8834 |
| İ | 2   | -130.63 | -61472.5 | 0.6455 |
| 1 | 3   | -118.84 | -55927.3 | 0.7986 |
| 1 | 4   | -118.34 | -55689.8 | 1.0000 |

# EJT-PRM95 prod crystals over weekend equilibrated mPROTON C6D6 {e:\bruk400data\2013\Sep} ejt 37





|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Tillo toport mad or     |                            |                         |                              |                   |                                |          |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------|----------------------------|-------------------------|------------------------------|-------------------|--------------------------------|----------|
| Acquisition Time (sec)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | 0.7340                  | Comment                    | EJT-PRM95 prod crysta   | als over weekend equilibrate | ed mF19CPD C6D6 ( | e:\bruk400data\2013\Sep) ejt 3 |          |
| The second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second secon | 23 Sep 2013 11:42:08    | Date Stamp                 | 23 Sep 2013 11:42:08    |                              |                   |                                |          |
| File Name                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | \\ss7a ds man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 400data\2013\Sep\data\e | t\nmr\2013-09-23-ejt-37\11   | l\fid             | Frequency (MHz)                | 376.50   |
| Nucleus                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 19F                     | Number of Transients       | 16                      | Origin                       | AV400             | Original Points Count          | 65536    |
| Owner                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Administrator           | Points Count               | 65536                   | Pulse Sequence               | zgig              | Receiver Gain                  | 4100.00  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 89285.71                | Solvent                    | BENZENE-d6              | Spectrum Offset (Hz)         | -37649.5977       | Spectrum Type                  | STANDARD |
| SW(cyclical) (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 09203.71                | 30ivent                    |                         |                              |                   |                                |          |



Non-Negative Value

1.44295704

1.48149800

1.00809872 0.89820582

Value

(ppm)

3493 .. -1301.44295704

9284 ... -1130.89820582

2 0336 .. -1181.48149800

3 2540 .. -1151.00809872

Absolute Value

2.36217000e+7

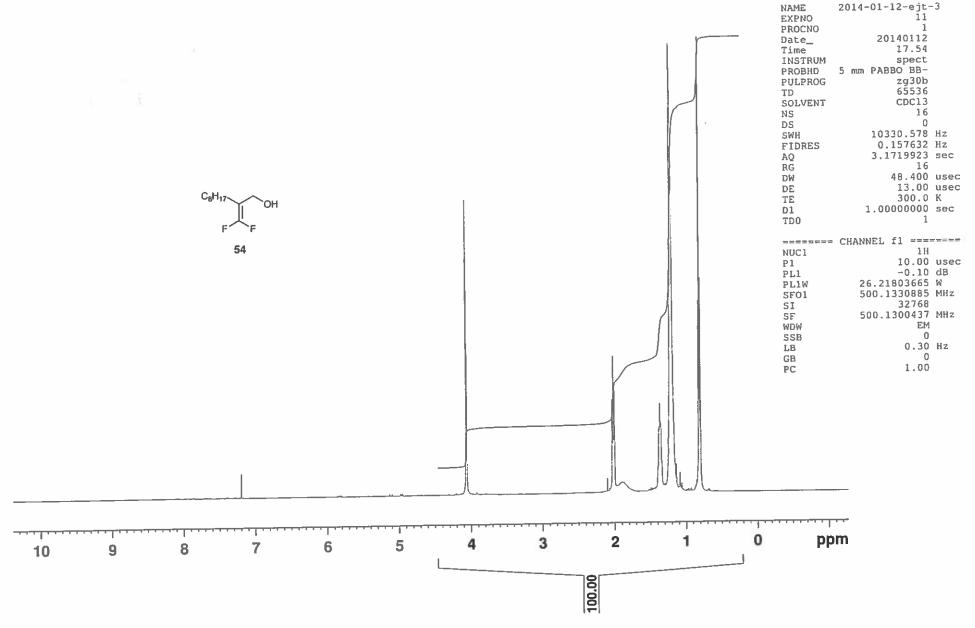
2.42526280e+7

1.65029200e+7

1.47039360e+7

# EJT-PRM115 product data allylic alcohol mPROTONnight CDCl3 /opt/oldbruk500data.11vii11/2014/Jan ejt 3





| Acquisition Time (se                    | ) 1.1010               | Com                                    | ment           | EJ.              | T-PRM1  | 15 product of  | data allylic a    | Icohol mCARI        | BONn   | ight CDCI3               | /opt/oldbruk   | 500data      | a.11vii11/ | 2014/Jan ejt 3 | }      |         |    |
|-----------------------------------------|------------------------|----------------------------------------|----------------|------------------|---------|----------------|-------------------|---------------------|--------|--------------------------|----------------|--------------|------------|----------------|--------|---------|----|
| Date                                    | 12 Jan 2014 17:5       | 50:56 Date                             | Stamp          |                  |         | 4 17:50:56     |                   |                     |        |                          | - 11           |              |            |                |        |         |    |
| ile Name                                | \\ss7a.ds.man.ac       | .uk\vol5\VOL3\L                        | SERS\SNMR      | DATA\BRL         | JK500DA | TABRUKS        | 00DATAV20         | 14\JAN\DAT          | A\EJT  | WMR\2014                 | I-01-12-EJT-   | 3\10\PI      | DATA\1\1   | R              |        |         |    |
| requency (MHz)                          | 125.76                 | Nuci                                   |                | 130              |         |                |                   | er of Transie       |        | 3072                     |                | 0            | rigin      |                | spect  |         |    |
| Original Points Coun                    | 32768                  | Own                                    | er             | VIII             |         |                | Points            | s Count             |        | 32768                    |                |              | Pulse Seq  |                | zgpg30 |         |    |
| Receiver Gain                           | 512.00                 | SW(                                    | cyclical) (Hz) | 297              | 761.90  |                | Solve             |                     |        | CHLORO                   | FORM-d         | S            | pectrum    | Offset (Hz)    | 12571. | 1670    |    |
| pectrum Type                            | STANDARD               | Swe                                    | ep Width (Hz,  | 297              | 761.00  |                | Temp              | erature (degi       | ree C) | 20.099                   |                |              |            |                |        |         |    |
| 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 | 56 54 52               | C <sub>8</sub> H <sub>17</sub><br>F 54 | ОН<br>3 46     | 44 4             |         | 40 38          | 36<br>Chemical Sh | 34 32<br>nift (ppm) |        | 29.3183<br>82<br>29.1956 | 95             | -24.4361     | 22,6233    | 20 1           | 8 16   | 14.0432 | 12 |
|                                         |                        |                                        |                |                  |         |                |                   |                     |        |                          | 41.1           |              |            |                |        |         |    |
|                                         | Jay   Listaba          | No (non)                               | (H-)           | Height           | i Na i  | (nnm)          | /H=\              | Height              | N∩     | (nnm)                    | (H2)           | He           | iant i     |                |        |         |    |
| Vo. (ppm) (                             | Hz) Height 66.0 0.7988 | No. (ppm)<br>4 27.50                   | (Hz)<br>3458.1 | Height<br>0.2238 | No.     | (ppm)<br>29.22 | (Hz)<br>3675.2    | Height 0.7842       | No.    | (ppm)<br>57.66           | (Hz)<br>7251.0 | Heig<br>0.15 |            |                |        |         |    |

29.20

0.4542

3073.0

24.44

3671.6

0.7282

31.82

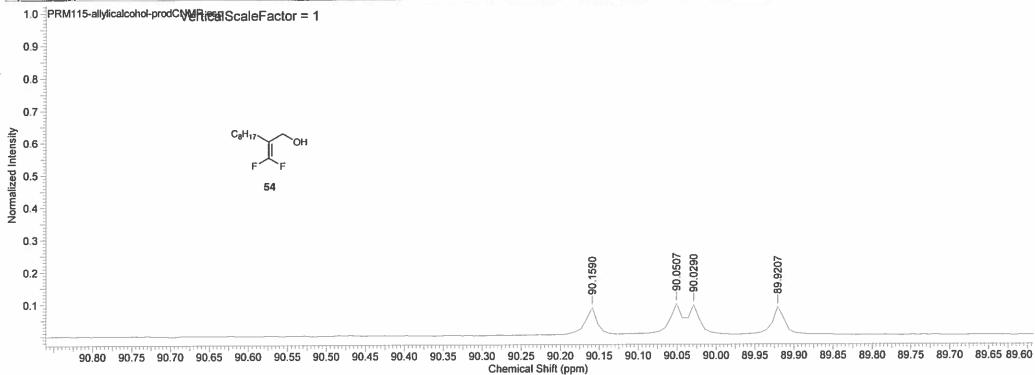
9

0.8907

4001.3

15/01/2014 15:52:04

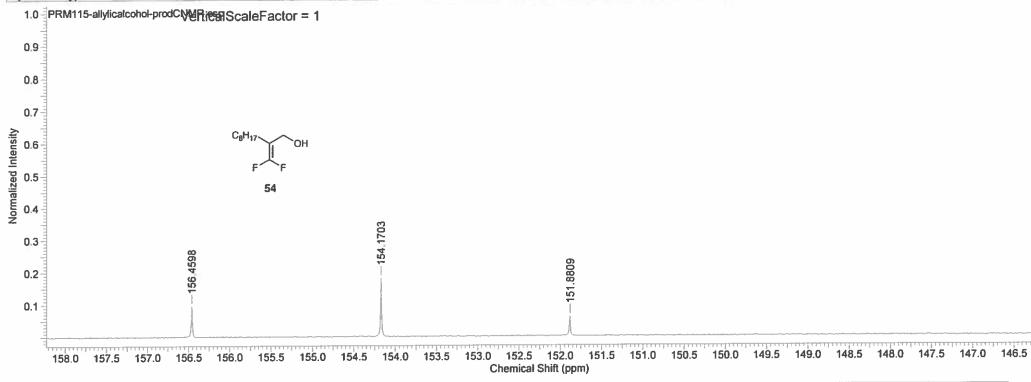
| Acquisition Time (sec) | 1.1010                   | Comment            | EJT-PRM115 product date | ta allylic alcohol mCARBONi | night CDCl3 /opt/oldbruk5 | 00data.11vii11/2014/Jan ejt 3 |            |
|------------------------|--------------------------|--------------------|-------------------------|-----------------------------|---------------------------|-------------------------------|------------|
| Date                   | 12 Jan 2014 17:50:56     | Date Stamp         | 12 Jan 2014 17:50:56    |                             |                           |                               |            |
| File Name              | \\ss7a.ds,man.ac.uk\vol5 | VOL3\USERS\SNMRDAT | AIBRUK500DATAIBRUK500   | DATA\2014\JAN\DATA\EJ       | TVNMR\2014-01-12-EJT-     | 3\10\PDATA\1\1R               |            |
| Frequency (MHz)        | 125.76                   | Nucleus            | 13C                     | Number of Transients        | 3072                      | Origin                        | spect      |
| Original Points Count  | 32768                    | Owner              | vnmr1                   | Points Count                | 32768                     | Pulse Sequence                | zgpg30     |
| Receiver Gain          | 512.00                   | SW(cyclical) (Hz)  | 29761.90                | Solvent                     | CHLOROFORM-d              | Spectrum Offset (Hz)          | 12571.1670 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)   | 29761.00                | Temperature (degree C       | 20.099                    |                               |            |



| No. | (ppm) | (Hz) Heigh   | No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)   | Height | No. (ppm) | (Hz)    | Height | No. | (ppm) | (Hz)    | Height |
|-----|-------|--------------|-----|-------|--------|--------|-----|-------|--------|--------|-----------|---------|--------|-----|-------|---------|--------|
| 1   | 14.04 | 1766.0 0.798 | 4   | 27.50 | 3458.1 | 0.2238 | 7   | 29.22 | 3675.2 | 0.7842 | 10 57.66  | 7251.0  | 0.1504 | 13  | 90.03 | 11321.9 | 0.0938 |
| 2   | 22.62 | 2845.1 1.000 | 5   | 27.52 | 3460.9 | 0.3816 | 8   | 29.32 | 3687.0 | 0.8407 | 11 57.70  | 7256.5  | 0.1568 | 14  | 90.05 | 11324.6 | 0.0980 |
| 3   | 24.44 | 3073.0 0.454 | 6   | 29.20 | 3671.6 | 0.7282 | 9   | 31.82 | 4001.3 | 0.8907 | 12 89.92  | 11308.2 | 0.0872 | 15  | 90.16 | 11338.2 | 0.0866 |

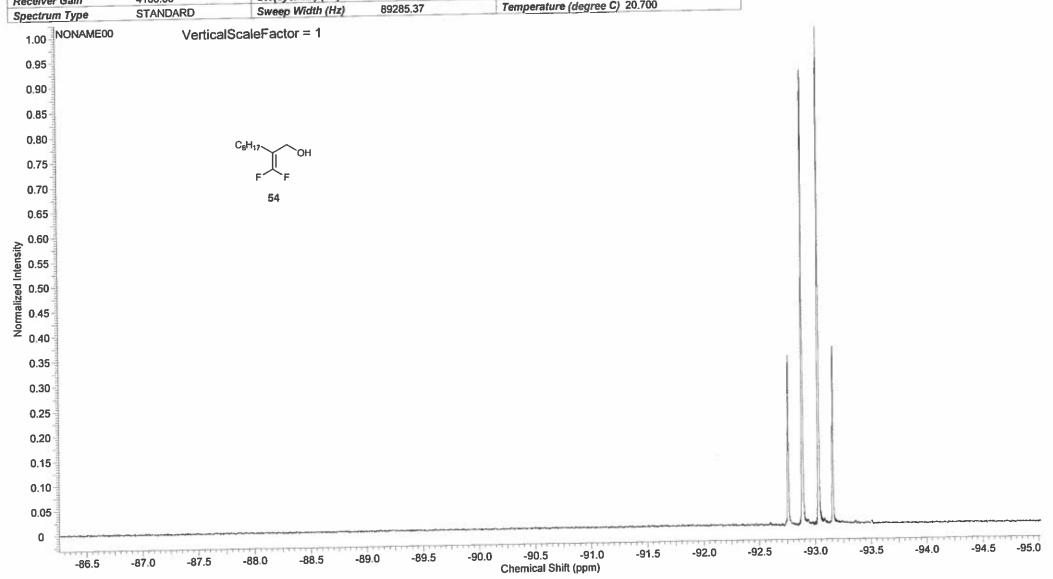
15/01/2014 15:52:22

| Acquisition Time (sec) | 1.1010                    | Comment            | EJT-PRM115 product dat | a allylic alcohol mCARBON | night CDCI3 /opt/oldbruk5 | 00data.11vii11/2014/Jan ejt 3 |            |
|------------------------|---------------------------|--------------------|------------------------|---------------------------|---------------------------|-------------------------------|------------|
| Date                   | 12 Jan 2014 17:50:56      | Date Stamp         | 12 Jan 2014 17:50:56   |                           |                           |                               |            |
| File Name              | \\ss7a.ds.man.ac.uk\vol5\ | VOL3\USERS\SNMRDAT | A\BRUK500DATA\BRUK500  | DATA\2014\JAN\DATA\EJ     | F\NMR\2014-01-12-EJT-:    | 3\10\PDATA\1\1R               |            |
| Frequency (MHz)        | 125.76                    | Nucleus            | 13C                    | Number of Transients      | 3072                      | Origin                        | spect      |
| Original Points Count  | 32768                     | Owner              | vnmr1                  | Points Count              | 32768                     | Pulse Sequence                | zgpg30     |
| Receiver Gain          | 512.00                    | SW(cyclical) (Hz)  | 29761.90               | Solvent                   | CHLOROFORM-d              | Spectrum Offset (Hz)          | 12571.1670 |
| Spectrum Type          | STANDARD                  | Sweep Width (Hz)   | 29761.00               | Temperature (degree C     | 20.099                    |                               |            |



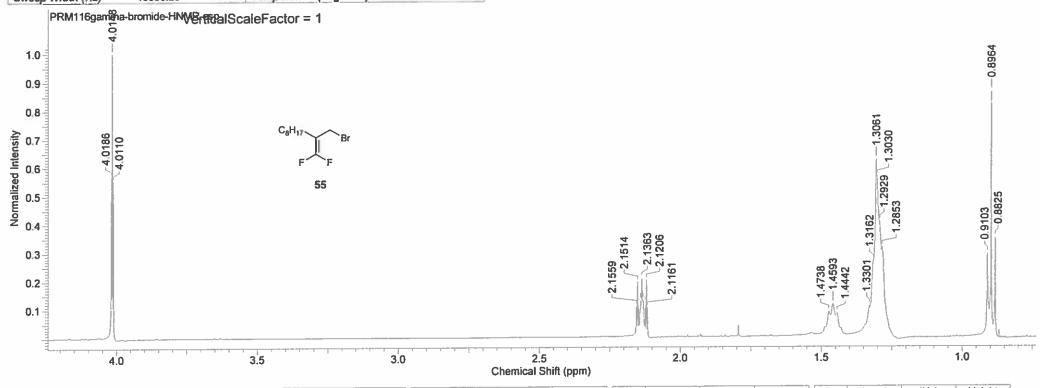
| No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)    | Height | No. | (ppm)  | (Hz)    | Height | No. | (ppm)  | (Hz)    | Height |
|-----|-------|--------|--------|-----|-------|--------|--------|-----|-------|---------|--------|-----|--------|---------|--------|-----|--------|---------|--------|
| 1   | 14.04 | 1766.0 | 0.7988 | 5   | 27.52 | 3460.9 | 0.3816 | 9   | 31.82 | 4001.3  | 0.8907 | 13  | 90.03  | 11321.9 | 0.0938 | 17  | 154.17 | 19388.1 | 0.1808 |
| 2   | 22.62 | 2845.1 | 1.0000 | 6   | 29.20 | 3671.6 | 0.7282 | 10  | 57.66 | 7251.0  | 0.1504 | 14  | 90.05  | 11324.6 | 0.0980 | 18  | 156.46 | 19676.0 | 0.0960 |
| 3   | 24.44 | 3073.0 | 0.4542 | 7   | 29.22 | 3675.2 | 0.7842 | 11  | 57.70 | 7256.5  | 0.1568 | 15  | 90.16  | 11338.2 | 0.0866 |     |        |         |        |
| 4   | 27.50 | 3458.1 | 0.2238 | 8   | 29.32 | 3687.0 | 0.8407 | 12  | 89.92 | 11308.2 | 0.0872 | 16  | 151.88 | 19100.2 | 0.0602 |     |        |         |        |

|                        |                         | Comment            | F.IT-PRM115E prod fra     | cs 94mg mF19CPD CDCl3             | (e:\bruk400data\2013\D    | ec) ejt 9            |             |
|------------------------|-------------------------|--------------------|---------------------------|-----------------------------------|---------------------------|----------------------|-------------|
| Acquisition time (ecc) |                         | Data Ctowns        | 18 Dec 2013 12:50:08      |                                   |                           |                      |             |
| Date File Name         | \\ss7a.ds,man.ac.uk\vol | SIVOL3IUSERSISNMRD |                           | DEC\DATA\EJT\NMR\2013             | 16 16-12-18-EJT-9\11\PDAT | Origin               | AV400       |
| Frequency (MHz)        | 376.50                  | Nucleus            | 19F                       | Number of Transients Points Count | 262144                    | Pulse Sequence       | zgig        |
| Original Points Count  | 65536                   | Owner (H=)         | Administrator<br>89285.71 | Solvent                           | CHLOROFORM-d              | Spectrum Offset (Hz) | -37649.5977 |
| Receiver Gain          | 4100.00<br>STANDARD     | SW(cyclical) (Hz)  | 89285.37                  | Temperature (degree C             | 20.700                    |                      |             |



20/01/2014 16:07:15

| Acquisition Time (sec) | 3.1719                  | Comment                    | EJT-PRM116 gamma-l       | oromide data mPROTONn      | ight CDCI3 (F:\bruks | 500_b_data\2014\Jan} eit 15 |          |
|------------------------|-------------------------|----------------------------|--------------------------|----------------------------|----------------------|-----------------------------|----------|
| Date                   |                         | Date Stamp                 | 13 Jan 2014 16:08:32     |                            |                      |                             |          |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | :500bdata\2014\Jan\data\ | ejt\nmr\2014-01-13-ejt-15\ | 10\fid               | Frequency (MHz)             | 500.13   |
| Nucleus                | 1H                      | Number of Transients       | 16                       | Origin                     | spect                | Original Points Count       | 32768    |
| Owner                  | Administrator           | Points Count               | 32768                    | Pulse Sequence             | zg30                 | Receiver Gain               | 20.20    |
| SW(cyclical) (Hz)      | 10330.58                | Solvent                    | CHLOROFORM-d             | Spectrum Offset (Hz)       | 3079.6614            | Spectrum Type               | STANDARD |
| Sweep Width (Hz)       | 10330.26                | Temperature (degree C      | 25.000                   |                            |                      |                             |          |



| No. | (ppm) | (Hz)  | Height | No. | (ppm)  | (Hz)  | Height | No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)   | Height |
|-----|-------|-------|--------|-----|--------|-------|--------|-----|-------|--------|--------|-----|-------|--------|--------|-----|-------|--------|--------|
| 1   | 0.88  | 441.4 | 0.3473 | 6   | 1.30   | 651.7 | 0.5638 | 11  | 1.46  | 729.8  | 0.1155 | 16  | 2.13  | 1066.2 | 0.1312 | 21  | 2.15  | 1076.0 | 0.1937 |
| 2   | 0.90  | 448.3 | 0.8616 | 7   | 1.31   | 653.2 | 0.6235 | 12  | 1.47  | 737.1  | 0.0883 | 17  | 2.13  | 1067.2 | 0.1312 | 22  | 2.16  | 1078.2 | 0.1086 |
| 3   | 0.91  | 455.2 | 0.2924 | 8   | 1.32   | 658.3 | 0.2676 | 13  | 2.12  | 1058.3 | 0.1030 | 18  | 2.14  | 1068.4 | 0.2079 | 23  | 4.01  | 2006.0 | 0.5535 |
| 4   | 1.29  | 642.8 | 0.3156 | 9   | 1.33   | 665.2 | 0.1092 | 14  | 2.12  | 1060.6 | 0.2010 | 19  | 2.14  | 1070.6 | 0.1279 | 24  | 4.01  | 2007.9 | 1.0000 |
| 5   | 1.29  | 646.6 | 0.4054 | 10  | 1.44   | 722.3 | 0.0831 | 15  | 2.12  | 1062.8 | 0.1131 | 20  | 2.15  | 1073.8 | 0.1106 | 25  | 4.02  | 2009.8 | 0.5684 |
| 9   | 1.25  | 040.0 | 0.4034 | 10  | 1,7474 | 722.0 | 0.0001 |     |       | 1000.0 |        |     |       |        |        | 1   |       |        |        |

15/01/2014 10:25:12

| Table   13 Jan 2014 20:50.08   Date Stamp   13 Jan 2014 20:50.08                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                            |                  |                    | 15    | 014\Jan} ejt     | 00_b_data\2        | (F:\bruk50     | ght CDCI3 | nCARBONni        | omide data π     | gamma-br     | PRM116     | EJT        | nt                           | Comme                         |           | 0912             | (sec) 1.         | sition Time                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Acquis                                                      |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------|------------------|--------------------|-------|------------------|--------------------|----------------|-----------|------------------|------------------|--------------|------------|------------|------------------------------|-------------------------------|-----------|------------------|------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------|
| Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   Second   S  |                            |                  |                    |       |                  |                    |                |           |                  |                  |              |            |            |                              |                               |           |                  | 13               | -0=                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                             |
| Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Section   Sect  |                            |                  |                    |       |                  |                    |                | 11Vid     | 11-13-ejt-15\1   | \nmr\2014-0      | lan\data\ejt | ata\2014\J | bruk500bd  | s\snmrdata\t                 | l5\vol3\user                  | ac.uk\vol | ss7a.ds.man.     | lls              | ame                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | ile Na                                                      |
| were Administrator Points Count 32768 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Pulse Sequence zepg30 Receiver Gain 4597.60 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse Sequence zepg30 Pulse |                            |                  |                    | Count |                  |                    |                |           |                  |                  |              |            | nts 309    | of Transien                  | Number                        |           | 3C               | 13               | us                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | ucleu                                                       |
| No.   Copm   (Hz)   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   No.   Copm   CH2   Height   Ch2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2   CH2  |                            |                  |                    |       | eiver Gain       | Rec                |                | zgpg30    | uence            | Pulse Sequ       |              | 8          | 327        | Count                        | Points C                      |           | dministrator     | A                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                             |
| 1.0   2014-01-13-ejt-15.011.esp   Verical Scale Factor = 1   2014-01-13-ejt-15.011.esp   Verical Scale Factor = 1   2014-01-13-ejt-15.011.esp   Verical Scale Factor = 1   2014-01-13-ejt-15.011.esp   Verical Scale Factor = 1   2014-01-13-ejt-15.011.esp   Verical Factor = 1   2014-01-13-ejt-15.011.esp   Verical Factor = 1   2014-01-13-ejt-15.011.esp   Verical Factor = 1   2014-01-13-ejt-15.011.esp   Verical Factor = 1   2014-01-13-ejt-15.011.esp   Verical Factor = 1   2014-01-13-ejt-15.011.esp   Verical Factor = 1   2014-01-13-ejt-15.011.esp   Verical Factor = 1   2014-01-13-ejt-15.011.esp   Verical Factor = 1   2014-01-13-ejt-15.011.esp   Verical Factor = 1   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-01-13-ejt-15.011.esp   2014-  |                            | }                | STANDAR            |       | ctrum Type       | Spec               | 715            | 12574.2   | Offset (Hz)      | Spectrum (       | lM-d         | OROFOR     | CHL        |                              | Solvent                       |           | 0030.03          | ) 30             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                             |
| 2014-01-13-ejt-15.011.esp Verifical Scale Factor = 1  1.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                            |                  |                    |       |                  |                    |                |           |                  |                  |              | 00         | ee C) 25.0 | ature (degre                 | Tempera                       |           | 0029.11          |                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                             |
| Chemical Shift (ppm)  No. (ppm) (Hz) Height No. (ppm) (Hz) Height No. (ppm) (Hz) Height No. (ppm) (Hz) Height No. (ppm) (Hz) Height No. (ppm) (Hz) Height No. (ppm) (Hz) Height No. (ppm) (Hz) Height No. (ppm) (Hz) 1 14.04 1766.2 0.3511 6 27.07 3404.8 0.2039 11 29.05 3653.1 0.5937 16 88.84 11172.6 0.0722 21 153.90 19354.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                            | 15               | 7 16               | 1     | 18               | 19                 |                | F.        |                  |                  | 24           |            | 26         | 27.795<br>27.0<br>27.0378 27 | 27.8685<br>27.8540<br>27.8102 | 29.0491   |                  | 21               | Tour hard bardard traduction from the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of the content of th | 0.9<br>0.8<br>0.7<br>0.6<br>0.5<br>0.4<br>0.3<br>0.2<br>0.1 |
| 1 14.04 1766.2 0.3511 6 27.07 3404.8 0.2039 11 29.05 3653.1 0.5937 16 88.84 11172.6 0.0722 21 153.90 19354.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                            | 13               | , 10               | ,     | 10               | 13                 | 20             | ۷1        |                  |                  |              | ∠5         | 20         | 21                           | 28                            | 29        | 30               | 31               | 32                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                             |
| 1 14.04 1766.2 0.3511 6 27.07 3404.8 0.2039 11 29.05 3653.1 0.5937 16 88.84 11172.6 0.0722 21 153.90 19354.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                            |                  |                    | Nto 1 | Majorhi          | (Hz)               | (ppm)          | No.       | Height           | (Hz)             | (ppm)        | No.        | Height     | (Hz)                         | (ppm)                         | No.       | Height           | (Hz)             | (mag)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | lo.                                                         |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Height                     |                  |                    | NO.   | neignt           | (*/                | /bbitti        |           |                  |                  |              |            |            |                              |                               |           |                  |                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                             |
| 2 22,04 2040.7 0.0050 7 27.00 0435.5 0.1040                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Height<br>0.0672           | 9354.6           | 153.90             |       |                  | 11172.6            | 88.84          | 16        | 0.5937           | 3653.1           | 29.05        | 11         | 0.2039     |                              |                               | 6         |                  |                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1                                                           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Height<br>0.0672<br>0.0605 | 9354.6<br>9356.4 | 153.90 1<br>153.92 |       |                  |                    | 88.84          | 16        | 0.5937<br>0.0268 | 3653.1<br>3661.4 |              |            |            | 3404.8                       | 27.07                         |           | 0.3511           | 1766.2           | 14.04                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | _                                                           |
| 4 27.04 3400.2 0.0841 9 27.85 3502.9 0.1310 14 29.26 3679.7 1.0000 19 89.13 11208.3 0.0664                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Height<br>0.0672           | 9354.6<br>9356.4 | 153.90 1<br>153.92 | 21 22 | 0.0722<br>0.0809 | 11172.6<br>11186.3 | 88.84<br>88.95 | 17        | 0.0268           | 3661.4           | 29.11        | 12         | 0.1549     | 3404.8<br>3495.5             | 27.07<br>27.80                | 7         | 0.3511<br>0.6830 | 1766.2<br>2846.7 | 14.04<br>22.64                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 2                                                           |

15

0.1670

31.83

4002.3

20

0.8875

151.60

19065.0

0.0455

27.05

5

3402.0

10

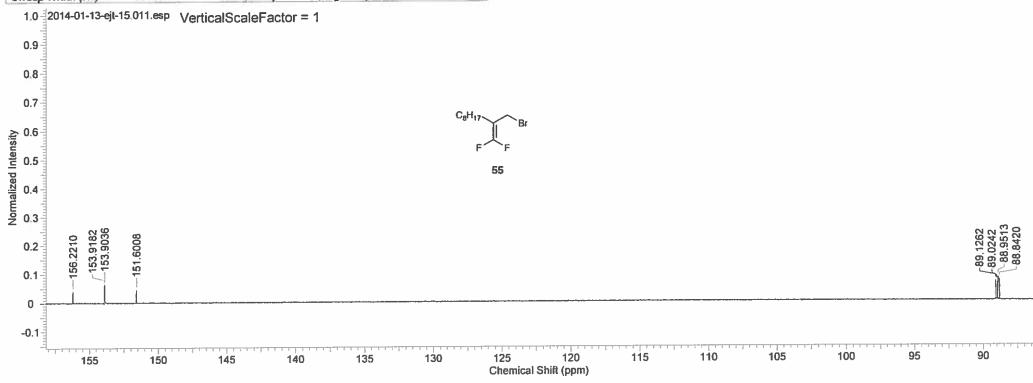
27.87

3504.7

0.2455

15/01/2014 10:24:55

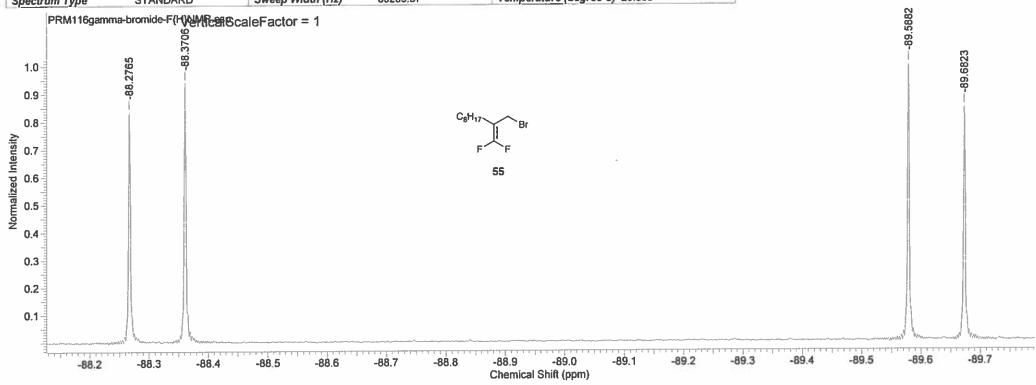
| Acquisition Time (sec) | 1.0912                  | Comment                    | EJT-PRM116 gamma-b       | romide data mCARBONni      | ght CDCl3 (F:\bruk50 | 00_b_data\2014\Jan}_ejt 15 |          |
|------------------------|-------------------------|----------------------------|--------------------------|----------------------------|----------------------|----------------------------|----------|
| Date                   | 13 Jan 2014 20:50:08    | Date Stamp                 | 13 Jan 2014 20:50:08     |                            |                      |                            |          |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 500bdata\2014\Jan\data\e | jl\nmr\2014-01-13-ejt-15\1 | 1\fid                | Frequency (MHz)            | 125,76   |
| Nucleus                | 13C                     | Number of Transients       | 3096                     | Origin                     | spect                | Original Points Count      | 32768    |
| Owner                  | Administrator           | Points Count               | 32768                    | Pulse Sequence             | zgpg30               | Receiver Gain              | 4597.60  |
| SW(cyclical) (Hz)      | 30030.03                | Solvent                    | CHLOROFORM-d             | Spectrum Offset (Hz)       | 12574.2715           | Spectrum Type              | STANDARD |
| Sweep Width (Hz)       | 30029.11                | Temperature (degree C      | 25.000                   |                            |                      |                            |          |



| No. | (ppm)  | (Hz)    | Height |
|-----|--------|---------|--------|
| 1   | 88.84  | 11172.6 | 0.0722 |
| 2   | 88.95  | 11186.3 | 0.0809 |
| 3   | 89.02  | 11195.5 | 0.0630 |
| 4   | 89.13  | 11208.3 | 0.0664 |
| 5   | 151.60 | 19065.0 | 0.0455 |
| 6   | 153.90 | 19354.6 | 0.0672 |
| 7   | 153.92 | 19356.4 | 0.0605 |
| 8   | 156.22 | 19646.0 | 0.0411 |

20/01/2014 15:51:13

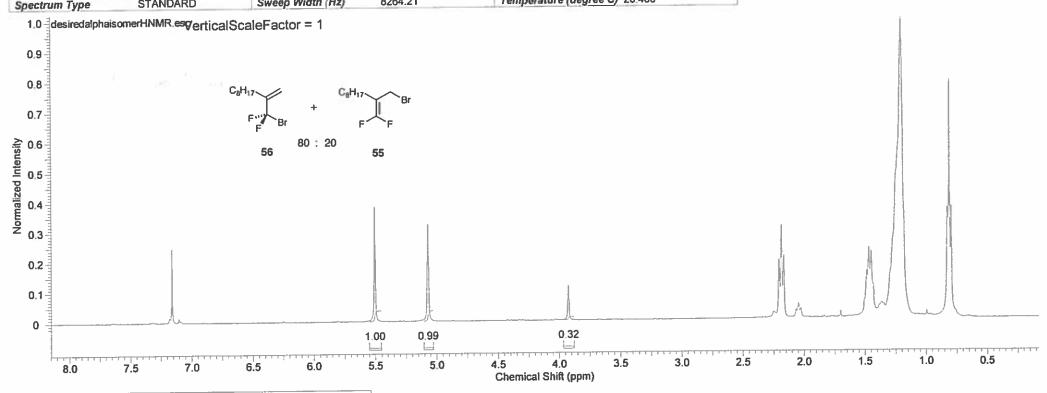
| Acquisition Time (sec) | 0.7340                  | Comment            | EJT-PRM116 f3+4 117   | mg mF19CPD CDCl3 (e:\bi | uk400data\2014\Jan} ejt | 42                   |             |
|------------------------|-------------------------|--------------------|-----------------------|-------------------------|-------------------------|----------------------|-------------|
| Date                   | 13 Jan 2014 12:33:04    | Date Stamp         | 13 Jan 2014 12:33:04  |                         |                         |                      |             |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\VOL3\USERS\SNMRD | ATA\BRUK400DATA\2014\ | JANIDATA/EJT/NMR/2014   | L-01-13-EJT-42\11\PDA   | TA\1\1R              |             |
| Frequency (MHz)        | 376.50                  | Nucleus            | 19F                   | Number of Transients    | 16                      | Origin               | AV400       |
| Original Points Count  | 65536                   | Owner              | Administrator         | Points Count            | 262144                  | Pulse Sequence       | zgig        |
| Receiver Gain          | 4100.00                 | SW(cyclical) (Hz)  | 89285.71              | Solvent                 | CHLOROFORM-d            | Spectrum Offset (Hz) | -37649.5977 |
| Spectrum Type          | STANDARD                | Sweep Width (Hz)   | 89285.37              | Temperature (degree C   | 20.800                  |                      |             |



| No. | (ppm)  | (Hz)     | Height |
|-----|--------|----------|--------|
| 1   | -89.68 | -33765.3 | 0.8449 |
| 2   | -89.59 | -33729.8 | 1.0000 |
| 3   | -88.37 | -33271.4 | 0.9398 |
| 4   | -88.28 | -33236.0 | 0.8364 |

13/01/2014 13:10:24

| Acquisition Time (sec) | 3.9649                  | Comment            | EJT-PRM120 reflux o/n tol-d8 mPROTON CDCl3 {e:\bruk400data\2014\Jan} ejt 28 |                       |              |                      |               |  |  |
|------------------------|-------------------------|--------------------|-----------------------------------------------------------------------------|-----------------------|--------------|----------------------|---------------|--|--|
| Date                   | 10 Jan 2014 10:46:24    | Date Stamp         | 10 Jan 2014 10:46:24                                                        |                       |              |                      |               |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\VOL3\USERS\SNMRD | ATA\BRUK400DATA\2014                                                        | VAN/DATA/EJTWMR/2014  |              | TA\1\1R              |               |  |  |
| Frequency (MHz)        | 400.13                  | Nucleus            | 1H                                                                          | Number of Transients  | 16           | Origin               | AV400         |  |  |
| Original Points Count  |                         | Owner              | Administrator                                                               | Points Count          | 32768        | Pulse Sequence       | zg3 <b>0b</b> |  |  |
| Receiver Gain          | 128.00                  | SW(cyclical) (Hz)  | 8264.46                                                                     | Solvent               | CHLOROFORM-d | Spectrum Offset (Hz) | 2421.3662     |  |  |
| Cantrum Tuna           | STANDARD                | Sweep Width (Hz)   | 8264.21                                                                     | Temperature (degree C | 20,400       |                      |               |  |  |



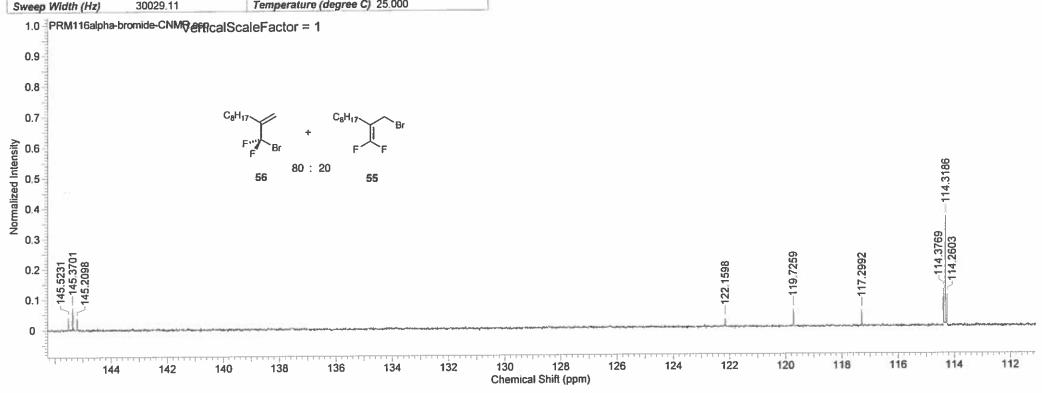
| No. | (ppm)             | Value      | Absolute Value | Non-Negative Value |
|-----|-------------------|------------|----------------|--------------------|
| 1   | 3791 <b>3.</b> 96 | 0.31848073 | 6.23530000e+6  | 0.31848073         |
| 2   | 0303 5.10         | 0.99194330 | 1.94205280e+7  | 0.99194330         |
| 3   | 4545 <b>5</b> .55 | 0.99989295 | 1.95761680e+7  | 0.99989295         |

15/01/2014 12:18:01

| Acquisition Time (sec)                                                                                              | 1.0912                 | Comment                                      | EJT-PRM116l      | alpha-bror  | nide data mC                            | ARBONnig             | ht CDC   | CI3 (F:\bruk5 | 00_b_data\2        | 014\Jan} ejt | 16        |                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |         |          |
|---------------------------------------------------------------------------------------------------------------------|------------------------|----------------------------------------------|------------------|-------------|-----------------------------------------|----------------------|----------|---------------|--------------------|--------------|-----------|------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|----------|
| Date                                                                                                                | 14 Jan 2014 01:48:48   | Date Stamp                                   | 14 Jan 2014 01   |             |                                         |                      |          |               |                    |              |           |                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |         |          |
| ile Name                                                                                                            | \\ss7a.ds.man.ac.uk\vc | l5\vol3\users\snmrdata\bruk                  | 500bdata\2014\Ja | in\data\ejt | \nmr\2014-01                            | <u>-13-ej</u> t-16\1 | 1\fid    |               |                    | quency (Mi   |           | 125.76_          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |         |          |
| lucieus                                                                                                             | 13C                    | Number of Transients                         | 3096             |             | Origin                                  |                      | spe      |               | Ori                | ginal Points | s Count   | 32768            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |         |          |
| Owner                                                                                                               | Administrator          | Points Count                                 | 32768            |             | Pulse Seque                             | ence                 | zgp      |               |                    | ceiver Gain  |           | 4096.00          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |         |          |
| SW(cyclical) (Hz)                                                                                                   | 30030.03               | Solvent                                      | CHLOROFORM       | VI-d        | Spectrum O                              | ffset (Hz)           | 125      | 74.2715       | Sp                 | ectrum Type  | 8         | STANDA           | RD                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |         |          |
| Sweep Width (Hz)                                                                                                    | 30029.11               | Temperature (degree C                        | 25.000           |             |                                         |                      |          |               |                    |              |           |                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |         |          |
| 0.9 0.8 0.5 0.4 0.3 0.9 0.2 0.1 0.1 0.9 0.9 0.2 0.1 0.1 0.9 0.9 0.2 0.1 0.1 0.9 0.9 0.9 0.9 0.9 0.9 0.9 0.9 0.9 0.9 | comide-CNMP €FRCalSo   | C <sub>8</sub> H <sub>17</sub> F Br F 80: 20 | Br<br>55         |             | *************************************** | 31.8256 31.8402      | -29.7268 |               |                    |              | 711111111 | minifim          | herri la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central de la central | 14,0663 |          |
| 54 52                                                                                                               | 50 48                  | 46 44 42                                     | 40 38            | 36          | 34<br>Chemical Sh                       |                      | 30       | 28            | 26 2               | 4 22         | 20        | 18               | 16                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 14      | 1        |
|                                                                                                                     |                        |                                              | *-T-1A A4        |             | /LI=\                                   | Llaiabi              | N/m      | (nnm)         | (Hz)               | Height       | No.       | (ppm)            | (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Height  | -        |
| lo. (ppm) (Hz                                                                                                       |                        |                                              | feight No.       | (ppm)       | (Hz)                                    | Height               | No.      |               | 6714.1             | 0.1016       | 21        | 119.73           | 15056.5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 0.0576  | $\dashv$ |
| 1 14.07 1768                                                                                                        |                        |                                              | .0437 11         | 29.27       | 3680.6                                  | 0.1341               |          |               | 14369.1            | 0.1016       | 22        | 122.16           | 15362.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 0.0376  |          |
| 2 22.64 2846                                                                                                        |                        |                                              | .4405 12         | 29.36       | 3691.6                                  | 0.9545               | 17       |               |                    |              | 1         |                  | 18261.3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 0.0288  | $\dashv$ |
| 3 22.65 2848                                                                                                        |                        |                                              | .1222 13         | 29.73       | 3738.4                                  | 0.3351               | 18       |               | 14376.5            | 0.3611       | 23        | 145.21           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |         | $\dashv$ |
| 4 25.19 3167                                                                                                        | 7.4 0.0763 9           |                                              | .6740 14         | 31.83       | 4002.3                                  | 0.1738               | 19       |               | 14383.8<br>14751.3 | 0.1226       | 24<br>25  | 145.37<br>145.52 | 18281.4<br>18300.7                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.0736  |          |
|                                                                                                                     |                        | 29.21 3673.3 0                               | .5448   15       | 31.84       | 4004.1                                  | 0.9721               | 20       |               |                    |              |           |                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |         |          |

15/01/2014 12:16:32

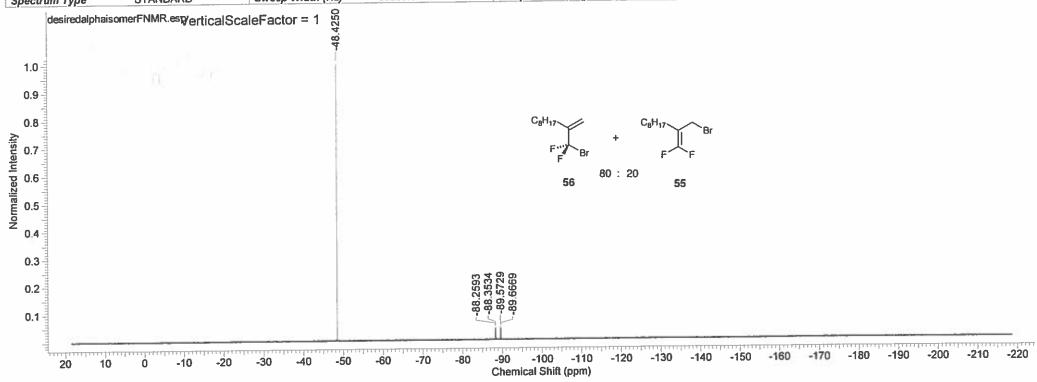
| Acquisition Time (sec) | 1.0912                  | Comment                    | EJT-PRM116I alpha-bromide data mCARBONnight CDCl3 {F:\bruk500_b_data\2014\Jan} ejt 16 |                             |            |                       |          |  |
|------------------------|-------------------------|----------------------------|---------------------------------------------------------------------------------------|-----------------------------|------------|-----------------------|----------|--|
| Date                   | 14 Jan 2014 01:48:48    | Date Stamp                 | 14 Jan 2014 01:48:48                                                                  |                             |            |                       |          |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 500bdata\2014\Jan\data\                                                               | ejt\nmr\2014-01-13-ejt-16\1 | 1\fid      | Frequency (MHz)       | 125.76   |  |
| Nucleus                | 13C                     | Number of Transients       | 3096                                                                                  | Origin                      | spect      | Original Points Count | 32768    |  |
| Owner                  | Administrator           | Points Count               | 32768                                                                                 | Pulse Sequence              | zgpg30     | Receiver Gain         | 4096.00  |  |
| SW(cyclical) (Hz)      | 30030.03                | Solvent                    | CHLOROFORM-d                                                                          | Spectrum Offset (Hz)        | 12574.2715 | Spectrum Type         | STANDARD |  |
| Sweep Width (Hz)       | 30029.11                | Temperature (degree C      | 25.000                                                                                |                             |            |                       |          |  |



| No. | (ppm)  | (Hz)    | Height |
|-----|--------|---------|--------|
| 1   | 114.26 | 14369.1 | 0.1056 |
| 2   | 114.32 | 14376.5 | 0.3611 |
| 3   | 114.38 | 14383.8 | 0.1226 |
| 4   | 117.30 | 14751.3 | 0.0533 |
| 5   | 119.73 | 15056.5 | 0.0576 |
| 6   | 122.16 | 15362.6 | 0.0286 |
| 7   | 145.21 | 18261.3 | 0.0397 |
| 8   | 145.37 | 18281.4 | 0.0736 |
| 9   | 145.52 | 18300.7 | 0.0430 |

13/01/2014 13:10:16

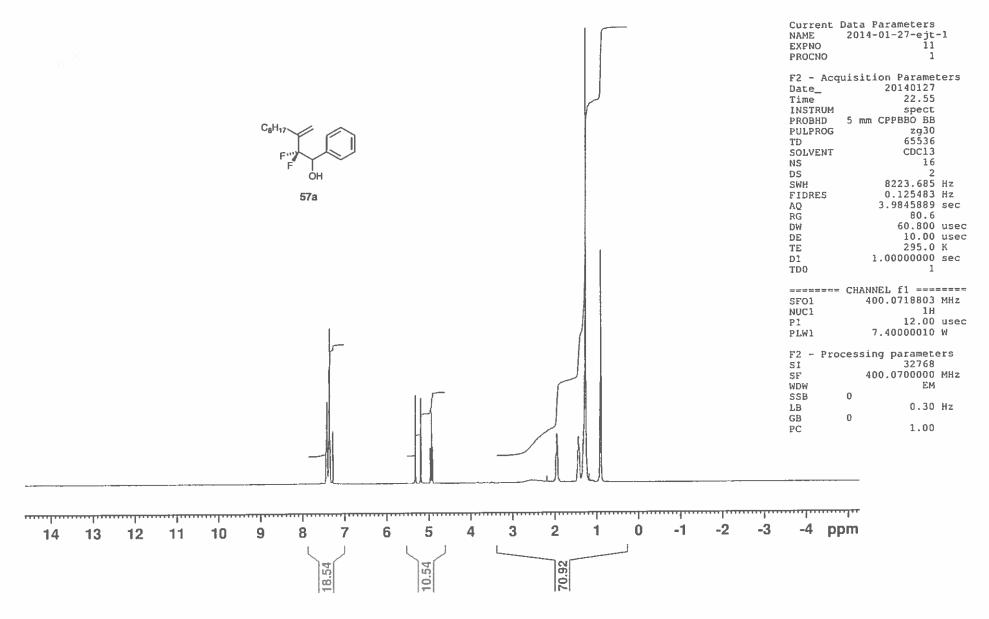
| AV400       |
|-------------|
| zgig        |
| -37649.5977 |
|             |
|             |

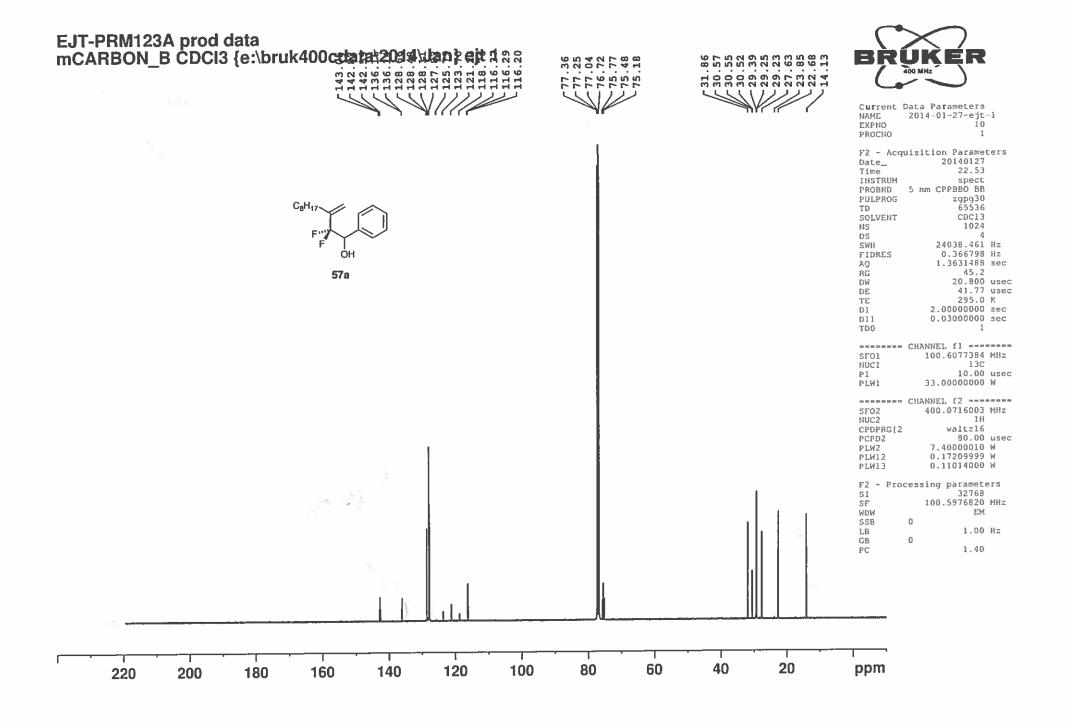


| No. | (ppm)  | (Hz)     | Height |
|-----|--------|----------|--------|
| 1   | -89.67 | -33759.5 | 0.0402 |
| 2   | -89.57 | -33724.0 | 0.0467 |
| 3   | -88.35 | -33264.9 | 0.0441 |
| 4   | -88.26 | -33229.5 | 0.0391 |
| 5   | -48.43 | -18231.9 | 1.0000 |

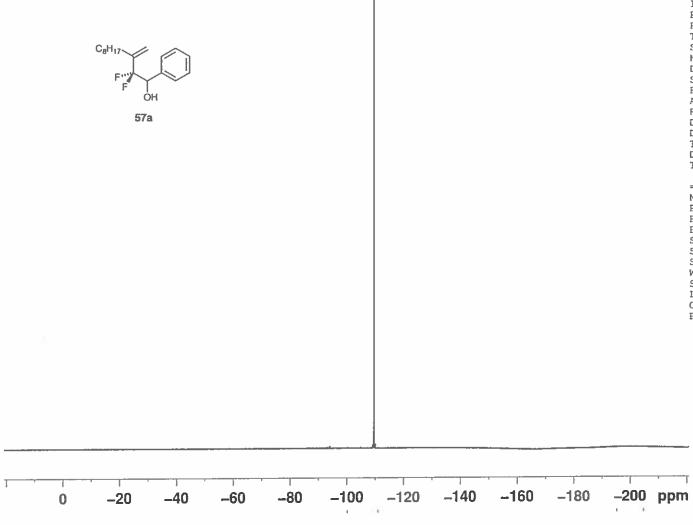
## EJT-PRM123A prod data mPROTON\_A\_night CDCl3 {e:\bruk400cdata\2014\Jan} ejt 1







EJT-PRM123A f25-43 29mg m19F CDC13 /opt/oldbruk500data.11vii11/2014/Jan ejt 34



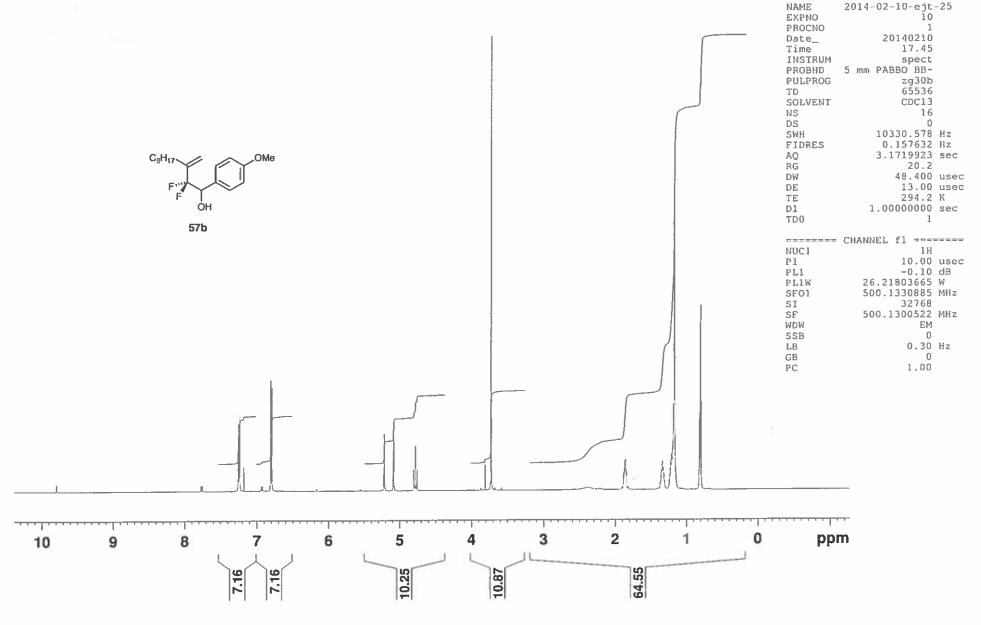


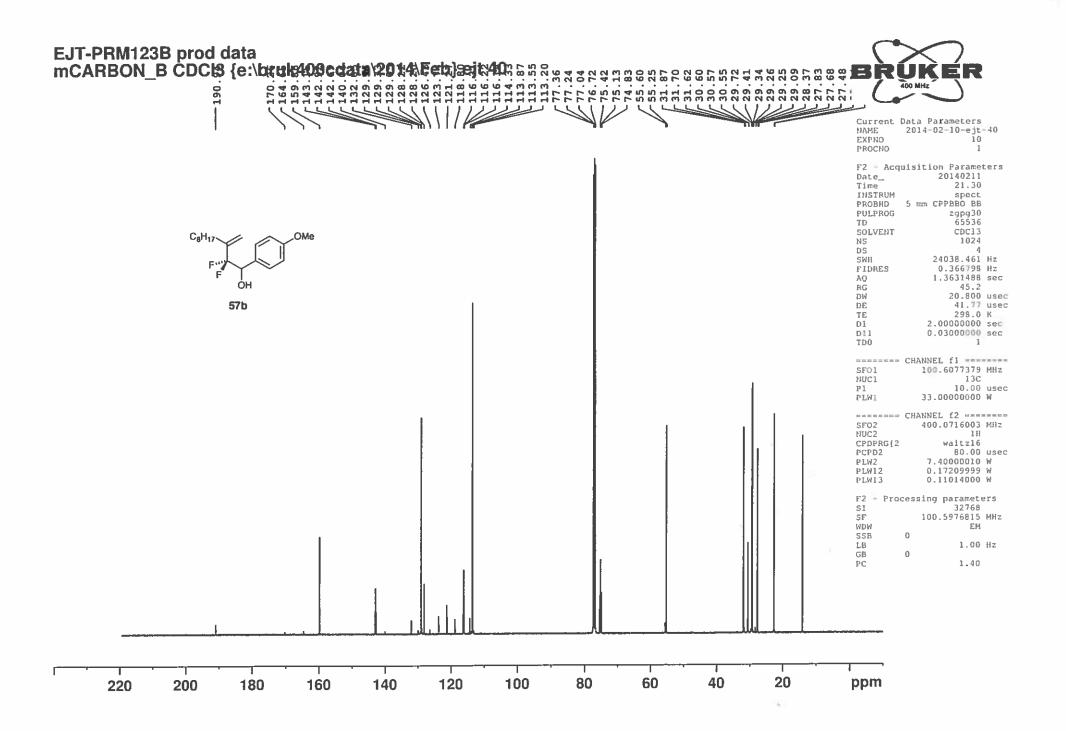
| NAME    | 2014-01-27-ejt | -34 |
|---------|----------------|-----|
| EXPNO   | 11             |     |
| PROCNO  | 1              |     |
| Date_   | 20140127       |     |
| Time    | 14.55          |     |
| INSTRUM | spect          |     |
| PROBHD  | 5 mm PABBO BB- |     |
| PULPROG | zgflqn         |     |
| TD      | 131072         |     |
| SOLVENT | CDC13          |     |
| NS      | 16             |     |
| DS      | 4              |     |
| SWH     | 113636.367     | Hz  |
| FIDRES  | 0.866977       | Ηz  |
| AQ      | 0.5767668      | sec |
| RG      | 203            |     |
| DW      | 4.400          | use |
| DE      | 6.50           |     |
| TE      | 300.0          |     |
| D1      | 1.00000000     | sec |
| TD0     | 1              |     |
|         |                |     |

| ======= | CHANNEL fl ==== |      |
|---------|-----------------|------|
| NUC1    | 19F             |      |
| P1      | 12.38           | used |
| PL1     | -0.10           | dB   |
| PL1W    | 25.70395851     | W    |
| SFO1    | 470.5453180     | MHz  |
| 51      | 65536           |      |
| SF      | 470.5923770     | MHz  |
| WDW     | EM              |      |
| SSB     | 0               |      |
| LB      | 0.30            | Hz   |
| GB      | 0               |      |
| PC      | 1.00            |      |
|         |                 |      |

# EJT-PRM123B prod data mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Feb ejt 25







EJT-PRM123B prod data m19FCPD CDC13 /opt/oldbruk500data.11vii11/2014/Feb ejt 25 2014-02-10-ejt-25 NAME 12 EXPNO PROCNO 1 20140210 Date\_ 17.50 Time INSTRUM spect PROBHD 5 mm PABBO BB-PULPROG zgfhigqn TD 131072 SOLVENT CDC13 NS 16 DS 4 SWH 113636.367 Hz 0.866977 Hz FIDRES 0.5767668 sec AQ RG 32 57b DW 4.400 usec 6.50 usec DE 294.3 K ΤE 1.00000000 sec D1 0.03000000 sec D11 0.00002000 sec D12 TDO ====== CHANNEL f1 ====== NUC1 12.38 usec P1 -0.10 dB PL1 25.70395851 W PL1W SF01 470.5453180 MHz ====== CHANNEL f2 ======= CPDPRG2 waltz16 NUC2 1H 80.00 usec PCPD2 PL2 0.00 dB 17.23 dB PL12 PL2W 25.62124252 W PL12W 0.48484197 W SFO2 500.1320005 MHz 65536 SI 470.5923770 MHz SF WDW EM SSB 0 0.30 Hz LB GB

-140

-160

-180

-80

-60

-40

-20

0

-100

-120

1.1

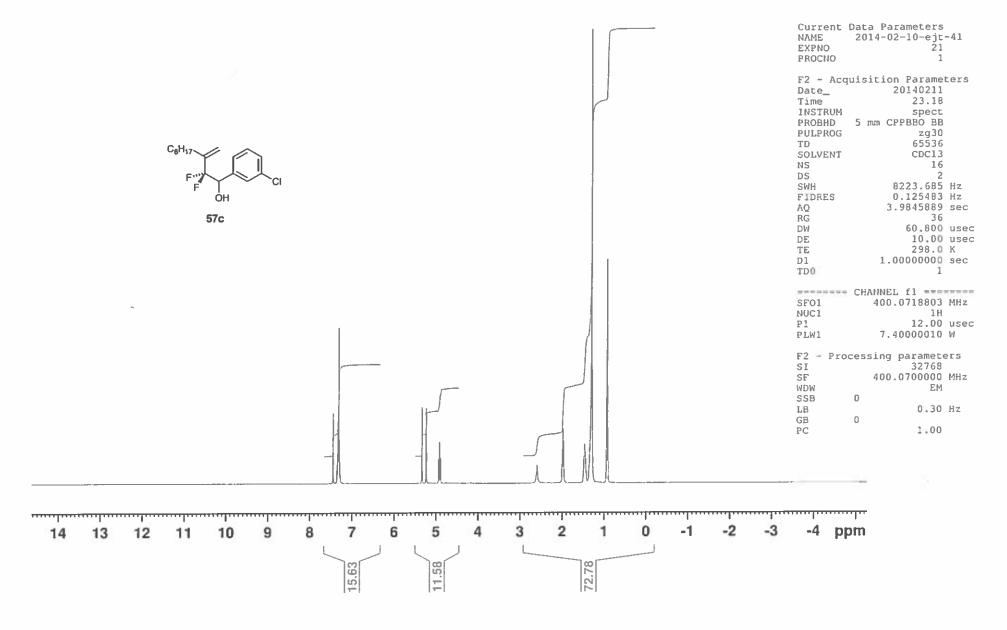
-PC

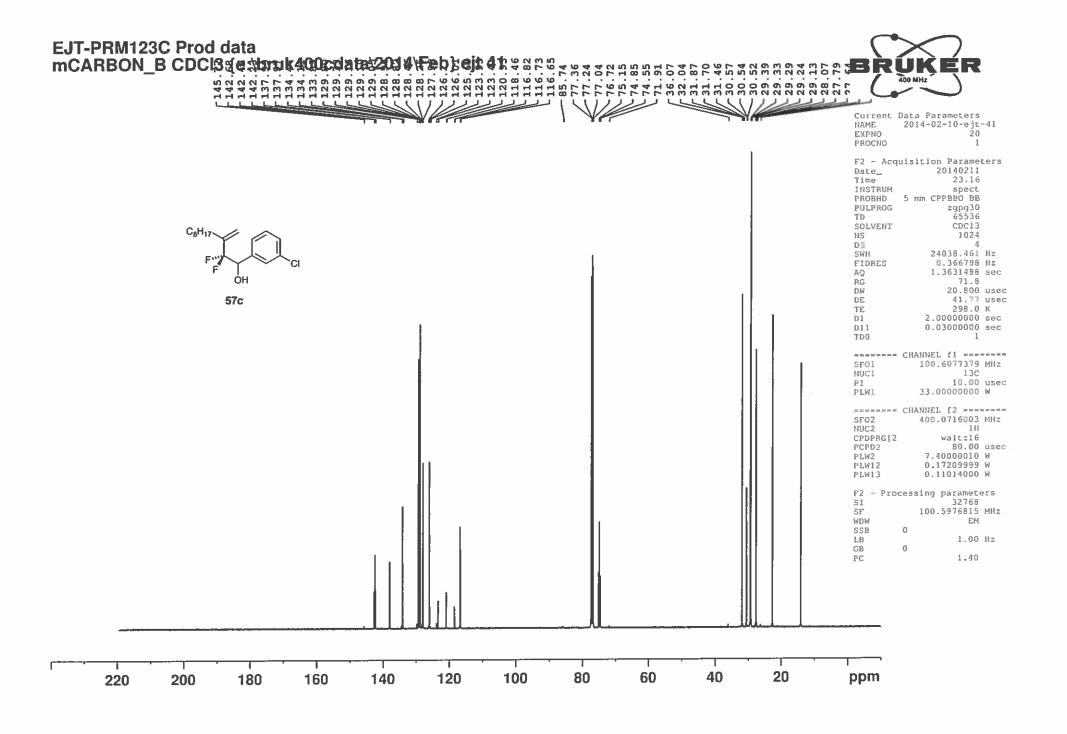
-200 ppm

1.00

## EJT-PRM123C Prod data mPROTON\_A\_night CDCl3 {e:\bruk400cdata\2014\Feb} ejt 41

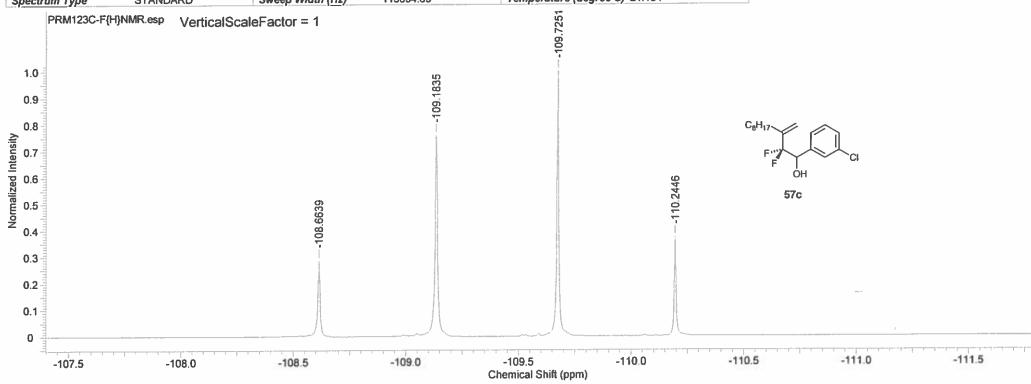






18/02/2014 16:44:47

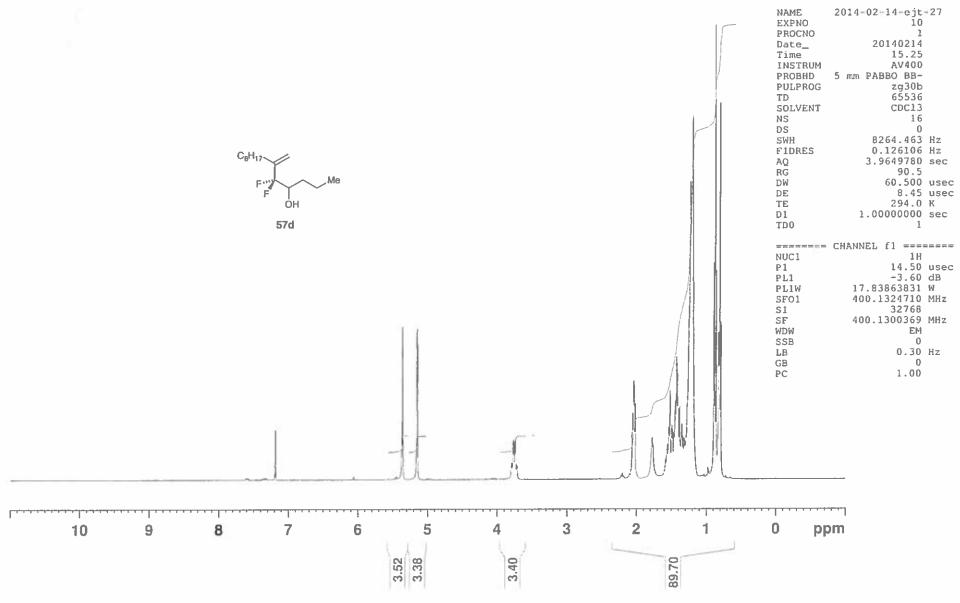
| Acquisition Time (sec) | 0.5767                   | Comment            | DIT-PRM123C prod m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Feb ejt 10 |                        |                       |                      |             |
|------------------------|--------------------------|--------------------|----------------------------------------------------------------------------|------------------------|-----------------------|----------------------|-------------|
| Date                   | 11 Feb 2014 09:33:52     | Date Stamp         | 11 Feb 2014 09:33:52                                                       |                        |                       |                      |             |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | SVOL3\USERS\SNMRDA | TA\BRUK500DATA\BRUK5                                                       | 00DATA\2014\FEB\DATA\E | EJT\NMR\2014-02-11-EJ | T-10\12\PDATA\1\1R   |             |
| Frequency (MHz)        | 470.59                   | Nucleus            | 19F                                                                        | Number of Transients   | 16                    | Origin               | spect       |
| Original Points Count  | 65536                    | Owner              | vnmr1                                                                      | Points Count           | 65536                 | Pulse Sequence       | zgfhigan    |
| Receiver Gain          | 32.00                    | SW(cyclical) (Hz)  | 113636.37                                                                  | Solvent                | CHLOROFORM-d          | Spectrum Offset (Hz) | -47059.0234 |
| Spectrum Type          | STANDARD                 | Sween Width (Hz)   | 113634.63                                                                  | Temperature (degree C) | 21.184                |                      |             |

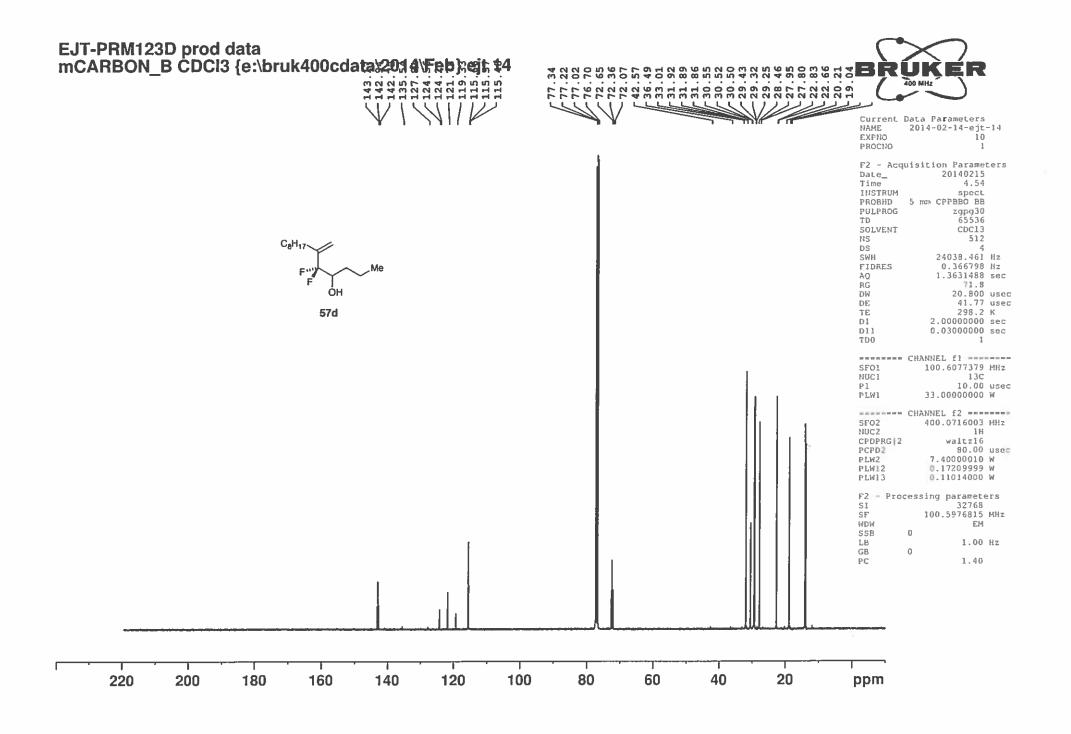


| No. | (ppm)   | (Hz)     | Height |
|-----|---------|----------|--------|
| 1   | -110.24 | -51880.3 | 0.3719 |
| 2   | -109.73 | -51635.8 | 1.0000 |
| 3   | -109.18 | -51380.9 | 0.7599 |
| 4   | -108.66 | -51136.4 | 0.2865 |

# EJT-PRM123D prod f12-26 48mg mPROTON CDCl3 {e:\bruk400data\2014\Feb} ejt 27







EJT-PRM123D crude 60mg m19F CDC13 /opt/oldbruk500data.11vii11/2014/Feb ejt 3 C<sub>8</sub>H<sub>17</sub> 57d -100 -120 -160 -180 -20 -40 -60 -80 -140 -200 ppm 0

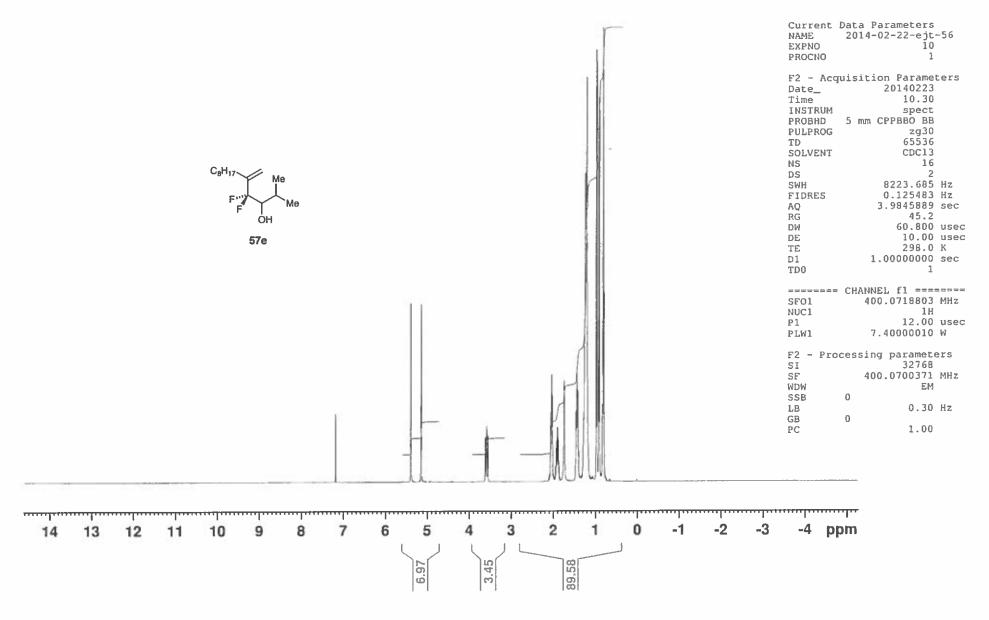


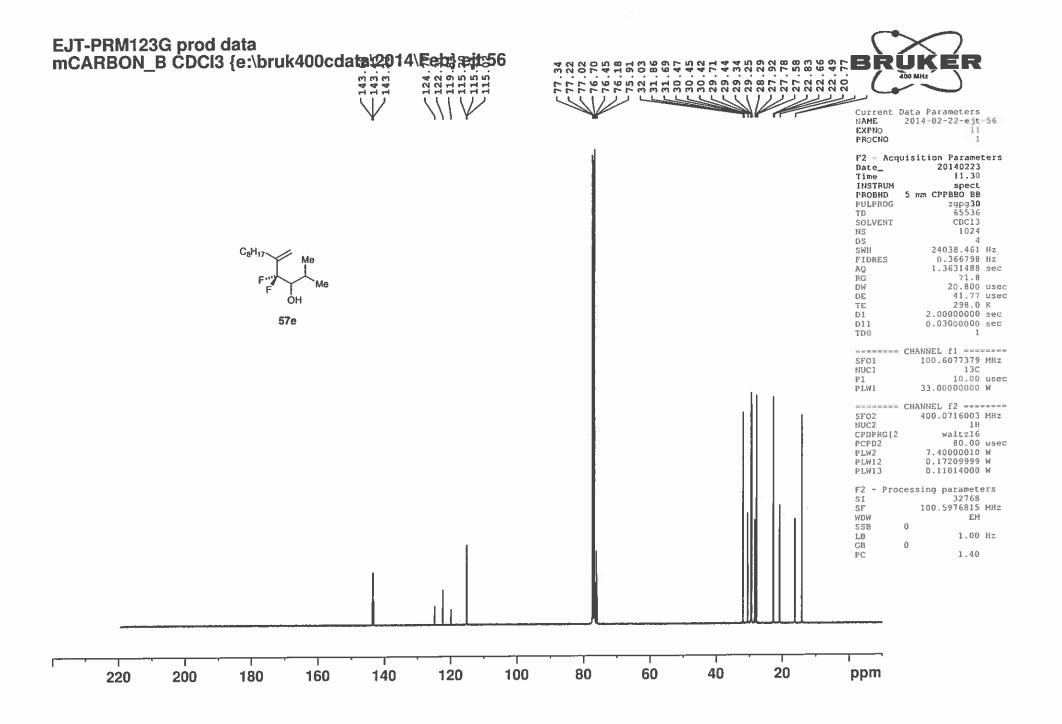
| NAME    | 2014-02-14-ejt- | -3   |
|---------|-----------------|------|
| EXPNO   | 11              |      |
| PROCNO  | 1               |      |
| Date_   | 20140214        |      |
| Time    | 11.18           |      |
| INSTRUM | spect           |      |
| PROBHD  | 5 mm PABBO BB-  |      |
| PULPROG | zgflan          |      |
| TD      | 131072          |      |
| SOLVENT | CDC13           |      |
| NS      | 16              |      |
| DS      | 4               |      |
| SWH     | 113636.367      | Hz   |
| FIDRES  | 0.866977        | Ηz   |
| AQ      | 0.5767668       | sec  |
| RG      | 203             |      |
| DW      | 4.400           | used |
| DE      | 6.50            |      |
| TE      | 300.0           |      |
| D1      | 1.00000000      | sec  |
| TD0     | 1               |      |
|         |                 |      |

| =    | CHANNEL | £  | 1  | ===: |     |
|------|---------|----|----|------|-----|
| NUC1 |         |    |    | 19F  |     |
| P1   |         |    | 12 | .38  | use |
| PL1  |         |    | -0 | .10  | dB  |
| PL1W | 25.7    | 03 | 95 | 851  | W   |
| SF01 | 470.    | 54 | 53 | 180  | MHz |
| SI   |         |    | 65 | 536  |     |
| SF   | 470.    | 59 | 23 | 770  | MHz |
| WDW  |         |    |    | EM   |     |
| SSB  |         |    |    | - 0  |     |
| LB   |         |    | 0  | .30  | Hz  |
| GB   |         |    |    | 0    |     |
| PC   |         |    | 1  | .00  |     |
|      |         |    |    |      |     |

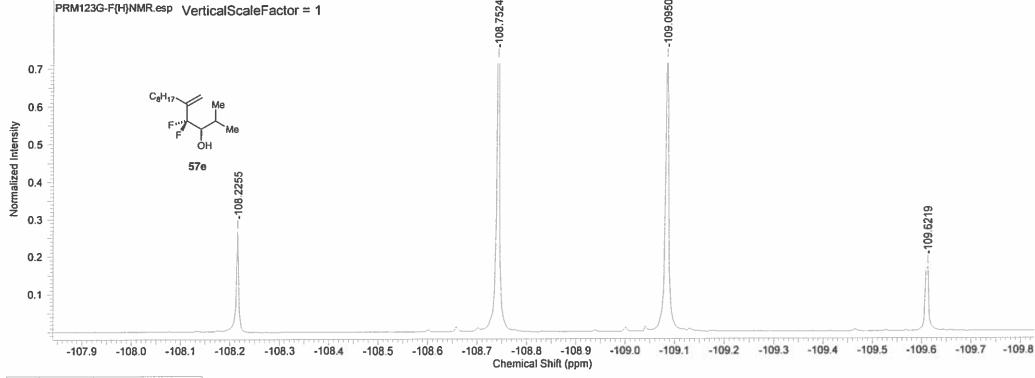
## EJT-PRM123G prod data mPROTON\_A\_night CDCl3 {e:\bruk400cdata\2014\Feb} ejt 56







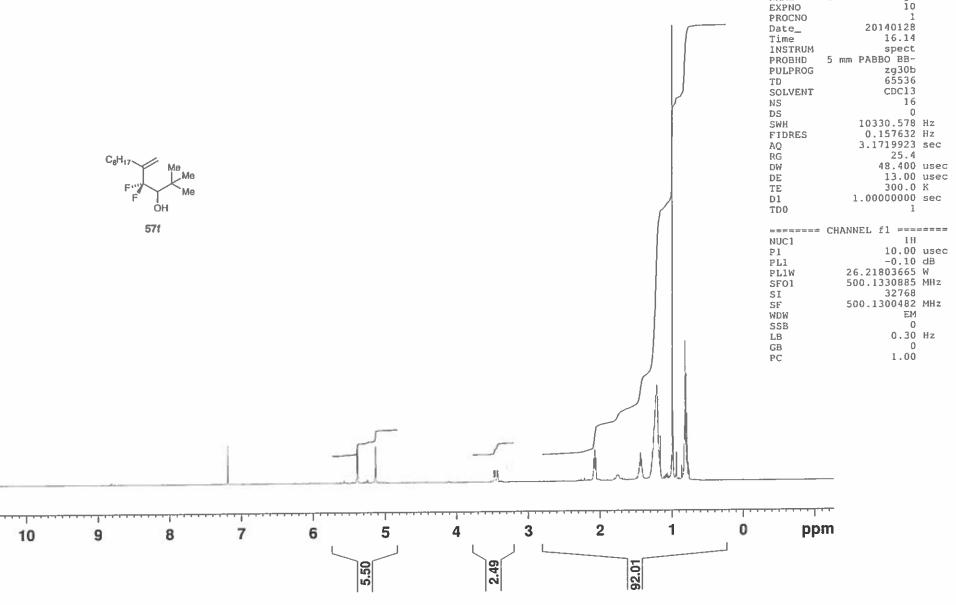
|                        |                                   |                           |                         |                            |                       |                       | 24/      | 02/2014 15:06:4 |
|------------------------|-----------------------------------|---------------------------|-------------------------|----------------------------|-----------------------|-----------------------|----------|-----------------|
| Acquisition Time (sec) | 0.5767                            | Comment                   | EJT-PRM123G prod n      | n19FCPD CDCl3 /opt/oldbr   | uk500data.11vii11/201 | 14/Feb ejt 56         |          |                 |
| Date                   | 23 Feb 2014 18:54:56              | Date Stamp                | 23 Feb 2014 18:54:56    |                            |                       |                       |          |                 |
| File Name              | \\ss7a.ds.man.ac.uk\vol           | 5\vol3\users\snmrdata\bru | k500data\bruk500data\20 | 14\Feb\data\ejt\nmr\2014-0 | )2-23-ejt-56\12\fid   | Frequency (MHz)       | 470.59   |                 |
| Nucleus                | 19F                               | Number of Transients      | 16                      | Origin                     | spect                 | Original Points Count | 65536    |                 |
| Owner                  | vnmr1                             | Points Count              | 65536                   | Pulse Sequence             | zgfhigqn              | Receiver Gain         | 32.00    |                 |
| SW(cyclical) (Hz)      | 113636.37                         | Solvent                   | CHLOROFORM-d            | Spectrum Offset (Hz)       | -47059.0234           | Spectrum Type         | STANDARD |                 |
| Sweep Width (Hz)       | 113634.63                         | Temperature (degree C     | 27.000                  |                            |                       |                       |          |                 |
| PRM123G-F{H}           | NMR.esp VerticalSc                | aleFactor = 1             |                         | 108.7524                   | 109,0950              |                       |          |                 |
| 0.7                    |                                   |                           |                         |                            |                       |                       |          |                 |
| 0.6                    | C <sub>8</sub> H <sub>17</sub> Me |                           |                         |                            |                       |                       |          |                 |

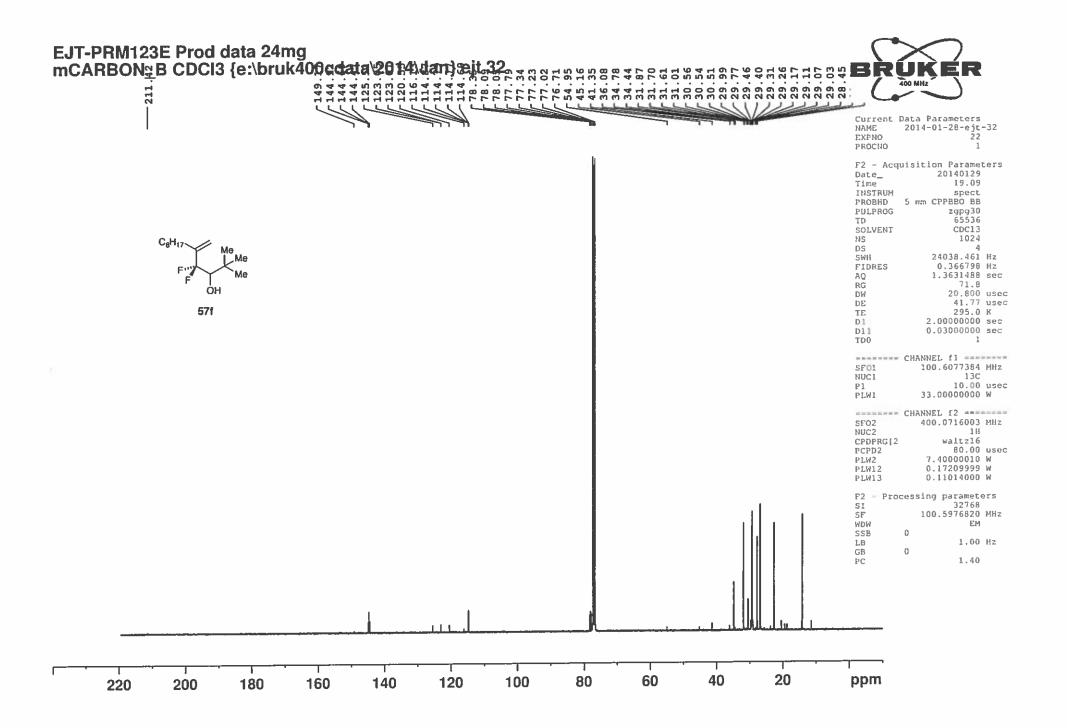


| No. | (ppm)   | (Hz)     | Height |
|-----|---------|----------|--------|
| 1   | -109.62 | -51587.2 | 0.1688 |
| 2   | -109.10 | -51339.3 | 0.8761 |
| 3   | -108.75 | -51178.0 | 1.0000 |
| 4   | -108.23 | -50930.1 | 0.2675 |



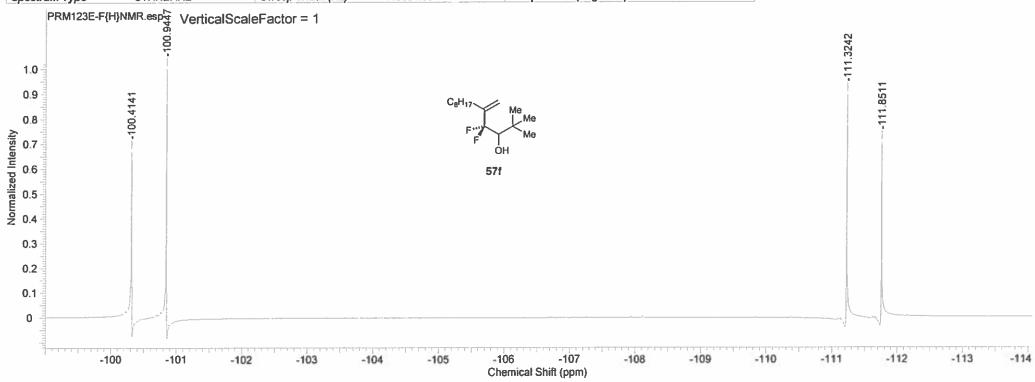






30/01/2014 11:37:52

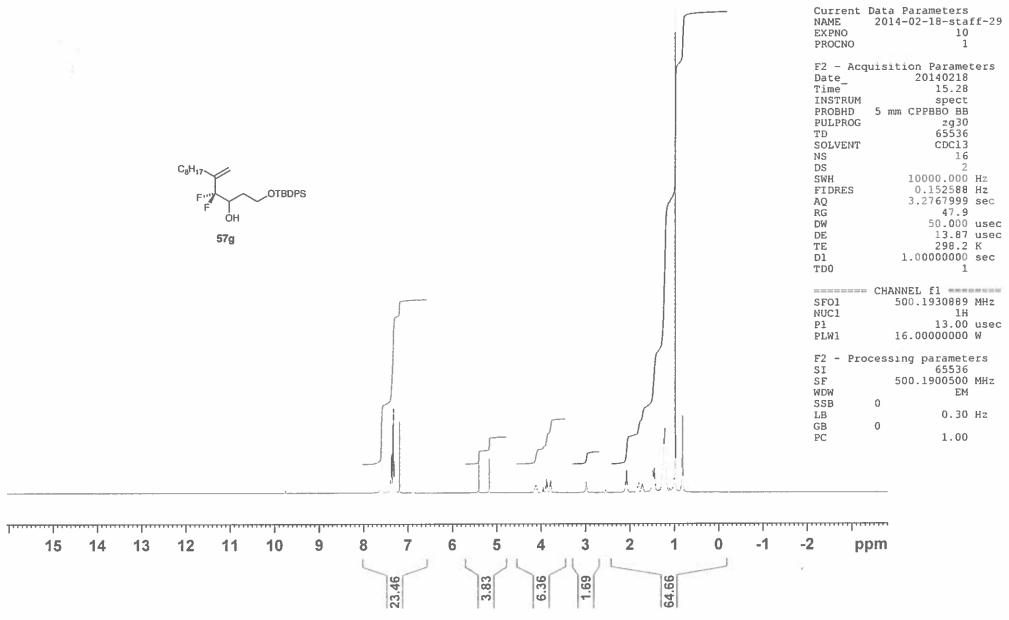
| Acquisition Time (sec) | 0.5767                   | Comment            | EJT-PRM123E f8-15 24mg m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Jan ejt 29 |                         |                      |                      |             |  |
|------------------------|--------------------------|--------------------|----------------------------------------------------------------------------------|-------------------------|----------------------|----------------------|-------------|--|
| Date                   | 28 Jan 2014 16:19:12     | Date Stamp         | 28 Jan 2014 16:19:12                                                             |                         |                      |                      |             |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | IVOL3\USERS\SNMRDA | TA\BRUK500DATA\BRUK5                                                             | 500DATA\2014\JAN\DATA\E | JT\NMR\2014-01-28-EJ | T-29\12\PDATA\1\1R   |             |  |
| Frequency (MHz)        | 470.59                   | Nucleus            | 19F                                                                              | Number of Transients    | 16                   | Origin               | spect       |  |
| Original Points Count  | 65536                    | Owner              | vnmr1                                                                            | Points Count            | 65536                | Pulse Sequence       | zgfhigqn    |  |
| Receiver Gain          | 32.00                    | SW(cyclical) (Hz)  | 113636.37                                                                        | Solvent                 | CHLOROFORM-d         | Spectrum Offset (Hz) | -47059.0234 |  |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)   | 113634.63                                                                        | Temperature (degree C   | 27.000               |                      |             |  |



| No. | (ppm)   | (Hz)     | Height |
|-----|---------|----------|--------|
| 1   | -111.85 | -52636.3 | 0.7016 |
| 2   | -111.32 | -52388.3 | 0.8938 |
| 3   | -100.94 | -47503.8 | 1.0000 |
| 4   | -100.41 | -47254.1 | 0.6694 |

P. Mears
EJT-PRM 120 prod F31-41
0214-029
mPROTON CDCI3 {E:\bruk500cdata\2014\Feb} staff 29





220

200

180

160

140

120

100

80

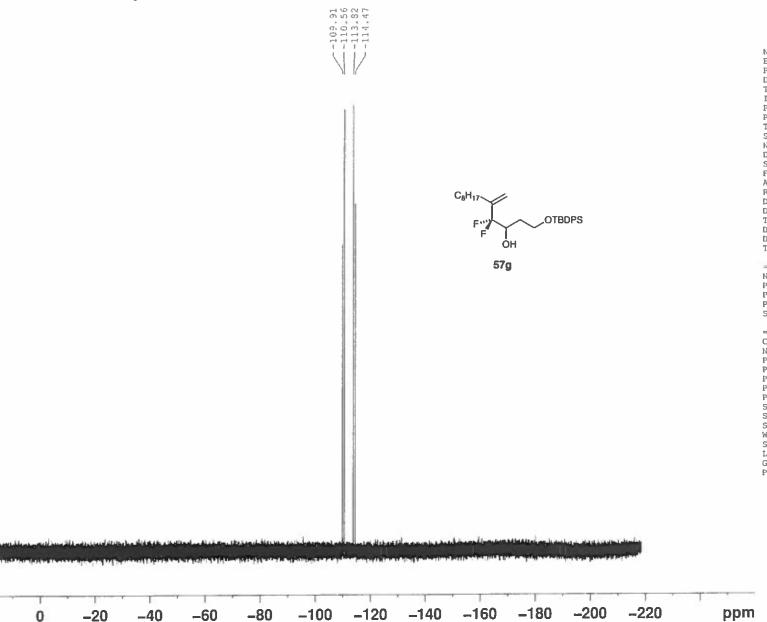
60

40

20

ppm

## EJT-PRM120 f95-113 24mg mF19CPD CDCl3 {e:\bruk400data\2014\Feb} ejt 1

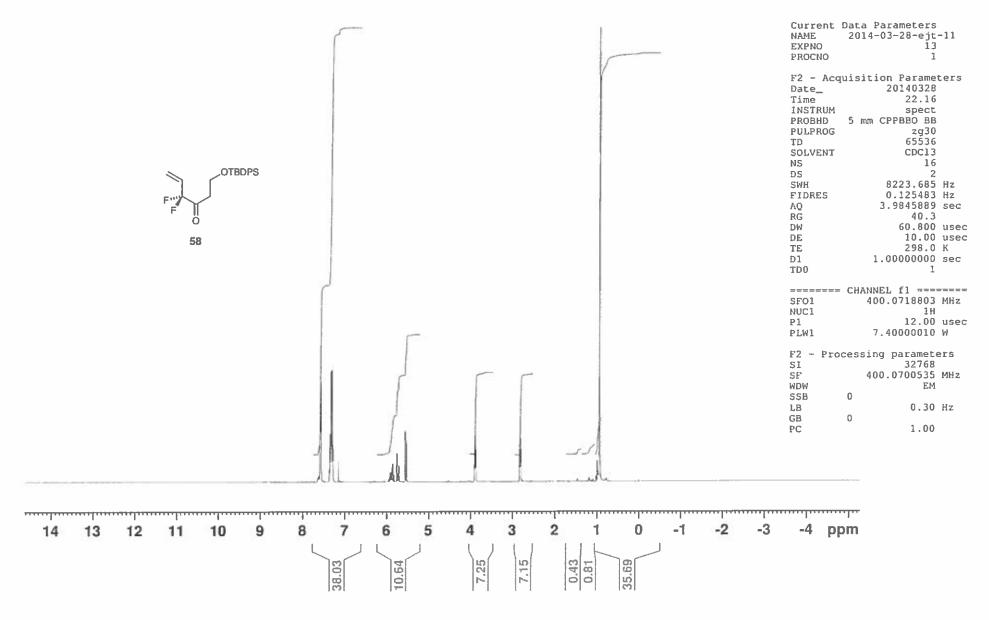


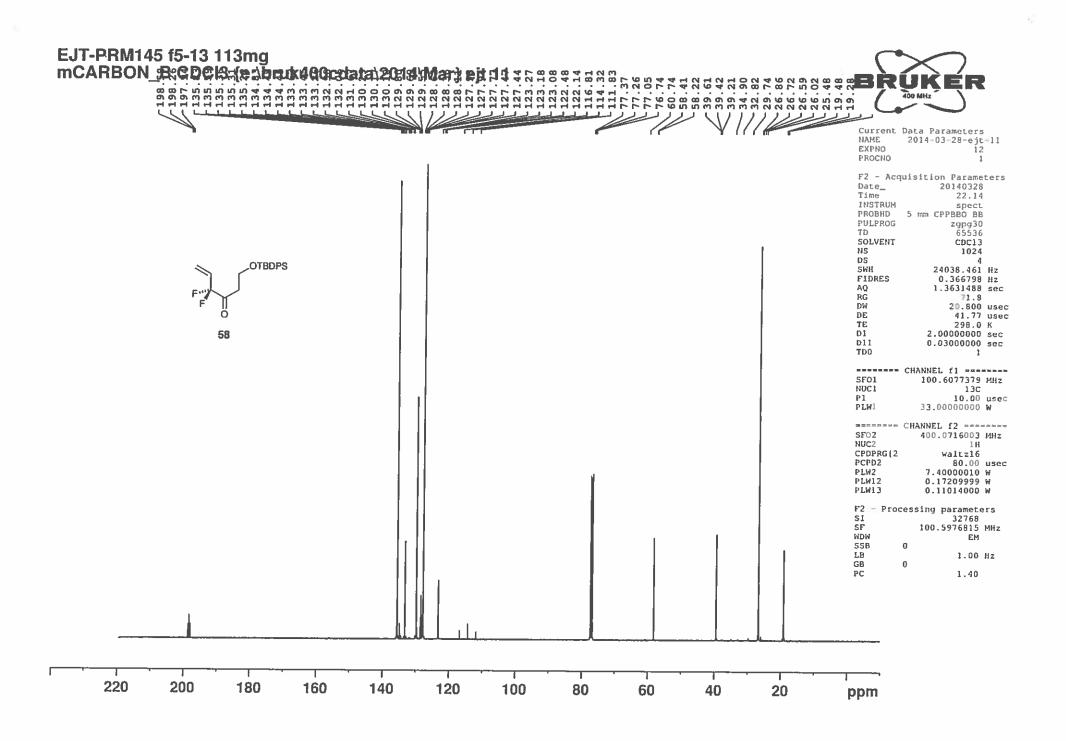


| NAME EXPNO PROCNO Date_ Time INSTRUM PROBHD PULPROG TD SOLVENT NS DS SSWH FIDRES AQ RG DW DE TE TE TE TE TE TE TE TE TE TE TE TE TE | 294.3<br>1.00000000                                            | Hz<br>Hz<br>sec<br>usec<br>K<br>sec<br>sec |
|-------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------|--------------------------------------------|
| TDO                                                                                                                                 | 1                                                              |                                            |
| NUC1<br>P1<br>PL1<br>PL1W<br>SFOI                                                                                                   | CHANNEL fl 19F<br>10.70<br>-5.00<br>27.00716019<br>376.4607164 | usec<br>dB<br>W                            |
| CPDPRG2 NUC2 PLC2 PL12 PL12 PL12W SFO2 SI SF NDW SSB LB GB GB                                                                       | CHANNEL f2 ====                                                |                                            |

## EJT-PRM145 f5-13 113mg mPROTON\_A\_night CDCl3 {e:\bruk400cdata\2014\Mar} ejt 11

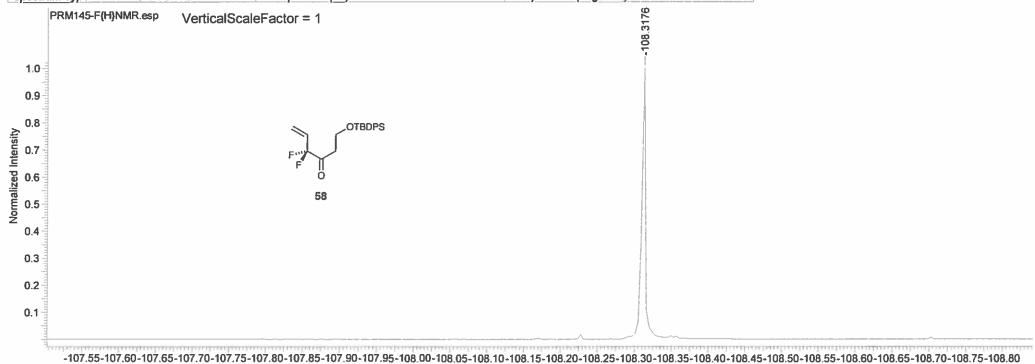






07/04/2014 13:54:05

| Acquisition Time (sec) | 0.5767                     | Comment                                                                                                                  | EJT-PRM145 f3-7 40mg m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 5 |                        |              |                      |             |  |
|------------------------|----------------------------|--------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------|------------------------|--------------|----------------------|-------------|--|
| Date                   | 26 Mar 2014 14:26:08       | Date Stamp                                                                                                               | 26 Mar 2014 14:26:08                                                          |                        |              |                      |             |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol5\\ | Nss7a.ds.man.ac.uk/vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2014\MAR\DATA\EJT\NMR\2014-03-26-EJT-5\12\PDATA\1\1R |                                                                               |                        |              |                      |             |  |
| Frequency (MHz)        | 470.59                     | Nucleus                                                                                                                  | 19F                                                                           | Number of Transients   | 16           | Origin               | spect       |  |
| Original Points Count  | 65536                      | Owner                                                                                                                    | vnmr1                                                                         | Points Count           | 65536        | Pulse Sequence       | zgfhigqn    |  |
| Receiver Gain          | 575.00                     | SW(cyclical) (Hz)                                                                                                        | 113636.37                                                                     | Solvent                | CHLOROFORM-d | Spectrum Offset (Hz) | -47059.0234 |  |
| Spectrum Type          | STANDARD                   | Sweep Width (Hz)                                                                                                         | 113634.63                                                                     | Temperature (degree C) | 27.000       |                      |             |  |

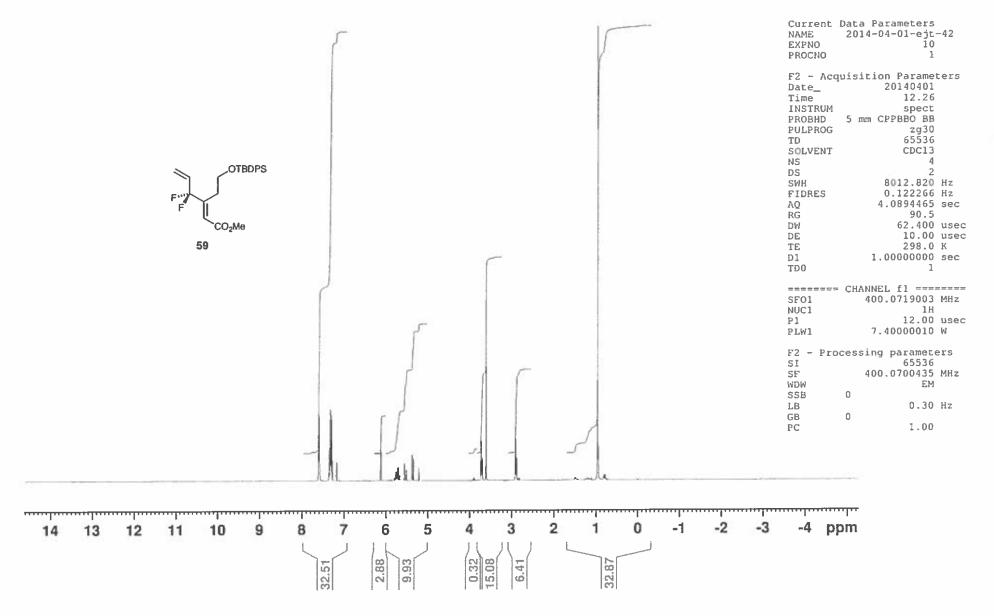


Chemical Shift (ppm)

| No. | (ppm)   | (Hz)     | Height |
|-----|---------|----------|--------|
| 1   | -108.32 | -50973.4 | 1.0000 |

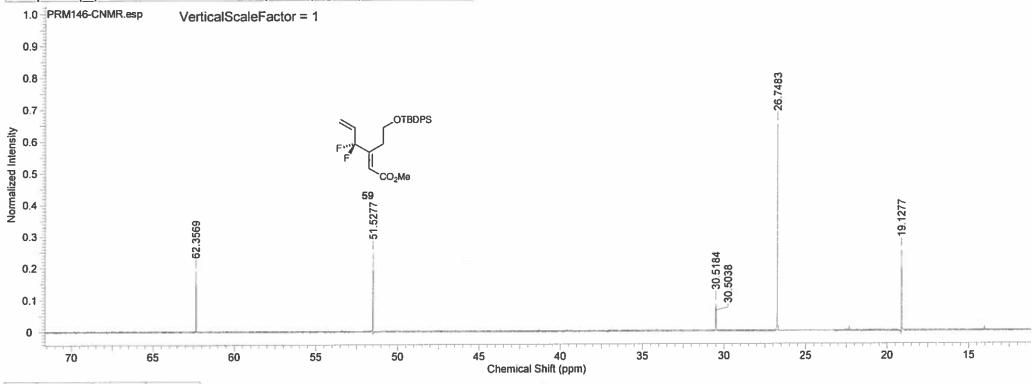
## EJT-PRM146 phosphoranylidene f14-24 20mg mPROTON\_A CDCl3 {e:\bruk400cdata\2014\Apr} ejt 42





07/04/2014 15:31:32

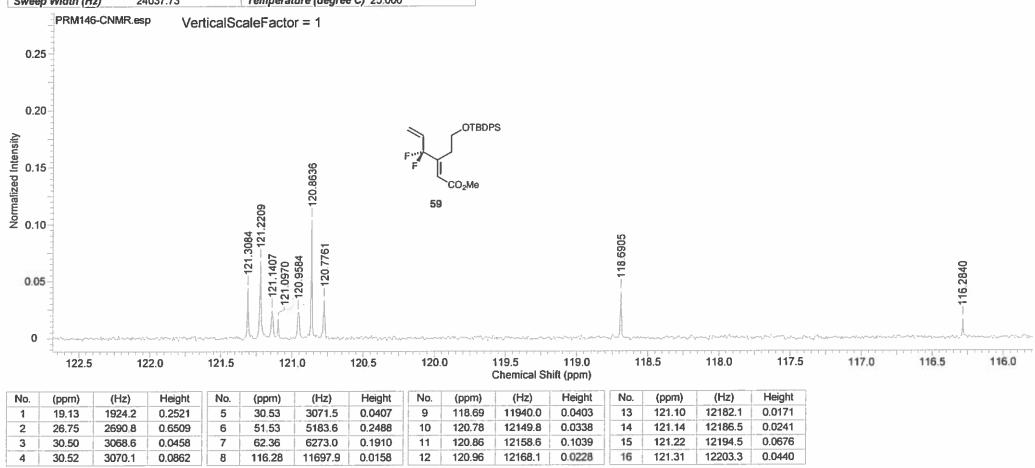
| Acquisition Time (sec) | 1.3631               | Comment                      | EJT-PRM146 prod al    | Ikene mCARBON_B CDCl3        | {e:\bruk400cdata\2014\A | pr} ejt 24            |          |
|------------------------|----------------------|------------------------------|-----------------------|------------------------------|-------------------------|-----------------------|----------|
| Date                   | 03 Apr 2014 19:05:5  | 2                            |                       | Date Stamp                   | 03 Apr 2014 19:05:52    |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\ | vol5\vol3\users\snmrdata\bru | k400cdata\2014\Apr\da | ata\ejt\nmr\2014-04-03-ejt-2 | 4\10\fid                | Frequency (MHz)       | 100.60   |
| Nucleus                | 13C                  | Number of Transients         | 1024                  | Origin                       | spect                   | Original Points Count | 32768    |
| Owner                  | nmrsu                | Points Count                 | 32768                 | Pulse Sequence               | zgpg30                  | Receiver Gain         | 45.20    |
| SW(cyclical) (Hz)      | 24038.46             | Solvent                      | CHLOROFORM-d          | Spectrum Offset (Hz)         | 10052.8125              | Spectrum Type         | STANDARD |
| Sweep Width (Hz)       | 24037.73             | Temperature (degree C)       | 25.000                |                              |                         |                       |          |



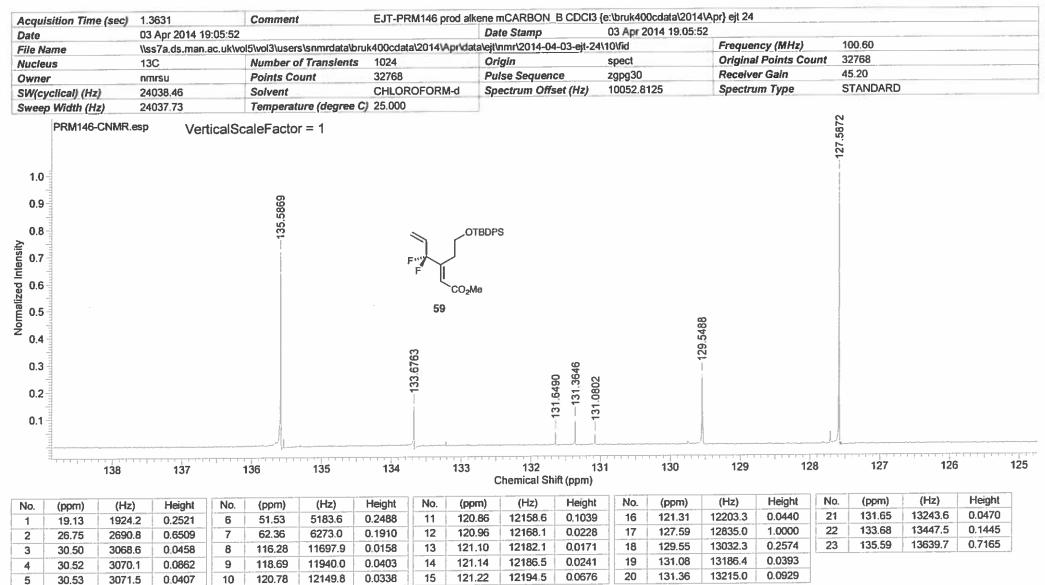
| No. | (ppm) | (Hz)   | Height |
|-----|-------|--------|--------|
| 1   | 19.13 | 1924.2 | 0.2521 |
| 2   | 26.75 | 2690.8 | 0.6509 |
| 3   | 30.50 | 3068.6 | 0.0458 |
| 4   | 30.52 | 3070.1 | 0.0862 |
| 5   | 30.53 | 3071.5 | 0.0407 |
| 6   | 51.53 | 5183.6 | 0.2488 |
| 7   | 62.36 | 6273.0 | 0.1910 |

07/04/2014 15:34:44

| Acquisition Time (sec) | 1.3631                | Comment EJT-PRM146 prod alkene mCARBON_B CDCl3 (e:\bruk400cdata\2014\Apr) ejt 24 |                        |                      |                      |                       |          |  |  |
|------------------------|-----------------------|----------------------------------------------------------------------------------|------------------------|----------------------|----------------------|-----------------------|----------|--|--|
| Date                   | 03 Apr 2014 19:05:52  |                                                                                  |                        | Date Stamp           | 03 Apr 2014 19:05:52 |                       |          |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\w | ol5\vol3\users\snmrdata\bru                                                      | ik400cdata\2014\Apr\da | 4\10\fid             | Frequency (MHz)      | 100.60                |          |  |  |
| Nucleus                | 13C                   | Number of Transients                                                             | 1024                   | Origin               | spect                | Original Points Count | 32768    |  |  |
| Owner                  | nmrsu                 | Points Count                                                                     | 32768                  | Pulse Sequence       | zgpg30               | Receiver Gain         | 45.20    |  |  |
| SW(cyclical) (Hz)      | 24038.46              | Solvent                                                                          | CHLOROFORM-d           | Spectrum Offset (Hz) | 10052.8125           | Spectrum Type         | STANDARD |  |  |
| Sween Width (Hz)       | 24037 73              | Temperature (degree C                                                            | 1 25 000               |                      |                      |                       |          |  |  |

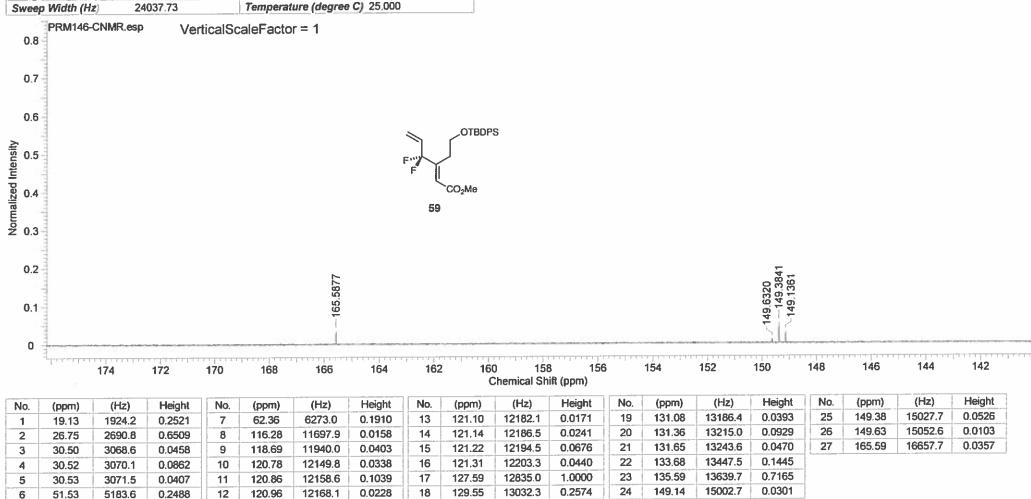


07/04/2014 15:41:55



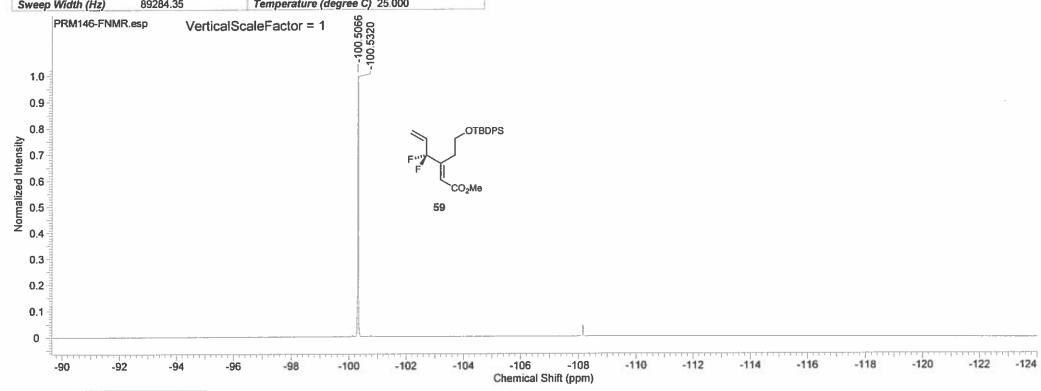
07/04/2014 15:45:55

| Acquisition Time (sec) | 1.3631                 | Comment                     |                        |                               |                      |                       |          |
|------------------------|------------------------|-----------------------------|------------------------|-------------------------------|----------------------|-----------------------|----------|
| Date                   | 03 Apr 2014 19:05:52   |                             |                        | Date Stamp                    | 03 Apr 2014 19:05:52 |                       |          |
|                        | \\ss7a.ds.man.ac.uk\vo | xi5\voi3\users\snmrdata\bru | ik400cdata\2014\Apr\da | ata\ejt\nmr\2014-04-03-ejt-24 | 4\10\fid             | Frequency (MHz)       | 100,60   |
| Nucleus                | 13C                    | Number of Transients        | 1024                   | Origin                        | spect                | Original Points Count | 32768    |
| Owner                  | nmrsu                  | Points Count                | 32768                  | Pulse Sequence                | zgpg30               | Receiver Gain         | 45.20    |
| SW(cyclical) (Hz)      | 24038.46               | Solvent                     | CHLOROFORM-d           | Spectrum Offset (Hz)          | 10052.8125           | Spectrum Type         | STANDARD |
| Surger Midth (Un)      | 24027.73               | Temperature (degree C       | 25 000                 |                               |                      | -                     |          |



07/04/2014 16:11:28

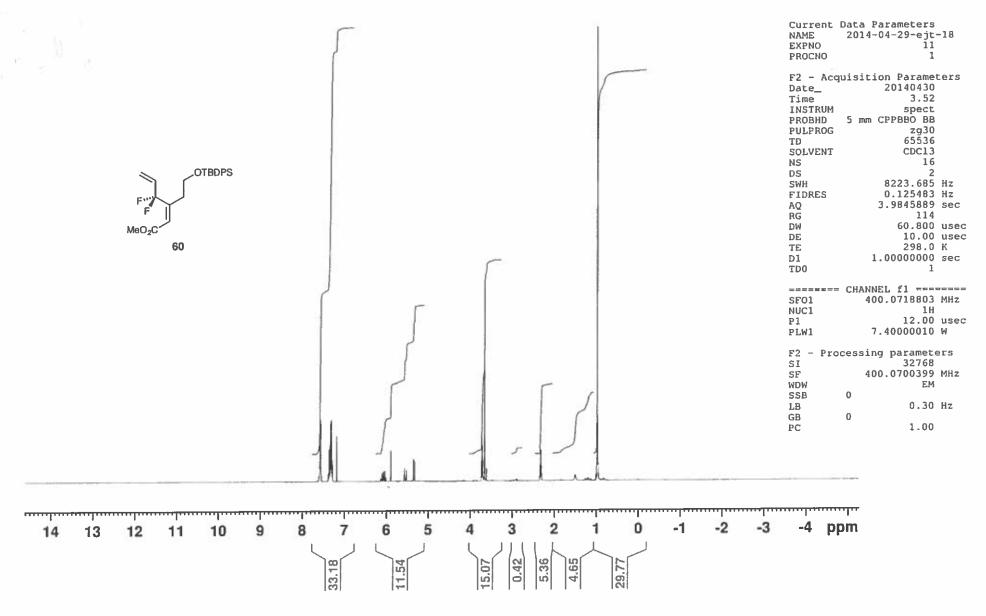
| Acquisition Time (sec) | 0.7340                 | Comment                     | EJT-PRM146 phosphoranylidene f14-24 20mg mF19_cryo CDCl3 {e:\bruk400cdata\2014\Apr} ejt 42 |                              |             |                       |          |  |
|------------------------|------------------------|-----------------------------|--------------------------------------------------------------------------------------------|------------------------------|-------------|-----------------------|----------|--|
| Date                   | 01 Apr 2014 12:29:04   | Date Stamp                  | 01 Apr 2014 12:29:04                                                                       |                              |             |                       |          |  |
| File Name              | \\ss7a.ds.man.ac.uk\vo | l5\vol3\users\snmrdata\bruk | 400cdata\2014\Apr\data                                                                     | alejt\nmr\2014-04-01-ejt-42\ | 11\fid      | Frequency (MHz)       | 376.44   |  |
| Nucleus                | 19F                    | Number of Transients        | 4                                                                                          | Origin                       | spect       | Original Points Count | 65536    |  |
| Owner                  | nmrsu                  | Points Count                | 65536                                                                                      | Pulse Sequence               | zg          | Receiver Gain         | 16.00    |  |
| SW(cyclical) (Hz)      | 89285.71               | Solvent                     | CHLOROFORM-d                                                                               | Spectrum Offset (Hz)         | -37644.8594 | Spectrum Type         | STANDARD |  |
| Sween Width (Hz)       | 80284 35               | Temperature (degree C)      | 25,000                                                                                     |                              |             |                       |          |  |

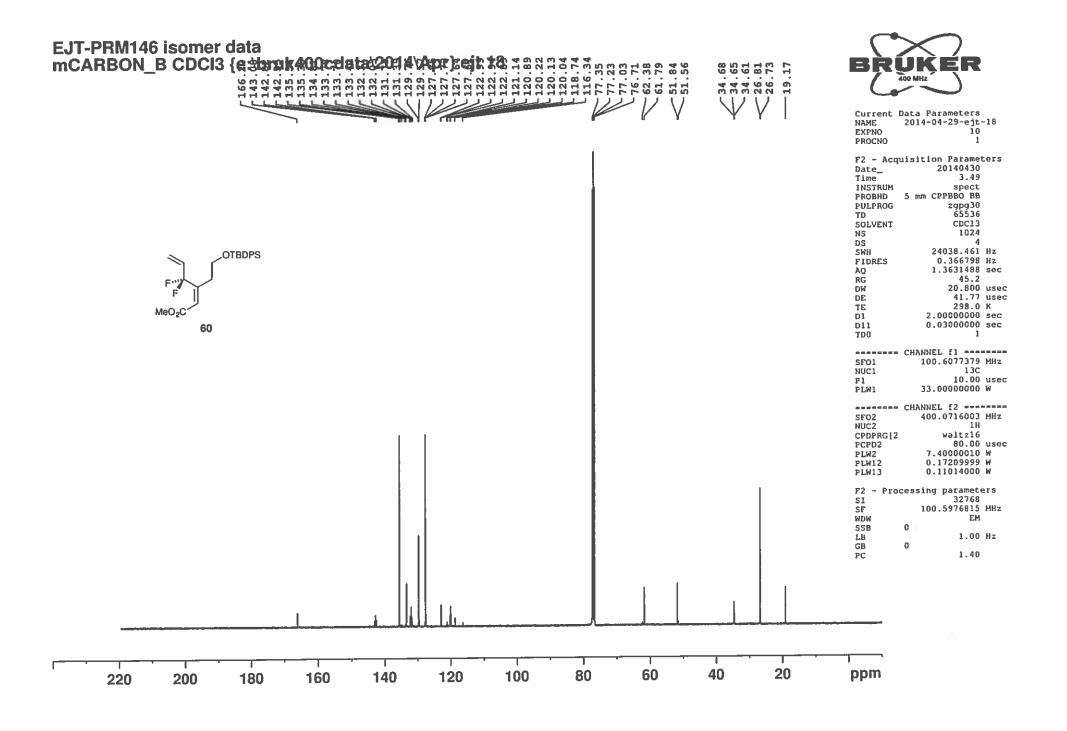


|   | No. | (ppm)   | (Hz)     | Height |
|---|-----|---------|----------|--------|
|   | 1   | -100.53 | -37844.4 | 0.9733 |
| ļ | 2   | -100.51 | -37834.9 | 1.0000 |

## EJT-PRM146 isomer data mPROTON\_A\_night CDCl3 {e:\bruk400cdata\2014\Apr} ejt 18







|                        | I IIIO I GPOIL HAD DI   |                    |                                                                       |                               |                       |                      |             |  |  |
|------------------------|-------------------------|--------------------|-----------------------------------------------------------------------|-------------------------------|-----------------------|----------------------|-------------|--|--|
| Acquisition Time (sec) | 0.7340                  | Comment            | EJT-PRM146 f44-48 40mg mF19CPD CDCl3 {e:\bruk400data\2014\May} ejt 23 |                               |                       |                      |             |  |  |
| Date                   | 19 May 2014 19:08:00    | Date Stamp         | 19 May 2014 19:08:00                                                  |                               |                       |                      |             |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5/VOL3/USERS/SNMRD | ATA\BRUK400DATA\2014\                                                 | MAY/DATA/EJT/NMR/2014         | 4-05-19-EJT-23\22\PDA |                      |             |  |  |
| Frequency (MHz)        | 376.50                  | Nucleus            | 19F                                                                   | Number of Transients          | 16                    | Origin               | AV400       |  |  |
| Original Points Count  | 65536                   | Owner              | Administrator                                                         | Points Count                  | 262144                | Pulse Sequence       | zgig        |  |  |
| Receiver Gain          | 4100.00                 | SW(cyclical) (Hz)  | 89285.71                                                              | Solvent                       | CHLOROFORM-d          | Spectrum Offset (Hz) | -37649.5977 |  |  |
| Spectrum Type          | STANDARD                | Sweep Width (Hz)   | 89285.37                                                              | Temperature (degree C) 22.600 |                       |                      |             |  |  |

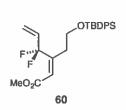
2014-05-19-EJT-23.022.001.1R.esp VerticalScaleFactor 1

-75

-80

-85

-90

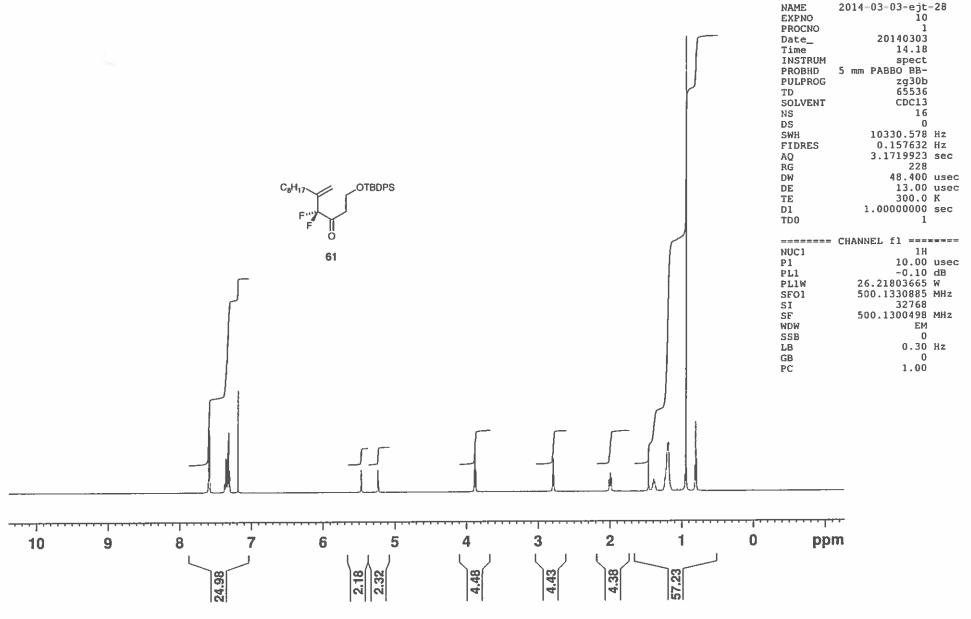


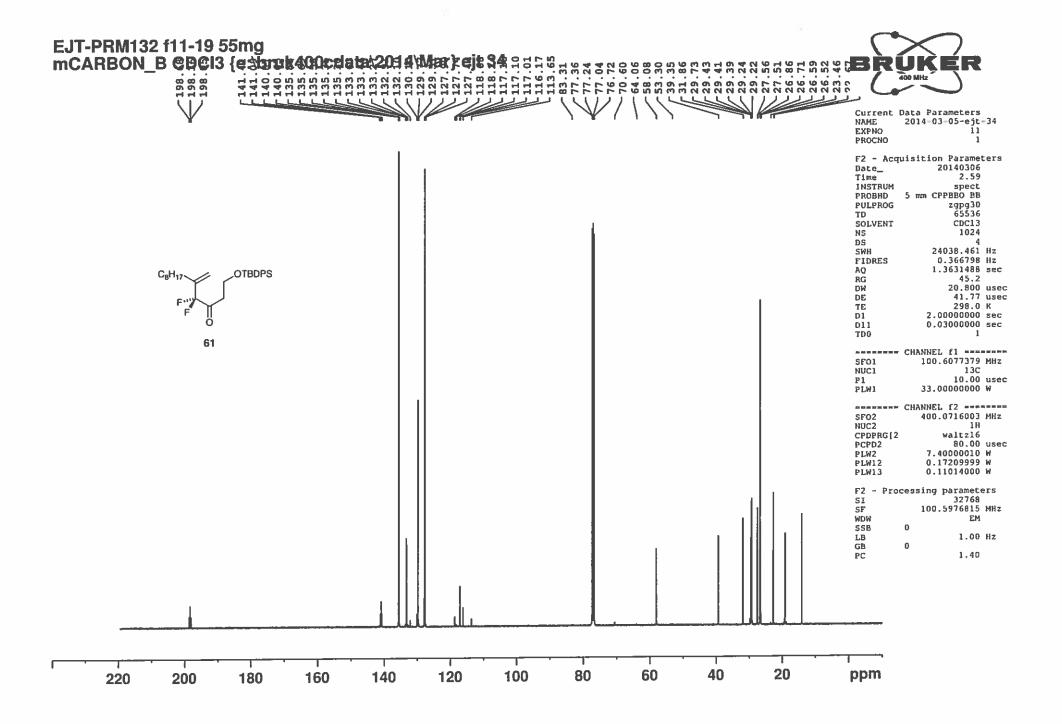
-95

-100









|                        |                          |                    |                                                                             |                       |                       |                      | •           |  |  |
|------------------------|--------------------------|--------------------|-----------------------------------------------------------------------------|-----------------------|-----------------------|----------------------|-------------|--|--|
| Acquisition Time (sec) | 0.5767                   | Comment            | EJT-PRM132 f5-10 7mg m19F CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 28 |                       |                       |                      |             |  |  |
| Date                   | 03 Mar 2014 14:21:52     | Date Stamp         | 03 Mar 2014 14:21:52                                                        |                       |                       |                      |             |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | IVOL3\USERS\SNMRDA | TAIBRUK500DATAIBRUK5                                                        | 500DATA\2014\MAR\DATA | \EJT\NMR\2014-03-03-E | EJT-28\11\PDATA\1\1R |             |  |  |
| Frequency (MHz)        | 470.59                   | Nucleus            | 19F                                                                         | Number of Transients  | 16                    | Origin               | spect       |  |  |
| Original Points Count  | 65536                    | Owner              | vnmr1                                                                       | Points Count          | 65536                 | Pulse Sequence       | zgflqn      |  |  |
| Receiver Gain          | 362.00                   | SW(cyclical) (Hz)  | 113636.37                                                                   | Solvent               | CHLOROFORM-d          | Spectrum Offset (Hz) | -47059.0234 |  |  |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)   | 113634.63                                                                   | Temperature (degree C | 27.000                |                      |             |  |  |

-109.7398

PRM132-FNMR.esp

EJT-PRM133 f16-21 4mg mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 7 NAME 2014-03-07-ejt-7 **EXPNO** ĩo PROCNO Date\_ 20140307 15.20 Time INSTRUM spect PROBHD 5 mm PABBO BB-**PULPROG** zg30b TD 65536 SOLVENT CDC13 NS 16 0 DS 10330.578 Hz SWH FIDRES 0.157632 Hz 3.1719923 sec AQ OTBDPS RG 287 48.400 usec DW DE 13.00 usec F TE 298.0 K 1.00000000 sec D1 1 TD0 62 ----- CHANNEL fl -----NUC1 10.00 usec P1 PL1 -0.10 dB 26.21803665 W PL1W 500.1330885 MHz SF01 32768 SI 500.1300487 MHz SF WDW E.M 0 SSB 0.30 Hz LB GB - 0 PC 1.00

10

9

25.16

1.28

2

3.27

56.51

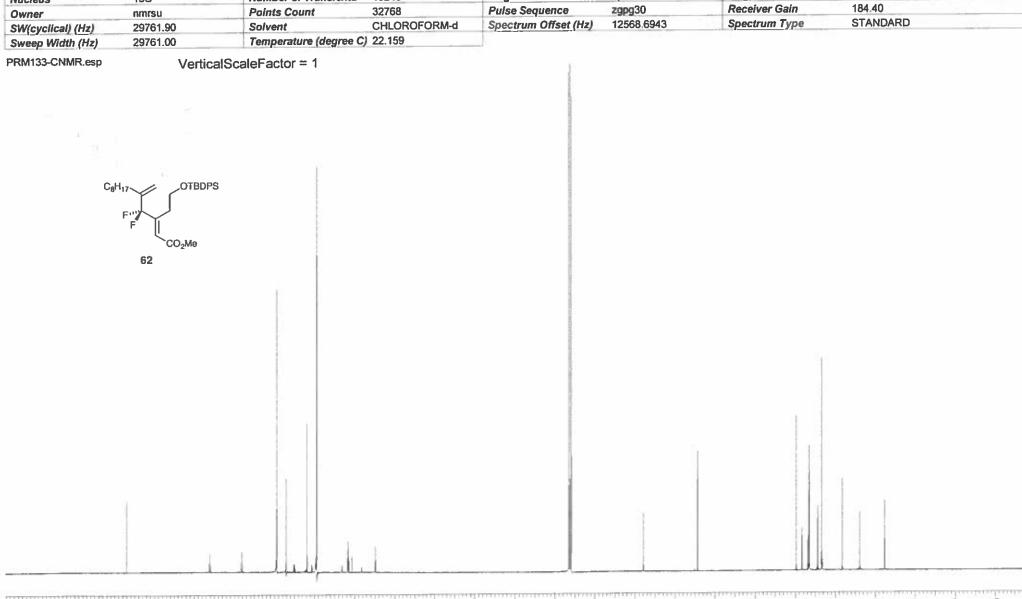
2.66

0.57

0

ppm

|                        |                         | The second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second secon |                                                                                    | 4                             |            |                       |          |  |  |
|------------------------|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------|-------------------------------|------------|-----------------------|----------|--|--|
| Acquisition Time (sec) | 1,1010                  | Comment                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | P. Mears EJT-PRM133prod 0614-032 mCARBON CDCl3 (E:\bruk500cdata\2014\Jun) staff 42 |                               |            |                       |          |  |  |
| Date                   | 20 Jun 2014 07:19:44    | Date Stamp                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 20 Jun 2014 07:19:44                                                               |                               |            |                       |          |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 15\vol3\users\snmrdata\bruk                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | <500cdata\2014\Jun\data                                                            | a\staff\nmr\2014-06-19-staff- | 42\12\fid  | Frequency (MHz)       | 125.77   |  |  |
| Nucleus                | 13C                     | Number of Transients                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 10240                                                                              | Origin                        | spect      | Original Points Count | 32768    |  |  |
| Owner                  | nmrsu                   | Points Count                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 32768                                                                              | Pulse Sequence                | zgpg30     | Receiver Gain         | 184.40   |  |  |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | CHLOROFORM-d                                                                       | Spectrum Offset (Hz)          | 12568,6943 | Spectrum Type         | STANDARD |  |  |
| 0 147-141-111-1        | 20764.00                | Tompomium (doggo C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 1 22 150                                                                           |                               |            |                       |          |  |  |



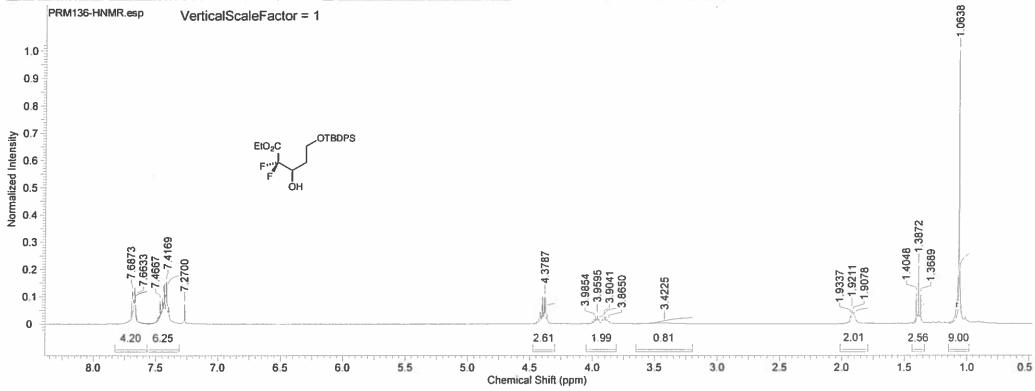
| Acquisition Time (sec) | 0.7340                 | Comment                     | EJT-PRM133 f14-21    | 17mg mF19CPD CDCl3 (e        | :\bruk400adata\2014\Jur | ) ejt 28              |          |
|------------------------|------------------------|-----------------------------|----------------------|------------------------------|-------------------------|-----------------------|----------|
| Date                   | 17 Jun 2014 12:50:24   |                             |                      | Date Stamp                   | 17 Jun 2014 12:50:24    | 4,000 to to -         |          |
| File Name              | \\ss7a.ds.man.ac.uk\vo | ol5\vol3\users\snmrdata\bru | k400adata\2014\Jun\d | ata\ejt\nmr\2014-06-17-ejt-2 | 8\12\fid                | Frequency (MHz)       | 376.50   |
| Nucleus                | 19F                    | Number of Transients        |                      | Origin                       | AV400                   | Original Points Count | 65536    |
| Owner                  | nmrsu                  | Points Count                | 65536                | Pulse Sequence               | zgig                    | Receiver Gain         | 2050.00  |
| SW(cyclical) (Hz)      | 89285.71               | Solvent                     | CHLOROFORM-d         | Spectrum Offset (Hz)         | -37649.5977             | Spectrum Type         | STANDARD |
| Sweep Width (Hz)       | 89284.35               | Temperature (degree C       | 22.400               |                              |                         |                       |          |

PRM133-F{H}NMR.esp

VerticalScaleFactor = 1

02/04/2014 17:04:51

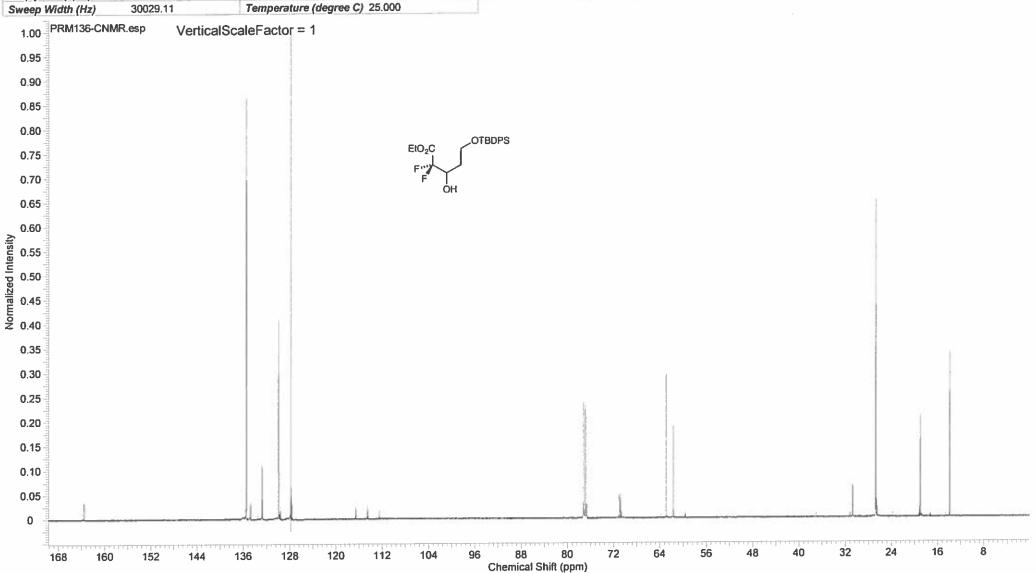
| Acquisition Time (sec) | 3.9649               | Comment           | EJT-PRM136 prod    | mPROTON CDCI3 (e:\bruk400 | Odata\2014\Mar} ejt 44 | Date                  | 14 Mar 2014 11:46:08           |
|------------------------|----------------------|-------------------|--------------------|---------------------------|------------------------|-----------------------|--------------------------------|
| Date Stamp             | 14 Mar 2014 11:46:08 | File Name         | \\ss7a.ds.man.ac.u | k\vol5\VOL3\USERS\SNMRDA  | TA\BRUK400DATA\20      | 14\MAR\DATA\EJT\MR\20 | 014-03-14-EJT-44\10\PDATA\1\1R |
| Frequency (MHz)        | 400.13               | Nucleus           | 1H                 | Number of Transients      | 16                     | Origin                | AV400                          |
| Original Points Count  | 32768                | Owner             | Administrator      | Points Count              | 32768                  | Pulse Sequence        | zg30b                          |
| Receiver Gain          | 128.00               | SW(cyclical) (Hz) | 8264.46            | Solvent                   | CHLOROFORM-d           | Spectrum Offset (Hz)  | 2464.6750                      |
| Spectrum Type          | STANDARD             | Sweep Width (Hz)  | 8264.21            | Temperature (degree C     | 21.400                 |                       |                                |



| No. | (ppm)     | Value      | Absolute Value | Non-Negative Value |
|-----|-----------|------------|----------------|--------------------|
| 1   | 9815 1.14 | 8 99984264 | 1.72771696e+8  | 8.99984264         |
| 2   | 3378 1.43 | 2.56114244 | 4.91667400e+7  | 2.56114244         |
| 3   | 7934 2.01 | 2.00694013 | 3.85276120e+7  | 2.00694013         |
| 4   | 1978 3.65 | 0.80761468 | 1.55039330e+7  | 0.80761468         |
| 5   | 3076 4.04 | 1.98614478 | 3.81284000e+7  | 1.98614478         |
| 6   | 3008 4.47 | 2.61058092 | 5.01158200e+7  | 2.61058092         |
| 7   | 3095 7.56 | 6.25181770 | 1.20017336e+8  | 6.25181770         |
| 8   | 5699 7.82 | 4.19923115 | 8.06134400e+7  | 4.19923115         |

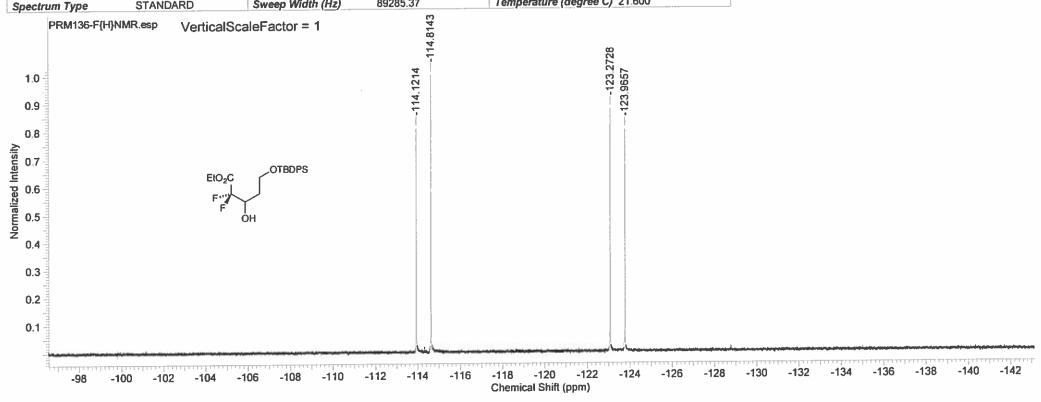
02/04/2014 16:39:43

| Acquisition Time (sec) | 1.0912                 | Comment                    | EJT-PRM136 Prod data mCARBONnight CDCl3 {F:\bruk500_b_data\2014\Mar} ejt 59 |                              |            |                       |          |
|------------------------|------------------------|----------------------------|-----------------------------------------------------------------------------|------------------------------|------------|-----------------------|----------|
| Date                   | 21 Mar 2014 21:41:20   | Date Stamp                 | 21 Mar 2014 21:41:20                                                        |                              |            |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\vo | 5\vol3\users\snmrdata\brul | <500bdata\2014\Mar\data                                                     | a\ejt\nmr\2014-03-21-ejt-59\ | 10\fid     | Frequency (MHz)       | 125.76   |
| Nucleus                | 13C                    | Number of Transients       | 3096                                                                        | Origin                       | spect      | Original Points Count | 32768    |
| Owner                  | Administrator          | Points Count               | 32768                                                                       | Pulse Sequence               | zgpg30     | Receiver Gain         | 5792.60  |
| SW(cyclical) (Hz)      | 30030.03               | Solvent                    | CHLOROFORM-d                                                                | Spectrum Offset (Hz)         | 12566.0234 | Spectrum Type         | STANDARD |
|                        |                        |                            |                                                                             |                              |            |                       |          |



02/04/2014 17:33:27

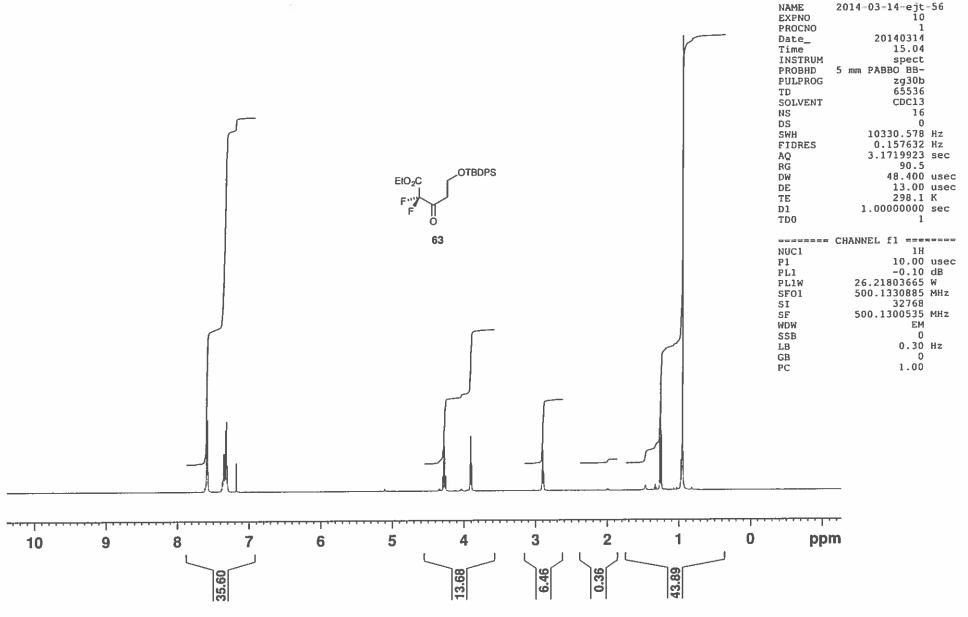
| Acquisition Time (sec) | 0.7340               | Comment           | EJT-PRM136 prod mF     | 19CPD CDCl3 (e:\bruk400d | ata\2014\Mar} ejt 44 | Date                 | 14 Mar 2014 11 46:08          |
|------------------------|----------------------|-------------------|------------------------|--------------------------|----------------------|----------------------|-------------------------------|
| Date Stamp             | 14 Mar 2014 11:46:08 | File Name         | \\ss7a.ds.man.ac.uk\vo | 15\VOL3\USERS\SNMRDA     | TA\BRUK400DATA\2014  | WARIDATA/EJTWMR/20   | 14-03-14-EJT-44\11\PDATA\1\1R |
| Frequency (MHz)        | 376.50               | Nucleus           | 19F                    | Number of Transients     | 16                   | Origin               | AV400                         |
| Original Points Count  | 65536                | Owner             | Administrator          | Points Count             | 262144               | Pulse Sequence       | zgig                          |
| Receiver Gain          | 4100.00              | SW(cyclical) (Hz) | 89285.71               | Solvent                  | CHLOROFORM-d         | Spectrum Offset (Hz) | -37649.5977                   |
| Canadana Tuno          | STANDADD             | Sween Width (Hz)  | 89285.37               | Temperature (degree C    | 21.600               |                      |                               |

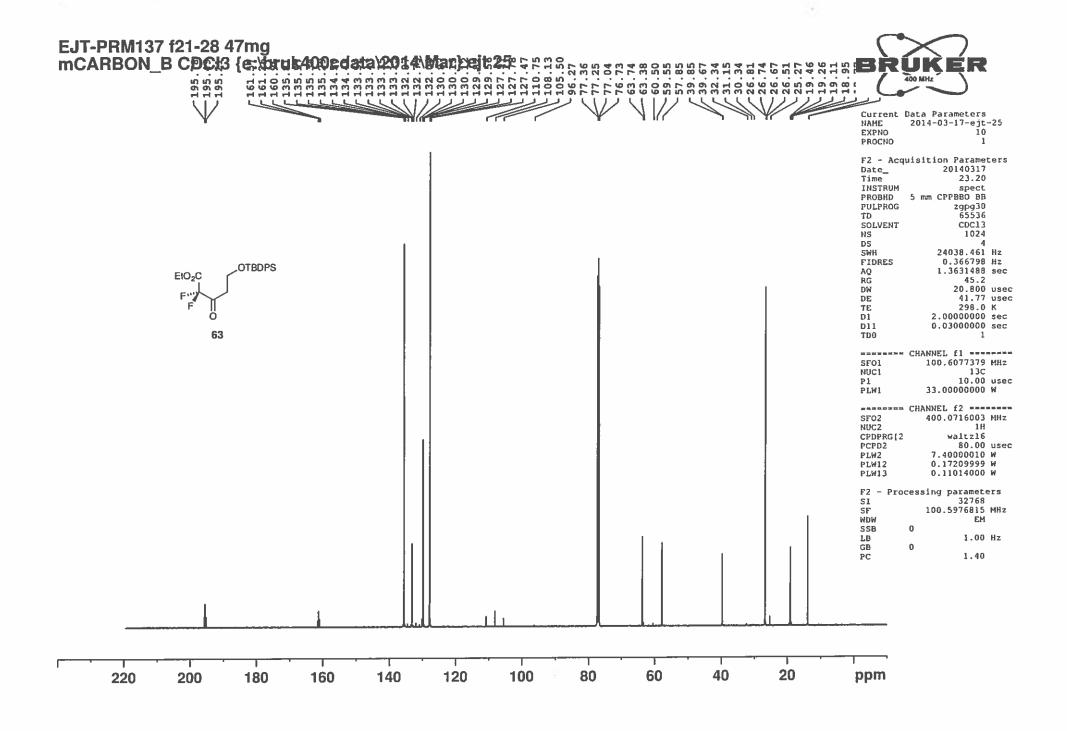


| į | No. | (ppm)   | (Hz)     | Height |
|---|-----|---------|----------|--------|
| İ | 1   | -123.97 | -46672.9 | 0.8015 |
| 1 | 2   | -123.27 | -46412.0 | 0.8765 |
|   | 3   | -114.81 | -43227.4 | 1.0000 |
| - | 4   | -114.12 | -42966.5 | 0.8086 |

EJT-PRM137 DMP f21-26 22mg mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 56

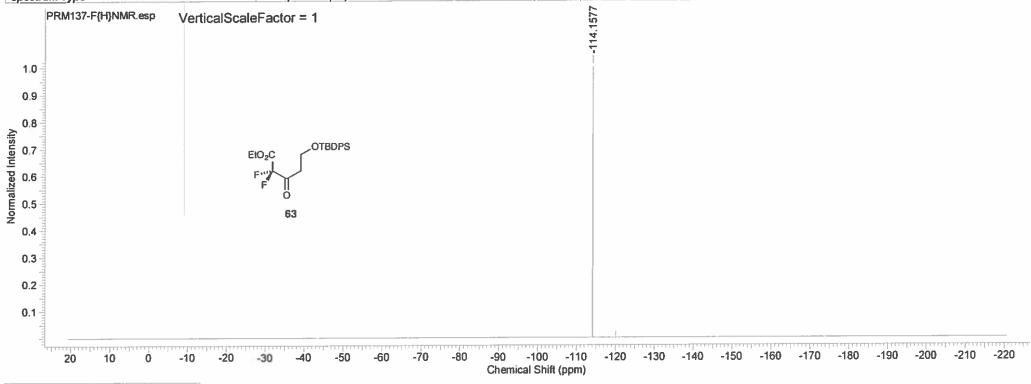






07/04/2014 11:10:45

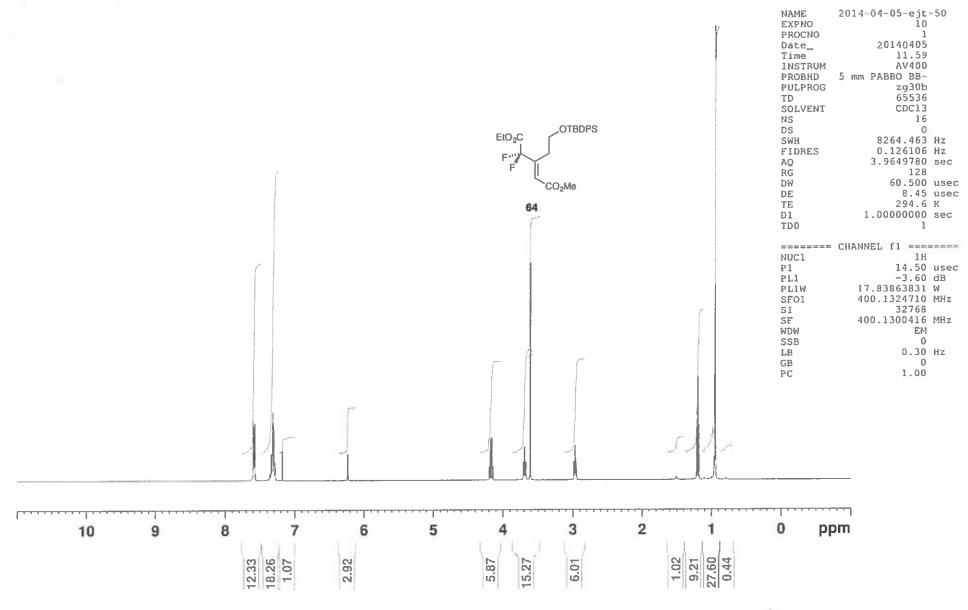
| Acquisition Time (sec) | 0.5767                    | Comment           | EJT-PRM137 DMP f21-26 22mg m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 56 |                       |                       |                      |             |  |
|------------------------|---------------------------|-------------------|--------------------------------------------------------------------------------------|-----------------------|-----------------------|----------------------|-------------|--|
| Date                   | 14 Mar 2014 15:08:48      | Date Stamp        | 14 Mar 2014 15:08:48                                                                 |                       |                       |                      |             |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol5\ | VOL3\USERS\SNMRDA | A\BRUK500DATA\BRUK50                                                                 | ODATA\2014\MAR\DATA\E | JT\NMR\2014-03-14-EJT | -56\12\PDATA\1\1R    |             |  |
| Frequency (MHz)        | 470.59                    | Nucleus           | 19F                                                                                  | Number of Transients  | 16                    | Origin               | spect       |  |
| Original Points Count  | 65536                     | Owner             | vnmr1                                                                                | Points Count          | 65536                 | Pulse Sequence       | zgfhigqn    |  |
| Receiver Gain          | 912.00                    | SW(cyclical) (Hz) | 113636.37                                                                            | Solvent               | CHLOROFORM-d          | Spectrum Offset (Hz) | -47059.0234 |  |
| Spectrum Type          | STANDARD                  | Sweep Width (Hz)  | 113634.63                                                                            | Temperature (degree C | 27.000                |                      |             |  |

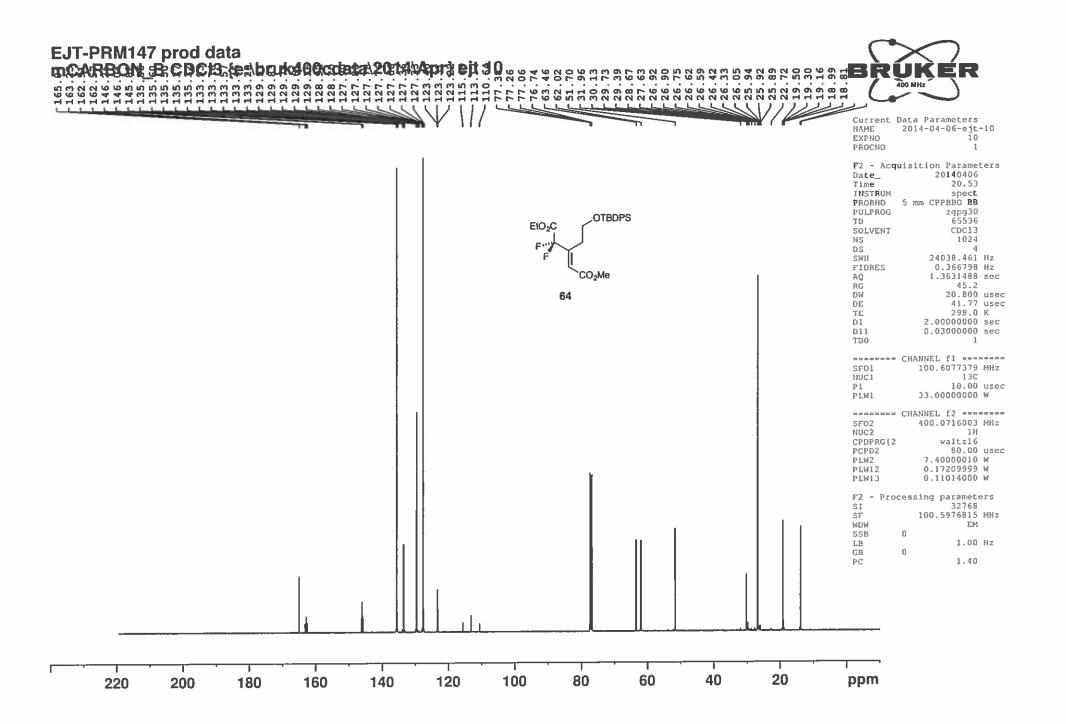


| No. | (ppm)   | (Hz)     | Height |
|-----|---------|----------|--------|
| 1   | -114.16 | -53721.7 | 1.0000 |

# EJT-PRM147 f17-27 31mg mPROTON CDCl3 {e:\bruk400data\2014\Apr} ejt 50

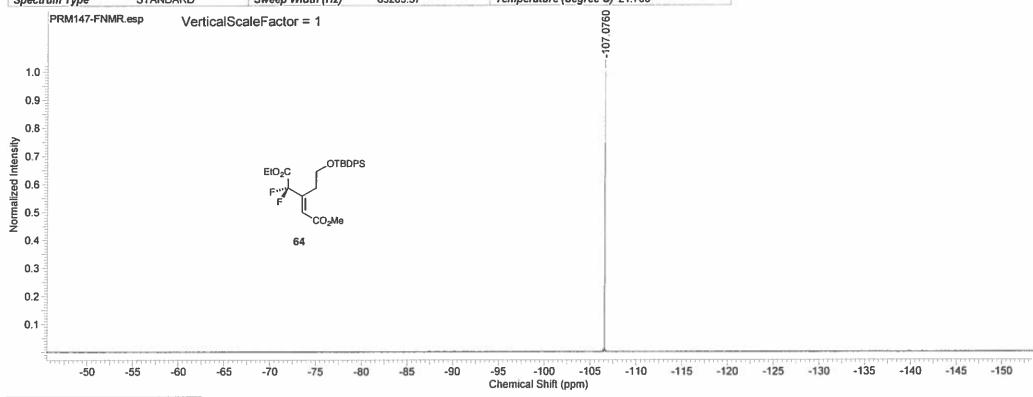






07/04/2014 17:01:40

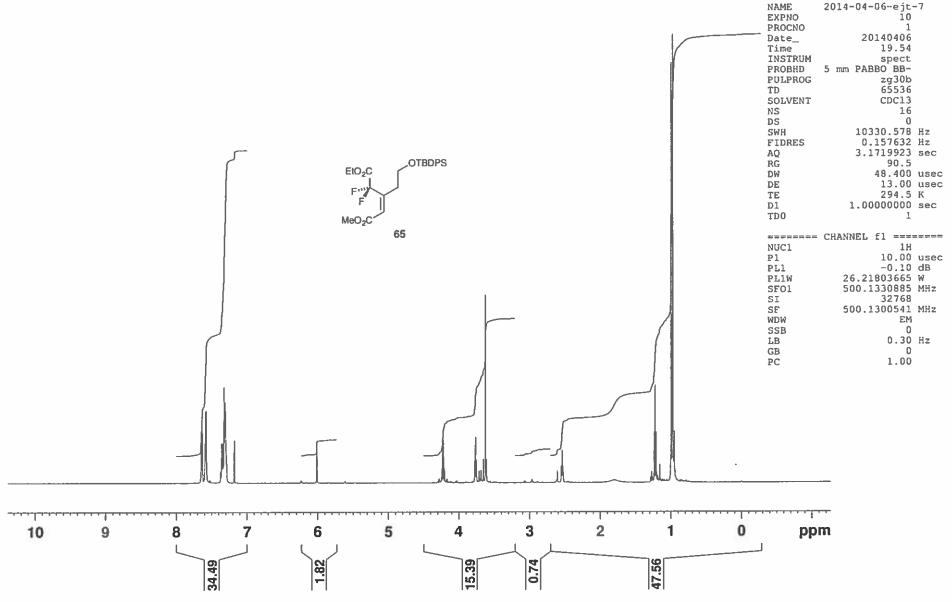
| Acquisition Time (sec) | 0.7340               | Comment           | EJT-PRM147 f17-2    | 7 31mg mF19 CDCl3 {e:\bruk4 | 00data\2014\Apr} ejt 50 | Date                   | 05 Apr 2014 12:01:20          |
|------------------------|----------------------|-------------------|---------------------|-----------------------------|-------------------------|------------------------|-------------------------------|
| Date Stamp             | 05 Apr 2014 12:01:20 | File Name         | \\ss7a.ds.man.ac.ul | klvol5\VOL3\USERS\SNMRDA    | TA\BRUK400DATA\201      | 14/APR/DATA/EJT/NMR/20 | 14-04-05-EJT-50\12\PDATA\1\1R |
| Frequency (MHz)        | 376.50               | Nucleus           | 19F                 | Number of Transients        | 16                      | Origin                 | AV400                         |
| Original Points Count  | 65536                | Owner             | Administrator       | Points Count                | 262144                  | Pulse Sequence         | zg                            |
| Receiver Gain          | 4100.00              | SW(cyclical) (Hz) | 89285.71            | Solvent                     | CHLOROFORM-d            | Spectrum Offset (Hz)   | -37649.5977                   |
| Spectrum Type          | STANDARD             | Sweep Width (Hz)  | 89285.37            | Temperature (degree C       | 21.700                  |                        |                               |

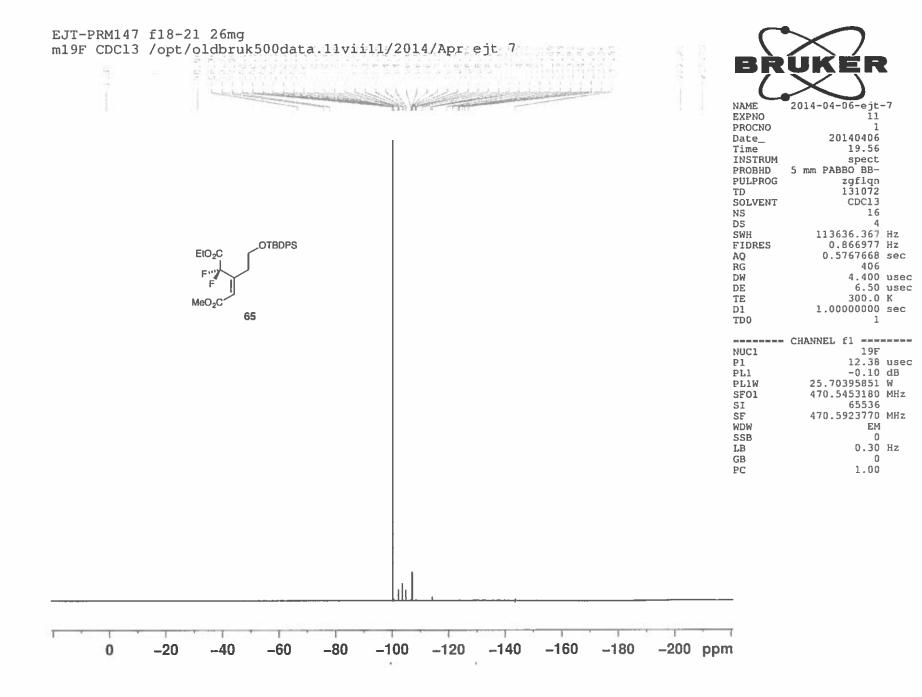


| No. | (ppm)   | (Hz)     | Height |
|-----|---------|----------|--------|
| 1   | -107.08 | -40313.9 | 1.0000 |

EJT-PRM147 f18-21 26mg mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Apr ejt 7

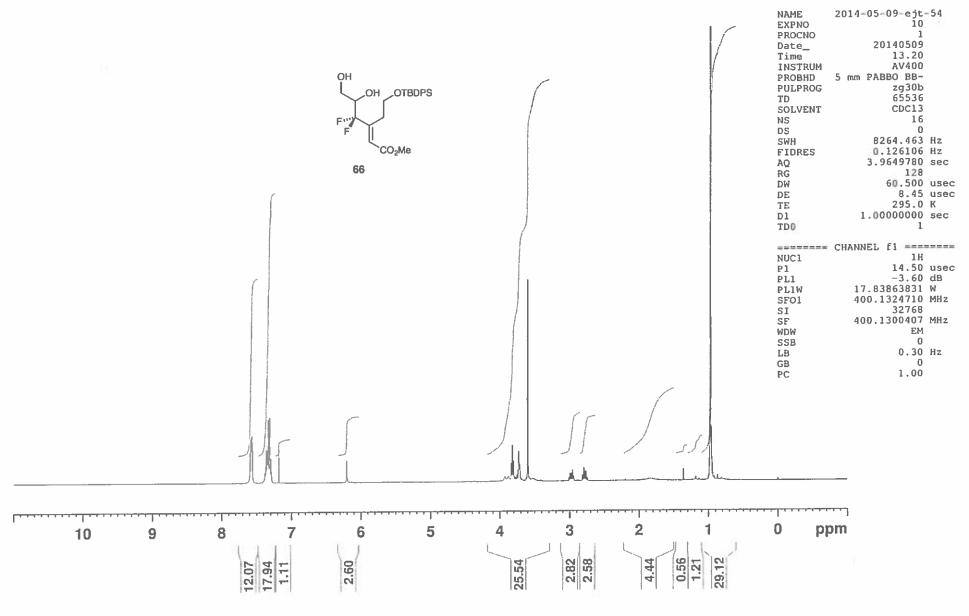


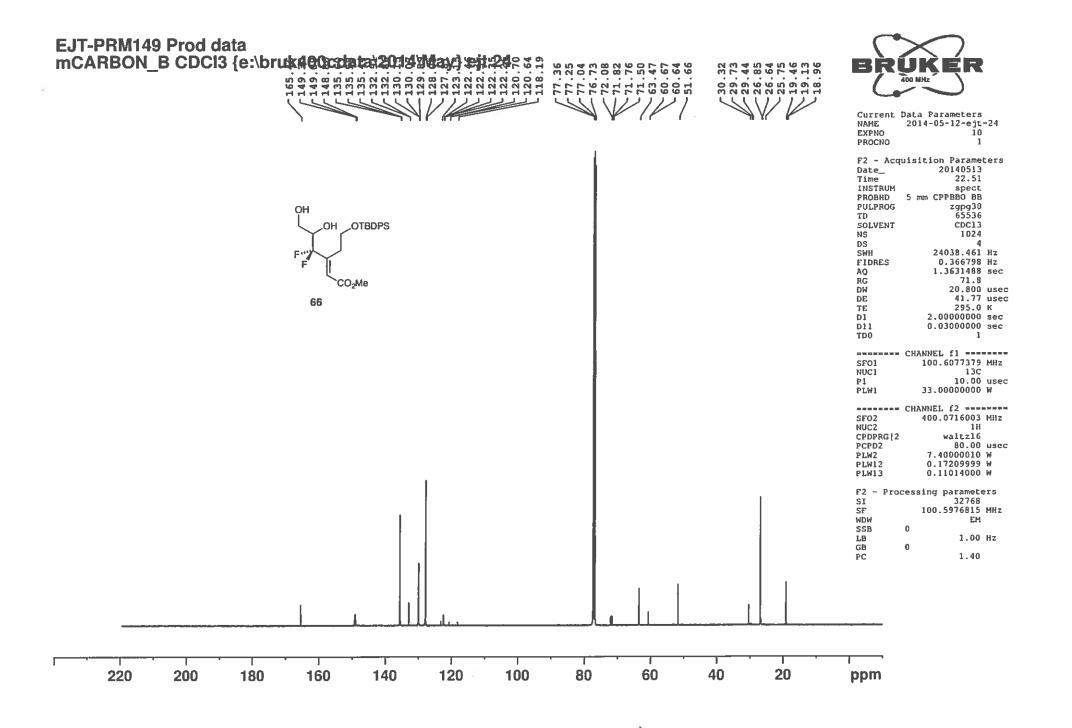




# EJT-PRM149F f17-34 38mg mPROTON CDCl3 {e:\bruk400data\2014\May} ejt 54

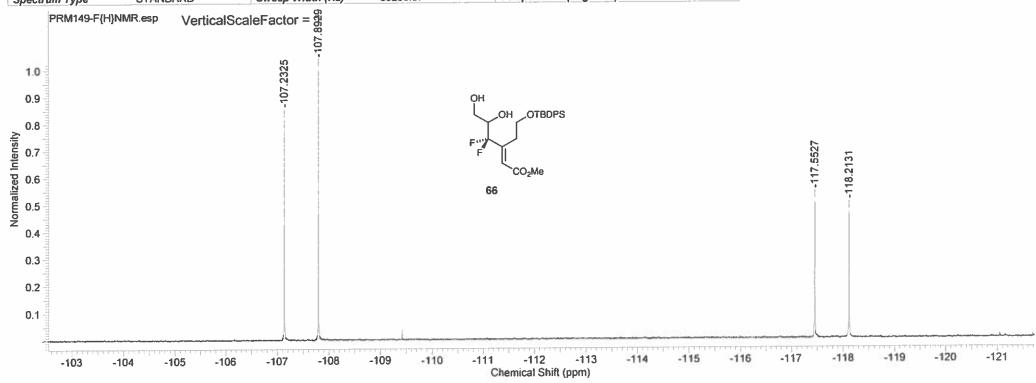






21/05/2014 12:04:27

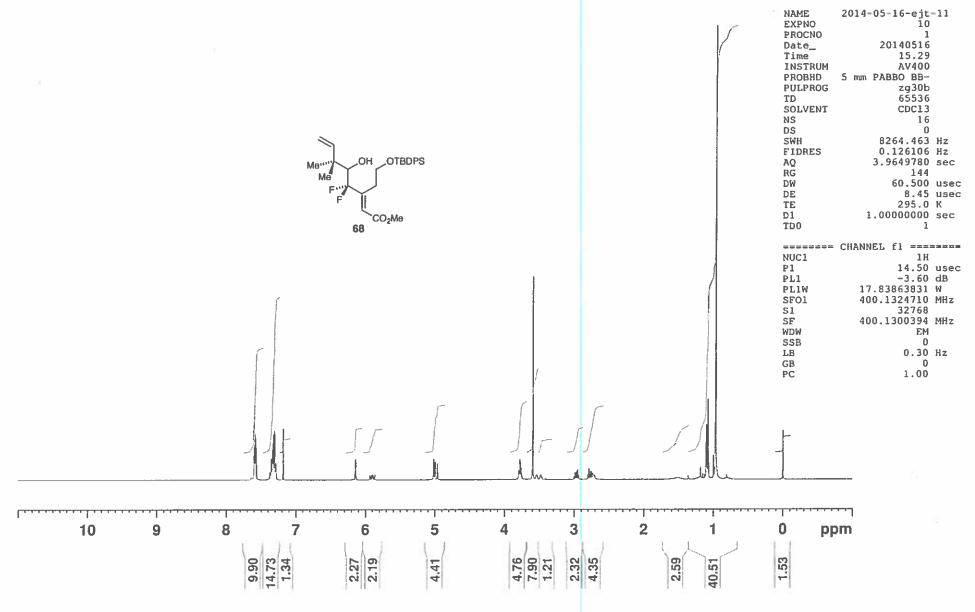
| Acquisition Time (sec) | 0.7340                   | Comment            | EJT-PRM149F f17-34 3  | 8mg mF19CPD CDCl3 (e:\ | bruk400data\2014\May} e | jt 54                |             |
|------------------------|--------------------------|--------------------|-----------------------|------------------------|-------------------------|----------------------|-------------|
| Date                   | 09 May 2014 13:22:24     | Date Stamp         | 09 May 2014 13:22:24  |                        |                         |                      |             |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | SIVOL3IUSERSISNMRD | ATA\BRUK400DATA\2014\ | MAY\DATA\EJT\NMR\2014  | I-05-09-EJT-54\11\PDAT  | A\1\1R               |             |
| Frequency (MHz)        | 376.50                   | Nucleus            | 19F                   | Number of Transients   | 16                      | Origin               | AV400       |
| Original Points Count  | 65536                    | Owner              | Administrator         | Points Count           | 262144                  | Pulse Sequence       | zgig        |
| Receiver Gain          | 4100.00                  | SW(cyclical) (Hz)  | 89285.71              | Solvent                | CHLOROFORM-d            | Spectrum Offset (Hz) | -37649.5977 |
| Spectrum Type          | STANDARD                 | Sweep Width (Hz)   | 89285.37              | Temperature (degree C  | 22.200                  |                      |             |



| No. | (ppm)   | (Hz)     | Height |
|-----|---------|----------|--------|
| 1   | -118.21 | -44507.0 | 0.4667 |
| 2   | -117.55 | -44258.4 | 0.5046 |
| 3   | -107.89 | -40621.5 | 1.0000 |
| 4   | -107.23 | -40372.8 | 0.8148 |

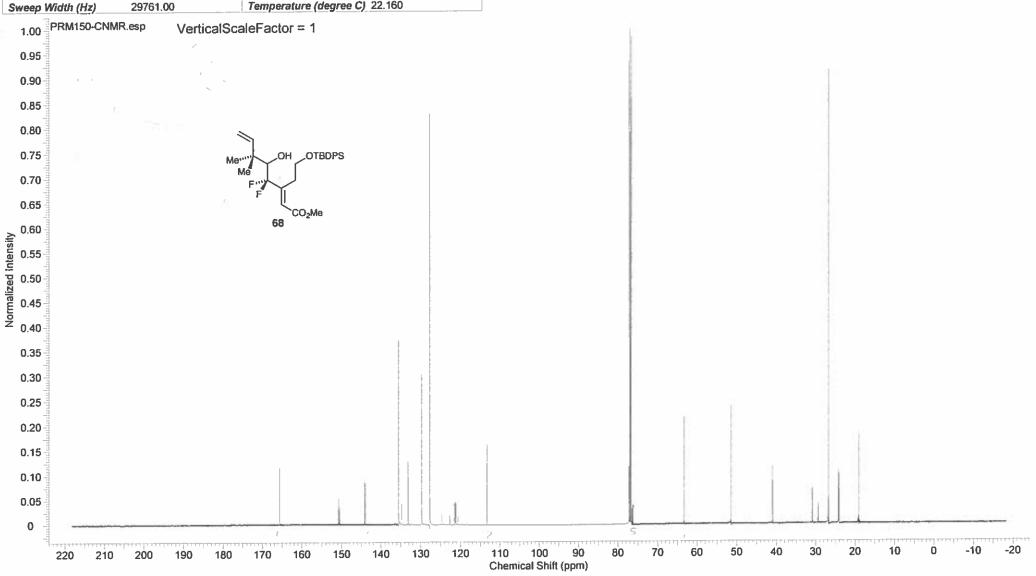
# EJT-PRM150 Zn allylation f5-15 20mg mPROTON CDCl3 {e:\bruk400data\2014\May} ejt 11





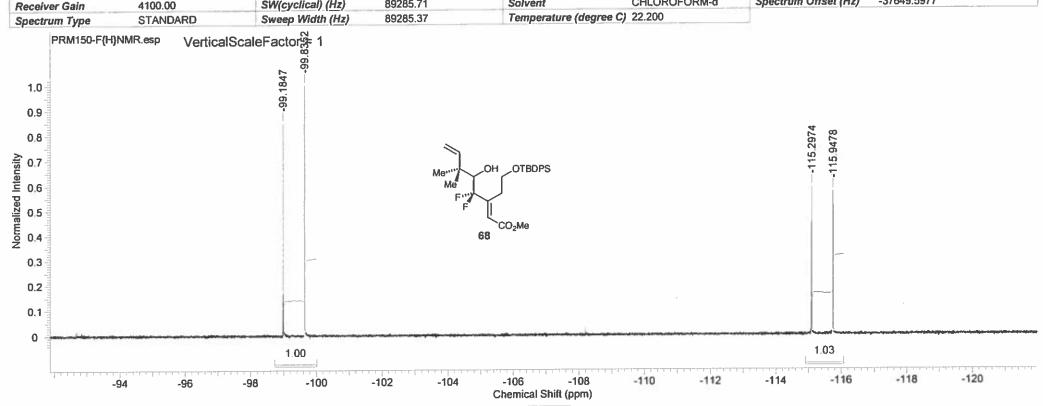
23/05/2014 19:19:14

| Acquisition Time (sec) | 1,1010                  | Comment                    | P. Mears EJT-PRM150 Prod 0514-049 mCARBON CDCl3 (E:\bruk500cdata\2014\May) staff 17 |                             |            |                       |          |  |  |
|------------------------|-------------------------|----------------------------|-------------------------------------------------------------------------------------|-----------------------------|------------|-----------------------|----------|--|--|
| Date                   | 21 May 2014 15:30:24    | Date Stamp                 | 21 May 2014 15:30:24                                                                |                             |            |                       |          |  |  |
|                        | \\ss7a ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 500cdata\2014\May\data                                                              | \staff\nmr\2014-05-21-staff | -17\12\fid | Frequency (MHz)       | 125.77   |  |  |
| Nucleus                | 13C                     | Number of Transients       | 2048                                                                                | Origin                      | spect      | Original Points Count | 32768    |  |  |
| Owner                  | nmrsu                   | Points Count               | 32768                                                                               | Pulse Sequence              | zgpg30     | Receiver Gain         | 184.40   |  |  |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                    | CHLOROFORM-d                                                                        | Spectrum Offset (Hz)        | 12568.6943 | Spectrum Type         | STANDARD |  |  |
| 347(09011001) [112]    |                         |                            | 1 00 400                                                                            | i                           |            |                       |          |  |  |



28/05/2014 17:03:52

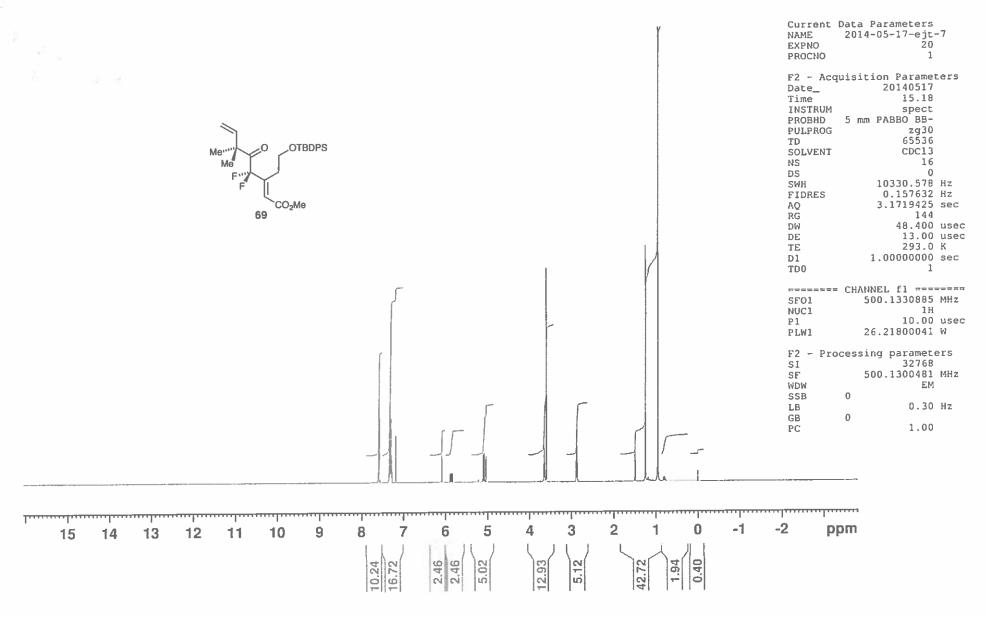
| Acquisition Time (sec) | 0.7340                  | Comment             | EJT-PRM150 Zn allylati | on f5-15 20mg mF19CPD C | DCI3 (e:\bruk400data\20 | 14\May} ejt 11       |             |
|------------------------|-------------------------|---------------------|------------------------|-------------------------|-------------------------|----------------------|-------------|
| Date                   | 16 May 2014 15:30:24    | Date Stamp          | 16 May 2014 15:30:24   |                         |                         |                      |             |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\VOL3\USERS\SNMRDA | ATA\BRUK400DATA\2014\A | MAY\DATA\EJT\NMR\2014-  | 05-16-EJT-11\11\PDAT    | 4\1\1R               |             |
| Frequency (MHz)        | 376.50                  | Nucleus             | 19F                    | Number of Transients    | 16                      | Origin               | AV400       |
| Original Points Count  | 65536                   | Owner               | Administrator          | Points Count            | 262144                  | Pulse Sequence       | zgig        |
| Receiver Gain          | 4100.00                 | SW(cyclical) (Hz)   | 89285.71               | Solvent                 | CHLOROFORM-d            | Spectrum Offset (Hz) | -37649.5977 |
| Snectrum Type          | STANDARD                | Sweep Width (Hz)    | 89285.37               | Temperature (degree C   | 22.200                  |                      |             |



| No. | (ppm)   | Value      | Absolute Value | Non-Negative Value | No. | (ppm)   | (Hz)     | Height |
|-----|---------|------------|----------------|--------------------|-----|---------|----------|--------|
| 1   | 2702115 | 1.03150678 | 1.04263719e+6  | 1.03150678         | 1   | -115.95 | -43654.2 | 0.5707 |
| 2   | 207598. | 0.99985164 | 1.01064050e+6  | 0.99985164         | 2   | -115.30 | -43409.3 | 0.5886 |
|     |         |            |                |                    | 3   | -99.84  | -37587.8 | 1.0000 |
|     |         |            |                |                    | 4   | -99.18  | -37342.9 | 0.8471 |

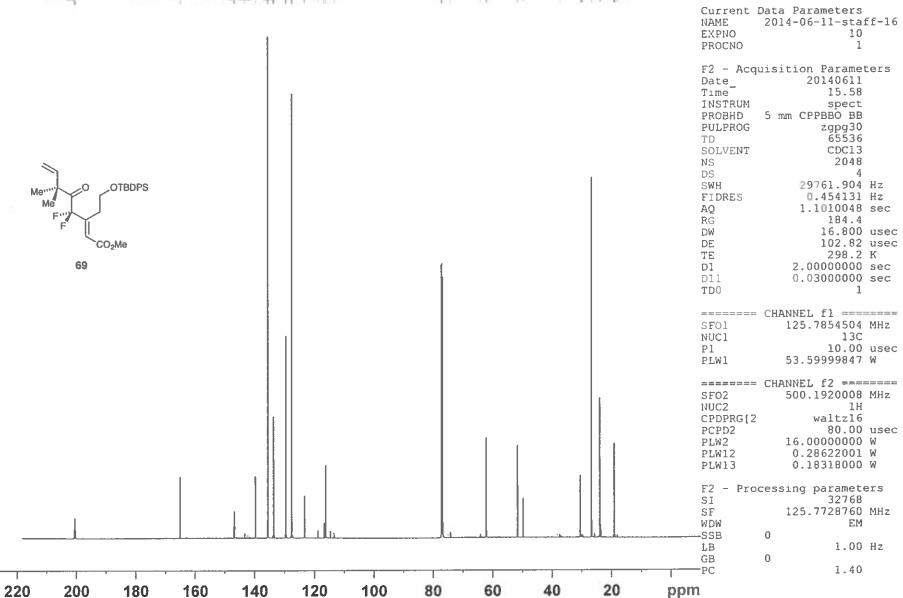
## EJT-PRM151 f4-12 11mg mPROTON CDCl3 {E:\bruk500adata\2014\May} ejt 7





P. Mears
EJT151 prod data
0614-017
2048 scans
mCARBON CDCL3 (E:\bruk500cdata\2014\Jun) staff 16



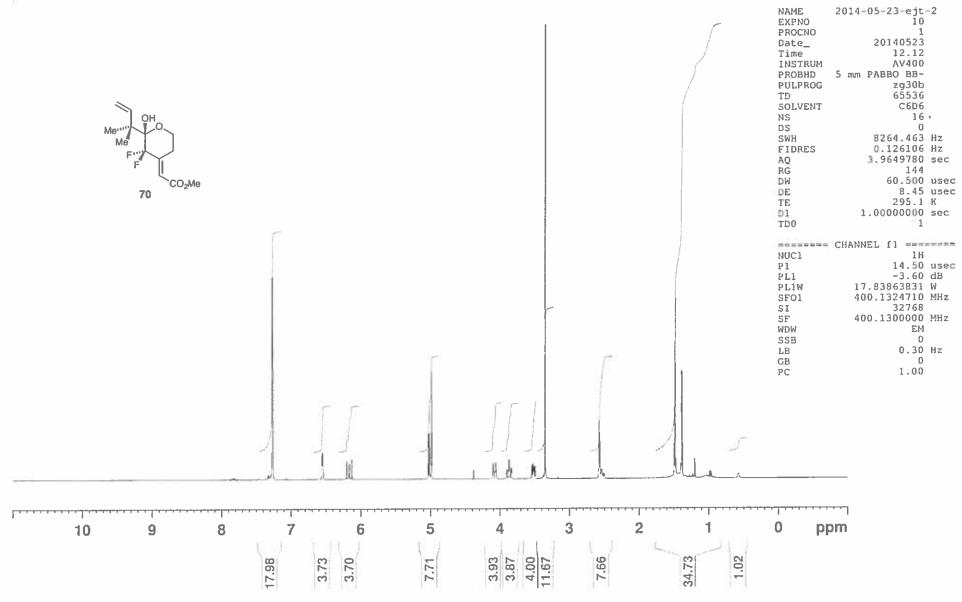


| Acquisition Time (sec) | 0.5767               | Comment                | EJT-PRM151 f4-12 1   | 11mg m19F CDCl3 (E:\bruk     | (500adata\2014\May) ejt 7 | 7                     |          |
|------------------------|----------------------|------------------------|----------------------|------------------------------|---------------------------|-----------------------|----------|
| Date                   | 17 May 2014 15:21:52 |                        |                      | Date Stamp                   | 17 May 2014 15:21:52      |                       |          |
|                        |                      |                        | k500adata\2014\May\c | lata\ejt\nmr\2014-05-17-ejt- | 7\22\fid                  | Frequency (MHz)       | 470.59   |
| Nucleus                | 19F                  | Number of Transients   | 16                   | Origin                       | spect                     | Original Points Count | 65536    |
| Owner                  | nmrsu                | Points Count           | 65536                | Pulse Sequence               | zgfiqn                    | Receiver Gain         | 362.00   |
| SW(cyclical) (Hz)      | 113636.37            | Solvent                | CHLOROFORM-d         | Spectrum Offset (Hz)         | -47059.0234               | Spectrum Type         | STANDARD |
| Sweep Width (Hz)       | 113634.63            | Temperature (degree C) | 20.000               |                              |                           |                       |          |

PRM151-FNMR.esp

# EJT-PRM152 HF.py f3-11 15mg mPROTON C6D6 {e:\bruk400data\2014\May} ejt 2

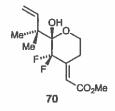


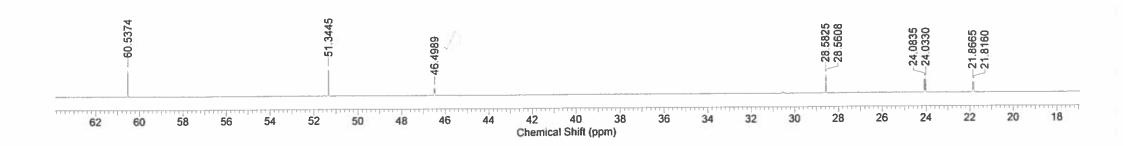


|                        | THIS TOPOIL HOS OF      |                            |                         | The second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second secon |                   |                                |          |
|------------------------|-------------------------|----------------------------|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------|--------------------------------|----------|
| Acquisition Time (sec) | 1.1010                  | Comment                    | P. Mears EJT-PRM152     | HF.py 83-11 0514-053 m <sup>(2)</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | CARBON C6D6 (E:\b | ruk500cdata\2014\May} staff 28 |          |
| Date                   | 23 May 2014 20:35:28    |                            | 23 May 2014 20:35:28    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                   |                                |          |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 500cdata\2014\May\data\ | staff\nmr\2014-05-23-staff                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | -28\12\fid        | Frequency (MHz)                | 125.77   |
| Nucleus                | 13C                     | Number of Transients       | 5120                    | Origin                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | spect             | Original Points Count          | 32768    |
| Owner                  | nmrsu                   | Points Count               | 32768                   | Pulse Sequence                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | zgpg30            | Receiver Gain                  | 184.40   |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                    | BENZENE-d6              | Spectrum Offset (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 12662.5273        | Spectrum Type                  | STANDARD |
| Sweep Width (Hz)       | 29761.00                | Temperature (degree C      | 25.149                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                   |                                |          |

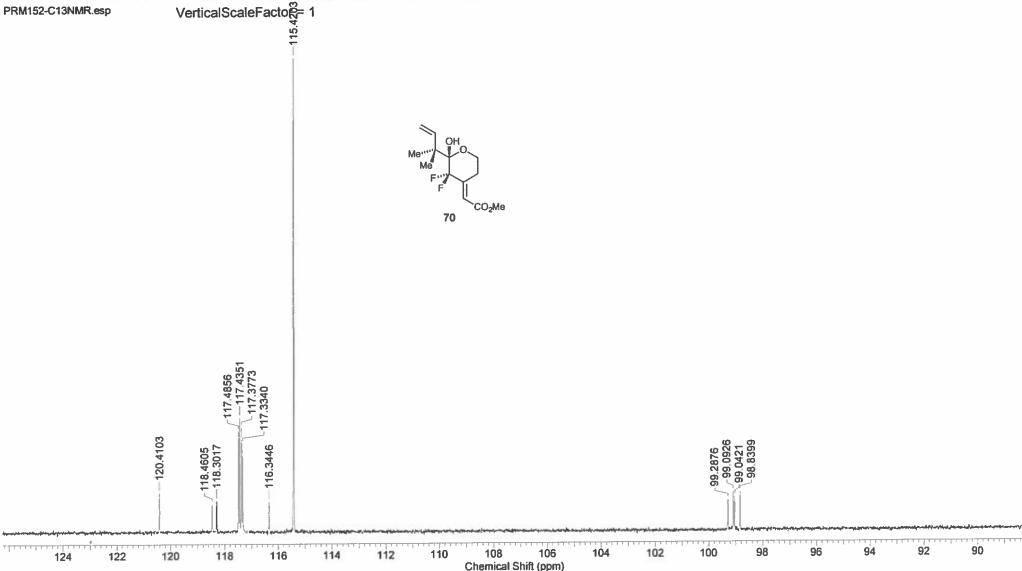
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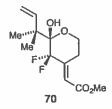
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ P. Mears EJT-PRM152 HF.py 83-11 0514-053 mCARBON C6D6 (E:\bruk500cdata\2014\May) staff 28 Acquisition Time (sec) 1.1010 Comment 23 May 2014 20:35:28 23 May 2014 20:35:28 Date Stamp Date \\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2014\\May\data\staff\nmr\2014-05-23-staff-28\12\\fid Frequency (MHz) 125.77 File Name Original Points Count 32768 Origin spect Number of Transients 5120 13C Nucleus 184.40 Receiver Gain 32768 **Pulse Sequence** zgpg30 **Points Count** Owner nmrsu **STANDARD** Spectrum Offset (Hz) 12662.5273 Spectrum Type BENZENE-d6 Solvent SW(cyclical) (Hz) 29761.90 Temperature (degree C) 25.149 29761.00 Sweep Width (Hz) VerticalScaleFacto8 1

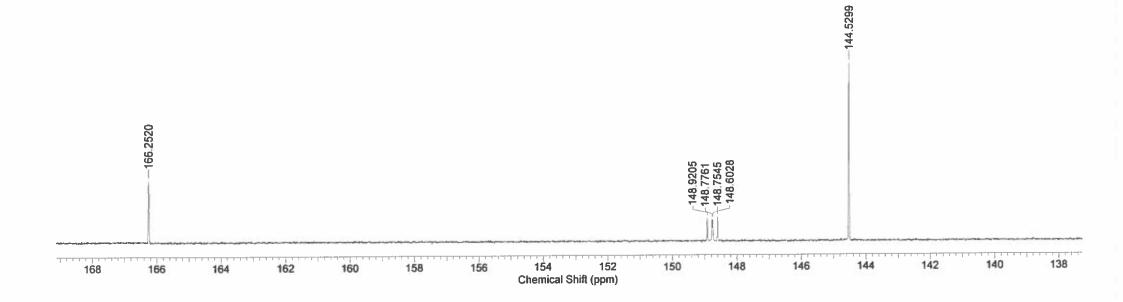


| Acquisition Time (sec) | 1.1010                  | Comment                    | P. Mears EJT-PRM152     | HF.py 83-11 0514-053 mC     | CARBON C6D6 (E:\ | ruk500cdata\2014\May) staff 28 | 3.00     |
|------------------------|-------------------------|----------------------------|-------------------------|-----------------------------|------------------|--------------------------------|----------|
| Date                   | 23 May 2014 20:35:28    | Date Stamp                 | 23 May 2014 20:35:28    |                             |                  |                                |          |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 500cdata\2014\May\data\ | staff\nmr\2014-05-23-staff- | -28\12\fid       | Frequency (MHz)                | 125.77   |
| Nucleus                | 13C                     | Number of Transients       | 5120                    | Origin                      | spect            | Original Points Count          | 32768    |
| Owner                  | nmrsu                   | Points Count               | 32768                   | Pulse Sequence              | zgpg30           | Receiver Gain                  | 184.40   |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                    | BENZENE-d6              | Spectrum Offset (Hz)        | 12662.5273       | Spectrum Type                  | STANDARD |
| Sween Width (Hz)       | 29761 00                | Temperature (degree C)     | 25.149                  |                             |                  |                                |          |

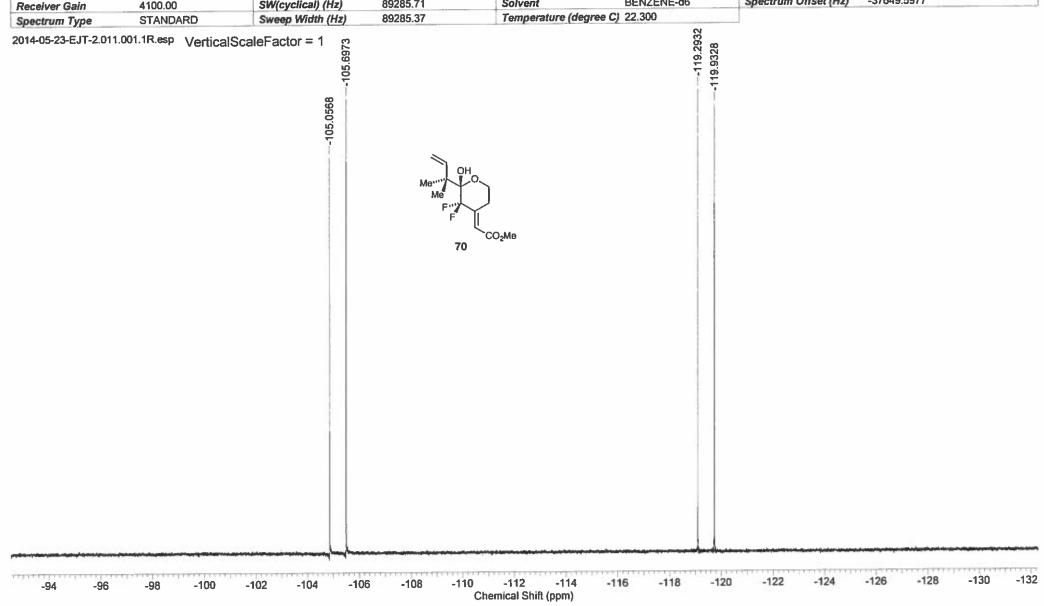
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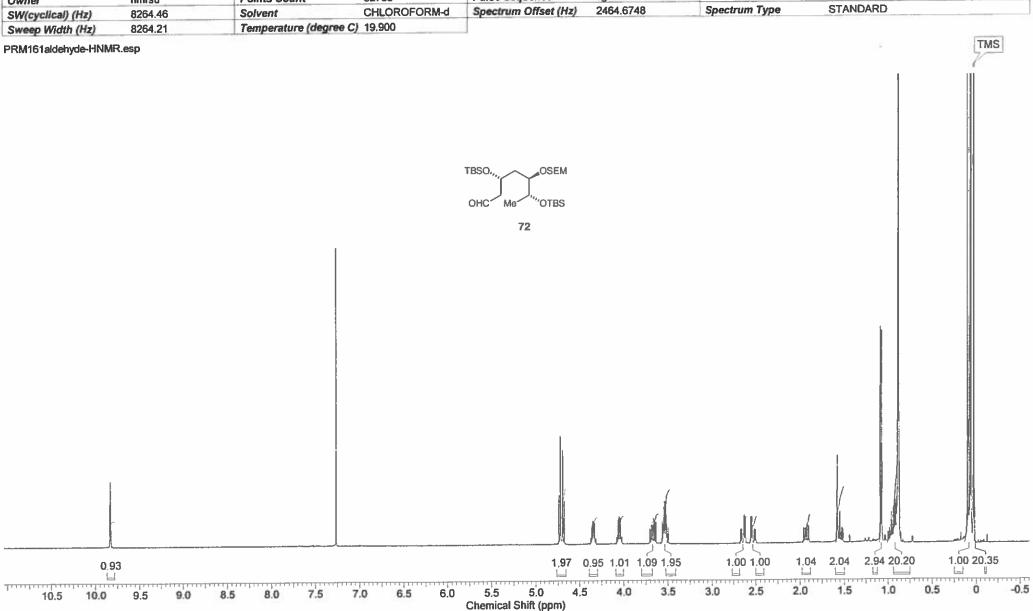




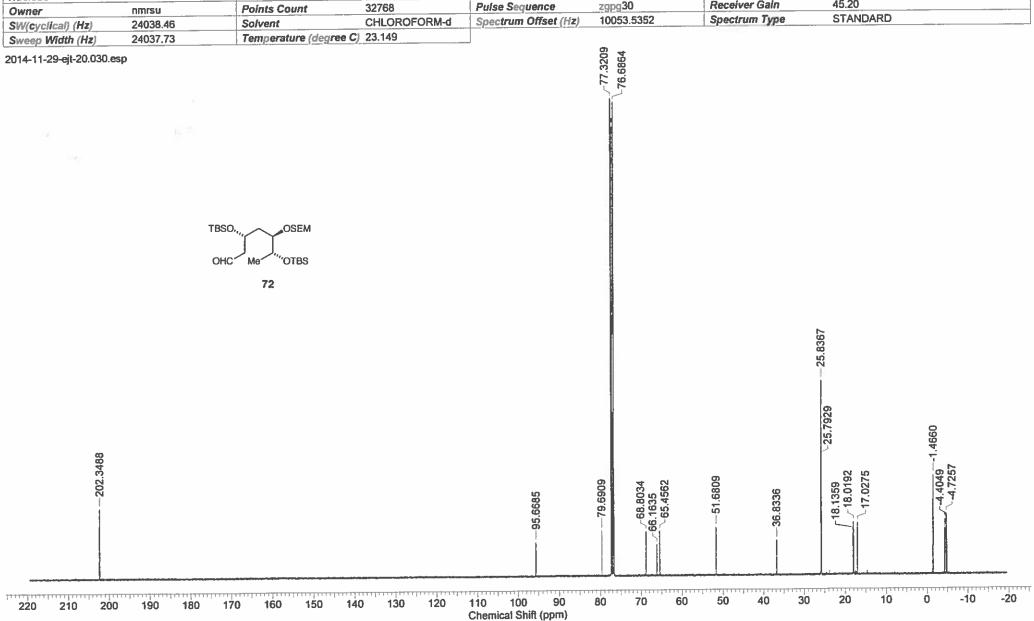
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| Acquisition Time (sec) | 0.7340                  | Comment            | EJT-PRM152 HF.py f3-  | 11 15mg mF19CPD C6D6  | (e:\bruk400data\2014) | May) ept 2           |             |
| Date                   | 23 May 2014 12:14:08    | Date Stamp         | 23 May 2014 12:14:08  |                       |                       |                      |             |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5/VOL3/USERS/SNMRD | ATA\BRUK400DATA\2014\ | MAY\DATA\EJT\NMR\201  | 4-05-23-EJT-2\11\PD   | ATA\1\1R             |             |
| Frequency (MHz)        | 376.50                  | Nucleus            | 19F                   | Number of Transients  | 16                    | Origin               | AV400       |
| Original Points Count  | 65536                   | Owner              | Administrator         | Points Count          | 262144                | Pulse Sequence       | zgig        |
| Receiver Gain          | 4100.00                 | SW(cyclical) (Hz)  | 89285.71              | Solvent               | BENZENE-d6            | Spectrum Offset (Hz) | -37649.5977 |
| Construct Tune         | STANDARD                | Swaan Width (Hz)   | 89285 37              | Temperature (degree C | 22.300                |                      |             |



|                        | rina report mas o     |                                                                                 |                      | 2011110 2211101111111111111111111111111 |                      | W                     |          |  |  |  |
|------------------------|-----------------------|---------------------------------------------------------------------------------|----------------------|-----------------------------------------|----------------------|-----------------------|----------|--|--|--|
| Acquisition Time (sec) | 3.9649                | Comment EJT-PRM161 f15-35 289mg mPROTON CDCl3 (e:\bruk400adata\2015\Feb) ejt 22 |                      |                                         |                      |                       |          |  |  |  |
| Date                   | 25 Feb 2015 16:36:16  |                                                                                 |                      | Date Stamp                              | 25 Feb 2015 16:36:16 |                       |          |  |  |  |
| File Name              | liss7a ds man.ac.uklw | ol5\vol3\users\snmrdata\bru                                                     | k400adata\2015\Feb\d | lata\ejt\nmr\2015-02-25-ejt-2           | 22\10\fid            | Frequency (MHz)       | 400.13   |  |  |  |
| Nucleus                | 1H                    | Number of Transients                                                            | F 7/45               | Origin                                  | AV400                | Original Points Count | 32768    |  |  |  |
| Owner                  | nmrsu                 | Points Count                                                                    | 32768                | Pulse Sequence                          | zg30b                | Receiver Gain         | 144.00   |  |  |  |
| SW(cyclical) (Hz)      | 8264.46               | Solvent                                                                         | CHLOROFORM-d         | Spectrum Offset (Hz)                    | 2464.6748            | Spectrum Type         | STANDARD |  |  |  |
| Sween Width (Hz)       | 8264.21               | Temperature (degree C)                                                          | 19 900               |                                         |                      |                       |          |  |  |  |

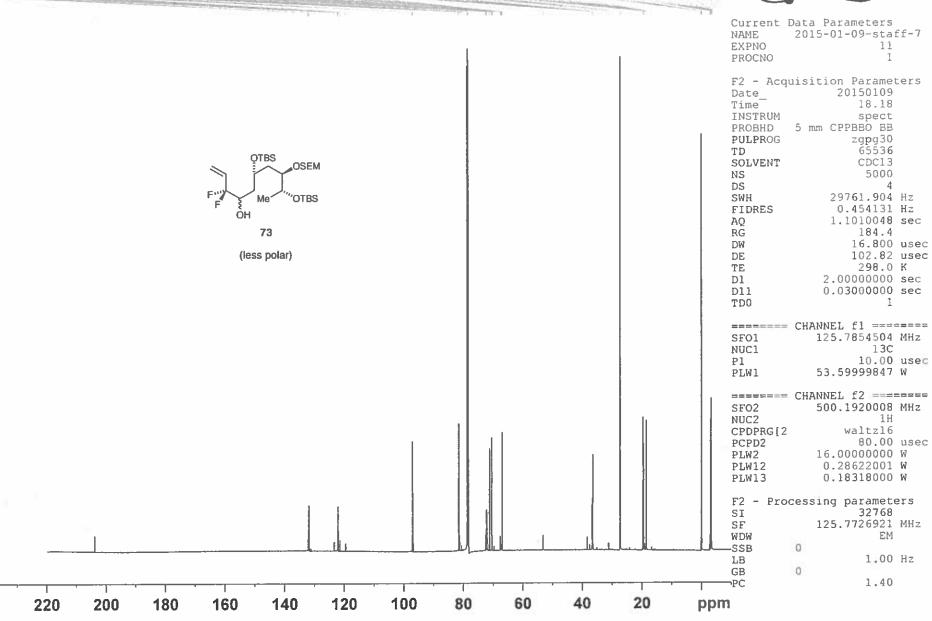


|                        | LING LEDOLF MING O   | reaced by resultant        |                       | The second second            |                        |                       |                 |
|------------------------|----------------------|----------------------------|-----------------------|------------------------------|------------------------|-----------------------|-----------------|
| Acquisition Time (sec) | 1.3631               | Comment                    | EJT-PRM161 aldehyd    | e mCARBON_B CDCl3 (e:        | \bruk400cdata\2014\Nov | /} ejt 20             |                 |
| Date                   | 29 Nov 2014 17:23:12 |                            |                       | Date Stamp                   | 29 Nov 2014 17:23:12   |                       |                 |
| File Name              |                      | d5\vol3\users\snmrdata\bru | k400cdata\2014\Nov\da | ta\eit\nmr\2014-11-29-ejt-20 | 0\30\fid               | Frequency (MHz)       | 100.60          |
|                        | 13C                  | Number of Transients       | 1024                  | Origin                       | spect                  | Original Points Count | 32768           |
| Nucleus                |                      |                            | 32768                 | Pulse Sequence               | zgpg30                 | Receiver Gain         | 45.20           |
| Owner                  | nmrsu                | Points Count               |                       |                              | 10053.5352             | Spectrum Type         | STANDARD        |
| SW(cyclical) (Hz)      | 24038.46             | Solvent                    | CHLOROFORM-d          | Spectrum Offset (Hz)         | 10000.0002             | opeculain Type        | O F H TO F H TO |
| Sweep Width (Hz)       | 24037.73             | Temperature (degree C)     | 23.149                |                              |                        |                       |                 |



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM166 f12+13 34mg clean front diastereomer? mPROTON CDCl3 (e \u00bcruk400adata\u00e42015\u00bclan) ejt 2 Acquisition Time (sec) 3.9649 Comment 08 Jan 2015 13:17:52 Date Stamp 08 Jan 2015 13:17:52 Date Frequency (MHz) 400.13 \\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jan\data\ejt\nmr\2015-01-08-ejt-2\13\fid 32768 File Name Original Points Count Origin AV400 16 Number of Transients 1H Nucleus 101.00 Receiver Gain zg30b Pulse Sequence 32768 **Points Count** nmrsu STANDARD Owner 2464.9270 Spectrum Type Spectrum Offset (Hz) CHLOROFORM-d 8264.46 Solvent SW(cyclical) (Hz) Temperature (degree C) 23.000 8264.21 Sweep Width (Hz) PRM166-frontdiast-HNMR.esp 73 (less polar) 6.36 7.19 9.34 3,5922.37 1.002.10 1.42 1.87 1.30 0.96 1.25 2.29 2,35 1.05 1.04 1.0 -0.5 0.5 2.0 1.5 3.0 2.5 3.5 4.5 4.0 5.0 5.5 6.0 Chemical Shift (ppm)





|                                          |                         | Comment                    | EJT-PRM166 f12+13      | 34mg clean front diastereоп  | ner? mF19CPD CDCl3 | (e:\bruk400adata\2015\Jan) e | jt 2     |
|------------------------------------------|-------------------------|----------------------------|------------------------|------------------------------|--------------------|------------------------------|----------|
| Date                                     | 08 Jan 2015 13:22:08    | Date Stamp                 | 08 Jan 2015 13:22:08   |                              |                    |                              |          |
| File Name                                | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 400adata\2015\Jan\data | vejt\nmr\2015-01-08-ejt-2\15 | 5Vid               | Frequency (MHz)              | 376.50   |
| Nucleus                                  | 19F                     | Number of Transients       | 16                     | Origin                       | AV400              | Original Points Count        | 65536    |
| Owner                                    | nmrsu                   | Points Count               | 65536                  | Pulse Sequence               | zgig               | Receiver Gain                | 2050.00  |
| SW(cyclical) (Hz)                        | 89285.71                | Solvent                    | CHLOROFORM-d           | Spectrum Offset (Hz)         | -37649.5977        | Spectrum Type                | STANDARD |
|                                          | 89284.35                | Temperature (degree C      | 23.000                 |                              |                    |                              |          |
| Sweep Width (Hz) PRM166-frontdiast-F{H}N | MR.esp  OTBS OSEM       |                            | 73.000                 |                              | -114.5298          |                              |          |
|                                          |                         |                            |                        |                              |                    |                              |          |
|                                          |                         |                            |                        |                              |                    |                              |          |
|                                          |                         |                            |                        |                              |                    |                              |          |
|                                          |                         |                            |                        |                              | 1 1 1 1            |                              |          |
|                                          |                         | 1                          | 11 1 11                |                              |                    |                              |          |

-110 -111 -112 Chemical Shift (ppm)

-112

-113

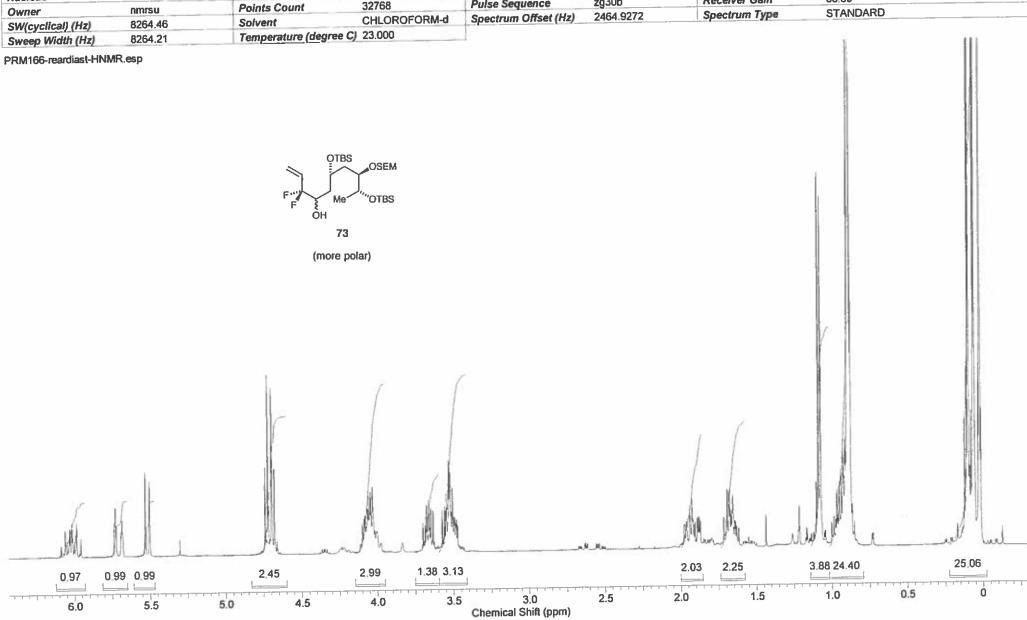
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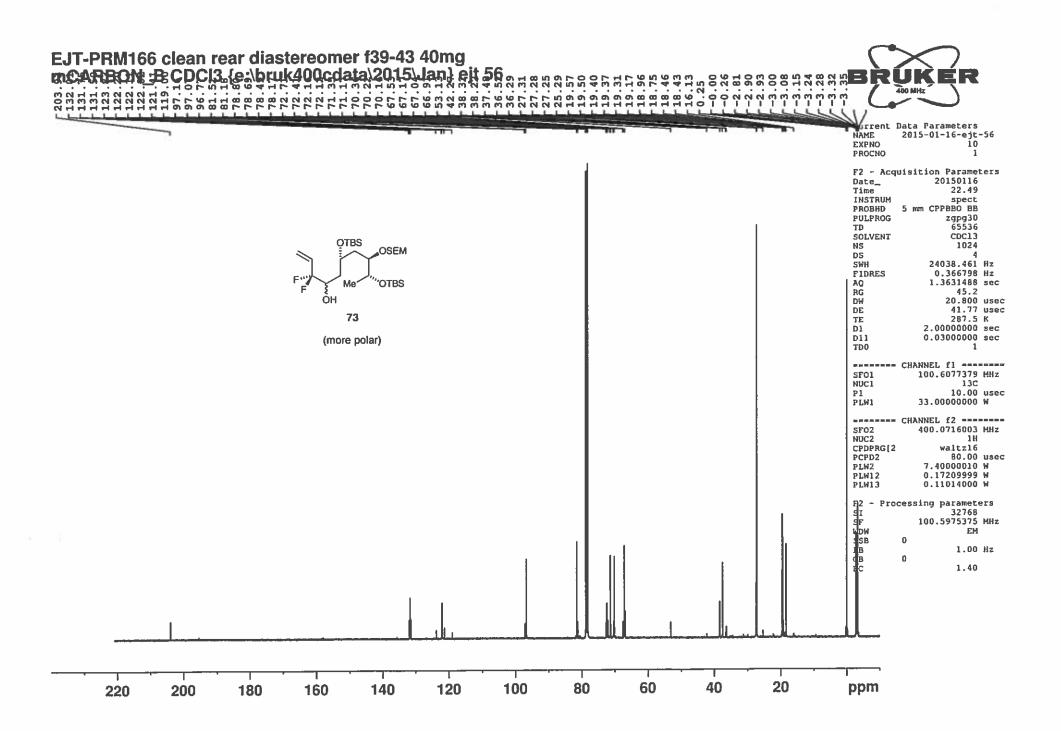
-104 -

-105

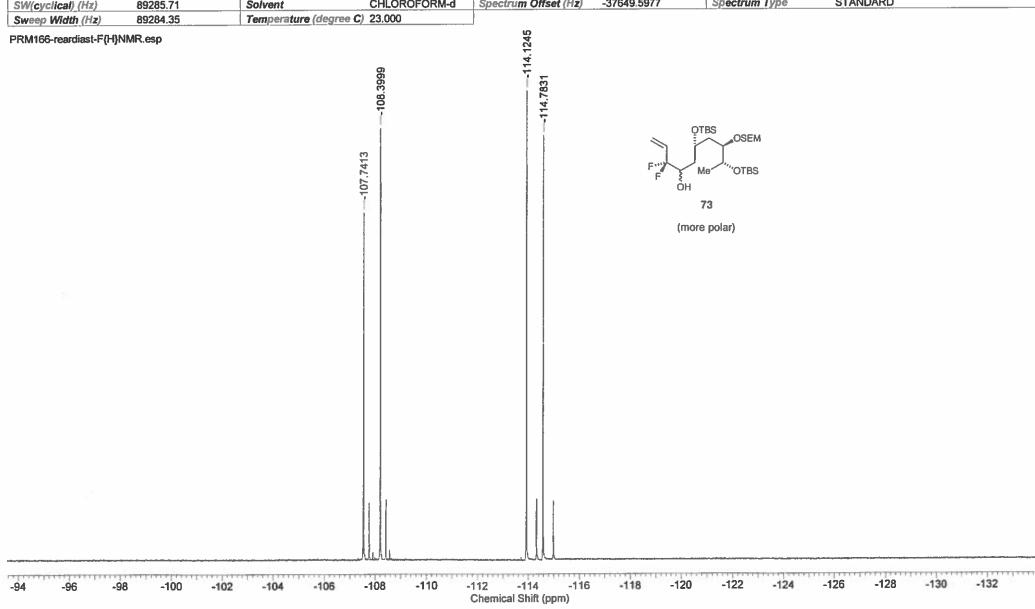
-114 -115 -116 -117 -118 -119 -120 -121 -122

|                        | I his report was c   | reated by ACD/Milli  | (11000301700              |                              |                        | 1 -3 04               |          |
|------------------------|----------------------|----------------------|---------------------------|------------------------------|------------------------|-----------------------|----------|
| Acquisition Time (sec) | 3.9649               | Comment              | EJT-PRM166 f39-43         | 40mg mPROTON CDCI3 (         | e:\bruk400adata\2015\0 | an) ejt 34            |          |
|                        |                      |                      |                           | Date Stamp                   | 16 Jan 2015 11:35:28   |                       |          |
| Date                   | 16 Jan 2015 11:35:28 |                      | J. 400 - John St. Control |                              | 14\10\fid              | Frequency (MHz)       | 400.13   |
| File Name              |                      |                      |                           | ata\ejt\nmr\2015-01-16-ejt-3 | AV400                  | Original Points Count | 32768    |
| Nucleus                | 1H                   | Number of Transients | 16                        | Origin                       |                        |                       | 80.60    |
|                        | mm2011               | Points Count         | 32768                     | Pulse Sequence               | zg30b                  | Receiver Gain         |          |
| Owner                  | nmrsu                |                      | CHLOROFORM-d              | Spectrum Offset (Hz)         | 2464.9272              | Spectrum Type         | STANDARD |
| SW(cyclical) (Hz)      | 8264.46              | Solvent              |                           | Openium email                |                        |                       |          |
|                        |                      |                      | 1 72 000                  |                              |                        |                       |          |

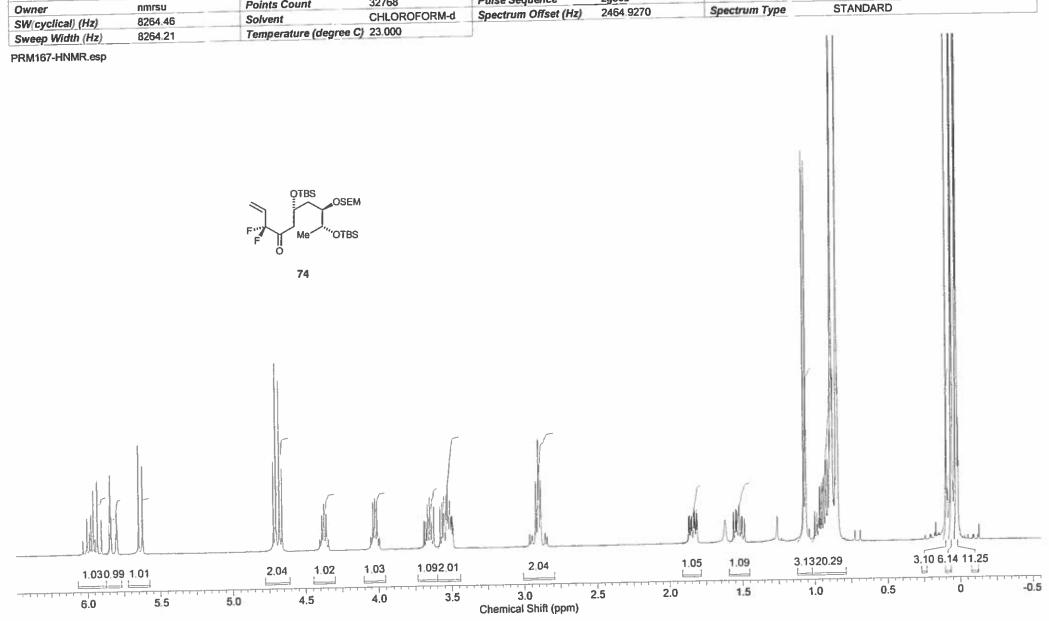


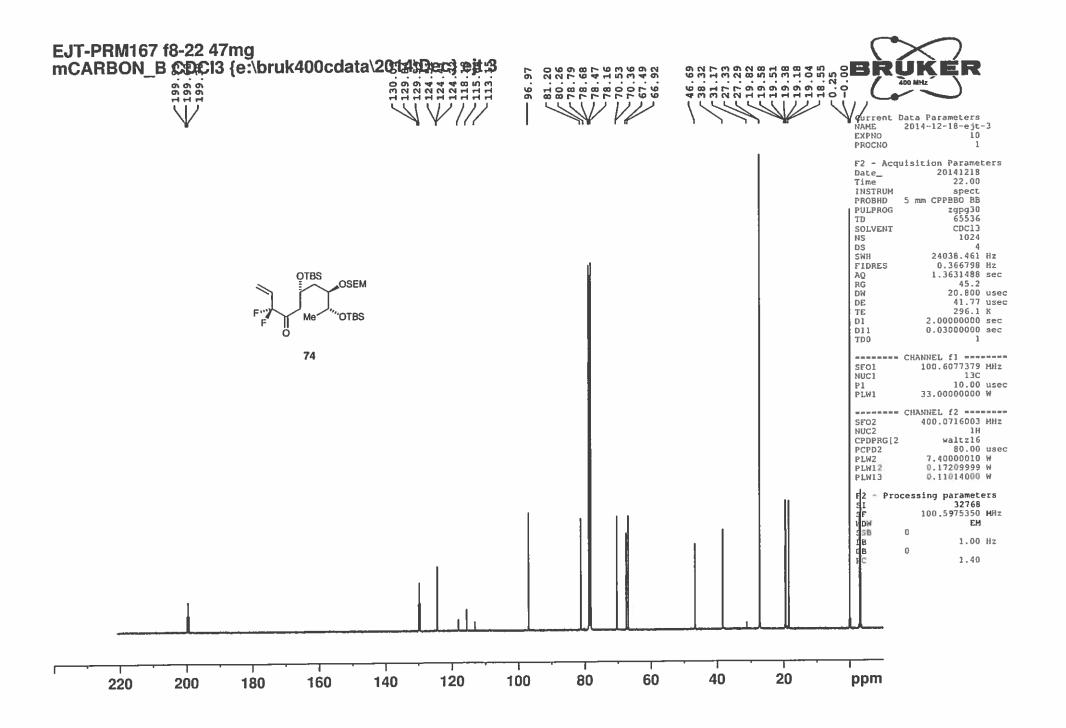


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|------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------|------------------------|-----------------------------|----------------------|-----------------------|----------|--|--|--|--|--|
| Acquisition Time (sec) | 0.7340                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Comment EJT-PRM166 (39-43 40mg mF19CPD CDCl3 (e:\bruk400adata\2015\Jan) ejt 34 |                        |                             |                      |                       |          |  |  |  |  |  |
| Date                   | 16 Jan 2015 11:39:44                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                |                        | Date Stamp                  | 16 Jan 2015 11:39:44 |                       |          |  |  |  |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vo                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | ol5\vol3\users\snmrdata\bru                                                    | ık400adata\2015\Jan\da | ta\ejt\nmr\2015-01-16-ejt-3 | 34\12\fid            | Frequency (MHz)       | 376.50   |  |  |  |  |  |
| Nucleus                | 19F                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Number of Transients                                                           | 16                     | Origin                      | AV400                | Original Points Count | 65536    |  |  |  |  |  |
| Owner                  | nmrsu                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Points Count                                                                   | 65536                  | Pulse Sequence              | zgig                 | Receiver Gain         | 322.00   |  |  |  |  |  |
| SW(cyclical) (Hz)      | 89285.71                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | Solvent                                                                        | CHLOROFORM-d           | Spectrum Offset (Hz)        | -37649.5977          | Spectrum Type         | STANDARD |  |  |  |  |  |
| Owner Madela (Ma)      | 00204.25                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | Tomporatura (doggo C                                                           | 22,000                 |                             |                      |                       |          |  |  |  |  |  |

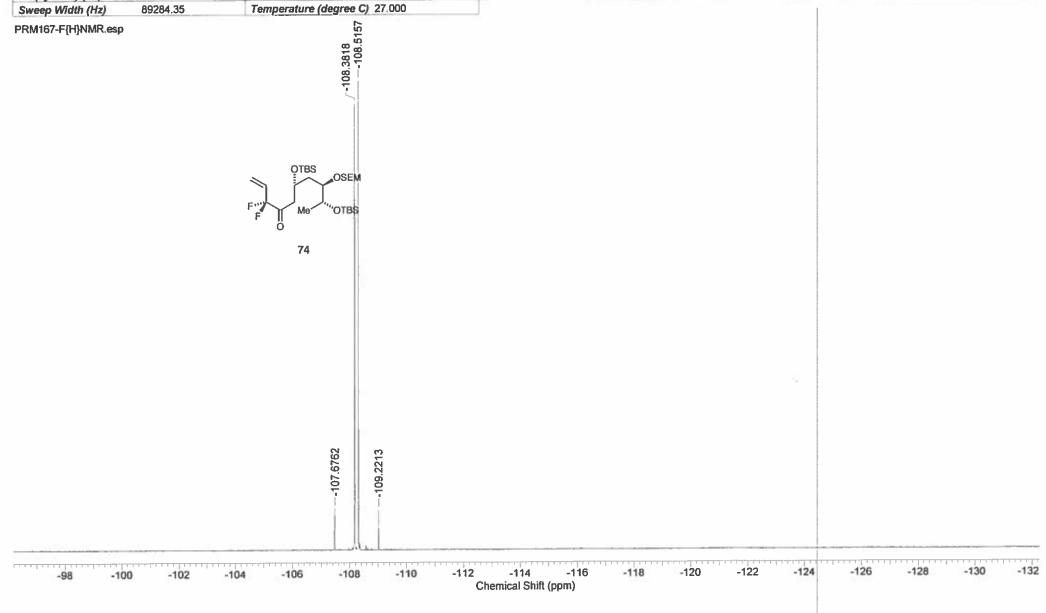


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM167 f8-22 47mg mPROTON CDCl3 (e:\bruk400adata\2014\Dec) ejt 59 Acquisition Time (sec) 3,9649 Comment 18 Dec 2014 14:13:20 Date Stamp 18 Dec 2014 14:13:20 400.13 Date \\ss7a.ds.man.ac.uk\\vol5\\vol3\\users\\snmrdata\\bruk400adata\\2014\\Dec\\data\\ejt\\nmr\\2014-12-18-ejt-59\\10\\fid Frequency (MHz) 32768 File Name Original Points Count AV400 Origin Number of Transients 16 1H 90.50 Nucleus Receiver Gain zg30b Pulse Sequence 32768 **Points Count** nmrsu STANDARD Owner Spectrum Offset (Hz) Spectrum Type 2464.9270 CHLOROFORM-d Solvent 8264.46 SW(cyclical) (Hz) Temperature (degree C) 23.000 8264.21 Sweep Width (Hz)

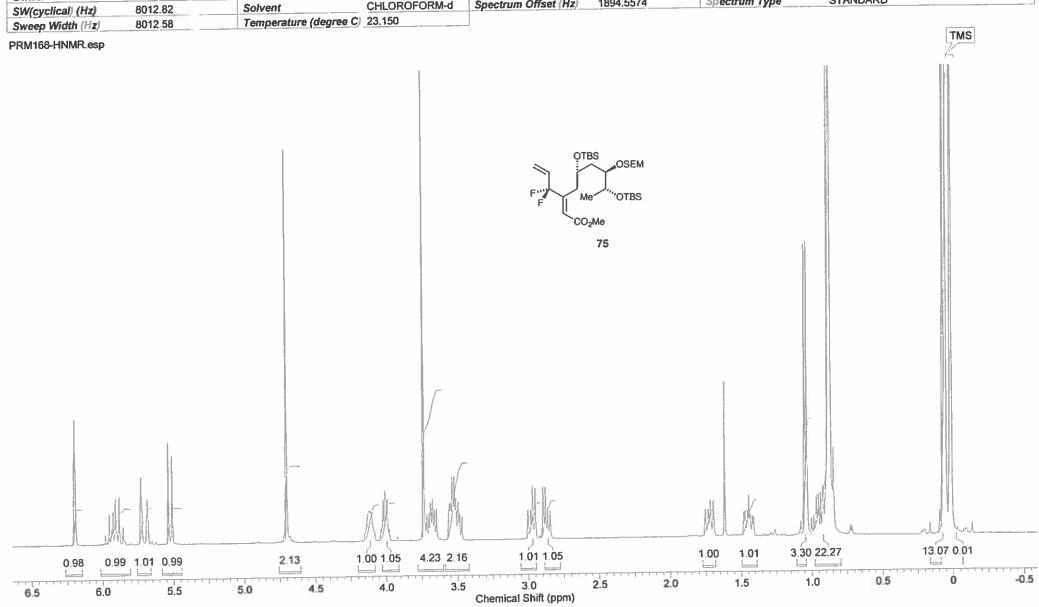


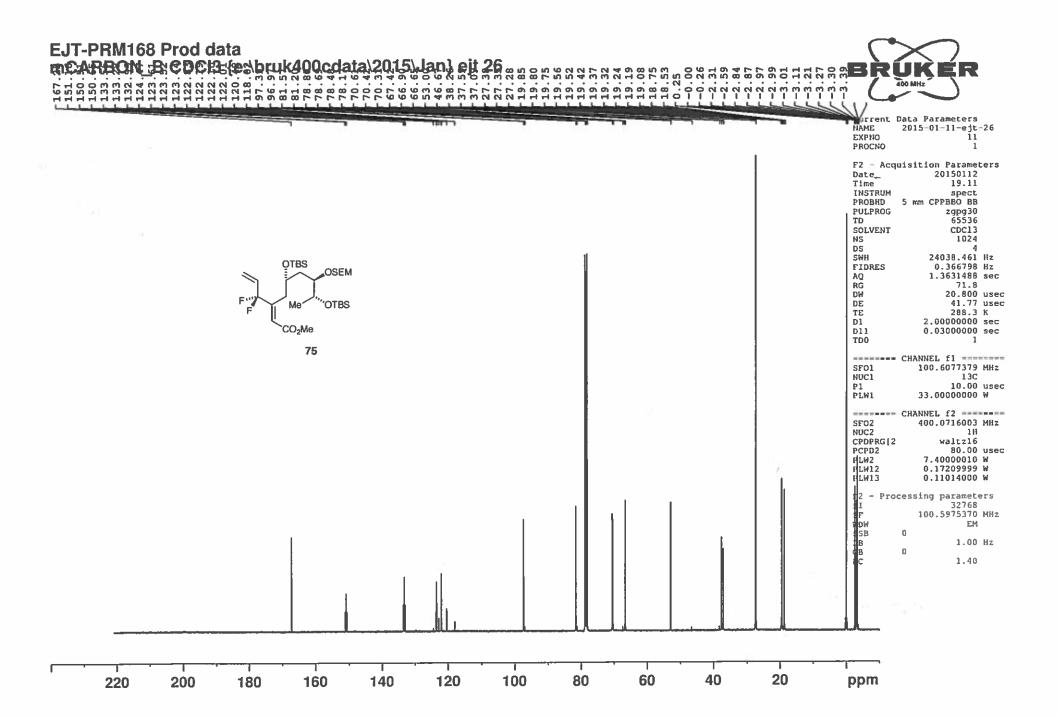


| ec 2014 14:17:36    | - ///                     |                                   | Date Stamp                                 | 40 D 0044 4447-00                                                |                                                                             |                                                                                                                                                       |
|---------------------|---------------------------|-----------------------------------|--------------------------------------------|------------------------------------------------------------------|-----------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
|                     |                           |                                   | Date Stamp                                 | 18 Dec 2014 14:17:36                                             |                                                                             |                                                                                                                                                       |
| a.ds.man.ac.uk\vol! | 5\vol3\users\snmrdata\bru | k400adata\2014\Dec\da             | ata\ejt\nmr\2014-12-18-ejt-5               | i9\12\fid                                                        | Frequency (MHz)                                                             | 376.50                                                                                                                                                |
|                     | Number of Transients      | 16                                | Origin                                     | AV400                                                            | Original Points Count                                                       | 65536                                                                                                                                                 |
| su                  | Points Count              | 65536                             | Pulse Sequence                             | zgig                                                             | Receiver Gain                                                               | 2050.00                                                                                                                                               |
| 35.71               | Solvent                   | CHLOROFORM-d                      | Spectrum Offset (Hz)                       | -37649.5977                                                      | Spectrum Type                                                               | STANDARD                                                                                                                                              |
| su                  |                           | Number of Transients Points Count | Number of Transients 16 Points Count 65536 | Number of Transients 16 Origin Points Count 65536 Pulse Sequence | Number of Transients 16 Origin AV400 Points Count 65536 Pulse Sequence zgig | Number of Transients     16     Origin     AV400     Original Points Count       Points Count     65536     Pulse Sequence     zgig     Receiver Gain |

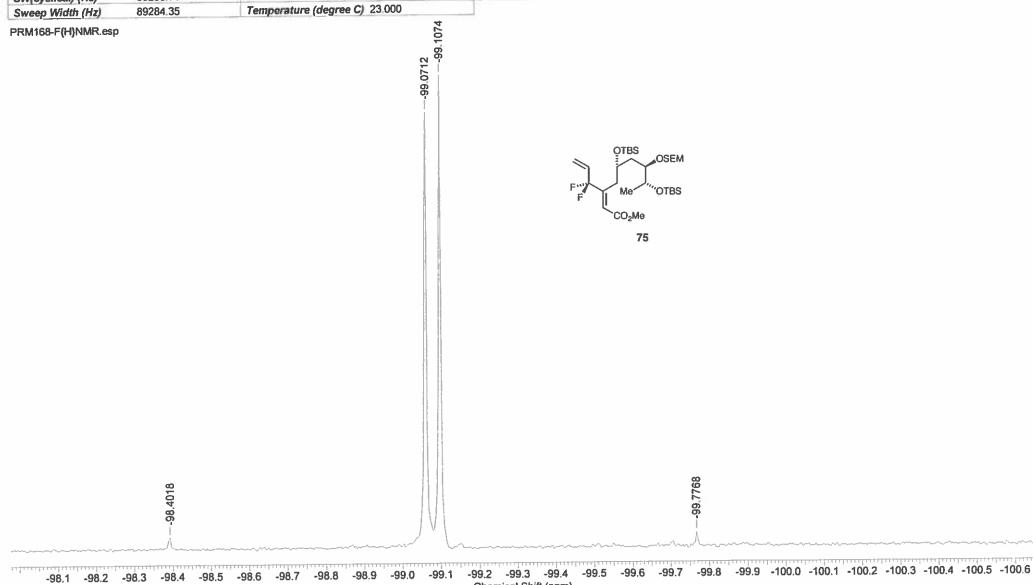


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|------------------------|----------------------|-----------------------------|------------------------|-----------------------------|-------------------------|-----------------------|----------|
| Acquisition Time (sec) |                      | Comment                     | EJT-PRM168 f7-9 38     | mg mPROTON_A CDCl3          | {e:\bruk400cdata\2015\J | an) ejt 10            |          |
|                        | 07 Jan 2015 16:34:08 |                             |                        | Date Stamp                  | 07 Jan 2015 16:34:08    |                       |          |
| Date                   | 07 Jan 2015 10.34.00 | ol5\vol3\users\snmrdata\bru | L400cdata\2015\ lan\d: | ata\eit\nmr\2015-01-07-eit- | -10\10\fid              | Frequency (MHz)       | 400.07   |
| File Name              |                      |                             |                        | Origin                      | spect                   | Original Points Count | 32768    |
| Nucleus                | 1H                   | Number of Transients        |                        |                             |                         | Receiver Gain         | 64.00    |
| Owner                  | nmrsu                | Points Count                | 32768                  | Puise Sequence              | zg <b>30</b>            |                       |          |
| SW(cyclical) (Hz)      | 8012.82              | Solvent                     | CHLOROFORM-d           | Spectrum Offset (Hz)        | 1894.5574               | Spectrum Type         | STANDARD |
| Sween Width (Hz)       | 8012.58              | Temperature (degree C)      | 23.150                 |                             |                         |                       |          |



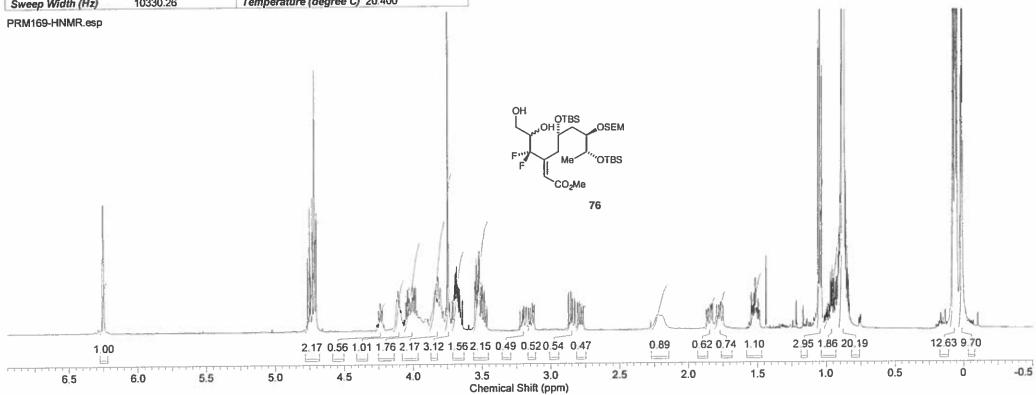


|                        |                      |                      |                        |                              |                         | The state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the s |          |
|------------------------|----------------------|----------------------|------------------------|------------------------------|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|
| Acquisition Time (sec) | 0.7340               | Comment              | EJT-PRM189 f17-33      | 124mg mF19CPD CDCl3 {        | e:\bruk400adata\2015\Ja | in) ejt 29                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |          |
| Date                   | 10 Jan 2015 15:32:16 |                      |                        | Date Stamp                   | 10 Jan 2015 15:32:16    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |          |
|                        |                      |                      | ik400adata\2015\Jan\da | ata\ejt\nmr\2015-01-10-ejt-2 | 9\12\fid                | Frequency (MHz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 376.50   |
|                        |                      |                      |                        | Origin                       | AV400                   | Original Points Count                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 65536    |
| Nucleus                | 19F                  | Number of Transients |                        |                              |                         | Receiver Gain                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 287.00   |
| Owner                  | nmrsu                | Points Count         | 65536                  | Pulse Sequence               | zgig                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | STANDARD |
| SW(cyclical) (Hz)      | 89285.71             | Solvent              | CHLOROFORM-d           | Spectrum Offset (Hz)         | -37649,5977             | Spectrum Type                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | STANDARD |
| 011 07 011 011 111     |                      |                      |                        |                              |                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |          |



Chemical Shift (ppm)

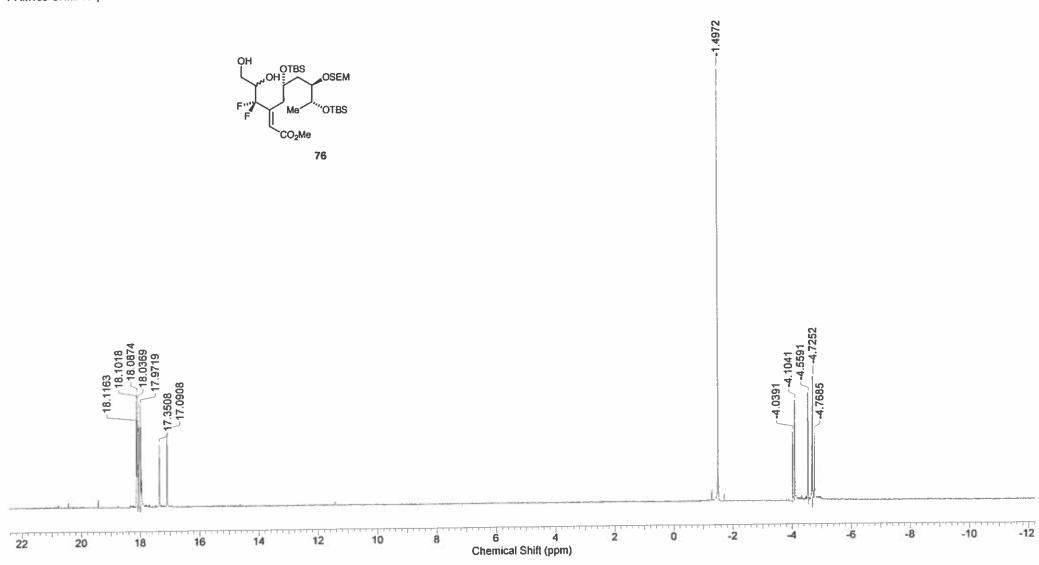
| Acquisition Time (sec) | 3,1719               | Comment               | EJT-PRM169 f28-36     | 44mg mPROTON CDCI3            | {E:\bruk500adata\2015\J | an) <u>e</u> it 10    |          |
|------------------------|----------------------|-----------------------|-----------------------|-------------------------------|-------------------------|-----------------------|----------|
| Date                   | 12 Jan 2015 13:05:04 |                       |                       | Date Stamp                    | 12 Jan 2015 13:05:04    |                       |          |
| File Name              |                      |                       | uk500adata\2015\Jan\d | lata\ejt\nmr\2015-01-12-ejt-1 | 10\20\fid               | Frequency (MHz)       | 500.13   |
| Nucleus                |                      |                       |                       | Origin                        | spect                   | Original Points Count | 32768    |
|                        | nmrsu                | Points Count          | 32768                 | Pulse Sequence                | zg30                    | Receiver Gain         | 50.80    |
| Owner CM/ovelines (NZ) | 10330.58             | Solvent               | CHLOROFORM-d          | Spectrum Offset (Hz)          | 3081,5532               | Spectrum Type         | STANDARD |
| SW(cyclical) (Hz)      | 10330.30             | Temperature (degree C |                       | 1                             |                         |                       |          |



| No. | (ppm)     | Value      | Absolute Value | Non-Negative Value | No. | (ppm)     | Value      | Absolute Value | Non-Negative Value |
|-----|-----------|------------|----------------|--------------------|-----|-----------|------------|----------------|--------------------|
| 1   |           | 9.70469666 | 1.55986125e+10 | 9.70469666         | 12  | 1107 3.16 | 0.51732343 | 8.31507520e+8  | 0.51732343         |
| 2   | 0363 0.10 |            | 2.03028726e+10 | 12.63145828        | 13  | 1687 3.23 | 0.49489146 | 7.95451968e+8  | 0.49489146         |
| 3   | 3486 0.90 |            | 3.24516250e+10 | 20.18981934        | 14  | 4552 3.56 | 2.15453339 | 3.46303770e+9  | 2.15453339         |
| 4   | 9102 1.01 |            | 2.98496614e+9  | 1.85710049         | 15  | 5323 3.71 | 1.56468415 | 2.51495782e+9  | 1.56468415         |
| 5   | 0235 1.06 |            | 4.74843597e+9  | 2.95424557         | 16  | 7205 3.76 | 3.11513853 | 5.00704358e+9  | 3.11513853         |
| 6   | 4679 1.57 | 1.09587038 | 1.76142106e+9  | 1.09587038         | 17  | 7679 3.88 | 2.17377329 | 3.49396250e+9  | 2.17377329         |
| 7   | 101-11-1  | D.74124676 | 1.19142528e+9  | 0.74124676         | 18  | 9501 4.06 | 1.75517964 | 2.82114611e+9  | 1.75517964         |
| В   | 3096 1.88 |            | 1.00238470e+9  | 0.62363493         | 19  | 0657 4.14 | 1.01384950 | 1.62958682e+9  | 1.01384950         |
| 9   |           | 0.89462709 | 1.43795750e+9  | 0.89462709         | 20  | 1993 4.28 | 0.56165135 | 9.02756928e+8  | 0.56165135         |
| 10  |           | 0.47494268 | 7.63387776e+8  | 0.47494268         | 21  | 5814 4.78 | 2.17071009 | 3.48903910e+9  | 2.17071009         |
| 11  |           | 0.53880036 | 8 66027904e+8  | 0.53880036         | 22  | 2189 6.27 | 1.00053573 | 1.60818714e+9  | 1.00053573         |

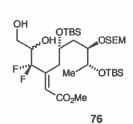
|                        | mo report mae or       | 1                          |                          | 4 0445 050 CADDON          | CDCI2 (E-thout-600) | edata\2015\ lan\ etaff 10 |          |
|------------------------|------------------------|----------------------------|--------------------------|----------------------------|---------------------|---------------------------|----------|
| Acquisition Time (sec) | 1.1010                 | Comment                    | EJT-PRM 169 128-36 4     | 14mg 0115 062 mCARBO       | CDCI3 (E.WIGKSOO)   | cdata\2015\Jan) staff 10  |          |
| Date                   | 14 Jan 2015 02:48:32   | Date Stamp                 | 14 Jan 2015 02:48:32     |                            |                     | 1                         | 405.77   |
| File Name              | Nes7a de man ac uk\vol | 5\vol3\users\snmrdata\bruk | :500cdata\2015\Jan\data\ | staff\nmr\2015-01-13-staff | -10\11\fid          | Frequency (MHz)           | 125.77   |
|                        |                        | Number of Transients       | 5000                     | Origin                     | spect               | Original Points Count     | 32768    |
| Nucleus                | 13C                    |                            |                          | Pulse Sequence             | zgpg30              | Receiver Gain             | 184.40   |
| Owner                  | nmrsu                  | Points Count               | 32768                    |                            |                     | - 1                       | STANDARD |
| SW(cyclical) (Hz)      | 29761.90               | Solvent                    | CHLOROFORM-d             | Spectrum Offset (Hz)       | 12571.4053          | Spectrum Type             | STANDARD |
| Sweep Width (Hz)       | 29761.00               | Temperature (degree C      | 24.997                   |                            |                     |                           |          |

PRM169-CNMR.esp

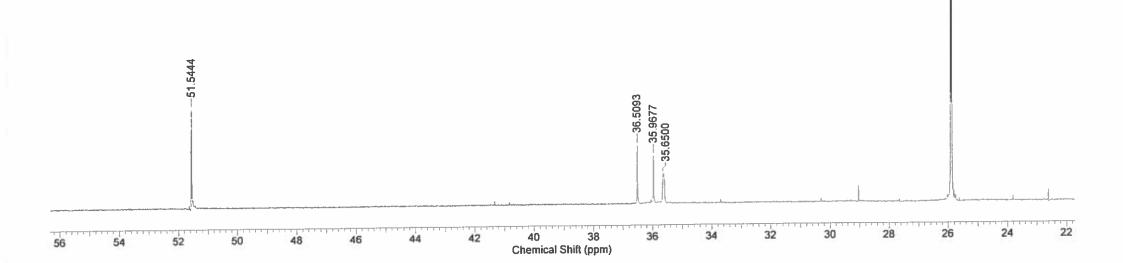


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|------------------------|------------------------|----------------------------|-------------------------|----------------------------|-----------------------|-------------------------|----------|
| Acquisition Time (sec) | 1.1010                 | Comment                    | EJT-PRM 169 f28-36 4    | 4mg 0115 062 mCARBON       | I CDCI3 (E:\bruk500cd | lata\2015\Jan) staff 10 |          |
| Date                   | 14 Jan 2015 02:48:32   | Date Stamp                 | 14 Jan 2015 02:48:32    |                            |                       |                         |          |
| File Name              | Nes7a de man ac uk\vol | 5\vol3\users\snmrdata\bruk | 500cdata\2015\Jan\data\ | staff\nmr\2015-01-13-staff | -10\11\fid            | Frequency (MHz)         | 125.77   |
| 7 (74                  | 13C                    | Number of Transients       | 5000                    | Origin                     | spect                 | Original Points Count   | 32768    |
| Nucleus                |                        | Points Count               | 32768                   | Pulse Sequence             | zgpg30                | Receiver Gain           | 184.40   |
| Owner                  | nmrsu                  |                            | CHLOROFORM-d            | Spectrum Offset (Hz)       | 12571.4053            | Spectrum Type           | STANDARD |
| SW(cyclical) (Hz)      | 29761.90               | Solvent                    |                         | Specaani Onset (112)       | 12011.1000            | 7,                      |          |
| Sweep Width (Hz)       | 29761.00               | Temperature (degree C)     | 24.997                  | J                          |                       |                         |          |

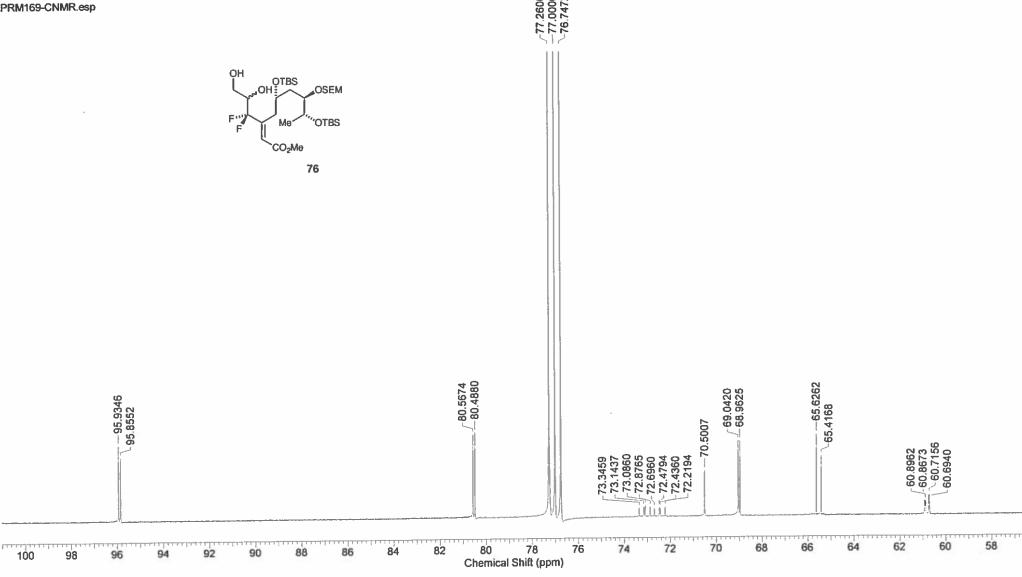




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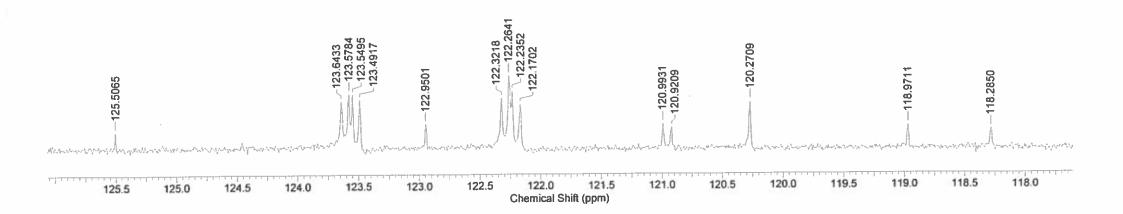


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM 169 f28-36 44mg 0115 062 mCARBON CDCl3 (E:\bruk500cdata\2015\Jan) staff 10 Comment Acquisition Time (sec) 1.1010 14 Jan 2015 02:48:32 Date Stamp 14 Jan 2015 02:48:32 Date \\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Jan\data\staff\nmr\2015-01-13-staff-10\11\\fid Frequency (MHz) 125.77 File Name Original Points Count 32768 Origin spect Number of Transients 5000 13C Nucleus zgpg30 Receiver Gain 184.40 **Pulse Sequence** 32768 Points Count Owner nmrsu **STANDARD** Spectrum Offset (Hz) 12571.4053 Spectrum Type CHLOROFORM-d 29761.90 Solvent SW(cyclical) (Hz) Temperature (degree C) 24.997 29761.00 Sweep Width (Hz) PRM169-CNMR.esp OTBS OSEM OTBS



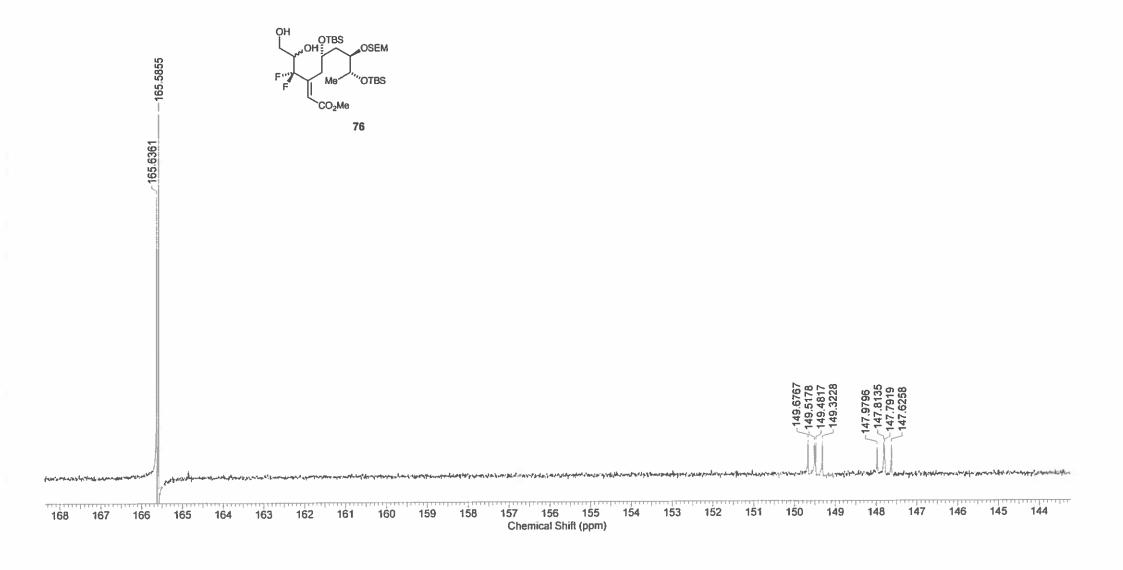
| Acquisition Time (sec) | 1.1010                  | Comment                    | EJT-PRM 169 f28-36 4     | 4mg 0115 062 mCARBON       | I CDC13 {E:\bruk500 | cdata\2015\Jan} staff 10 |          |
|------------------------|-------------------------|----------------------------|--------------------------|----------------------------|---------------------|--------------------------|----------|
| Date                   | 14 Jan 2015 02:48:32    | Date Stamp                 | 14 Jan 2015 02:48:32     |                            |                     | (6.18-81)                |          |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | :500cdata\2015\Jan\data\ | staff\nmr\2015-01-13-staff | -10\11\fid          | Frequency (MHz)          | 125.77   |
| Nucleus                | 13C                     | Number of Transients       | 5000                     | Origin                     | spect               | Original Points Count    | 32768    |
| Owner                  | nmrsu                   | Points Count               | 32768                    | Pulse Sequence             | zgpg30              | Receiver Gain            | 184.40   |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                    | CHLOROFORM-d             | Spectrum Offset (Hz)       | 12571.4053          | Spectrum Type            | STANDARD |
| Sweep Width (Hz)       | 29761.00                | Temperature (degree C      | 24.997                   |                            |                     |                          |          |

PRM169-CNMR.esp

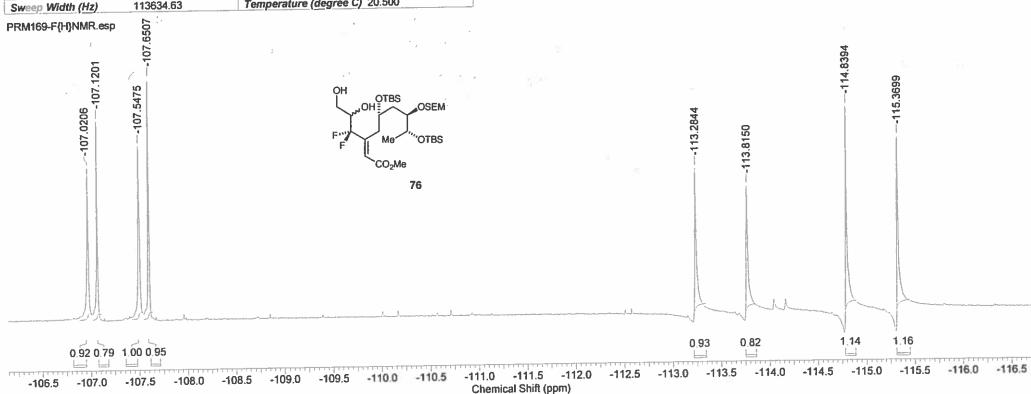


| Acquisition Time (sec) | 1.1010                  | Comment                    | EJT-PRM 169 f28-36 4     | 4mg 0115 062 mCARBON       | I CDCI3 (E:\bruk500 | cdata\2015\Jan} staff 10 |          |
|------------------------|-------------------------|----------------------------|--------------------------|----------------------------|---------------------|--------------------------|----------|
| Date                   | 14 Jan 2015 02:48:32    | Date Stamp                 | 14 Jan 2015 02:48:32     |                            |                     |                          |          |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | :500cdata\2015\Jan\data\ | staff\nmr\2015-01-13-staff | -10\11\fid          | Frequency (MHz)          | 125.77   |
| Nucleus                | 13C                     | Number of Transients       | 5000                     | Origin                     | spect               | Original Points Count    | 32768    |
| Owner                  | nmrsu                   | Points Count               | 32768                    | Pulse Sequence             | zgpg30              | Receiver Gain            | 184.40   |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                    | CHLOROFORM-d             | Spectrum Offset (Hz)       | 12571.4053          | Spectrum Type            | STANDARD |
| Sweep Width (Hz)       | 29761.00                | Temperature (degree C      | 24.997                   |                            |                     |                          |          |

PRM169-CNMR.esp

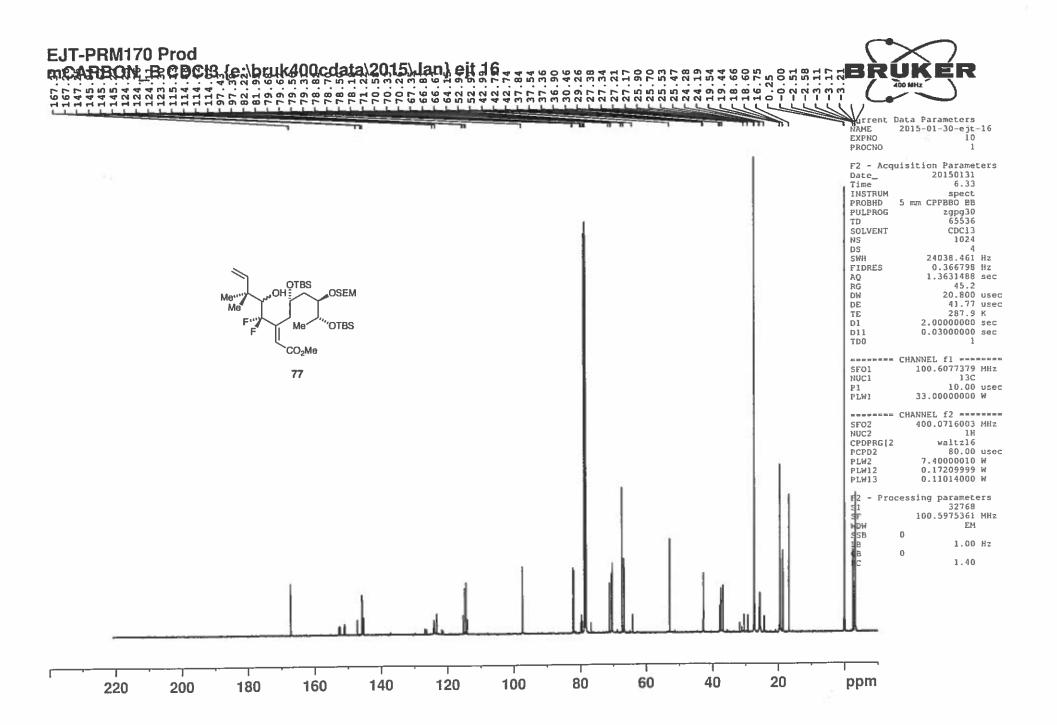


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|                        | 0.5767                 | Comment                     | EJT-PRM169 (28-36 4    | 4mg m19FCPD CDCl3 (E:       | Wruk500adatav2015Wan | ) ejt 10              |          |
| Acquisition Time (sec) | 12 Jan 2015 13:09:20   |                             |                        | Date Stamp                  | 12 Jan 2015 13:09:20 |                       |          |
| - 5010                 | 12 Jan 2015 15.05.20   | x5\vol3\users\snmrdata\brul | 600adata\2015\ lan\dat | a\eit\nmr\2015-01-12-eit-10 | \23\fid              | Frequency (MHz)       | 470.59   |
| File Name              | \\ss7a.ds.man.ac.uk\vc |                             |                        | Origin                      | spect                | Original Points Count | 65536    |
| Nucleus                | 19F                    | Number of Transients        |                        |                             | zgfhiggn             | Receiver Gain         | 575.00   |
| Owner                  | nmrsu                  | Points Count                | 65536                  | Pulse Sequence              |                      | Spectrum Type         | STANDARD |
| SW(cyclical) (Hz)      | 113636.37              | Solvent                     | CHLOROFORM-d           | Spectrum Offset (Hz)        | -47059.0234          | Spectrum Type         | OTATO    |
| Sweep Width (Hz)       |                        | Temperature (degree C)      | 20.500                 | ]                           |                      |                       |          |
| PRM169-F{H}NMR.esp     | 1507                   |                             | ,                      |                             |                      |                       |          |

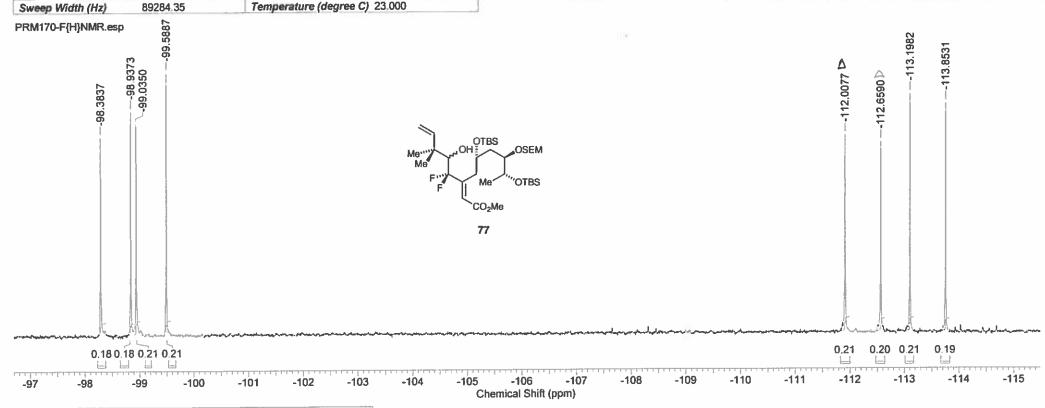


| No. | (ppm)   | Value                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Absolute Value | Non-Negative Value |
|-----|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|--------------------|
| 1   | 4979115 | 1,16230905                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 2.03938675e+9  | 1.16230905         |
| 2   | 9359114 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1.99388979e+9  | 1.13637888         |
| 3   | 9101113 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1.43967245e+9  | 0.82051349         |
| 4   | 3913113 | The second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second secon | 1.62383578e+9  | 0.92547381         |
| 5   | 5915107 | The second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second secon | 1.66191501e+9  | 0.94717634         |
| 6   | 5948107 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1.75054810e+9  | 0.99769104         |
| 7   | 1681107 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1.39409690e+9  | 0.79453856         |
| 8   | D656106 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1.62046221e+9  | 0.92355108         |

|                   | 3.9649     |             | Comment     | t               | EJT-PRM         | /1170 f75-87 | 27mg mPROTON CDC           | 3 (e:\bruk400adat                                 | la\2015\ | Uan) ejt 38                 |                |                 |             |
|-------------------|------------|-------------|-------------|-----------------|-----------------|--------------|----------------------------|---------------------------------------------------|----------|-----------------------------|----------------|-----------------|-------------|
| Date              | 21 Jan 201 | 5 14:06:56  |             | -110            |                 |              | Date Stamp                 | 21 Jan 2015                                       | 14:06:5  |                             |                |                 |             |
|                   |            | an.ac.uk\vo | i5\vol3\use | rs/snmrdata/bru | uk400adata      | \2015\Jan\c  | lata\ejt\nmr\2015-01-21-ej | 1-38\10\fid                                       |          | Frequency (I                | MHz) 40        | 00.13           |             |
| Nucleus           | 1H         |             |             | of Transients   | 16              |              | Origin                     | AV400                                             |          | Original Poir               |                | 2768            |             |
|                   | nmrsu      |             | Points Co   | ount            | 32768           |              | Pulse Sequence             | zg30b                                             |          | Receiver Gai                |                | 01.00           |             |
| SW(cyclical) (Hz) | 8264.46    |             | Solvent     |                 |                 | FORM-d       | Spectrum Offset (Hz)       | 2464.9270                                         |          | Spectrum Ty                 | pe S           | TANDARD         |             |
| Sweep Width (Hz)  | 8264.21    |             | Temperat    | ture (degree C  | 23.000          |              |                            |                                                   |          |                             |                |                 |             |
| RM170-HNMR.esp    |            |             |             |                 |                 |              | Me"" OH E Me               | OSEM<br>'''OTBS                                   |          |                             |                |                 |             |
|                   |            |             |             |                 |                 |              | CO₂Me                      |                                                   |          |                             | 1              |                 |             |
|                   |            |             |             |                 |                 |              | 77                         |                                                   |          |                             |                |                 |             |
|                   |            |             |             |                 |                 |              | 0.51 0.54 0.980.99         |                                                   | ^~~~     | 1.29 1.31 E                 |                |                 | 20.70       |
| 1.00 1.00         |            | 2.02        | 1.98        | 0.54            | 1 2 1 1 7 7 1 4 | 89 2.73      |                            | <del>, , , , , , , , , , , , , , , , , , , </del> | <u> </u> | 7-1 - 1 - 7 - 1 - 7 - 1 - 1 | 3.06 3.2120.68 | 2 1 1 1 1 1 1 1 | <del></del> |
|                   | 5.5        | 5.0         |             | 4.5             | 4.0             | 3.5          | 3.0                        | 2.5                                               | 2.0      | 1.5                         | 1.0            | 0.5             | 0           |



| Acquisition Time (sec) | 0.7340                | Comment                     | EJT-PRM170 f75-87    | 27mg mF19CPD CDCl3 (e        | e:\bruk400adata\2015\Jar | ı) ejt 38             |          |
|------------------------|-----------------------|-----------------------------|----------------------|------------------------------|--------------------------|-----------------------|----------|
| Date                   | 21 Jan 2015 14:11:12  |                             |                      | Date Stamp                   | 21 Jan 2015 14:11:12     |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bru | k400adata\2015\Jan\d | ata\ejt\nmr\2015-01-21-ejt-3 | 38\12\fid                | Frequency (MHz)       | 376.50   |
| Nucleus                | 19F                   | Number of Transients        |                      | Origin                       | AV400                    | Original Points Count | 65536    |
| Owner                  | nmrsu                 | Points Count                | 65536                | Pulse Sequence               | zgig                     | Receiver Gain         | 406.00   |
| SW(cyclical) (Hz)      | 89285.71              | Solvent                     | CHLOROFORM-d         | Spectrum Offset (Hz)         | -37649.5977              | Spectrum Type         | STANDARD |
| 0 145-44- (14-1        | 00384.35              | Tomporatura (dograda C      | 1 22 000             |                              |                          |                       |          |

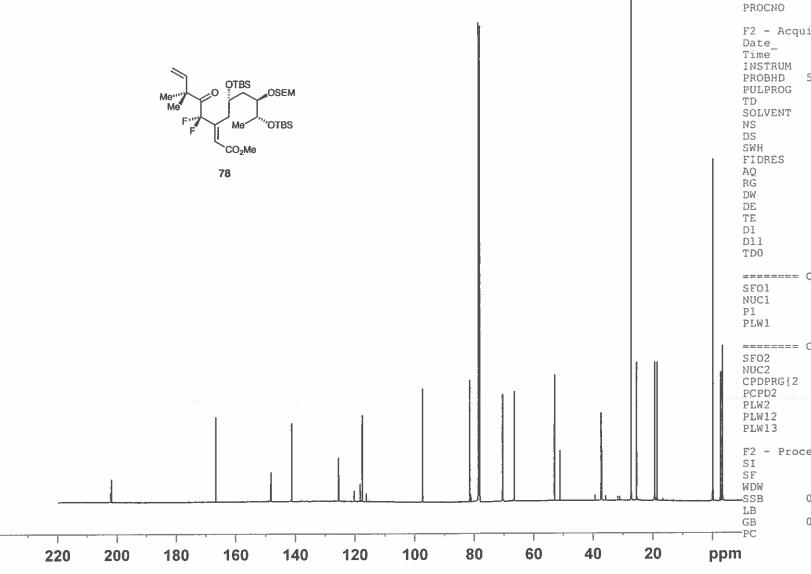


| No. | (ppm)    | Value      | Absolute Value | Non-Negative Value |
|-----|----------|------------|----------------|--------------------|
| 1   | 9327113  | 0.18757442 | 3.96218432e+8  | 0.18757442         |
| 2   | 2709113  | 0.20678121 | 4.36789440e+8  | 0.20678121         |
| 3   | 7358112  | 0.19675171 | 4.15603872e+8  | 0.19675171         |
| 4   | 0951111  | 0.21439180 | 4.52865504e+8  | 0.21439180         |
| 5   | 571799.5 | 0.21261145 | 4.49104832e+8  | 0.21261145         |
| 6   | 108598.9 | 0.20801891 | 4.39403872e+8  | 0.20801891         |
| 7   | 995898.8 | 0.18103851 | 3.82412448e+8  | 0.18103851         |
| 8   | 478398.3 | 0.17934489 | 3.78834976e+8  | 0.17934489         |

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM171 f3-9 50mg mPROTON\_A CDCl3 (e:\bruk400cdata\2015\Feb) ejt 6 Acquisition Time (sec) 4.0894 Comment 04 Feb 2015 16:06:24 Date Stamp 04 Feb 2015 16:06:24 Date \\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Feb\data\eji\nmr\2015-02-04-ejt-6\10\fid Frequency (MHz) 400.07 File Name Original Points Count 32768 Origin spect Number of Transients 4 1H Nucleus zg30 Receiver Gain 32.00 Pulse Sequence **Points Count** 32768 nmrsu Owner Spectrum Type STANDARD Spectrum Offset (Hz) 1894.0684 CHLOROFORM-d SW(cyclical) (Hz) 8012.82 Solvent Temperature (degree C) 14.793 8012.58 Sweep Width (Hz) PRM171-HNMR.esp **OTBS** OSEM OTBS 78 23.23 7.74 3.78 22.47 1,96 2.12 2.14 4.33 2.23 2.13 0.99 1.00 3.0 2.5 1.5 0.5 Ó -0.5 2.0 1.0 3.5 4.5 4.0 6.5 6.0 5.5 5.0 Chemical Shift (ppm)

0215-106 Mears P. EJT-PRM 171 f3-9

50 mg
mCARBON CDCl3 (E:\bruk500cdata\2015\Feb) staff=22





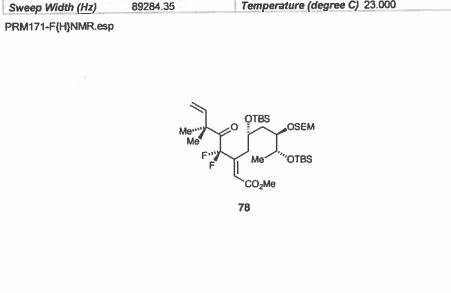
| Current I<br>NAME<br>EXPNO<br>PROCNO                                                     |          |        |        |        |          |                  |                      |                                            |                                             | st                                                                                                                                     |                       | ff-22                                       |
|------------------------------------------------------------------------------------------|----------|--------|--------|--------|----------|------------------|----------------------|--------------------------------------------|---------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|-----------------------|---------------------------------------------|
| F2 - Acquenter Time INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG DW DE TE D1 | 5 m      | um     | 2      | 2      | 2<br>90. | 0<br>P<br>7      | 1<br>Bz<br>640<br>11 | 5 SB G G C C C C C C C C C C C C C C C C C | 02<br>0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 | 20<br>30<br>30<br>30<br>30<br>30<br>30<br>40<br>30<br>40<br>30<br>30<br>30<br>30<br>30<br>30<br>30<br>30<br>30<br>30<br>30<br>30<br>30 | 54 tB0638441840220    | Hz<br>Hz<br>sec<br>usec<br>usec<br>K<br>sec |
| D11<br>TD0<br>======<br>SFO1<br>NUC1<br>P1<br>PLW1                                       | CHA      | 1<br>1 | N<br>2 | E<br>5 | L        | 7                | f<br>8               | 1 5.                                       | 4 5                                         | 50<br>L3                                                                                                                               | 1<br>4<br>C           | MHz<br>usec                                 |
| SFO2<br>NUC2<br>CPDPRG{2<br>PCPD2<br>PLW2<br>PLW12<br>PLW13                              | CHF      | 5      | 60     | 0      | 02       | 1<br>w<br>0<br>8 | 9:<br>a<br>0:<br>6:  | 2 i                                        | 0 (<br>t :<br>0 (<br>2 (                    | 00<br>1<br>21                                                                                                                          | 8<br>H<br>6<br>0<br>1 | MHz                                         |
| F2 - Proc<br>SI<br>SF<br>WDW<br>-SSB<br>LB                                               | ess<br>0 |        |        | _      |          | -                |                      | 3:                                         | 21<br>69                                    | 76<br>93<br>E                                                                                                                          | 8<br>4<br>M           | ers<br>MHz<br>Hz                            |
| <br>GB<br>-PC                                                                            | 0        |        |        |        |          |                  |                      |                                            |                                             | . 4                                                                                                                                    |                       | - 4 400                                     |

|                        | Timo topott mee -    |                       |                       |                             |                         |                       |          |
|------------------------|----------------------|-----------------------|-----------------------|-----------------------------|-------------------------|-----------------------|----------|
| Acquisition Time (sec) | 0.7340               | Comment               | EJT-PRM171 f4-18 5    | 7mg mF19CPD CDCl3 (e:       | \bruk400adata\2015\Feb) | ejt 55                |          |
| Date                   | 02 Feb 2015 12:45:52 |                       |                       | Date Stamp                  | 02 Feb 2015 12:45:52    |                       |          |
| File Name              |                      |                       | uk400adata\2015\Feb\d | ata\ejt\nmr\2015-02-02-ejt- | 55\13\fid               | Frequency (MHz)       | 376.50   |
| Nucleus                | 19F                  | Number of Transients  |                       | Origin                      | AV400                   | Original Points Count | 65536    |
| Owner                  | nmrsu                | Points Count          | 65536                 | Pulse Sequence              | zgig                    | Receiver Gain         | 203.00   |
| SW(cyclical) (Hz)      | 89285.71             | Solvent               | CHLOROFORM-d          | Spectrum Offset (Hz)        | -37649.5977             | Spectrum Type         | STANDARD |
| SVI(Cychical) (112)    | 00200.71             | Townsenture (deares C | 23.000                | 1                           | 10 - 20 - 1             |                       |          |

-100.1423

-100

-99



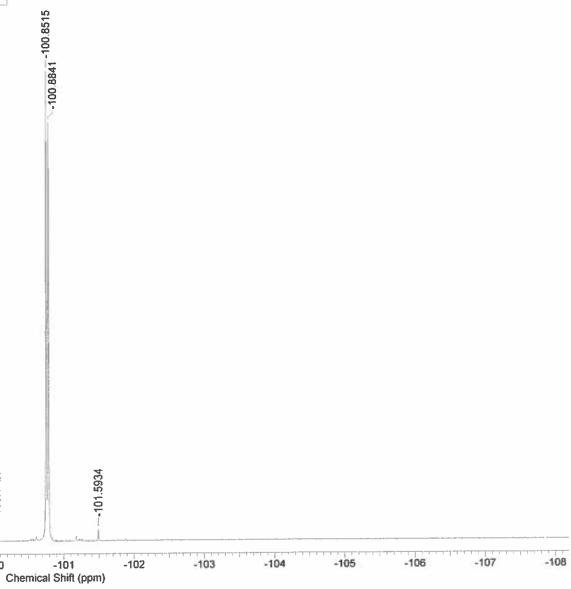
-95

-94

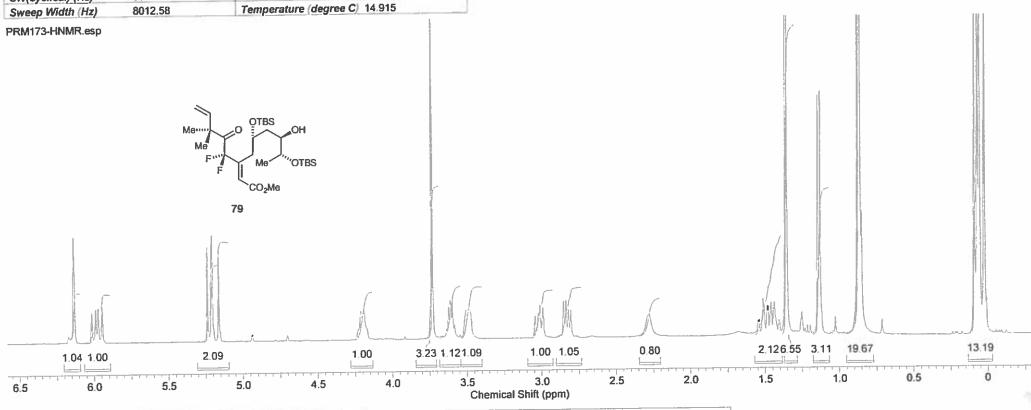
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-97

-98

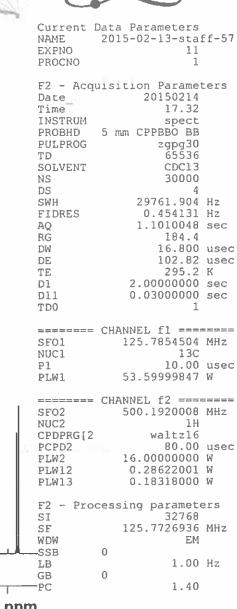


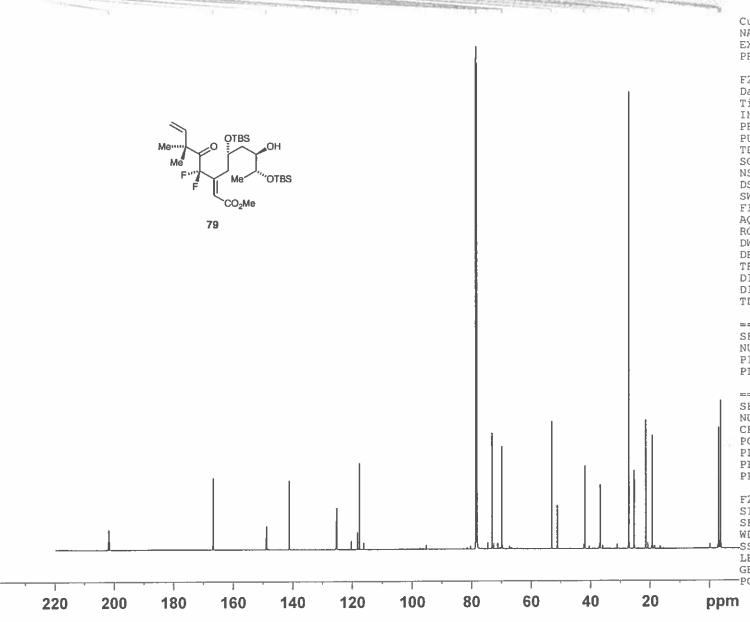
|                        | I III O I OPOIL II MO 4 |                          |                      |                               |                        |                       |          |
|------------------------|-------------------------|--------------------------|----------------------|-------------------------------|------------------------|-----------------------|----------|
| Acquisition Time (sec) | 4.0894                  | Comment                  | EJT-PRM173 f6-22 2   | 9mg mPROTON_A CDCI3           | {e:\bruk400cdata\2015\ | Feb) ejt 14           | 110      |
|                        | 12 Feb 2015 16:00:00    |                          |                      | Date Stamp                    | 12 Feb 2015 16:00:00   |                       |          |
| Date                   | 12 Feb 2013 10.00.00    | alet alette omredetetber | k400cdata\2015\Eeb\d | lata\ejt\nmr\2015-02-12-ejt-1 | 14\10\fid              | Frequency (MHz)       | 400.07   |
| File Name              |                         |                          |                      |                               | spect                  | Original Points Count | 32768    |
| Nucleus                | 1H                      | Number of Transients     |                      | Origin                        |                        |                       | 32.00    |
| Owner                  | nmrsu                   | Points Count             | 32768                | Pulse Sequence                | zg30                   | Receiver Gain         |          |
| SW(cyclical) (Hz)      | 8012.82                 | Solvent                  | CHLOROFORM-d         | Spectrum Offset (Hz)          | 1893.8241              | Spectrum Type         | STANDARD |
| SVV(Cychody (Vic)      | 0010.50                 | Tammamatura (dagrag C    | 14 015               |                               |                        |                       |          |



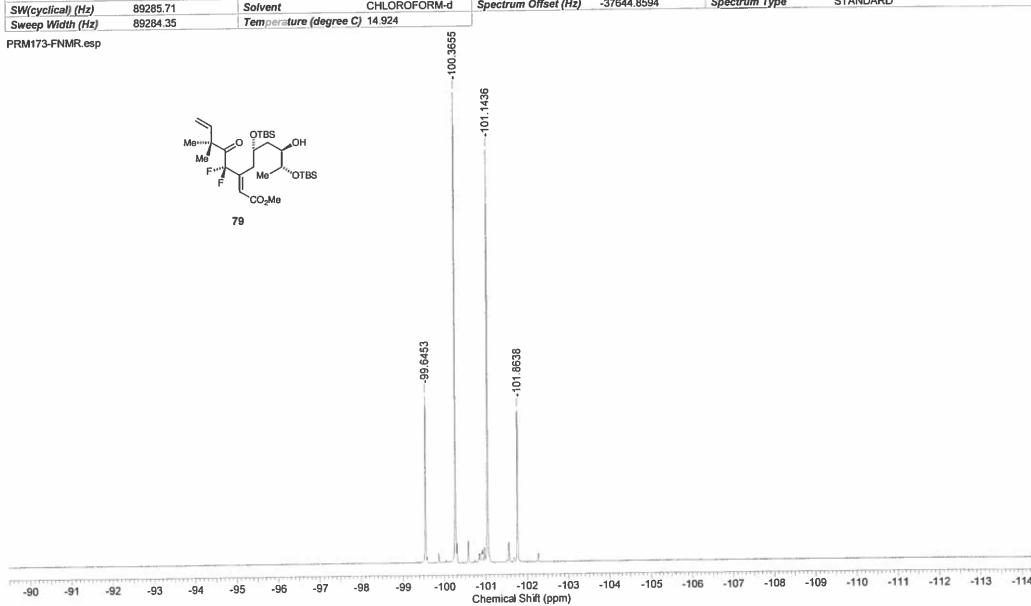
| NI- | (ppm)     | Value      | Absolute Value | Non-Negative Value | No. | (ppm)         | Value      | Absolute Value                          | Non-Negative Value |
|-----|-----------|------------|----------------|--------------------|-----|---------------|------------|-----------------------------------------|--------------------|
| No. | 0300 0.13 |            | 2.20347003e+10 | 13.19273376        | 9   | 4009 3.54     | 1.08516133 | 1.81245261e+9                           | 1.08516133         |
| 1   | 1         |            | 3.28596849e+10 | 19.67392731        |     |               | 1.11831653 | 1.86782886e+9                           | 1,11831653         |
| 2   | 7731 0.95 |            | 5.19691622e+9  | 3.11152554         |     |               | 3.23063946 | 5.39586202e+9                           | 3.23063946         |
| 3   | 0681 1.17 |            | 1.09395466e+10 | 6.54978418         | 12  |               | 0.99953032 | 1.66943040e+9                           | 0.99953032         |
| 4   | 2976 1.38 |            | 3.54885965e+9  | 2.12479234         | 13  |               | 2.08711100 | 3,48592358e+9                           | 2.08711100         |
| _   | 3850 1.57 | A          |                | 0.80205345         | 14  |               | 0.99999589 | 1.67020800e+9                           | 0.9999589          |
| 6   | -         | 0.80205345 | 1.74787955e+9  | 1.04649985         |     |               | 1.03641319 | 1.73103270e+9                           | 1.03641319         |
| 7   |           | 1.04649985 | 111 11 41      | 0.99720508         | 13  | 93-73 ,, 0.20 | 1.00041010 | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |                    |
| - 8 | 3256 3.09 | 0.99720508 | 1.66554675e+9  | 0.99720000         |     |               |            |                                         |                    |



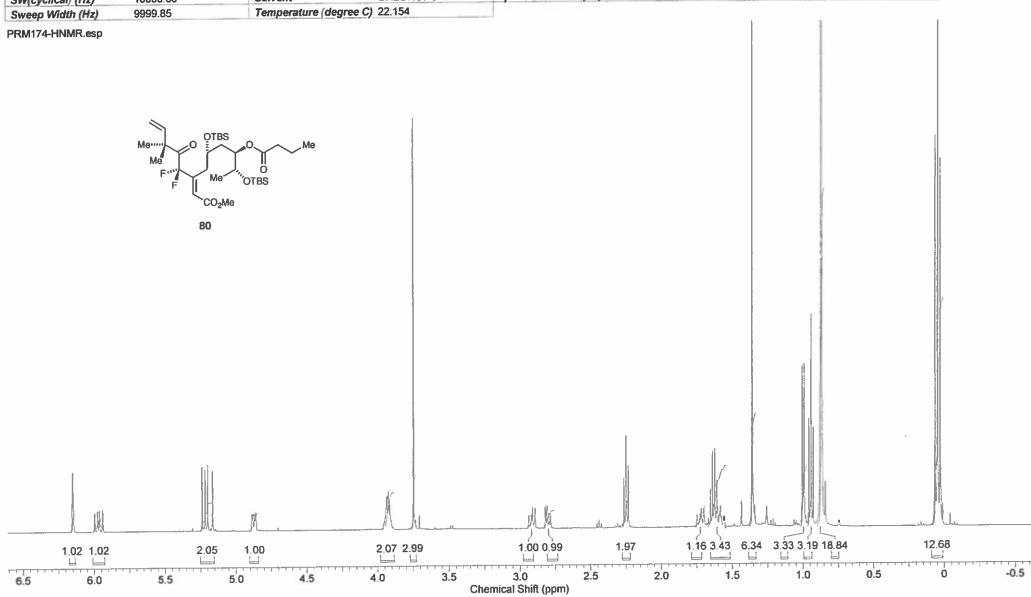




|                        | Tito toport mas -    |                      |                        |                              |                          | PARTICIA DA AMERICA   |          |
|------------------------|----------------------|----------------------|------------------------|------------------------------|--------------------------|-----------------------|----------|
| Acquisition Time (sec) | 0.7340               | Comment              | EJT-PRM173 f6-22 2     | 9mg mF19_cryo_zgbs CD0       | CI3 (e:\bruk400cdata\201 | by-eb) ejt 14         |          |
|                        | 12 Feb 2015 16:02:08 |                      |                        | Date Stamp                   | 12 Feb 2015 16:02:08     |                       |          |
| Date                   | 12 Feb 2015 10.02.00 | 453 - 153            | 1.400adata\2015\Eah\d: | ata\ejt\nmr\2015-02-12-ejt-1 | 4\11\fid                 | Frequency (MHz)       | 376.44   |
| File Name              |                      |                      |                        |                              |                          | Original Points Count | 65536    |
| Nucleus                | 19F                  | Number of Transients | 16                     | Origin                       | spect                    |                       |          |
| Owner                  | nmrsu                | Points Count         | 65536                  | Pulse Sequence               | zgbs                     | Receiver Gain         | 7,12     |
|                        |                      | Solvent              | CHLOROFORM-d           | Spectrum Offset (Hz)         | -37644.8594              | Spectrum Type         | STANDARD |
| SW(cyclical) (Hz)      | 89285.71             | Solvent              |                        |                              |                          |                       |          |



| Acquisition Time (sec) | 3.2768                                  | Comment                     | 0215 121 Mears P EJT     | -PRM174 F5-15 26 mg in C    | DCI3 mPROTON CDO | Cl3 (E:\bruk500cdata\2015\Feb) | staff 39 |
|------------------------|-----------------------------------------|-----------------------------|--------------------------|-----------------------------|------------------|--------------------------------|----------|
| Date                   | 24 Feb 2015 02:14:24                    | Date Stamp                  | 24 Feb 2015 02:14:24     |                             |                  |                                |          |
| File Name              | \\ss7a ds.man.ac.uk\vol                 | 5\vol3\users\snmrdata\bruk5 | 500cdata\2015\Feb\data\s | taff\nmr\2015-02-23-staff-3 | 9\10\PDATA\1\1r  | Frequency (MHz)                | 500.19   |
| Nucleus                | 1H                                      | Number of Transients        |                          | Origin                      | spect            | Original Points Count          | 32768    |
| Owner                  | nmrsu                                   | Points Count                | 65536                    | Pulse Sequence              | zg30             | Receiver Gain                  | 30.53    |
| SW(cyclical) (Hz)      | 10000.00                                | Solvent                     | CHLOROFORM-d             | Spectrum Offset (Hz)        | 3081.8008        | Spectrum Type                  | STANDARD |
| Greto Guidan (112)     | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |                             | 00.454                   |                             |                  |                                |          |

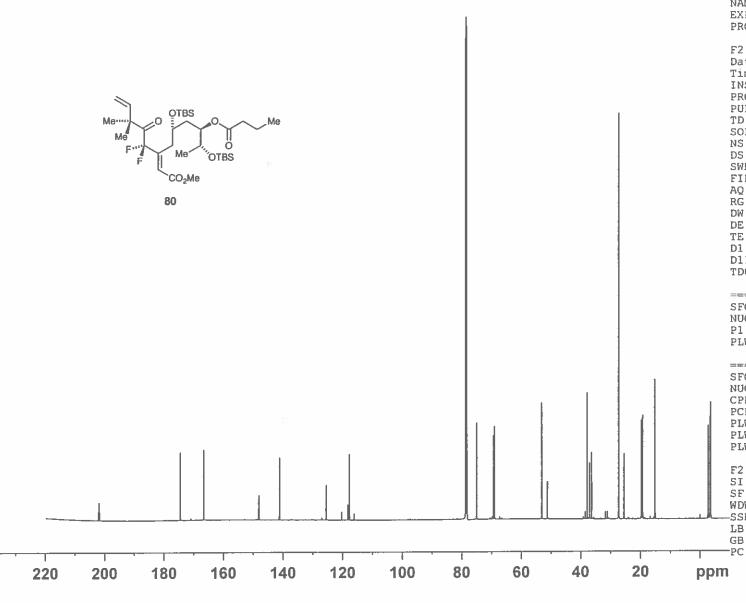


0215 121
Mears P
EJT-PRM174 F5-15
26 mg in CDC13
mCARBON CDC13 {E:\bruk500edata\2015\Feb|\_staff\_39

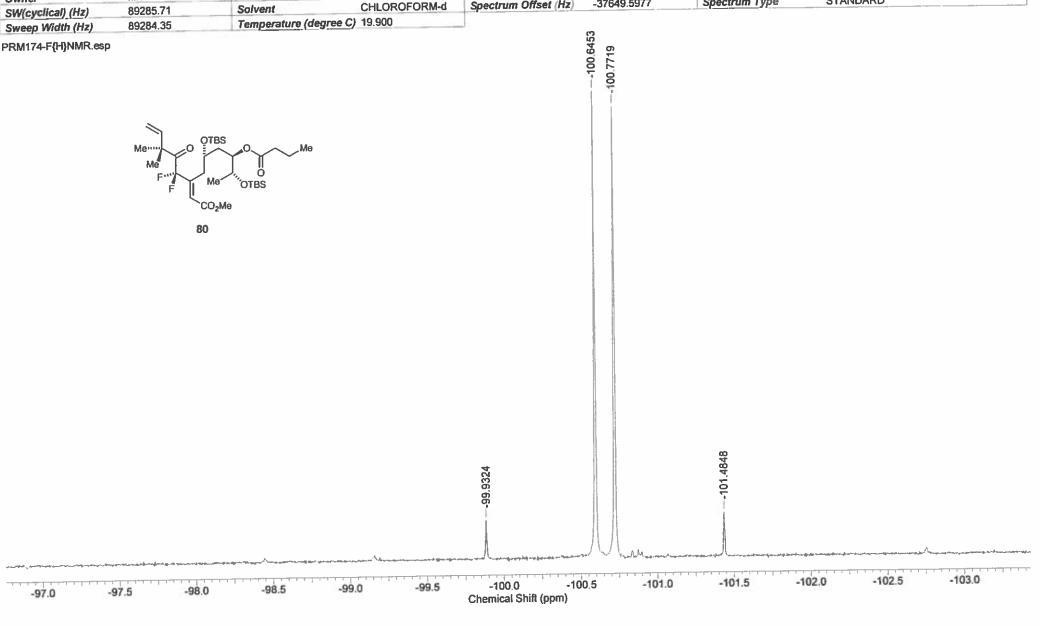
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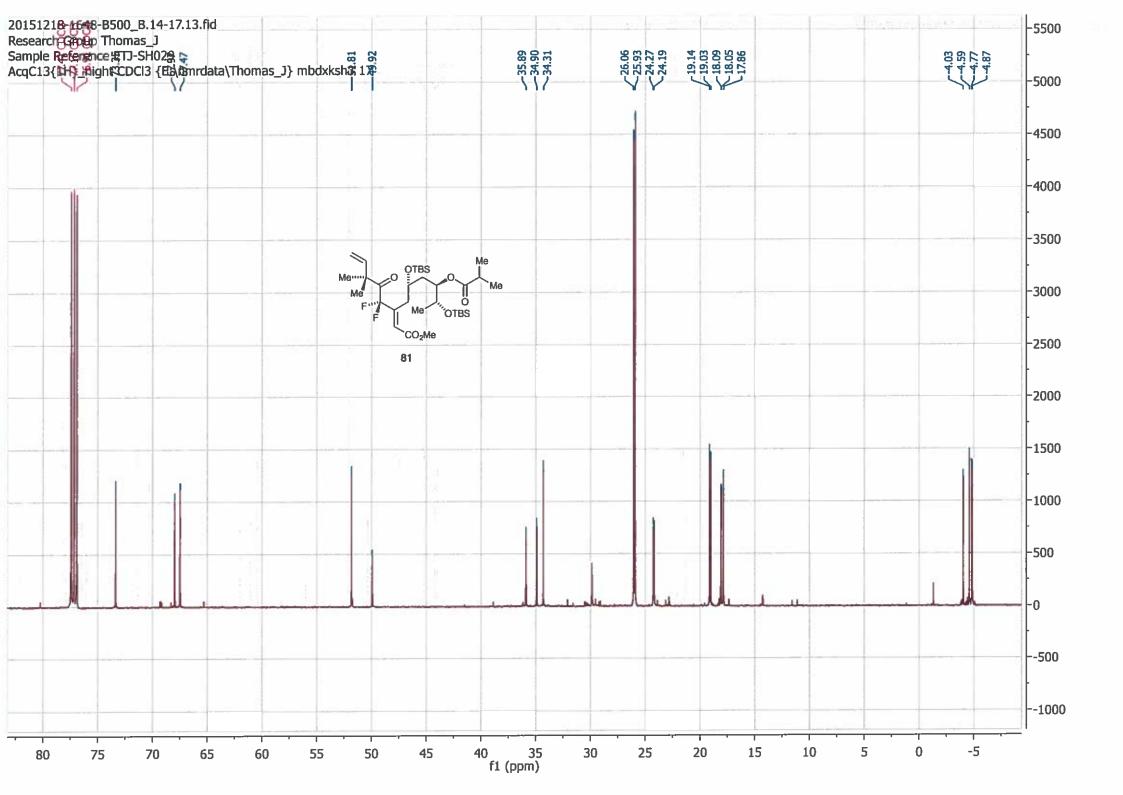


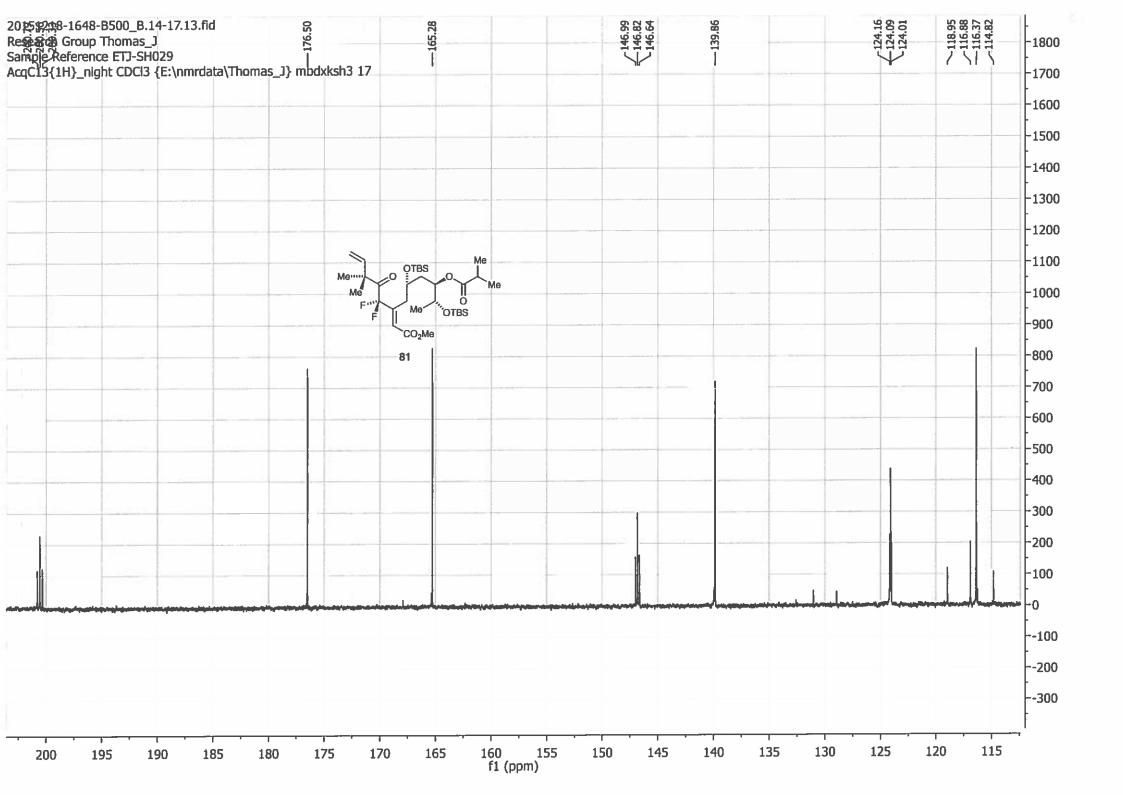
| in . |           |         |         |        |
|------|-----------|---------|---------|--------|
|      | Current 1 | Data Pa | rameter | s      |
|      | NAME      | 2015-0  | 2-23-st | aff-39 |
|      | EXPNO     |         | 1       | 1      |
|      | PROCNO    |         |         | 1      |
|      | 11100110  |         |         | •      |
|      | F2 - Acq  | nisitio | n Param | eters  |
|      | Date      | 1101616 | 2015022 | 04     |
|      | Time      |         | 10.1    |        |
|      | INSTRUM   |         |         |        |
|      |           |         | spec    |        |
|      | PROBHD    | 5 mm C  | PPBBO E |        |
|      | PULPROG   |         | zgpg.   |        |
|      | TD        |         | 6553    |        |
|      | SOLVENT   |         | CDC1    |        |
|      | NS        |         | 922     | 23     |
|      | DS        |         |         | 4      |
|      | SWH       | 2       | 9761.90 | )4 Hz  |
|      | FIDRES    |         | 0.45413 | 31 Hz  |
|      | AO        | 1       | .101004 | 8 sec  |
|      | RG        | _       | 184.    |        |
|      | DW        |         | 16 80   | 0 usec |
|      | DE        |         | 102.8   |        |
|      | TE        |         | 295.    |        |
|      |           | 2       | 0000000 |        |
|      | D1        |         |         |        |
|      | D11       | υ.      | 0300000 |        |
|      | TD0       |         |         | 1      |
|      |           | CUBBINE | T 61    |        |
|      | ======    |         | .785450 |        |
|      | SF01      | 125     |         |        |
|      | NUC1      |         | 13      |        |
|      | P1        |         |         | 0 usec |
|      | PLW1      | 53.     | 5999984 | 17 W   |
|      |           |         |         |        |
|      | ========  | CHANNE  | L f2 == | =====  |
|      | SFO2      | 500     | .192000 |        |
|      | NUC2      |         |         | H      |
| 1    | CPDPRG[2  |         | waltz1  |        |
| 1    | PCPD2     |         |         | 0 usec |
| ıl   | PLW2      | 16.     | 0000000 | 0 W    |
| ļ.   | PLW12     | 0.      | 2862200 | )1 W   |
|      | PLW13     | 0.      | 1831800 | 0 W    |
|      |           |         |         |        |
| ı    | F2 - Proc | cessino | parame  | eters  |
|      | SI        |         | 3276    |        |
| ı    | SF        | 125     | .772693 |        |
| ı    | WDW       |         |         | EM     |
|      | -SSB      | 0       |         | ***    |
|      | LB        | U       | 1.0     | 0 Hz   |
|      |           | 0       | 1.0     | , 0 HZ |
|      | GB<br>-PC | U       | 1.4     | 10     |
|      | FC        |         | 1.4     |        |
| DП   | ı         |         |         |        |
|      | -         |         |         |        |

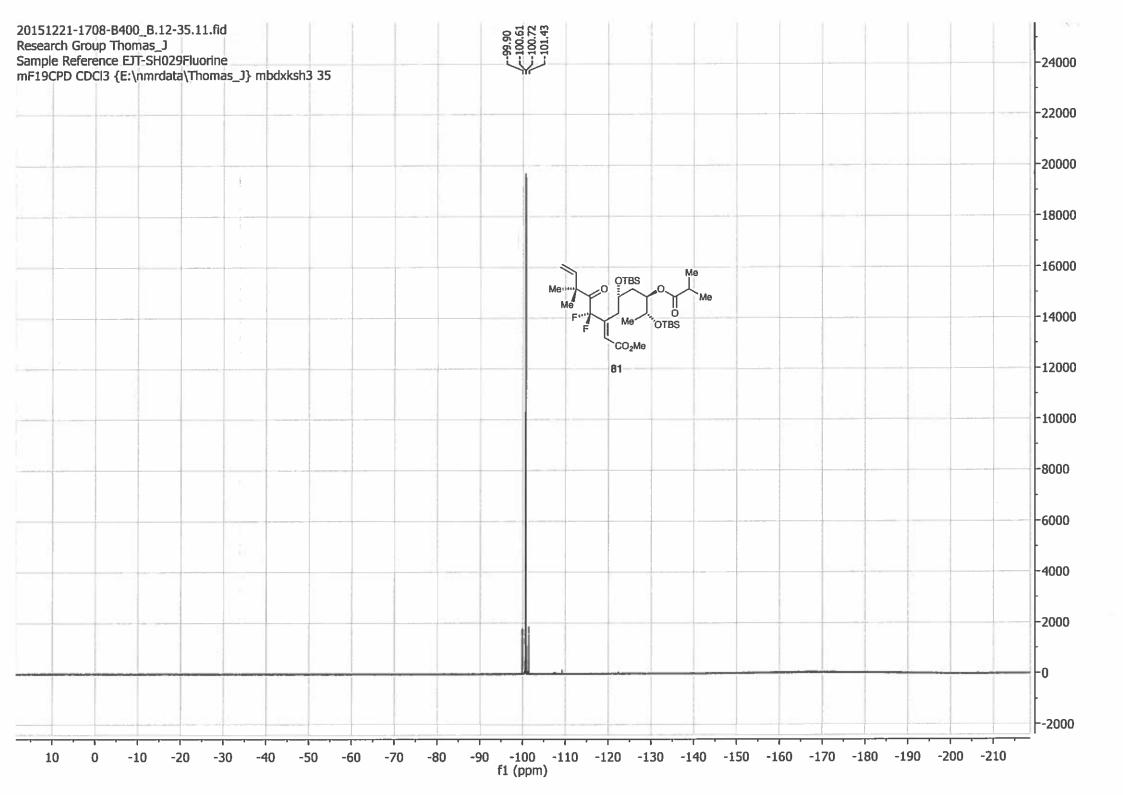


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM174 f5-15 26mg mF19CPD CDCl3 (e:\bruk400adata\2015\Feb) ejt 58 Comment Acquisition Time (sec) 0.7340 23 Feb 2015 15:30:08 Date Stamp 23 Feb 2015 15:30:08 Date Frequency (MHz) \lss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Feb\data\ejt\nmr\2015-02-23-ejt-58\12\fid 376.50 File Name Original Points Count 65536 AV400 Origin Number of Transients 16 19F Nucleus 203.00 Receiver Gain zgig Pulse Sequence 65536 **Points Count** nmrsu Owner **STANDARD** Spectrum Type Spectrum Offset (Hz) -37649.5977 CHLOROFORM-d Solvent 89285.71 SW(cyclical) (Hz) Temperature (degree C) 19.900 Sweep Width (Hz) 89284.35 -100,6453 PRM174-F{H}NMR.esp 100,7719 **OTBS** 

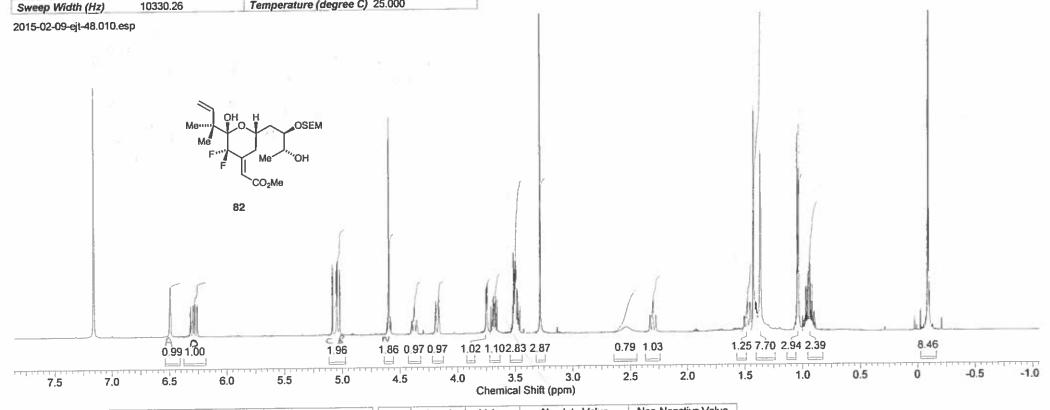








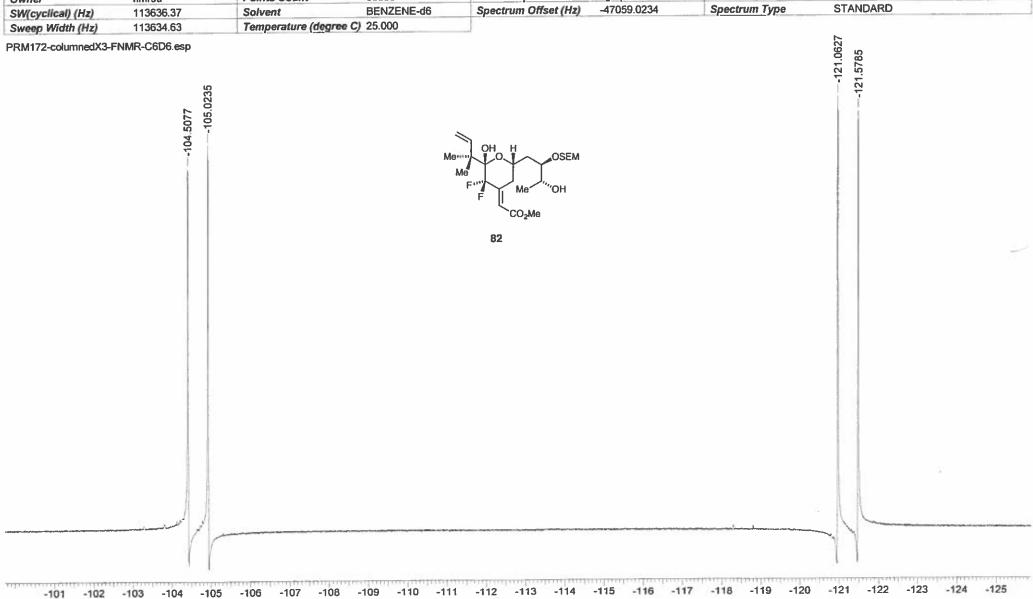
|                        | rino report mae e    | reaced by riverimin          |                    |                                | LOCOC (E-Vb-vd-COO-det    | -12016)Eab) ail 49    |          |
|------------------------|----------------------|------------------------------|--------------------|--------------------------------|---------------------------|-----------------------|----------|
| Acquisition Time (sec) | 3.1719               | Comment                      | EJT-PRM172 bis-    | TBS deprot. 24mg mPROTON       | A CODE (E: April K2009091 | accurated eli 40      |          |
| Date                   | 09 Feb 2015 14:24:00 |                              |                    | Date Stamp                     | 09 Feb 2015 14:24:00      | )                     | 1790     |
| Date                   | No.70 do man no ukhu | JE) w/3) us are/sommata/houl | k500adata\2015\Feb | \data\ejt\nmr\2015-02-09-ejt-4 | 18\10\fid                 | Frequency (MHz)       | 500.13   |
| File Name              |                      |                              |                    |                                |                           | Original Points Count | 32768    |
| Nucleus                | 1H                   | Number of Transients         | 16                 | Origin                         | spect                     |                       | .,       |
| Owner                  | nmrsu                | Points Count                 | 32768              | Pulse Sequence                 | zg30                      | Receiver Gain         | 90.50    |
|                        |                      |                              | BENZENE-d6         | Spectrum Offset (Hz)           | 3093,0591                 | Spectrum Type         | STANDARD |
| SW(cyclical) (Hz)      | 10330.58             | Solvent                      | BEINZEINE-00       | Spectrum Onset [112)           | 0000.0001                 |                       |          |
| O                      | 10330.26             | Temperature (degree C)       | 25 000             |                                |                           |                       |          |



| No.  | (ppm) 1      | Value   | Absolute Value | Non-Negative Value | No. | (ppm)     | Value        | Absolute Value | Non-Negative Value |
|------|--------------|---------|----------------|--------------------|-----|-----------|--------------|----------------|--------------------|
| 110. | 15990.028.4  |         | 2 23010775e+10 | 8.45782185         | 10  | 5335 3.72 | 1.10219407   | 2.90619930e+9  | 1.10219407         |
| 2    | 3718 1,002.3 |         | 6.31391744e+9  | 2.39459229         | 11  | 7208 3.79 | 1.01866615   | 2.68595789e+9  | 1.01866615         |
|      | 0027 1.082.9 |         | 7.76145357e+9  | 2.94357920         | 12  | 1260 4.22 | 0.96806675   | 2.55254042e+9  | 0.96806675         |
|      | 2804 1.447.7 |         | 2.03142328e+10 | 7.70429850         | 13  | 3233 4.42 | 0.97044659   | 2.55881549e+9  | 0.97044659         |
| 4    | 4463 1.521.2 |         | 3.28711808e+9  | 1,24665987         | 14  | 5590 4.63 |              | 4,90485555e+9  | 1.86019683         |
| 5    | 2401 2.361.0 |         | 2.72663706e+9  | 1.03409398         | 15  |           | 1.95728326   | 5.16084736e+9  | 1.95728326         |
| 6    |              |         | 2.07551309e+9  | 0.78715116         | 16  |           | 0.99992341   | 2.63653811e+9  | 0.99992341         |
| 7    | 4444 2.640.7 |         |                | 2.86838222         | 17  | 1099 6.54 |              | 2.62285389e+9  | 0.99473357         |
| 8    | 2388 3.312.8 |         | 7.56317850e+9  | 2.82843184         | ''- | 7000 0.01 | 0,00 11 0001 |                |                    |
| 9    | 4414 3.542.8 | 2843184 | 7.45783962e+9  | 2.02043104         | ]   |           |              |                |                    |

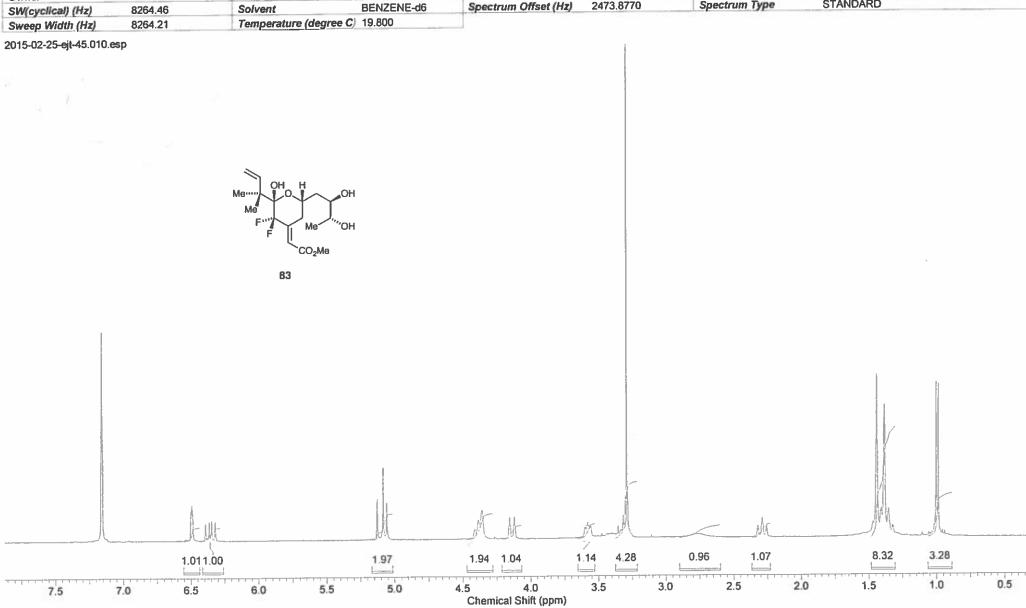
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ P.Mears EJT-PRM172 bis-TBS deprot mCARBON C6D6 (E:\bruk500cdata\2015\Feb) staff 26 Acquisition Time (sec) 1.1010 Comment 10 Feb 2015 01:44:32 10 Feb 2015 01:44:32 Date Stamp Date 125,77 \\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Feb\data\staff\nmr\2015-02-09-staff-26\21\fid Frequency (MHz) File Name Original Points Count 32768 spect Origin Number of Transients 10000 13C Nucleus 184.40 zgpg30 Receiver Gain Pulse Sequence 32768 **Points Count** Owner nmrsu STANDARD Spectrum Offset (Hz) 12661.5830 Spectrum Type BENZENE-d6 Solvent SW(cyclical) (Hz) 29761.90 Temperature (degree C) 22.161 29761.00 Sweep Width (Hz) PRM172-columnedX3-CNMR-C6D6.esp OSEM 82 51,3660 19.6710 85.6390 70,7195 67.0582 98.5076 18.3206 37.6452 67.2820 -113,9976 144.8405 34.2728 46.4554 166,3676 23.6861 99.5692 99.3236 24 16 0 -8 56 48 40 32 72 80 64 88 96 120 112 104 136 128 168 160 152 144 Chemical Shift (ppm)

| Acquisition Time (sec) | 0.5767            | Comment                         | EJT-PRM172 bis-    | TBS deprot. 24mg m19F C6D6      | 6 {E:\bruk500adata\2 | 2015\Feb} ejt 48      |          |
|------------------------|-------------------|---------------------------------|--------------------|---------------------------------|----------------------|-----------------------|----------|
| Date                   | 09 Feb 2015 14:3  | 4:40                            |                    | Date Stamp                      | 09 Feb 2015 14:3     | 4:40                  |          |
|                        | \\ss7a.ds.man.ac. | uk\vol5\vol3\users\snmrdata\bru | k500adata\2015\Fel | o\data\ejt\nmr\2015-02-09-ejt-4 | /8\12\fid            | Frequency (MHz)       | 470.59   |
| Nucleus                | 19F               | Number of Transients            |                    | Origin                          | spect                | Original Points Count | 65536    |
| Owner                  | nmrsu             | Points Count                    | 65536              | Pulse Sequence                  | zgflqn               | Receiver Gain         | 406.00   |
| SW(cyclical) (Hz)      | 113636.37         | Solvent                         | BENZENE-d6         | Spectrum Offset (Hz)            | -47059.0234          | Spectrum Type         | STANDARD |
| Sween Width (Ha)       | 11363/63          | Temperature (degree C           | 25 000             |                                 |                      |                       |          |

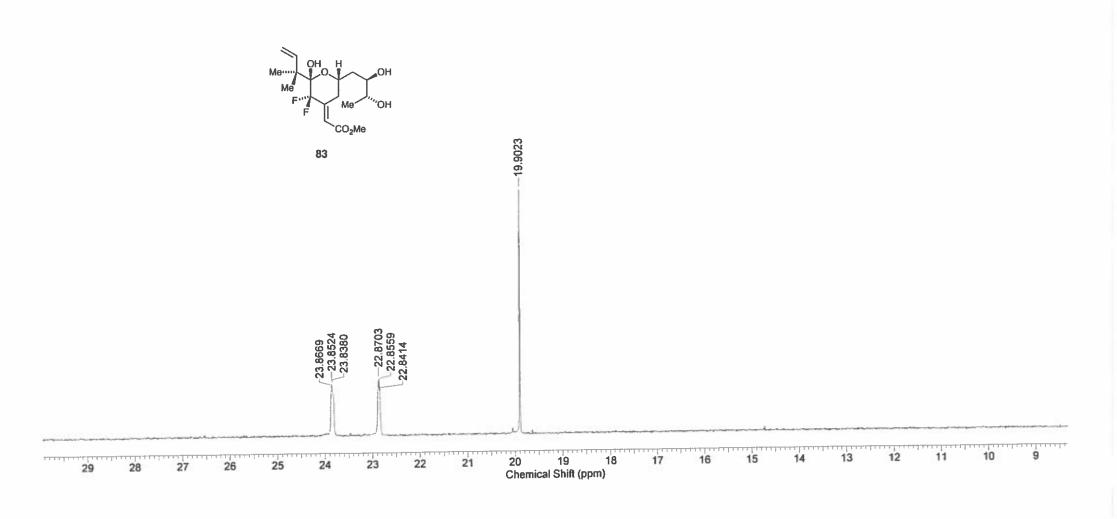


Chemical Shift (ppm)

|                        | Illia Leboir mas c    | cated by Aobitim             |                     |                                |                        | NULL I                |          |
|------------------------|-----------------------|------------------------------|---------------------|--------------------------------|------------------------|-----------------------|----------|
| Acquisition Time (sec) | 3.9649                | Comment                      | EJT-PRM175 f6-20    | 8 11mg mPROTON C6D6 (e:        | \bruk400adata\2015\Feb | ejt 45                |          |
| Date                   | 25 Feb 2015 18:31:28  |                              |                     | Date Stamp                     | 25 Feb 2015 18:31:28   |                       |          |
| File Name              | lles7a de man ac ukly | ol5\vol3\users\srimrdata\bri | ık400adata\2015\Fel | o\data\ejt\nmr\2015-02-25-ejt- | 45\10\fid              | Frequency (MHz)       | 400.13   |
| Nucleus                |                       | Number of Transients         |                     | Origin                         | AV400                  | Original Points Count | 32768    |
|                        |                       | Points Count                 | 32768               | Pulse Sequence                 | zg30b                  | Receiver Gain         | 128.00   |
| Owner                  | nmrsu<br>8264.46      | Solvent                      | BENZENE-d6          | Spectrum Offset (Hz)           | 2473.8770              | Spectrum Type         | STANDARD |
| SW(cyclical) (Hz)      | 8264.40               | Temperature (degree C)       |                     |                                |                        |                       |          |

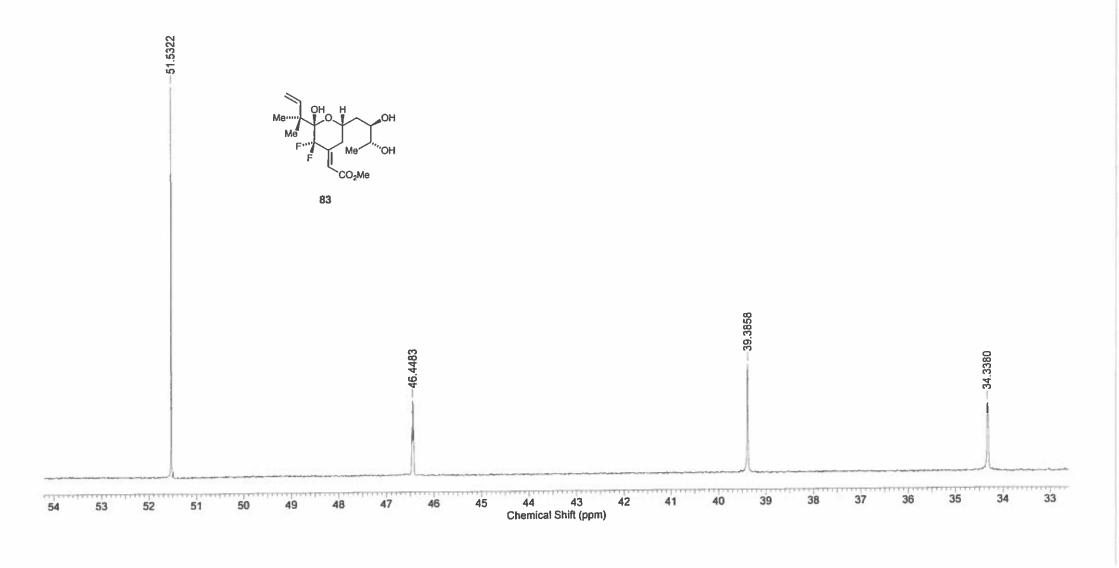


| Acquisition Time (sec) | 1.1010                  |                              |                             | 0 00 44 N                  | DOM CEDE IE-MarkED  | Ocdata)2015\Eah\ staff 53 |          |
|------------------------|-------------------------|------------------------------|-----------------------------|----------------------------|---------------------|---------------------------|----------|
| Comment                | Research Group EJT Ac   | ad/Staff/PDRA/PG/UG PDRA     | A 0215 129 EJT-PRM175 F     | 6-28 11mg Mears P. MCAR    | BON CODD (E. WILKSO | OCCIDITATED STATE SO      |          |
| Dete                   | 28 Feb 2015 19:50:24    | Date Stamp                   | 28 Feb 2015 19:50:24        |                            |                     |                           | 40E 77   |
|                        | Nee7a de man ac uklyol5 | lvol3\users\snmrdata\bruk50l | cdata\2015\Feb\data\staff\r | mr\2015-02-27-staff-53\11\ | fid                 | Frequency (MHz)           | 125.77   |
|                        |                         |                              | 8192                        | Origin                     | spect               | Original Points Count     | 32768    |
| Nucleus                | 13C                     | Number of Transients         |                             |                            | zgpg30              | Receiver Gain             | 184.40   |
| Owner                  | nmrsu                   | Points Count                 | 32768                       | Pulse Sequence             | - L                 |                           | STANDARD |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                      | BENZENE-d6                  | Spectrum Offset (Hz)       | 12660.7109          | Spectrum Type             | STANDARD |
| Sweep Width (Hz)       | 29761.00                | Temperature (degree C        | ) 22.153                    |                            |                     |                           |          |

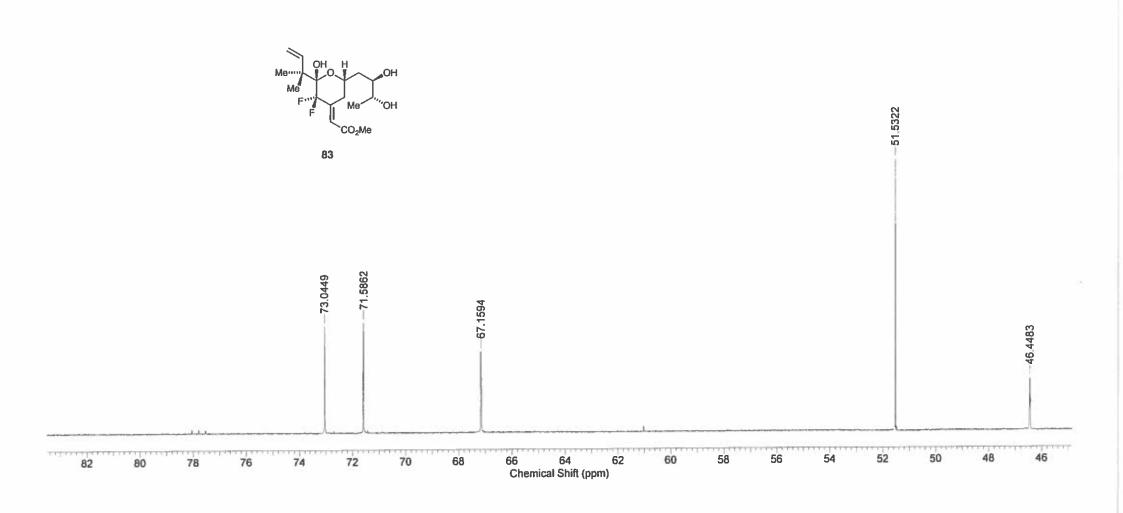


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

| Acquisition Time (sec) | 1.1010                   |                              |                             |                             |                     |                            |          |
|------------------------|--------------------------|------------------------------|-----------------------------|-----------------------------|---------------------|----------------------------|----------|
| Comment                | Research Group EJT Ac    | ad/Staff/PDRA/PG/UG PDR      | A 0215 129 EJT-PRM175 F     | F6-28 11mg Mears P. mCAR    | BON C6D6 (E:\bruk50 | 00cdata\2015\Feb} staff 53 |          |
| Date                   | 28 Feb 2015 19:50:24     | Date Stamp                   | 28 Feb 2015 19:50:24        |                             |                     |                            |          |
| File Name              | \\ss7a ds man ac.uk\vol5 | Nvol3\users\snmrdata\bruk500 | Ocdata\2015\Feb\data\staff\ | nmr\2015-02-27-staff-53\11\ | fid                 | Frequency (MHz)            | 125.77   |
| Nucleus                | 13C                      | Number of Transients         | 8192                        | Origin                      | spect               | Original Points Count      | 32768    |
|                        |                          | Points Count                 | 32768                       | Pulse Sequence              | zgpg30              | Receiver Gain              | 184.40   |
| Owner                  | nmrsu                    |                              | BENZENE-d6                  | Spectrum Offset (Hz)        | 12660.7109          | Spectrum Type              | STANDARD |
| SW(cyclical) (Hz)      | 29761.90                 | Solvent                      |                             | Spectrum Onset (112)        | 12000 100           | 72                         |          |
| Sweep Width (Hz)       | 29761.00                 | Temperature (degree C        | 22.153                      |                             |                     |                            |          |



| Acquisition Time (sec) | 1.1010                    |                              |                            |                             |                     |                           |          |
|------------------------|---------------------------|------------------------------|----------------------------|-----------------------------|---------------------|---------------------------|----------|
| Comment                | Research Group EJT Ac     | ad/Staff/PDRA/PG/UG PDRA     | 0215 129 EJT-PRM175 F      | 6-28 11mg Mears P. mCAR     | BON C6D6 (E:\bruk50 | Ocdata\2015\Feb} staff 53 |          |
| Date                   | 28 Feb 2015 19:50:24      | Date Stamp                   | 28 Feb 2015 19:50:24       |                             |                     |                           |          |
| File Name              | \\ss7a ds man ac uk\\vol5 | \vol3\users\snmrdata\bruk500 | cdata\2015\Feb\data\staff\ | nmr\2015-02-27-staff-53\11\ | fid                 | Frequency (MHz)           | 125.77   |
|                        | 13C                       | Number of Transients         | 8192                       | Origin                      | spect               | Original Points Count     | 32768    |
| Nucleus                |                           | Points Count                 | 32768                      | Pulse Sequence              | zgpg30              | Receiver Gain             | 184.40   |
| Owner                  | nmrsu                     | 7.01111                      | BENZENE-d6                 | Spectrum Offset (Hz)        | 12660.7109          | Spectrum Type             | STANDARD |
| SW(cyclical) (Hz)      | 29761.90                  | Solvent                      |                            | opecuam onset (nz)          | 12000100            | 1 -1 -1 -1 -1             |          |
| Sween Width (Hz)       | 29761.00                  | Temperature (degree C)       | 22.153                     |                             |                     |                           |          |



| Acquisition Time (sec) | 1.1010                   |                              |                             |                             |                      |                           |          |
|------------------------|--------------------------|------------------------------|-----------------------------|-----------------------------|----------------------|---------------------------|----------|
| Comment                | Research Group EJT Ac    | ad/Staff/PDRA/PG/UG PDR/     | \ 0215 129 EJT-PRM175 F     | 6-28 11mg Mears P. mCAR     | BON C6D6 (E:\bruk500 | ocdata\2015\Feb} staff 53 |          |
| Date                   | 28 Feb 2015 19:50:24     | Date Stamp                   | 28 Feb 2015 19:50:24        |                             |                      |                           |          |
| File Name              | \\ss7a.ds.man.ac.uk\vol5 | lvol3\users\snmrdata\bruk500 | cdata\2015\Feb\data\staff\r | nmr\2015-02-27-staff-53\11\ | fid                  | Frequency (MHz)           | 125.77   |
| Nucleus                | 13C                      | Number of Transients         | 8192                        | Origin                      | spect                | Original Points Count     | 32768    |
| Owner                  | nmrsu                    | Points Count                 | 32768                       | Pulse Sequence              | zgpg30               | Receiver Gain             | 184.40   |
| SW(cyclical) (Hz)      | 29761.90                 | Solvent                      | BENZENE-d6                  | Spectrum Offset (Hz)        | 12660.7109           | Spectrum Type             | STANDARD |
| Sweep Width (Hz)       | 29761.00                 | Temperature (degree C        | 22.153                      |                             |                      |                           |          |

PRM175-CNMR.esp

107.0

106.5

106.0

105.5

105.0

104.5

103.0

103.5

104.0

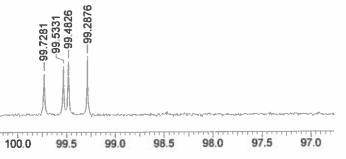
102.5

102.0

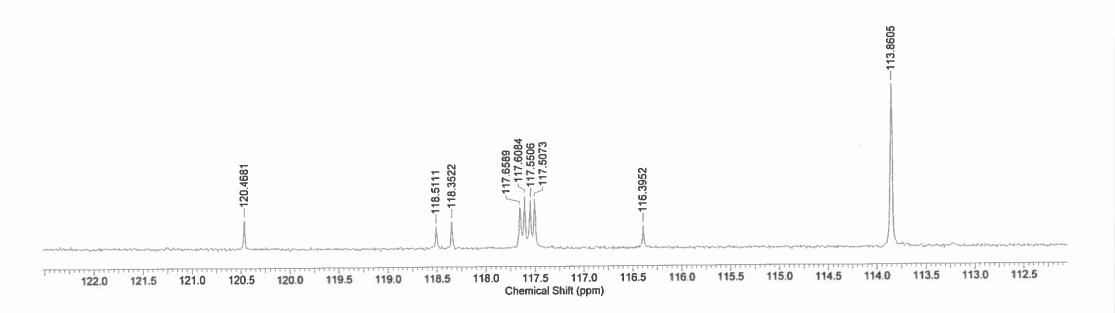
Chemical Shift (ppm)

101.5

101.0

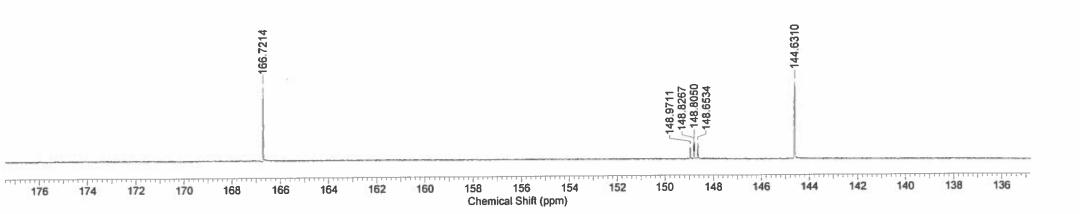


| Acquisition Time (sec) | 1.1010                   |                             |                              |                            |                      |                           |                                       |
|------------------------|--------------------------|-----------------------------|------------------------------|----------------------------|----------------------|---------------------------|---------------------------------------|
| Comment                | Research Group EJT Ac    | ad/Staff/PDRA/PG/UG PDRA    | 4 0215 129 EJT-PRM175 F      | 6-28 11mg Mears P. mCAR    | BON C6D6 (E:\bruk500 | ocdata\2015\Feb) staff 53 | · · · · · · · · · · · · · · · · · · · |
| Date                   | 28 Feb 2015 19:50:24     | Date Stamp                  | 28 Feb 2015 19:50:24         |                            |                      |                           |                                       |
| File Name              | \\ss7a ds man ac.uk\vol5 | vol3\users\snmrdata\bruk500 | ocdata\2015\Feb\data\staff\r | mr\2015-02-27-staff-53\11\ | fid                  | Frequency (MHz)           | 125.77                                |
| Nucleus                | 13C                      | Number of Transients        | 8192                         | Origin                     | spect                | Original Points Count     | 32768                                 |
| Owner                  | nmrsu                    | Points Count                | 32768                        | Pulse Sequence             | zgpg30               | Receiver Gain             | 184.40                                |
| SW(cyclical) (Hz)      | 29761.90                 | Solvent                     | BENZENE-d6                   | Spectrum Offset (Hz)       | 12660.7109           | Spectrum Type             | STANDARD                              |
| Sweep Width (Hz)       | 29761.00                 | Temperature (degree C       | 22.153                       |                            |                      |                           |                                       |

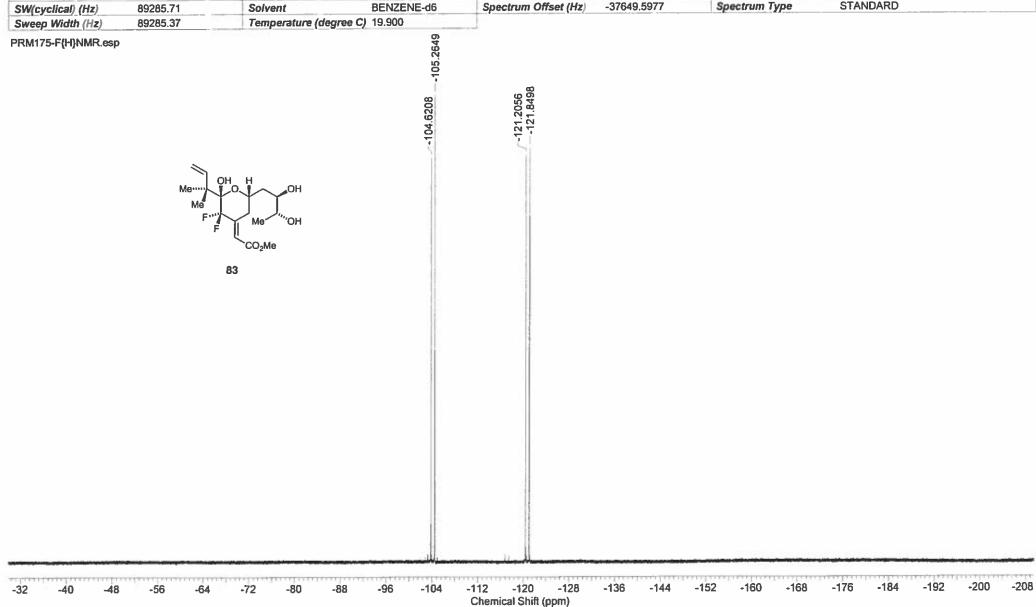


| Acquisition Time (sec) | 1,1010                   |                              |                             |                             |                      |                           |          |
|------------------------|--------------------------|------------------------------|-----------------------------|-----------------------------|----------------------|---------------------------|----------|
| Comment                | Research Group EJT Ac    | ad/Staff/PDRA/PG/UG PDR      | A 0215 129 EJT-PRM175 F     | 6-28 11mg Mears P. mCAR     | BON C6D6 (E:\bruk500 | ocdata\2015\Feb} staff 53 |          |
| Date                   | 28 Feb 2015 19:50:24     | Date Stamp                   | 28 Feb 2015 19:50:24        |                             |                      |                           |          |
| File Name              | \\ss7a ds.man.ac.uk\vol5 | \vol3\users\snmrdata\bruk50( | ocdata\2015\Feb\data\staff\ | nmr\2015-02-27-staff-53\11\ | fid                  | Frequency (MHz)           | 125.77   |
| Nucleus                | 13C                      | Number of Transients         | 8192                        | Origin                      | spect                | Original Points Count     | 32768    |
| Owner                  | nmrsu                    | Points Count                 | 32768                       | Pulse Sequence              | zgpg30               | Receiver Gain             | 184.40   |
| SW(cyclical) (Hz)      | 29761.90                 | Solvent                      | BENZENE-d6                  | Spectrum Offset (Hz)        | 12660.7109           | Spectrum Type             | STANDARD |
| Sweep Width (Hz)       | 29761.00                 | Temperature (degree C        | ) 22.153                    |                             |                      |                           |          |

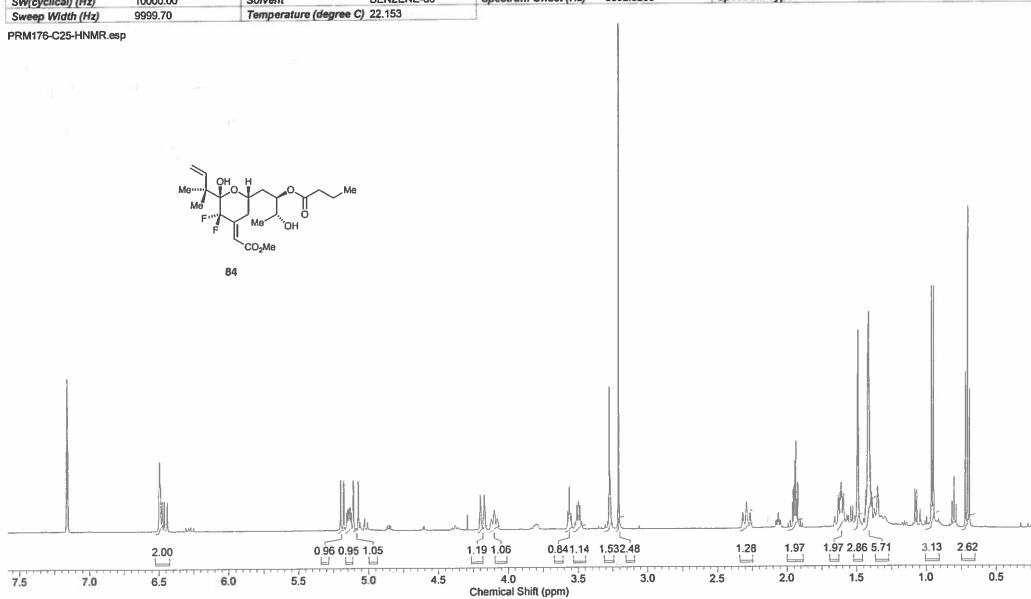
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|                        | 0.770.40              |                             | E IT DD14475 66 00   | 11mm ==E10CDD CEDE to:\       | aut 400 adata 2015 Eable | ii AE                 | •        |
|------------------------|-----------------------|-----------------------------|----------------------|-------------------------------|--------------------------|-----------------------|----------|
| Acquisition Time (sec) | 0.7340                | Comment                     | EJ1-PKM1/510-28      | 11mg mF19CPD C6D6 (e:\        | nukannanaran 154-en) e   | <u> </u>              |          |
| Date                   | 25 Feb 2015 18:46:24  |                             |                      | Date Stamp                    | 25 Feb 2015 18:46:24     |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bru | ık400adata\2015\Feb\ | data\ejt\nmr\2015-02-25-ejt-4 | 5\14\PDATA\1\1r          | Frequency (MHz)       | 376.50   |
| Nucleus                | 19F                   | Number of Transients        |                      | Origin                        | AV400                    | Original Points Count | 65536    |
| Owner                  | nmrsu                 | Points Count                | 262144               | Pulse Sequence                | zgig                     | Receiver Gain         | 322.00   |
| SW(cyclical) (Hz)      | 89285.71              | Solvent                     | BENZENE-d6           | Spectrum Offset (Hz)          | -37649.5977              | Spectrum Type         | STANDARD |
| Swoon Width (Hz)       | 80285 37              | Temperature (degree C       | 1 19 900             |                               |                          |                       |          |

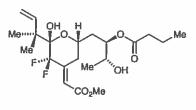


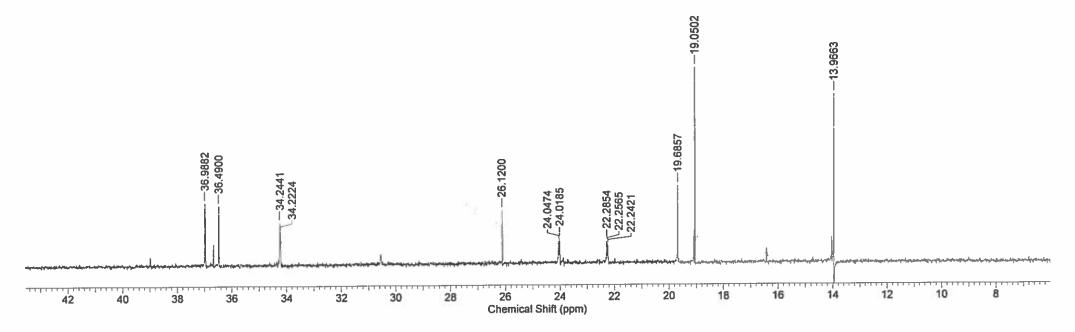
|                        | This report mas o     | routed by riebirini.        |                     |                               |                       |                        |          |
|------------------------|-----------------------|-----------------------------|---------------------|-------------------------------|-----------------------|------------------------|----------|
| Acquisition Time (sec) | 3.2768                | Comment                     | 0315 160 Mears P.   | EJT-PRM176 "C25" mPROT        | ON C6D6 (E:\bruk500cd | ata\2015\Mar} staff 56 | 7/2      |
| Date                   | 21 Mar 2015 20:43:44  |                             |                     | Date Stamp                    | 21 Mar 2015 20:43:44  |                        |          |
| File Name              | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bru | k500cdata\2015\Mar\ | data\staff\nmr\2015-03-20-sta | ff-56\10\fid          | Frequency (MHz)        | 500.19   |
| Nucleus                | 1H                    | Number of Transients        |                     | Origin                        | spect                 | Original Points Count  | 32768    |
| Owner                  | nmrsu                 | Points Count                | 32768               | Pulse Sequence                | zg30                  | Receiver Gain          | 61.38    |
| SW(cyclical) (Hz)      | 10000.00              | Solvent                     | BENZENE-d6          | Spectrum Offset (Hz)          | 3092.6208             | Spectrum Type          | STANDARD |
| Striction (112)        | 10000:00              |                             | 00.450              |                               |                       |                        |          |



| Acquisition Time (sec) | 1.1010                  | Comment                    | 0315 160 Mears P. EJT    | -PRM176 "C25" mCARB        | ON C6D6 (E:\bruk500 | Cdata\2015\Mar) staff 56 |          |
|------------------------|-------------------------|----------------------------|--------------------------|----------------------------|---------------------|--------------------------|----------|
| Date                   |                         | Date Stamp                 | 22 Mar 2015 05:45:36     |                            |                     |                          |          |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | :500cdata\2015\Mar\data\ | staff\nmr\2015-03-20-staff | -56\11\fid          | Frequency (MHz)          | 125.77   |
| Nucleus                | 13C                     | Number of Transients       | 10240                    | Origin                     | spect               | Original Points Count    | 32768    |
| Owner                  |                         | Points Count               | 32768                    | Pulse Sequence             | zgpg30              | Receiver Gain            | 184.40   |
|                        | nmrsu<br>29761.90       | Solvent                    | BENZENE-d6               | Spectrum Offset (Hz)       | 12661.6182          | Spectrum Type            | STANDARD |
| SW(cyclical) (Hz)      |                         | Temperature (degree C      |                          |                            |                     | 77                       |          |
| Sweep Width (Hz)       | 29761.00                | remperature (negree c)     | 7 22.107                 | J.                         |                     |                          |          |

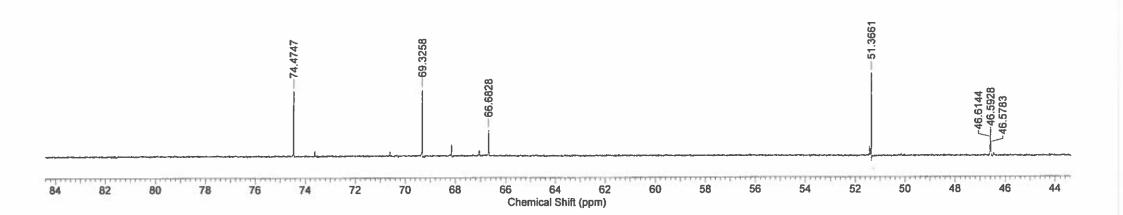
PRM176-C25-CNMR.esp





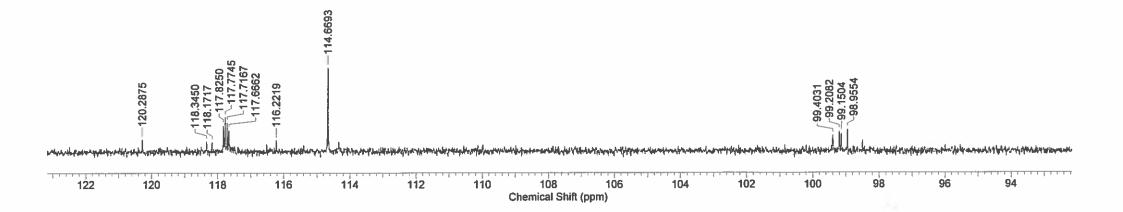
| Acquisition Time (sec) | 1.1010                  | Comment                    | 0315 160 Mears P. EJT-PRM176 "C25" mCARBON C6D6 {E:\bruk500cdata\2015\Mar} staff 56 |                            |            |                       |          |  |  |
|------------------------|-------------------------|----------------------------|-------------------------------------------------------------------------------------|----------------------------|------------|-----------------------|----------|--|--|
| Date                   | 22 Mar 2015 05:45:36    | Date Stamp                 | 22 Mar 2015 05:45:36                                                                |                            |            |                       |          |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 500cdata\2015\Mar\data\                                                             | staff\nmr\2015-03-20-staff | -56\11\fid | Frequency (MHz)       | 125.77   |  |  |
| Nucleus                | 13C                     | Number of Transients       | 10240                                                                               | Origin                     | spect      | Original Points Count | 32768    |  |  |
| Owner                  | nmrsu                   | Points Count               | 32768                                                                               | Pulse Sequence             | zgpg30     | Receiver Gain         | 184.40   |  |  |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                    | BENZENE-d6                                                                          | Spectrum Offset (Hz)       | 12661.6182 | Spectrum Type         | STANDARD |  |  |
| Sweep Width (Hz)       | 29761.00                | Temperature (degree C)     | 22.164                                                                              |                            |            |                       |          |  |  |

PRM176-C25-CNMR.esp



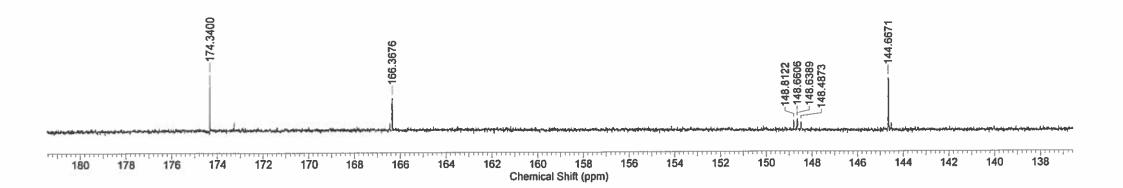
| Acquisition Time (sec) | 1,1010                  | Comment                    | 0315 160 Mears P. EJT-PRM176 "C25" mCARBON C6D6 {E:\bruk500cdata\2015\Mar} staff 56 |                            |            |                                         |          |  |  |
|------------------------|-------------------------|----------------------------|-------------------------------------------------------------------------------------|----------------------------|------------|-----------------------------------------|----------|--|--|
| Date                   | 22 Mar 2015 05:45:36    | Date Stamp                 | 22 Mar 2015 05:45:36                                                                |                            |            | 000000000000000000000000000000000000000 |          |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 500cdata\2015\Mar\data\                                                             | staff\nmr\2015-03-20-staff | -56\11\fid | Frequency (MHz)                         | 125.77   |  |  |
| Nucleus                | 13C                     | Number of Transients       | 10240                                                                               | Origin                     | spect      | Original Points Count                   | 32768    |  |  |
| Owner                  | nmrsu                   | Points Count               | 32768                                                                               | Pulse Sequence             | zgpg30     | Receiver Gain                           | 184.40   |  |  |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                    | BENZENE-d6                                                                          | Spectrum Offset (Hz)       | 12661.6182 | Spectrum Type                           | STANDARD |  |  |
| Sweep Width (Hz)       | 29761.00                | Temperature (degree C)     | 22.164                                                                              |                            |            |                                         |          |  |  |

PRM176-C25-CNMR.esp

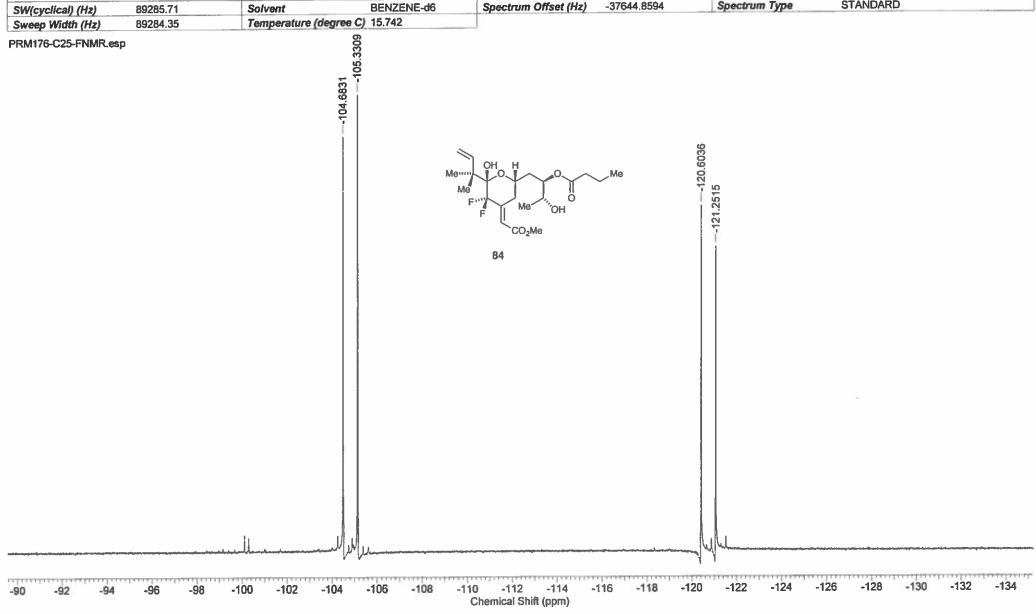


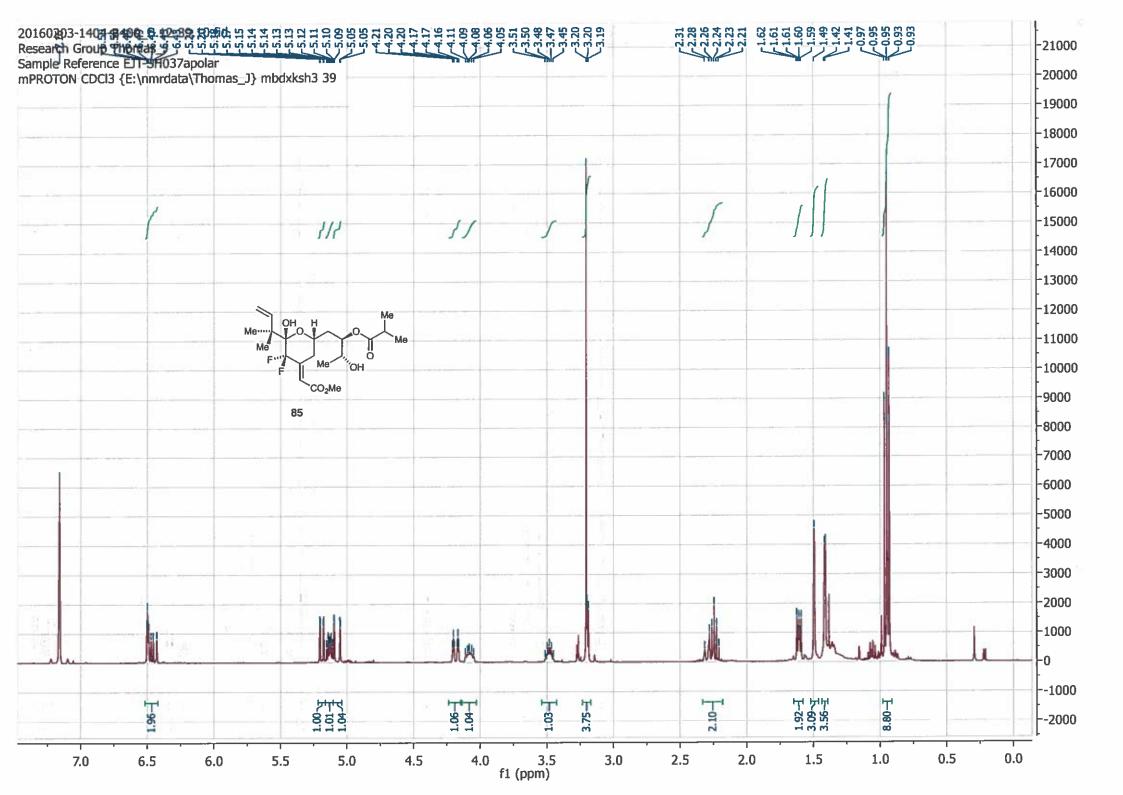
| Acquisition Time (sec) | 1.1010                  | Comment                    | 0315 160 Mears P. EJT-PRM176 "C25" mCARBON C6D6 {E:\bruk500cdata\2015\Mar} staff 56 |                            |            |                       |          |  |  |
|------------------------|-------------------------|----------------------------|-------------------------------------------------------------------------------------|----------------------------|------------|-----------------------|----------|--|--|
| Date                   | 22 Mar 2015 05:45:36    | Date Stamp                 | 22 Mar 2015 05:45:36                                                                |                            |            |                       | <u> </u> |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vol | 5\vol3\users\snmrdata\bruk | 500cdata\2015\Mar\data\                                                             | staff\nmr\2015-03-20-staff | -56\11\fid | Frequency (MHz)       | 125.77   |  |  |
| Nucleus                | 13C                     | Number of Transients       | 10240                                                                               | Origin                     | spect      | Original Points Count | 32768    |  |  |
| Owner                  | nmrsu                   | Points Count               | 32768                                                                               | Pulse Sequence             | zgpg30     | Receiver Gain         | 184.40   |  |  |
| SW(cyclical) (Hz)      | 29761.90                | Solvent                    | BENZENE-d6                                                                          | Spectrum Offset (Hz)       | 12661.6182 | Spectrum Type         | STANDARD |  |  |
| Sweep Width (Hz)       | 29761.00                | Temperature (degree C)     | 22.164                                                                              |                            |            |                       |          |  |  |

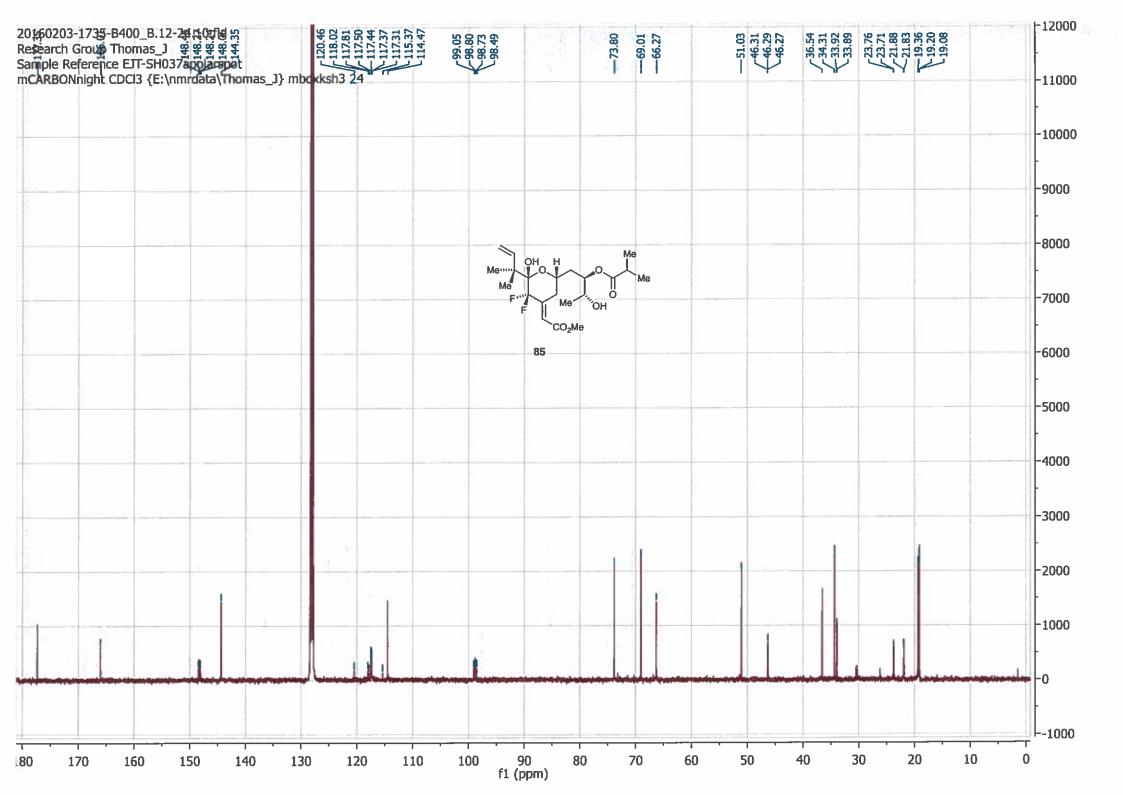
PRM176-C25-CNMR.esp

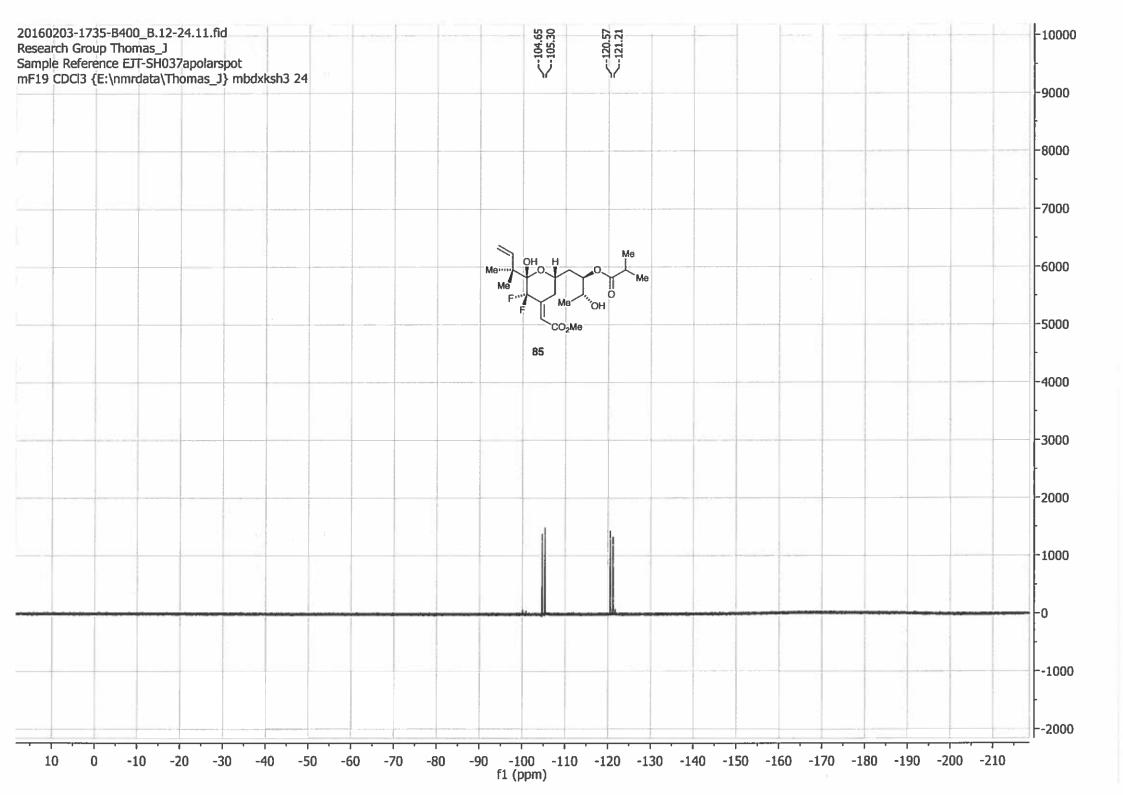


| Acquisition Time (sec) | 0.7340                 | .7340 Comment EJT-PRM176 2nd re-col. f4-12 7mg mF19_cryo_zgbs C6D6 {e:\bruk400cdata\2015\Feb} ejt 44 |                        |                            |                      |                       |          |  |  |  |  |
|------------------------|------------------------|------------------------------------------------------------------------------------------------------|------------------------|----------------------------|----------------------|-----------------------|----------|--|--|--|--|
|                        | 05 Mar 2015 17:46:40   |                                                                                                      |                        | Date Stamp                 | 05 Mar 2015 17:46:40 |                       |          |  |  |  |  |
|                        | \\ss7a.ds.man.ac.uk\vo | l5\vol3\users\snmrdata\bruk                                                                          | 400cdata\2015\Feb\data | Nejt\nmr\2015-03-05-ejt-44 | \11\fid              | Frequency (MHz)       | 376.44   |  |  |  |  |
| Nucleus                |                        | Number of Transients                                                                                 | 16                     | Origin                     | spect                | Original Points Count | 65536    |  |  |  |  |
| Owner                  | nmrsu                  | Points Count                                                                                         | 65536                  | Pulse Sequence             | zgbs                 | Receiver Gain         | 22.60    |  |  |  |  |
| SW(cyclical) (Hz)      | 89285.71               | Solvent                                                                                              | BENZENE-d6             | Spectrum Offset (Hz)       | -37644.8594          | Spectrum Type         | STANDARD |  |  |  |  |
| Curson Width /Uzl      | 80284 35               | Temperature (degree C)                                                                               | 15 742                 |                            |                      |                       |          |  |  |  |  |

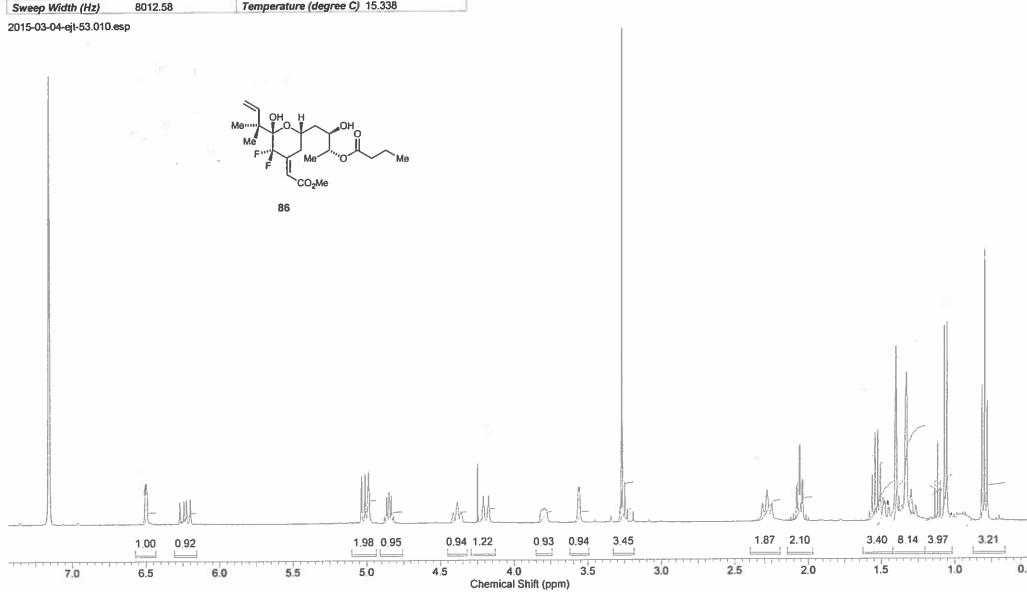








|                        | imo report i    | vas created by AOD/Min           |                    |                                |                    |                       | •        |
|------------------------|-----------------|----------------------------------|--------------------|--------------------------------|--------------------|-----------------------|----------|
| Acquisition Time (sec) | 4.0894          | Comment                          | EJT-PRM176 f6-1    | 7 6mg mPROTON_A C6D6 {         | e:\bruk400cdata\20 | 015\Feb} ejt 53       |          |
| Date                   | 04 Mar 2015 10: | :14:24                           |                    | Date Stamp                     | 04 Mar 2015 10:    | 14:24                 |          |
|                        | \\ss7a.ds.man.a | c.uk\vol5\vol3\users\snmrdata\br | uk400cdata\2015\Fe | b\data\ejt\nmr\2015-03-04-ejt- | -53\10\fid         | Frequency_(MHz)       | 400.07   |
| Nucleus                | 1H              | Number of Transients             |                    | Origin                         | spect              | Original Points Count | 32768    |
| Owner                  | nmrsu           | Points Count                     | 32768              | Pulse Sequence                 | zg30               | Receiver Gain         | 161.00   |
| SW(cyclical) (Hz)      | 8012.82         | Solvent                          | BENZENE-d6         | Spectrum Offset (Hz)           | 1903.3687          | Spectrum Type         | STANDARD |
| Sween Width (Hz)       | 8012 58         | Temperature (degree C            | 1 15 338           | -                              |                    |                       |          |



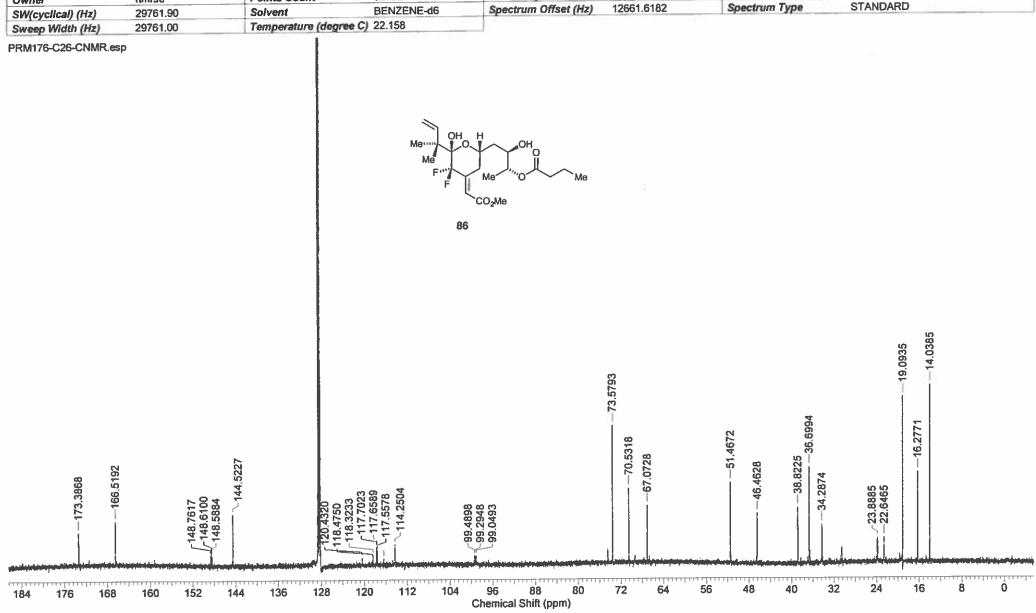
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ 0315 159 Mears P. EJT-PRM176 "C26" mCARBON C6D6 (E:\bruk500cdata\2015\Mar) staff 55 Acquisition Time (sec) 1.1010 Comment 21 Mar 2015 19:39:44 Date Stamp 21 Mar 2015 19:39:44 \\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Mar\data\staff\nmr\2015-03-20-staff-55\11\fid Frequency (MHz) 125.77 32768 Original Points Count Origin spect 10240 Number of Transients 13C Receiver Gain 184.40 Pulse Sequence zgpg30 32768 Points Count nmrsu STANDARD 12661.6182 Spectrum Type

Date

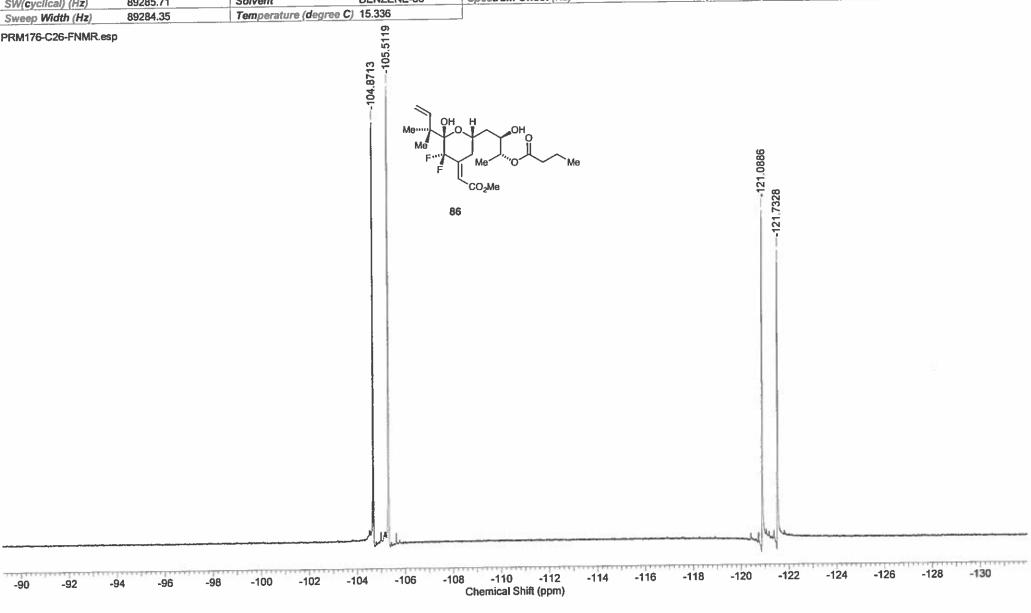
File Name

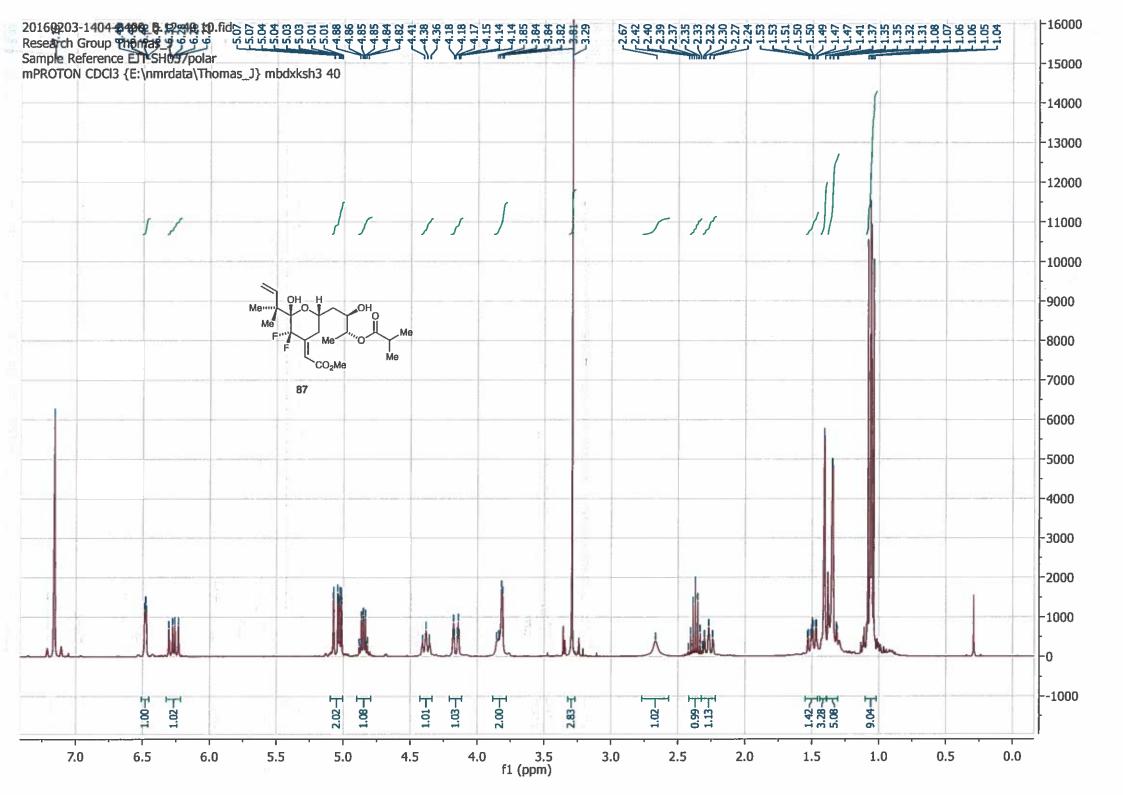
Nucleus

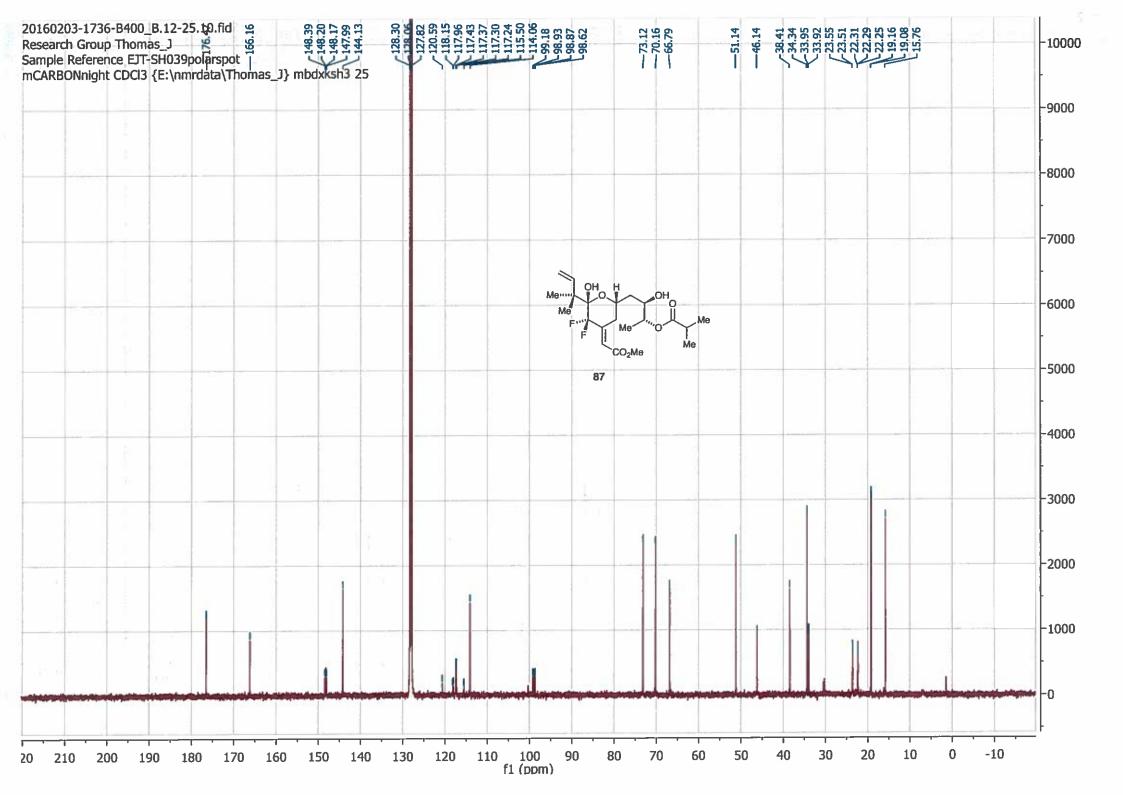
Owner

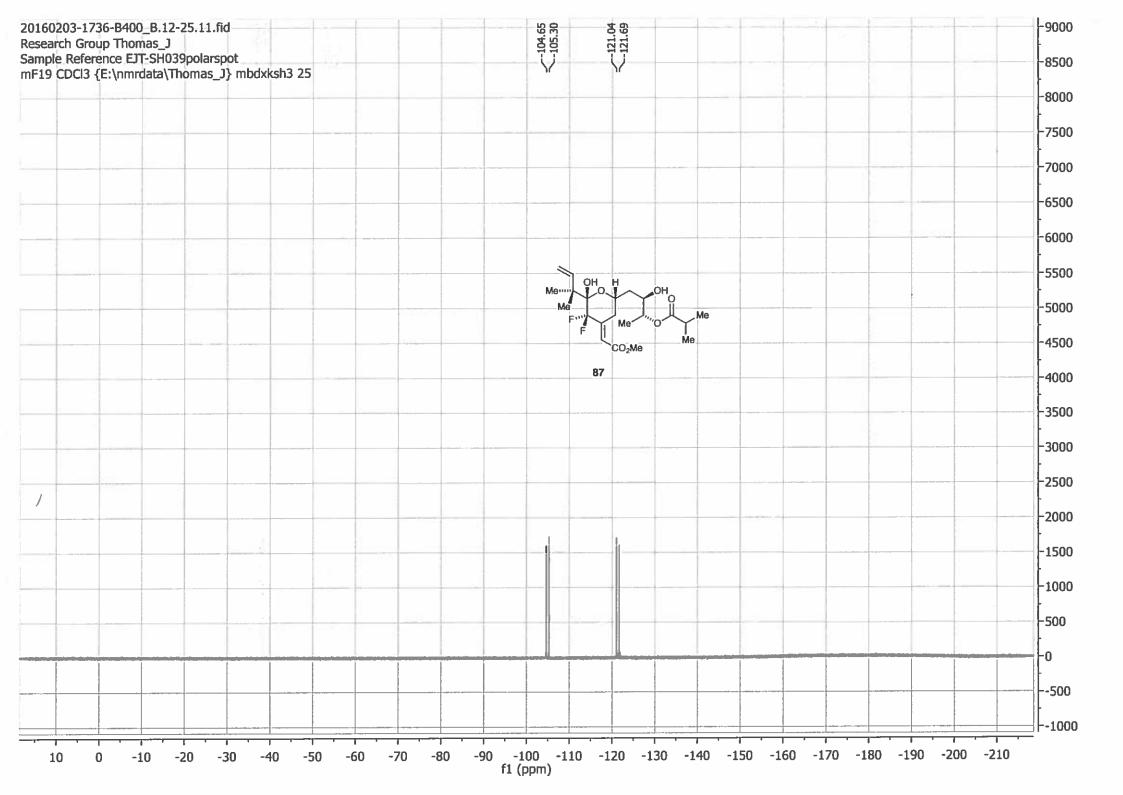


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM176 f6-17 6mg mF19\_cryo\_zgbs C6D6 {e:\bruk400cdata\2015\Feb} ejt 53 Acquisition Time (sec) 0.7340 Соттепт Date Stamp 04 Mar 2015 10:16:32 04 Mar 2015 10:16:32 Date Frequency (MHz) 376.44 \lss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Feb\data\ejt\nmr\2015-03-04-ejt-53\11\fid File Name Original Points Count 65536 Origin spect Number of Transients 16 Nucleus 20.20 Receiver Gain Pulse Sequence zgbs 65536 Points Count nmrsu Owner STANDARD Spectrum Type -37644.8594 BENZENE-d6 Spectrum Offset (Hz) Solvent SW(cyclical) (Hz) 89285.71 Temperature (degree C) 15.336 Sweep Width (Hz) 89284.35 -105,5119 PRM176-C26-FNMR.esp -104.8713 -121.0886 86







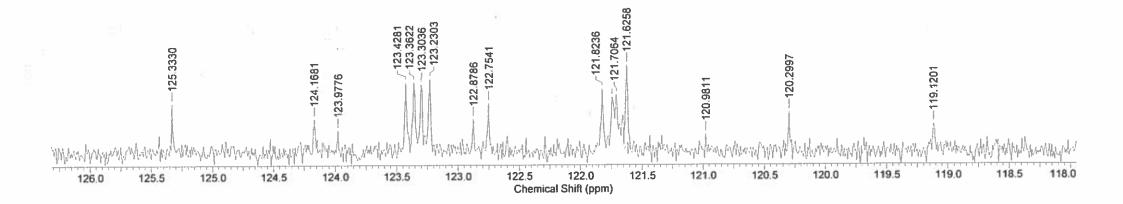


| Acquisition Time (sec) | 3.9649                    | Comment                                 | EJT-PRM184 f8-25 1     | 157mg mPROTON CDC13                | e:\bruk400adata\2015   | Jul} ejt 52                                                                                   |                                      |                            |
|------------------------|---------------------------|-----------------------------------------|------------------------|------------------------------------|------------------------|-----------------------------------------------------------------------------------------------|--------------------------------------|----------------------------|
| ate                    | 14 Jul 2015 19:25:0       |                                         |                        | Date Stamp                         | 14 Jul 2015 19:25:0    |                                                                                               |                                      |                            |
| ile Name               | \\ss7a.ds.man.ac.ul       | <\vol5\vol3\users\snmrdata\br           | uk400adata\2015\Jul\da | ata\ejt\nmr\2015-07-14-ejt-5       | 2\10\fid               | Frequency (MHz)                                                                               | 400.13                               |                            |
| lucieus                | 1H                        | Number of Transients                    | 16                     | Origin                             | AV400                  | Original Points Count                                                                         | 32768                                |                            |
| Owner                  | nmrsu                     | Points Count                            | 32768                  | Pulse Sequence                     | zg30b                  | Receiver Gain                                                                                 | 36,00                                |                            |
| W(cyclical) (Hz)       | 8264.46                   | Solvent                                 | CHLOROFORM-d           | Spectrum Offset (Hz)               | 2465.1792              | Spectrum Type                                                                                 | STANDARD                             |                            |
| weep Width (Hz)        | 8264.21                   | Temperature (degree C                   | 21.300                 |                                    |                        |                                                                                               |                                      |                            |
| RM184-aldehyde-HNMR    | esp                       |                                         |                        |                                    | -3.7377                |                                                                                               |                                      | 0.0749<br>0.0503<br>0.0452 |
|                        | CI<br>Me·····<br>Me<br>F' | OTBS OSEM  Me "OTBS  CO <sub>2</sub> Me |                        |                                    |                        |                                                                                               |                                      | \-0 0033                   |
| 1                      |                           |                                         |                        | 4,7367 4,7556<br>4,7292<br>14,7166 |                        |                                                                                               |                                      |                            |
| 9.5663                 |                           |                                         | 6.2539<br>6.1934       | 4.2791<br>4.2640 4.6989            |                        | 3.3040 3.4420<br>2.8224<br>2.8023<br>2.7884<br>2.6560<br>2.6384<br>2.6233<br>1.8360<br>1.7660 | 1,5385<br>1,5214<br>1,5126<br>1,4773 | 100                        |
| 1.84                   |                           |                                         | 0.99 1.00 4.14 1.62    | 4.14 2.29 5.72 2.36 2.19 1         | 1.95 1.02 0.94 1.01 1. | 04 0.97 1.19 2.18 0.56 2.96                                                                   | 3 24 5 31 0 52 6 62 3 94 3           | 7.50 23.51 1               |
|                        |                           |                                         |                        |                                    |                        |                                                                                               |                                      |                            |

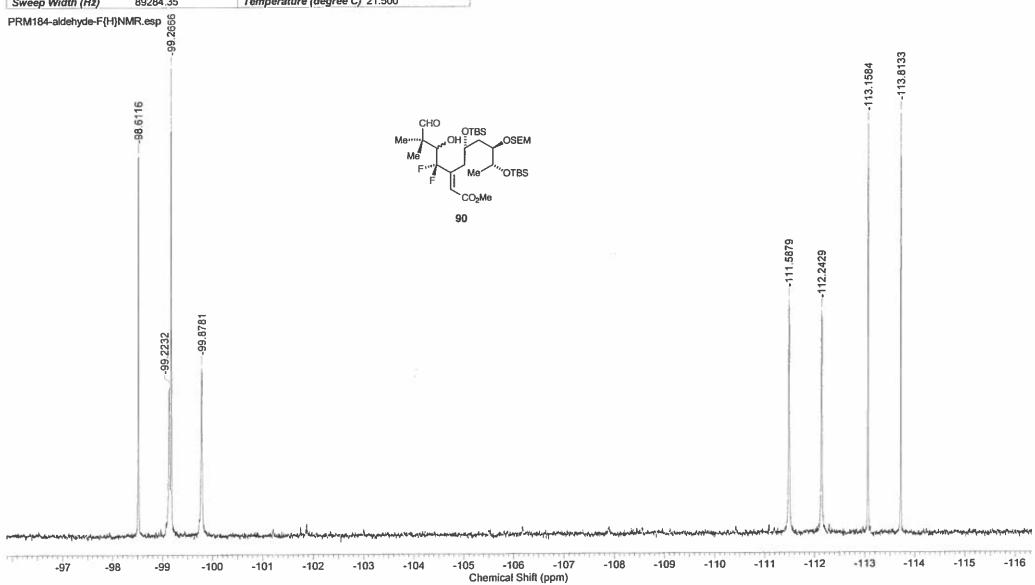
|                          |                                                              |                                                           | FIUCESSUI ACAU                                                                   | eniic Edition, i oi ii             | some introduction g            | O to www.acdiabs.c                | ommuni broce    |
|--------------------------|--------------------------------------------------------------|-----------------------------------------------------------|----------------------------------------------------------------------------------|------------------------------------|--------------------------------|-----------------------------------|-----------------|
|                          | 1.3566                                                       | Comment                                                   |                                                                                  | 157mg mCARBONnight CD              | UCIS (e:\bruk400adata\20       | 10 Null et 52                     |                 |
| Date                     | 14 Jul 2015 22:30:40                                         | Date Stamp                                                | 14 Jul 2015 22:30:40                                                             |                                    | 7/42/64                        | Frequency (MHz)                   | 100.61          |
|                          |                                                              |                                                           |                                                                                  | ta\ejt\nmr\2015-07-14-ejt-52       | V/400                          | Original Points Count             | 32768           |
| Nucleus                  | 13C                                                          | Number of Transients                                      | 3000                                                                             | Origin                             | AV400                          | Receiver Gain                     | 512.00          |
| Owner                    | nmrsu                                                        | Points Count                                              | 32768                                                                            | Pulse Sequence                     | zgpg30<br>10059.2100           | Spectrum Type                     | STANDARD        |
|                          | 24154.59                                                     | Solvent                                                   | CHLOROFORM-d                                                                     | Spectrum Offset (Hz)               | 10059.2100                     | Spectrum Type                     | STANDARD        |
| Sweep Width (Hz)         | 24153.85                                                     | Temperature (degree C)                                    | 22.900                                                                           |                                    |                                |                                   |                 |
| RM184-aldehyde-CNMR.     | esp                                                          |                                                           |                                                                                  |                                    | 77.3150<br>-77.0000<br>75.6850 | 25.9049                           |                 |
|                          | Me Me F                                                      | OTBS<br>OH OTBS<br>OSEM<br>Me "OTBS<br>CO <sub>2</sub> Me |                                                                                  |                                    |                                | 51.5257                           | 812             |
| <u>204.1223</u> 204.2835 | .165 7827                                                    | 165.6581                                                  |                                                                                  | 7578                               |                                | 49.4010 49.3571 -36.5210 -35.2682 | 19.6774         |
| 204                      | เรอบุลลักกรลี และเลือกในเรอบรอบรอบรอบรอบร<br>ได้ประชาชายายาย | 151.2469<br>150.9904<br>150.7926<br>148.6020<br>148.3602  | 125,3330<br>123,4281<br>123,3622<br>123,2303<br>122,7541<br>121,8236<br>121,6258 | L120.2997<br>L119.1201             | 74.3844                        | 200                               |                 |
| 220 210 200              | 190 180 170                                                  |                                                           | ) 130 120                                                                        | 110 100 90<br>Chemical Shift (ppm) | 80 70 60                       | 50 40 30                          | 20 10 0 -10 -20 |

| Acquisition Time (sec) | 1.3566                 | Comment                    | EJT-PRM184 f8-25 15     | EJT-PRM184 f8-25 157mg mCARBONnight CDCl3 {e:\bruk400adata\2015\Uul} ejt 52 |            |                       |          |  |  |  |
|------------------------|------------------------|----------------------------|-------------------------|-----------------------------------------------------------------------------|------------|-----------------------|----------|--|--|--|
| Date                   | 14 Jul 2015 22:30:40   | Date Stamp                 | 14 Jul 2015 22:30:40    |                                                                             |            |                       |          |  |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vo | l5\vol3\users\snmrdata\bru | k400adata\2015\Jul\data | \ejt\nmr\2015-07-14-ejt-52\                                                 | 13\fid     | Frequency (MHz)       | 100,61   |  |  |  |
| Nucleus                | 13C                    | Number of Transients       | 3000                    | Origin                                                                      | AV400      | Original Points Count | 32768    |  |  |  |
| Owner                  | nmrsu                  | Points Count               | 32768                   | Pulse Sequence                                                              | zgpg30     | Receiver Gain         | 512.00   |  |  |  |
| SW(cyclical) (Hz)      | 24154.59               | Solvent                    | CHLOROFORM-d            | Spectrum Offset (Hz)                                                        | 10059.2100 | Spectrum Type         | STANDARD |  |  |  |
| Sweep Width (Hz)       | 24153.85               | Temperature (degree C      | 22.900                  |                                                                             |            |                       |          |  |  |  |

PRM184-aldehyde-CNMR.esp



| Acquisition Time (sec) | 0.7340                | Comment                     | EJT-PRM184 f8-25 1     | 157mg mF19CPD CDCI3 (e                    | :\bruk400adata\2015\J | ul} ejt 52            |          |
|------------------------|-----------------------|-----------------------------|------------------------|-------------------------------------------|-----------------------|-----------------------|----------|
| Date                   | 14 Jul 2015 19:29:20  | Date Stamp                  | 14 Jul 2015 19:29:20   |                                           |                       |                       | 4        |
| File Name              | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bru | ık400adata\2015\Jul\da | ata\ejt\nmr\2015-07-14-ejt-5              | 2\12\fid              | Frequency (MHz)       | 376.50   |
| Nucleus                | 19F                   | Number of Transients        | 16                     | Origin                                    | AV400                 | Original Points Count | 65536    |
| Owner                  | nmrsu                 | Points Count                | 65536                  | Pulse Sequence                            | zgig                  | Receiver Gain         | 362.00   |
| SW(cyclical) (Hz)      | 89285.71              | Solvent                     | CHLOROFORM-d           | Spectrum Offset (Hz)                      | -37649.5977           | Spectrum Type         | STANDARD |
| Swoon Width (Ha)       | R0284 35              | Temperature (degree C       | 21 500                 | 3 - A - O - O - O - O - O - O - O - O - O |                       |                       |          |



| Acquisition Time (sec) | 3.9649                | Comment                                             | EJT-PRM185 f15-33                    | 118mg mPROTON CDCI3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | {e:\bruk400adata\2015\.                                                        | Jul} ejt 40                                    |                                        |                                                |
|------------------------|-----------------------|-----------------------------------------------------|--------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------|------------------------------------------------|----------------------------------------|------------------------------------------------|
| Date                   | 16 Jul 2015 16:08:48  |                                                     |                                      | Date Stamp                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 16 Jul 2015 16:08:48                                                           |                                                |                                        |                                                |
| ile Name               | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bru                         | ık400adata\2015\Jul\da               | talejt\nmr\2015-07-16-ejt-4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 0\10\fid                                                                       | Frequency (MHz)                                | 400.13                                 |                                                |
| lucleus                | 1H                    | Number of Transients                                | 16                                   | Origin                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | AV400                                                                          | Original Points Count                          | 32768                                  |                                                |
| Owner                  | nmrsu                 | Points Count                                        | 32768                                | Pulse Sequence                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | zg30b                                                                          | Receiver Gain                                  | 80.60                                  |                                                |
| SW(cyclical) (Hz)      | 8264.46               | Solvent                                             | CHLOROFORM-d                         | Spectrum Offset (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 2464.9270                                                                      | Spectrum Type                                  | STANDARD                               |                                                |
| Sweep Width (Hz)       | 8264.21               | Temperature (degree C)                              | 21.500                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                |                                                |                                        |                                                |
| RM185-HNMR.esp         |                       | Cu.                                                 |                                      | I                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                |                                                | —————————————————————————————————————— | 0.0818<br>0.0503<br>0.0503<br>0.0143<br>0.0125 |
|                        | Me·····<br>Me<br>F    | OH<br>OTBS<br>OSEM<br>Me OTBS<br>CO <sub>2</sub> Me | -4.7336                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                |                                                |                                        |                                                |
|                        |                       | 51                                                  |                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                |                                                | 71.0260                                |                                                |
| -7.2700                |                       |                                                     |                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                |                                                |                                        |                                                |
|                        | -6.2609               | -6.2545<br>-2010                                    | 7<br>8 ~4.7134                       | 245<br>0074<br>917<br>5<br>6<br>3.6980<br>3.5980<br>3.5246<br>3.5246                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 3.3595<br>3324<br>3324                                                         |                                                | -0.9195                                |                                                |
|                        |                       | 90                                                  | 4.1909<br>4.1909<br>4.0875<br>4.0402 | 3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3.8656<br>3. | 2.8811-3.<br>2.8628<br>2.8476<br>2.876<br>2.876<br>2.7304<br>-2.7128<br>2.6976 | 1.8297<br>1.7729<br>1.7729<br>1.7739<br>1.6549 | 2 (140)                                |                                                |
|                        | 1.07                  | 0.79 4                                              | 1.07 1.19 1.60 2.62 0.6              | 63 0.80 8.50 2.15 5.00 1.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 7 1.10 0.90 0.98 0.07 1.                                                       | 45 2.18 2.20 5.81 3                            | 3.238.57 0.40 3.97 3                   | 7.45 41.68                                     |
| 3.0 7.5                | 7.0 6.5               | 6.0 5.5                                             | 5.0 4.5                              | 4.0 3.5<br>Chemical Shift (ppm)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 3.0 2.5                                                                        | 2.0 1.5                                        | 1.0 0.5                                | Ó                                              |

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM185 Prod mCARBON\_B CDCl3 {e:\bruk400cdata\2015\Jul} ejt 20 Acquisition Time (sec) 1.3631 Comment Date Stamp 22 Jul 2015 23:41:04 Date 22 Jul 2015 23:41:04 \\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Jul\data\ejt\nmr\2015-07-22-ejt-20\10\fid Frequency (MHz) 100,60 File Name Original Points Count 32768 Origin Nucleus 13C Number of Transients 1024 spect zgpg30 45.20 Receiver Gain Points Count 32768 Pulse Sequence nmrsu Owner Spectrum Offset (Hz) 10050,6006 STANDARD SW(cyclical) (Hz) CHLOROFORM-d Spectrum Type 24038.46 Solvent Temperature (degree C) 17.967 24037.73 Sweep Width (Hz) 18.0119 25.8731 4.6236 PRM185-CNMR-2.esp OTBS OSEM OTBS 91 17.2900 68.8471 80.4055 51.4621 65.7187 95 8727 95 7779 65 2374 165.9962 165.8941 71.9099 70.0722 69.1169 36.2793 39.1234 22.9051 20.4038 5926 78.2616 75.75

80

Chemical Shift (ppm)

88

120

152

144

160

168

136

128

112

104

96

72

64

56

48

40

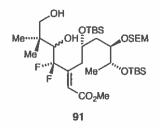
32

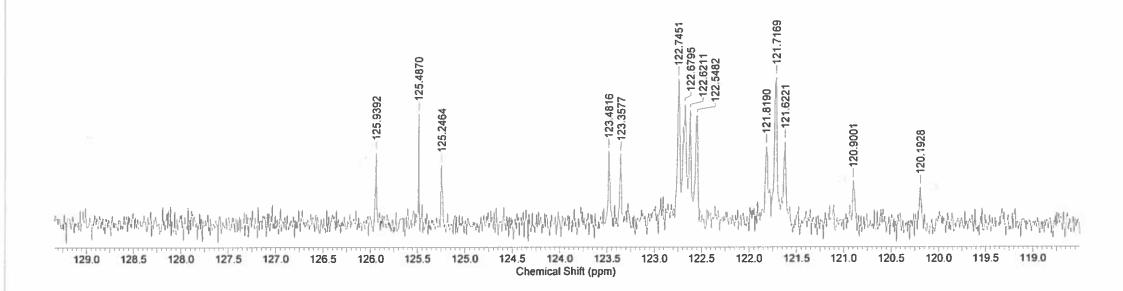
24

16

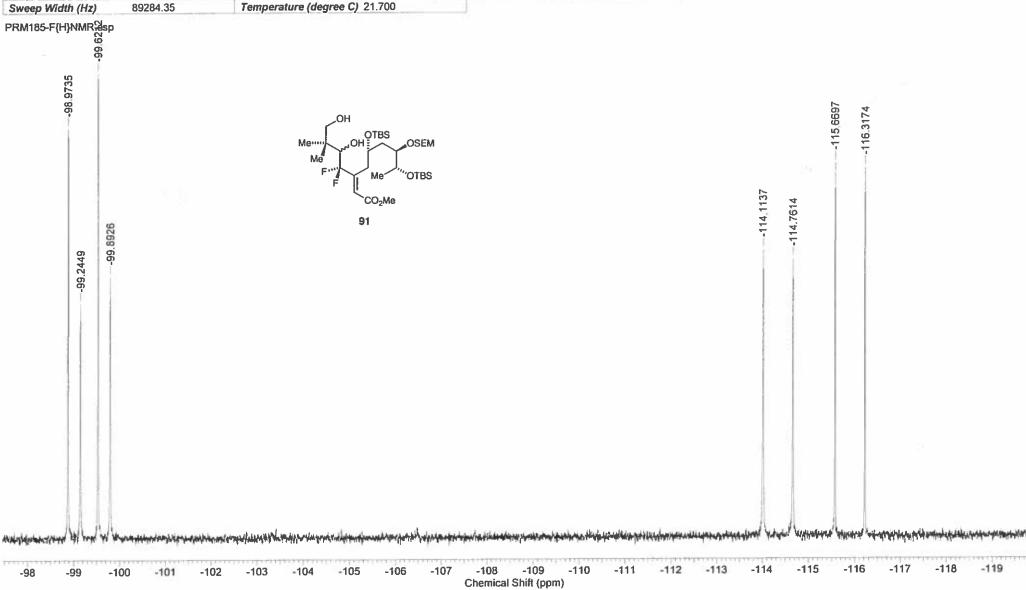
| Acquisition Time (sec) | 1.3631                | Comment                     | EJT-PRM185 Prod m      | CARBON_B CDCl3 {e:\bri       | uk400cdata\2015\Jul} ejt | 20                    |          |
|------------------------|-----------------------|-----------------------------|------------------------|------------------------------|--------------------------|-----------------------|----------|
| Date                   | 22 Jul 2015 23:41:04  |                             |                        | Date Stamp                   | 22 Jul 2015 23:41:04     |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bri | uk400cdata\2015\Jul\da | sta\ejt\nmr\2015-07-22-ejt-2 | 0\10\fid                 | Frequency (MHz)       | 100.60   |
| Nucleus                | 13C                   | Number of Transients        | 1024                   | Origin                       | spect                    | Original Points Count | 32768    |
| Owner                  | nmrsu                 | Points Count                | 32768                  | Pulse Sequence               | zgpg30                   | Receiver Gain         | 45.20    |
| SW(cyclical) (Hz)      | 24038.46              | Solvent                     | CHLOROFORM-d           | Spectrum Offset (Hz)         | 10050.6006               | Spectrum Type         | STANDARD |
| Sweep Width (Hz)       | 24037.73              | Temperature (degree C       | ) 17.967               | 100                          |                          |                       |          |

2015-07-22-ejt-20.010.esp





|                        | title repett mae a    |                             |                        |                              |                     |                       |          |
|------------------------|-----------------------|-----------------------------|------------------------|------------------------------|---------------------|-----------------------|----------|
| Acquisition Time (sec) | 0.7340                | Comment                     | EJT-PRM185 f15-33      | 118mg mF19CPD CDCI3 {        | e:\bruk400adata\201 | 5\Jul} ejt 40         |          |
| Date                   | 16 Jul 2015 16:13:04  | Date Stamp                  | 16 Jul 2015 16:13:04   |                              |                     |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bri | uk400adata\2015\Jul\da | atalejt\nmr\2015-07-16-ejt-4 | 0\12\fid            | Frequency (MHz)       | 376.50   |
| Nucleus                | 19F                   | Number of Transients        | 16                     | Origin                       | AV400               | Original Points Count | 65536    |
| Owner                  | nmrsu                 | Points Count                | 65536                  | Pulse Sequence               | zgig                | Receiver Gain         | 362.00   |
| SW(cyclical) (Hz)      | 89285.71              | Solvent                     | CHLOROFORM-d           | Spectrum Offset (Hz)         | -37649.5977         | Spectrum Type         | STANDARD |
| Courses Milelely (Ma)  | 90394 35              | Temperatura (degree C       | 21 700                 |                              |                     |                       |          |



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM189 f3-15 16mg mPROTON\_A CDCl3 {e:\bruk400cdata\2015\Jul\} ejt 32 Acquisition Time (sec) 4.0894 Comment 05 Aug 2015 12:46:08 Date Stamp 05 Aug 2015 12:46:08 Date \\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Jul\data\ejt\nmr\2015-08-05-ejt-32\10\fid Frequency (MHz) 400.07 File Name Original Points Count 32768 Origin Number of Transients spect Nucleus zg30 Receiver Gain 161.00 Pulse Seguence **Points Count** 32768 nmrsu Owner **STANDARD** 1894,3132 Spectrum Type CHLOROFORM-d Spectrum Offset (Hz) 8012.82 Solvent SW(cyclical) (Hz) Temperature (degree C) 18.208 Sweep Width (Hz) 8012.58 8760 8485 0.0087 PRM189-HNMR.esp o o CO2CH2CCI3 **OTBS** OSEM **OTBS** 93 -0.0625 -0.0502 -0.0435 1.3784 3,6326 4.8037 4.6961 1.0337 3.0324 4436 7.0078 7.0078 6.9882 0.9011 6.9699 2.13 2.14 1.39 1.26 6.66 3.45 23.35 23.52 4.382.16 2.16 2.13 2.11 2.13 1.03 4.26 1.00 1.03 1.5 7.0 2.5 2.0 1.0 0.5 -0.5 7.5 4.0 3.5 3.0

Chemical Shift (ppm)

6.5

8.0

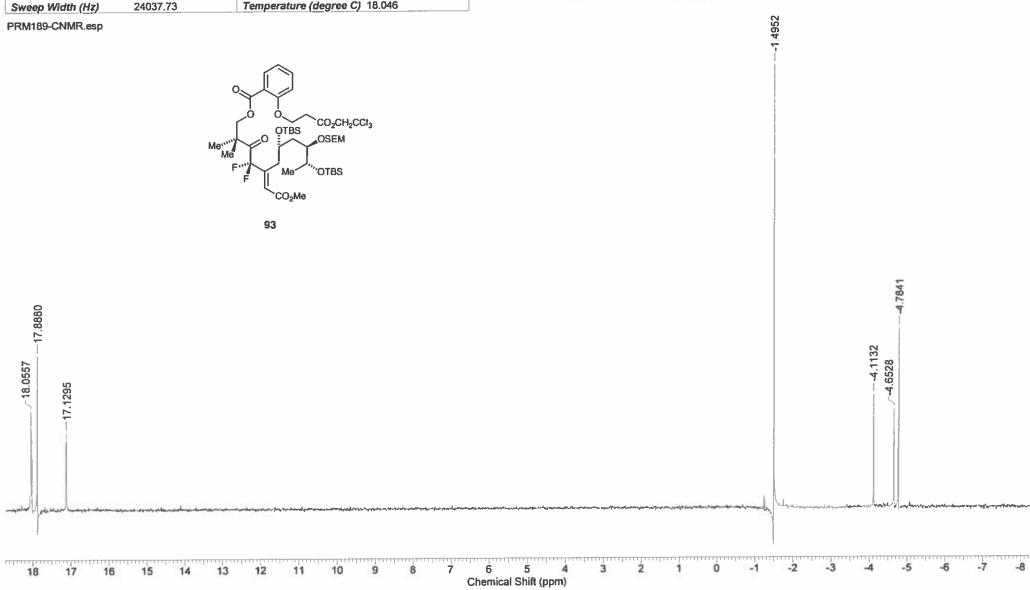
6.0

5.5

5.0

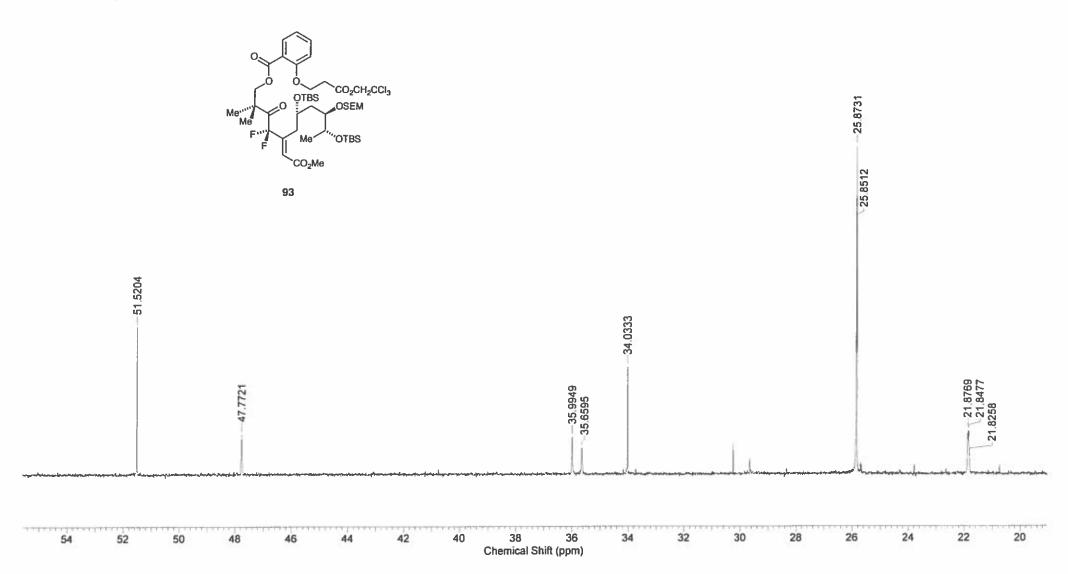
4.5

| Acquisition Time (sec) | 1.3631                | Comment                     | EJT-PRM189 prod m     | CARBON_A CDCl3 (e:\bru       | uk400cdata\2015\Aug} ejl | 54                    |          |
|------------------------|-----------------------|-----------------------------|-----------------------|------------------------------|--------------------------|-----------------------|----------|
| Date                   | 20 Aug 2015 16:00:16  |                             |                       | Date Stamp                   | 20 Aug 2015 16:00:16     |                       |          |
| File Name              | \\ss7a.ds.man.ac.uk\w | ol5\vol3\users\snmrdata\bru | uk400cdata\2015\Aug\d | lata\ejt\nmr\2015-08-20-ejt- | 54\11\fid                | Frequency (MHz)       | 100,60   |
| Nucleus                | 13C                   | Number of Transients        | 256                   | Origin                       | spect                    | Original Points Count | 32768    |
| Owner                  | nmrsu                 | Points Count                | 32768                 | Pulse Sequence               | zgpg30                   | Receiver Gain         | 71.80    |
| SW(cyclical) (Hz)      | 24038.46              | Solvent                     | CHLOROFORM-d          | Spectrum Offset (Hz)         | 10049.8672               | Spectrum Type         | STANDARD |
|                        | 0.4007.70             | T                           | 1 10 046              | 1922                         |                          |                       |          |



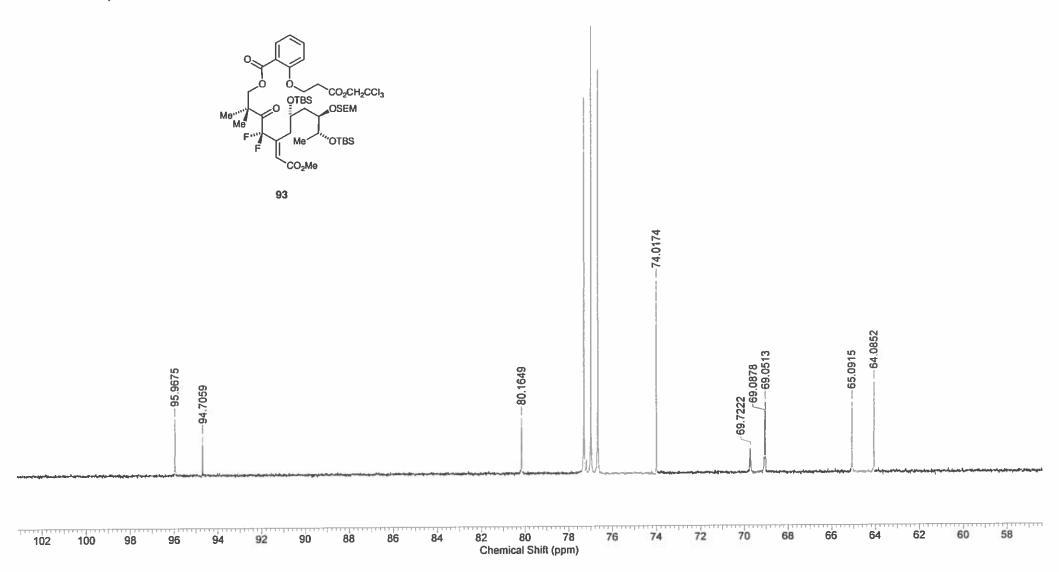
| Acquisition Time (sec) | 1.3631                | Comment                     | EJT-PRM189 prod m    | CARBON_A CDCI3 (e:\bru        | ik400cdata\2015\Aug} | ejt 54                |          |
|------------------------|-----------------------|-----------------------------|----------------------|-------------------------------|----------------------|-----------------------|----------|
| Date                   | 20 Aug 2015 16:00:16  | Set House                   |                      | Date Stamp                    | 20 Aug 2015 16:00:   | 16                    |          |
| File Name              | \\ss7a.ds.man.ac.uk\w | ol5\vol3\users\snmrdata\bru | k400cdata\2015\Aug\d | fatalejt\nmr\2015-08-20-ejt-: | 54\11\fid            | Frequency (MHz)       | 100.60   |
| Nucleus                | 13C                   | Number of Transients        | 256                  | Origin                        | spect                | Original Points Count | 32768    |
| Owner                  | nmrsu                 | Points Count                | 32768                | Pulse Sequence                | zgpg30               | Receiver Gain         | 71.80    |
| SW(cyclical) (Hz)      | 24038.46              | Solvent                     | CHLOROFORM-d         | Spectrum Offset (Hz)          | 10049.8672           | Spectrum Type         | STANDARD |
| Sween Width (Hz)       | 24037.73              | Temperature (degree C)      | 18.046               |                               |                      |                       |          |

PRM189-CNMR.esp



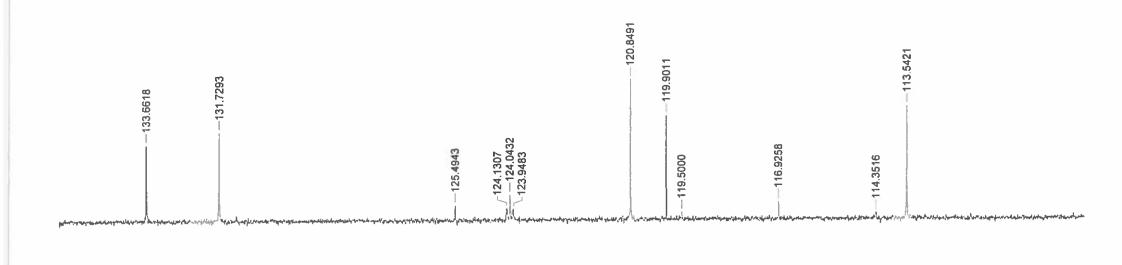
| Acquisition Time (sec) | 1.3631                | Comment                     | EJT-PRM189 prod m    | CARBON_A CDCl3 (e:\bru        | k400cdata\2015\Aug} ej | 54                    |          |
|------------------------|-----------------------|-----------------------------|----------------------|-------------------------------|------------------------|-----------------------|----------|
| Date                   | 20 Aug 2015 16:00:16  |                             |                      | Date Stamp                    | 20 Aug 2015 16:00:16   |                       |          |
|                        | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bru | k400cdata\2015\Aug\d | lata\ejt\nmr\2015-08-20-ejt-5 | 54\11\fid              | Frequency (MHz)       | 100.60   |
| Nucleus                | 13C                   | Number of Transients        | 256                  | Origin                        | spect                  | Original Points Count | 32768    |
| Owner                  | nmrsu                 | Points Count                | 32768                | Pulse Sequence                | zgpg30                 | Receiver Gain         | 71.80    |
| SW(cyclical) (Hz)      | 24038.46              | Solvent                     | CHLOROFORM-d         | Spectrum Offset (Hz)          | 10049.8672             | Spectrum Type         | STANDARD |
| Swaan Width (Hz)       | 24037.73              | Temperature (degree C)      | 18.046               |                               |                        |                       |          |

PRM189-CNMR.esp



| Acquisition Time (sec) | 1,3631                | Comment                     | EJT-PRM189 prod m     | CARBON_A CDCI3 (e:\bru       | ık400cdala\2015\Aug} e | ijt 54                |          |
|------------------------|-----------------------|-----------------------------|-----------------------|------------------------------|------------------------|-----------------------|----------|
| Date                   | 20 Aug 2015 16:00:16  |                             |                       | Date Stamp                   | 20 Aug 2015 16:00:1    | 6                     |          |
|                        | \\ss7a.ds.man.ac.uk\v | ol5\vol3\users\snmrdata\bru | ık400cdata\2015\Aug\d | lata\ejt\nmr\2015-08-20-ejt- | 54\11\fid              | Frequency (MHz)       | 100.60   |
| Nucleus                | 13C                   | Number of Transients        | 256                   | Origin                       | spect                  | Original Points Count | 32768    |
| Owner                  | nmrsu                 | Points Count                | 32768                 | Pulse Sequence               | zgpg30                 | Receiver Gain         | 71.80    |
| SW(cyclical) (Hz)      | 24038.46              | Solvent                     | CHLOROFORM-d          | Spectrum Offset (Hz)         | 10049.8672             | Spectrum Type         | STANDARD |
| Sweep Width (Hz)       | 24037.73              | Temperature (degree C)      | 18.046                |                              |                        | 150H                  |          |

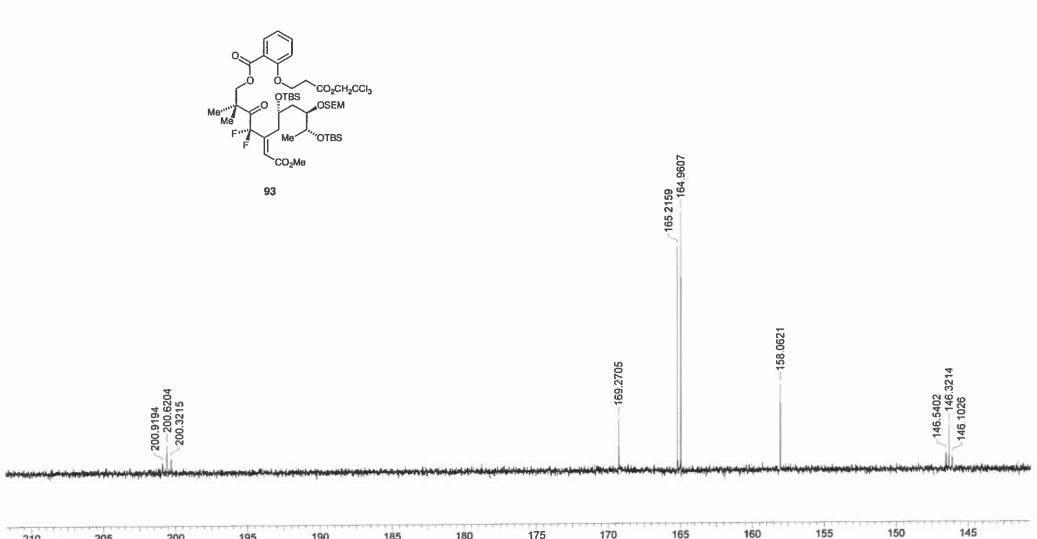
PRM189-CNMR.esp



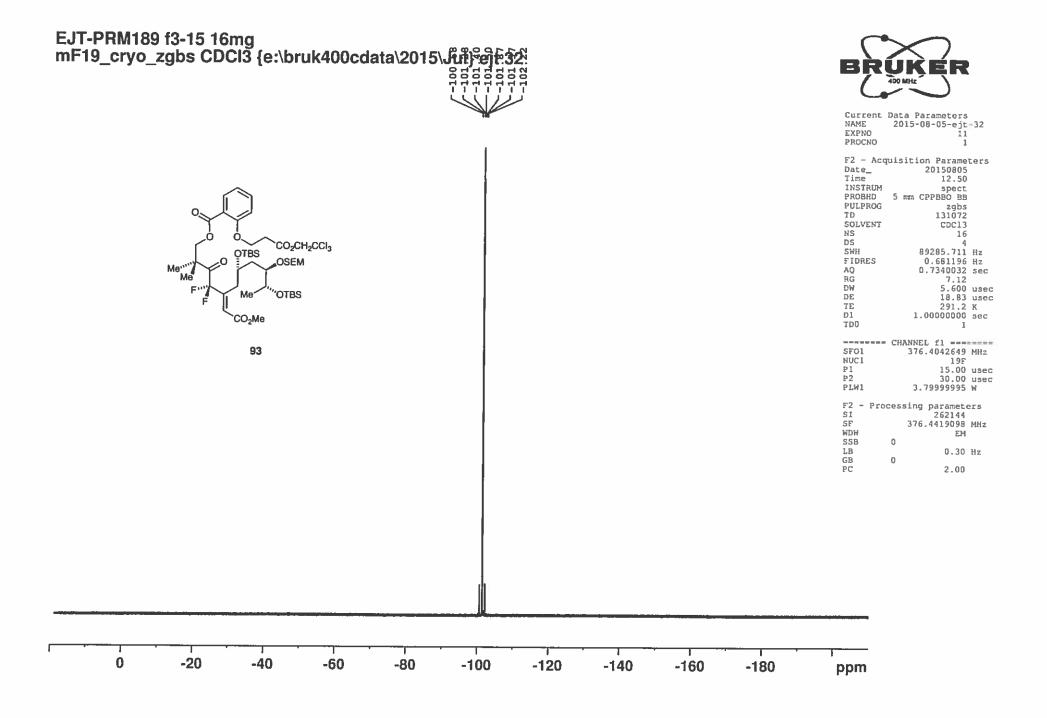
1 123 122 12 Chemical Shift (ppm) 

| Acquisition Time (sec) | 1.3631               | Comment                     | EJT-PRM189 prod m    | CARBON_A CDCI3 {e:\bru       | ik400cdata\2015\Aug} | ejt 54                |          |
|------------------------|----------------------|-----------------------------|----------------------|------------------------------|----------------------|-----------------------|----------|
| Date                   | 20 Aug 2015 16:00:10 | 3                           |                      | Date Stamp                   | 20 Aug 2015 16:00:   | 16                    |          |
|                        |                      | ol5\vol3\users\snmrdata\bru | k400cdata\2015\Aug\d | lata\ejt\nmr\2015-08-20-ejt- | 54\11\fid            | Frequency (MHz)       | 100.60   |
| Nucleus                | 13C                  | Number of Transients        | 256                  | Origin                       | spect                | Original Points Count | 32768    |
| Owner                  | nmrsu                | Points Count                | 32768                | Pulse Sequence               | zgpg30               | Receiver Gain         | 71.80    |
| SW(cyclical) (Hz)      | 24038.46             | Solvent                     | CHLOROFORM-d         | Spectrum Offset (Hz)         | 10049,8672           | Spectrum Type         | STANDARD |
| Sweep Width (Hz)       | 24037.73             | Temperature (degree C)      | 18.046               |                              |                      |                       |          |

PRM189-CNMR.esp



30 175 Chemical Shift (ppm)

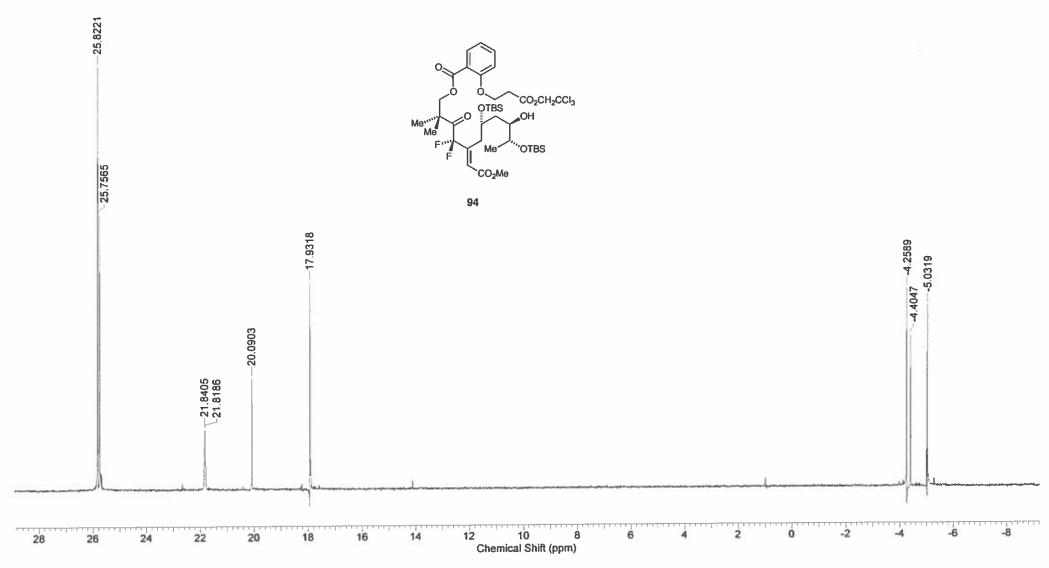


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM190 f7-19 11mg mPROTON CDCl3 {E:\bruk500adata\2015\Aug} ejt 43

| Acquisition Time (sec)                                             | 3.1719                        | Comment                        | EJT-PRM190 f7-19 1                              | 1mg mPROTON CDC13 (E                                                         | \bruk500adata\2015\A                           | ug} ejt 43            |                                       |
|--------------------------------------------------------------------|-------------------------------|--------------------------------|-------------------------------------------------|------------------------------------------------------------------------------|------------------------------------------------|-----------------------|---------------------------------------|
| Date                                                               | 13 Aug 2015 14:17             | :52                            |                                                 | Date Stamp                                                                   | 13 Aug 2015 14:17:                             | 52                    |                                       |
| ile Name                                                           | \\ss7a.ds.man.ac.u            | k\vol5\vol3\users\snmrdata\bru | ık500adata\2015\Aug\da                          |                                                                              |                                                | Frequency (MHz)       | 500.13                                |
| lucleus                                                            | 1H                            | Number of Transients           | 16                                              | Origin                                                                       | spect                                          | Original Points Count | 32768                                 |
| )wner                                                              | nmrsu                         | Points Count                   | 32768                                           | Pulse Sequence                                                               | zg30                                           | Receiver Gain         | 144.00                                |
| SW(cyclical) (Hz)                                                  | 10330.58                      | Solvent                        | CHLOROFORM-d                                    | Spectrum Offset (Hz)                                                         | 3081.2380                                      | Spectrum Type         | STANDARD                              |
| Sweep Width (Hz)                                                   | 10330.26                      | Temperature (degree C          | 25.000                                          |                                                                              |                                                |                       |                                       |
| RM190-HNMR.esp                                                     |                               | O OTBS                         | O <sub>2</sub> CH <sub>2</sub> CCI <sub>3</sub> |                                                                              |                                                |                       | 0.8724                                |
|                                                                    |                               | Me""Me                         | OTBS                                            |                                                                              |                                                |                       |                                       |
|                                                                    |                               |                                | .8034                                           | 3,6504                                                                       |                                                | 3912                  | 0.0876<br>0.0624<br>0.0542<br>-0.0290 |
| 7.6942<br>7.6905<br>7.6753<br>7.4824<br>7.4679<br>7.4660<br>7.4623 | -7.4478<br>-7.0116<br>-6.9750 | 6.1442                         | 4.4201                                          | 4.2361<br>4.2190<br>4.2020<br>4.2020<br>3.5994<br>3.5994<br>3.5988<br>3.5994 | 3.0283<br>3.0283<br>3.0150<br>2.8877<br>2.8619 | 1 2 E F               | 1.1239                                |
| 0.98 1.02                                                          | 2.05                          | 0.96                           | 2.05 2.05 2.13                                  | 1.04 3.00 1.03 1.20 2.                                                       | 17 0.88 1.05 O.                                | 88 2.21 2.59 6.03 3   |                                       |
| 8.0 7.5                                                            | 7.0 6.5                       | 6.0 5.5                        | 5.0 4.5                                         | 4.0 3.5<br>Chemical Shift (ppm)                                              | 3.0 2.5                                        | 2.0 1.5               | 1.0 0.5 0                             |

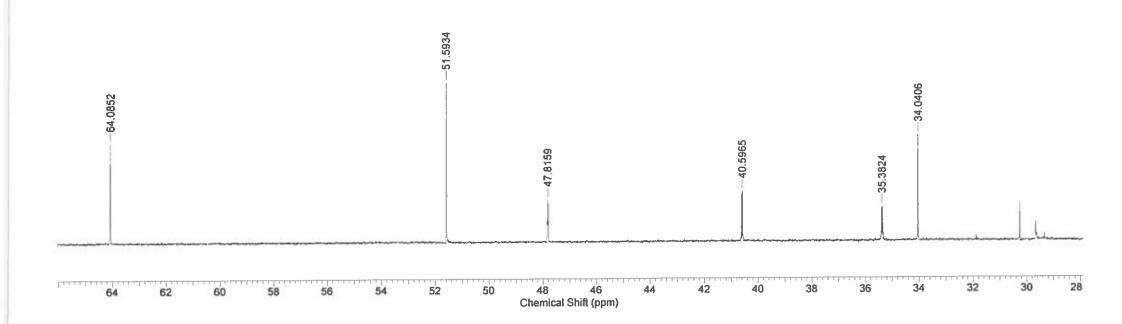
| Acquisition Time (sec) | 1.3631               | Comment                | EJT-PRM190 f13-46     | 54mg mCARBON_B CDCI          | 3 (e:\bruk400cdata\2015\ | Aug} ejt 6            |          |
|------------------------|----------------------|------------------------|-----------------------|------------------------------|--------------------------|-----------------------|----------|
| Date                   | 21 Aug 2015 22:58:24 |                        |                       | Date Stamp                   | 21 Aug 2015 22:58:24     |                       |          |
| File Name              |                      |                        | k400cdata\2015\Aug\da | ata\ejt\nmr\2015-08-21-ejt-6 | \21\fid                  | Frequency (MHz)       | 100.60   |
| Nucleus                | 13C                  | Number of Transients   | 1000                  | Origin                       | spect                    | Original Points Count | 32768    |
| Owner                  | nmrsu                | Points Count           | 32768                 | Pulse Sequence               | zgpg30                   | Receiver Gain         | 45.20    |
| SW(cyclical) (Hz)      | 24038.46             | Solvent                | CHLOROFORM-d          | Spectrum Offset (Hz)         | 10049,8789               | Spectrum Type         | STANDARD |
| Sweep Width (Hz)       | 24037.73             | Temperature (degree C) | 18.170                |                              |                          |                       |          |

PRM190-CNMR.esp



| Acquisition Time (sec) | 1.3631              | Comment                       | nment EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 {e:\bruk400cdata\2015\Aug} ejt 6 |                              |                     |                       |          |  |  |
|------------------------|---------------------|-------------------------------|-------------------------------------------------------------------------------|------------------------------|---------------------|-----------------------|----------|--|--|
| Date                   | 21 Aug 2015 22:58:2 | 4                             |                                                                               | Date Stamp                   | 21 Aug 2015 22:58:2 | 4                     |          |  |  |
|                        |                     | vol5\vol3\users\snmrdata\brul | <400cdata\2015\Aug\da                                                         | ata\ejt\nmr\2015-08-21-ejt-6 | 1\21\fid            | Frequency (MHz)       | 100.60   |  |  |
| Nucleus                | 13C                 | Number of Transients          | 1000                                                                          | Origin                       | spect               | Original Points Count | 32768    |  |  |
| Owner                  | nmrsu               | Points Count                  | 32768                                                                         | Pulse Sequence               | zgpg30              | Receiver Gain         | 45.20    |  |  |
| SW(cyclical) (Hz)      | 24038.46            | Solvent                       | CHLOROFORM-d                                                                  | Spectrum Offset (Hz)         | 10049.8789          | Spectrum Type         | STANDARD |  |  |
| Sweep Width (Hz)       | 24037.73            | Temperature (degree C)        | 18.170                                                                        |                              |                     |                       |          |  |  |

PRM190-CNMR.esp

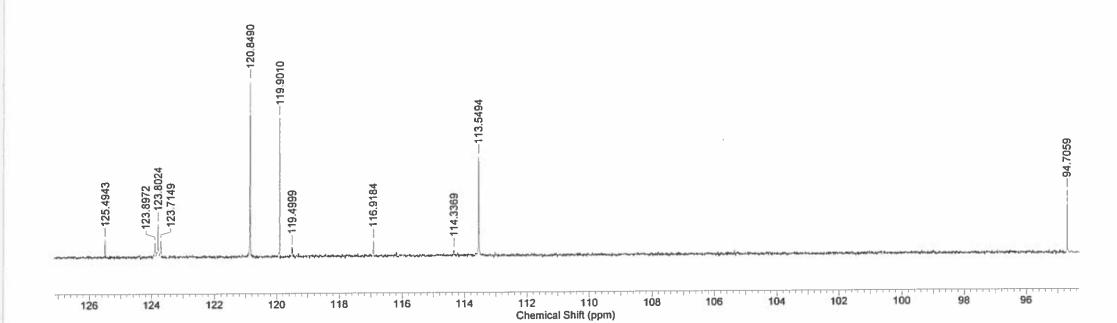


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/ EJT-PRM190 f13-46 54mg mCARBON\_B CDCl3 (e:\bruk400cdata\2015\Aug\ ejt 6 Acquisition Time (sec) 1.3631 Comment 21 Aug 2015 22:58:24 Date Stamp 21 Aug 2015 22:58:24 Date Frequency (MHz) 100.60 File Name Original Points Count 32768 Origin spect Number of Transients 1000 13C Nucleus zgpg30 Receiver Gain 45.20 Pulse Sequence 32768 Points Count nmrsu Owner **STANDARD** Spectrum Offset (Hz) 10049.8789 Spectrum Type CHLOROFORM-d 24038.46 Solvent SW(cyclical) (Hz) Temperature (degree C) 18.170 Sweep Width (Hz) 24037.73 PRM190-CNMR.esp CO2CH2CCI3 OTBS 94 64.0852 74 0247 68,4971 94.7059 -69.6712

96 94 92 90 88 86 84 82 80 78 76 74 72 70 68 66 64 Chemical Shift (ppm)

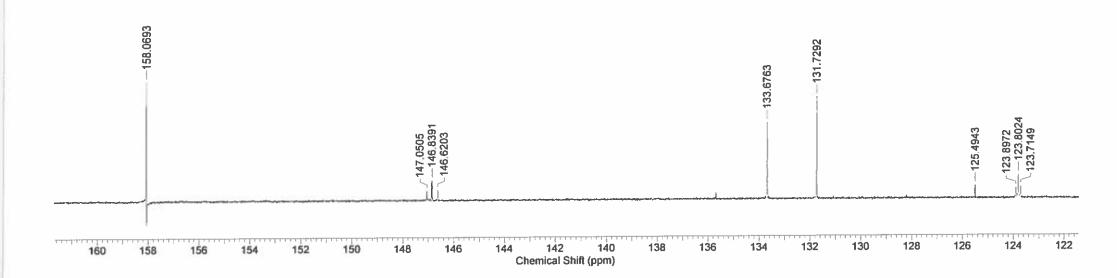
| Acquisition Time (sec) | 1.3631               | Comment EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 (e:\bruk400cdata\2015\Aug) ejt 6 |                      |                              |                      |                       |          |  |  |
|------------------------|----------------------|---------------------------------------------------------------------------------|----------------------|------------------------------|----------------------|-----------------------|----------|--|--|
| Date                   | 21 Aug 2015 22:58:24 |                                                                                 |                      | Date Stamp                   | 21 Aug 2015 22:58:24 |                       |          |  |  |
|                        |                      | i5\vol3\users\snmrdata\bruk                                                     | 400cdata\2015\Aug\da | ata\ejt\nmr\2015-08-21-ejt-6 | 1\21\fid             | Frequency (MHz)       | 100.60   |  |  |
| Nucleus                |                      | Number of Transients                                                            | 1000                 | Origin                       | spect                | Original Points Count | 32768    |  |  |
| Owner                  | nmrsu                | Points Count                                                                    | 32768                | Pulse Sequence               | zgpg30               | Receiver Gain         | 45.20    |  |  |
| SW(cyclical) (Hz)      | 24038.46             | Solvent                                                                         | CHLOROFORM-d         | Spectrum Offset (Hz)         | 10049.8789           | Spectrum Type         | STANDARD |  |  |
| Sweep Width (Hz)       | 24037.73             | Temperature (degree C)                                                          | 18.170               |                              |                      |                       |          |  |  |

PRM190-CNMR esp



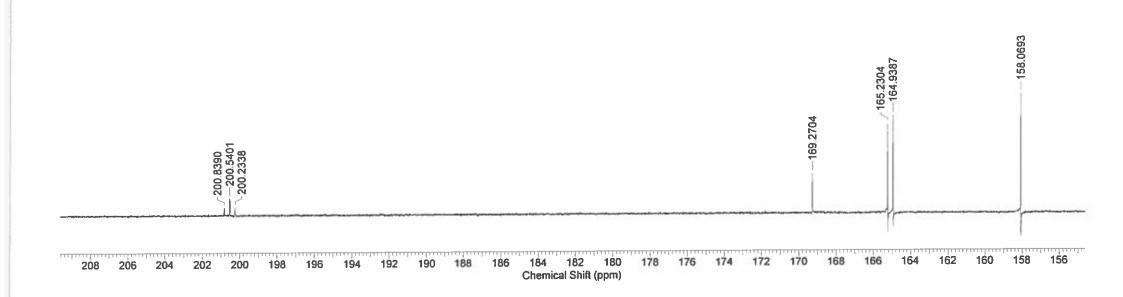
| Acquisition Time (sec) | 1,3631               | Comment                     | EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 (e:\bruk400cdata\2015\Aug} ejt 6 |                             |                      |                       |          |  |  |
|------------------------|----------------------|-----------------------------|-------------------------------------------------------------------------|-----------------------------|----------------------|-----------------------|----------|--|--|
| Date                   | 21 Aug 2015 22:58:24 |                             | 367.000.0                                                               | Date Stamp                  | 21 Aug 2015 22:58:24 |                       |          |  |  |
|                        |                      | l5\vol3\users\snmrdata\bruk | 400cdata\2015\Aug\da                                                    | ta\ejt\nmr\2015-08-21-ejt-6 | i\21\fid             | Frequency (MHz)       | 100.60   |  |  |
| Nucleus                | 13C                  | Number of Transients        | 1000                                                                    | Origin                      | spect                | Original Points Count | 32768    |  |  |
| Owner                  | nmrsu                | Points Count                | 32768                                                                   | Pulse Sequence              | zgpg30               | Receiver Gain         | 45.20    |  |  |
| SW(cyclical) (Hz)      | 24038.46             | Solvent                     | CHLOROFORM-d                                                            | Spectrum Offset (Hz)        | 10049.8789           | Spectrum Type         | STANDARD |  |  |
| Sweep Width (Hz)       | 24037.73             | Temperature (degree C)      | 18.170                                                                  |                             |                      |                       |          |  |  |

PRM190-CNMR.esp

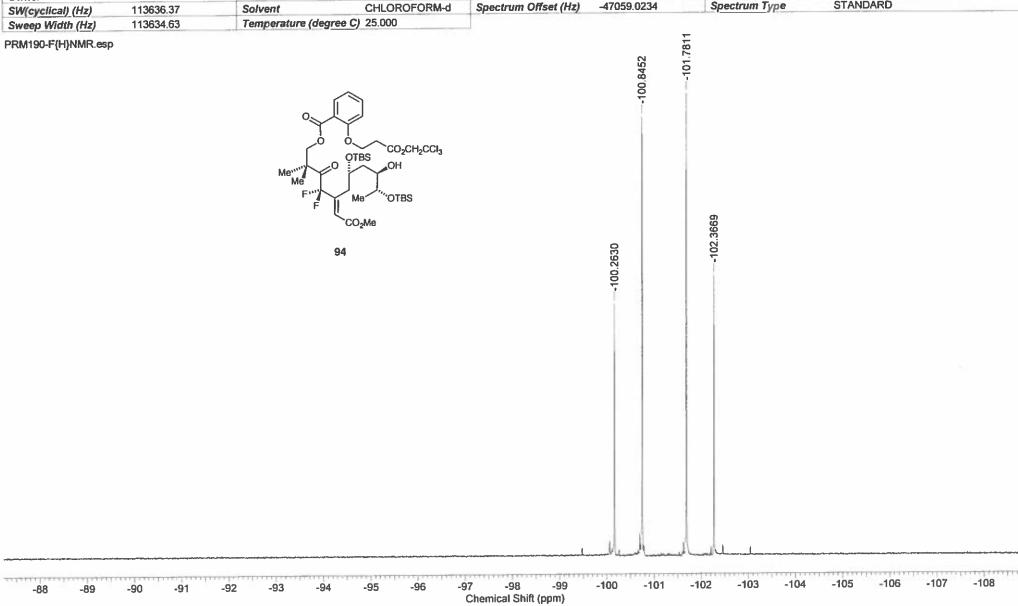


| Acquisition Time (sec) | 1,3631                 | Comment EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 (e:\bruk400cdata\2015\Aug) ejt 6 |                      |                              |                      |                       |                                         |  |  |
|------------------------|------------------------|---------------------------------------------------------------------------------|----------------------|------------------------------|----------------------|-----------------------|-----------------------------------------|--|--|
| Date                   | 21 Aug 2015 22:58:24   |                                                                                 |                      | Date Stamp                   | 21 Aug 2015 22:58:24 |                       | 211111111111111111111111111111111111111 |  |  |
| File Name              | \\ss7a.ds.man.ac.uk\vo | l5\vol3\users\snmrdata\bruk                                                     | 400cdata\2015\Aug\da | ntalejtlnmr\2015-08-21-ejt-6 | 1\21\fid             | Frequency (MHz)       | 100.60                                  |  |  |
| Nucleus                | 13C                    | Number of Transients                                                            | 1000                 | Origin                       | spect                | Original Points Count | 32768                                   |  |  |
| Owner                  | nmrsu                  | Points Count                                                                    | 32768                | Pulse Sequence               | zgpg30               | Receiver Gain         | 45.20                                   |  |  |
| SW(cyclical) (Hz)      | 24038.46               | Solvent                                                                         | CHLOROFORM-d         | Spectrum Offset (Hz)         | 10049.8789           | Spectrum Type         | STANDARD                                |  |  |
| Sweep Width (Hz)       | 24037.73               | Temperature (degree C)                                                          | 18.170               |                              |                      |                       |                                         |  |  |

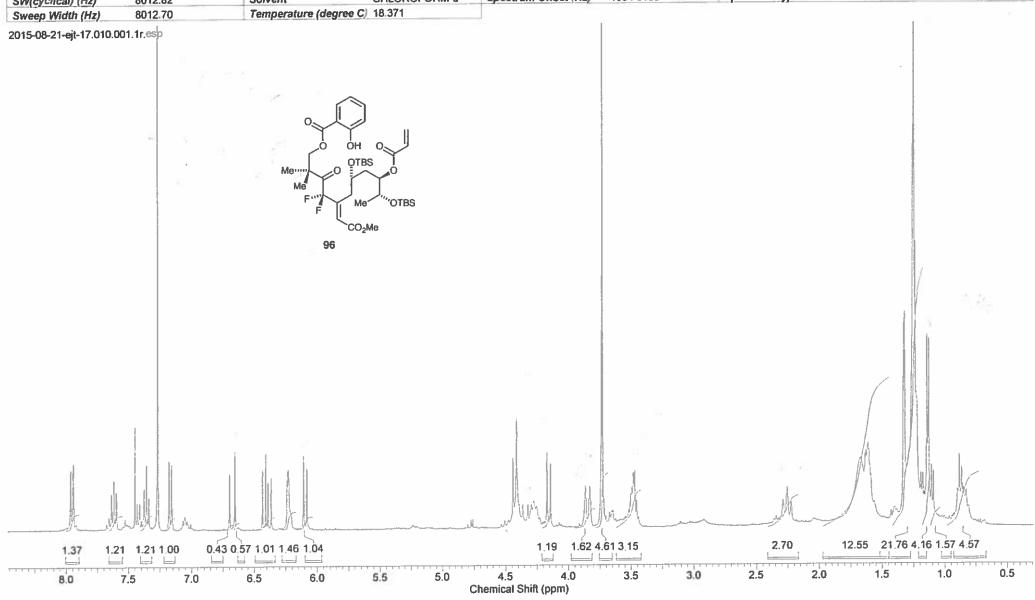
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|                        |                      | To be seen as        |                       | The state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the s |                      |                       |          |  |  |  |
|------------------------|----------------------|----------------------|-----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------|-----------------------|----------|--|--|--|
| Acquisition Time (sec) | 0.5767               | Comment              | EJT-PRM190 f7-19 1    | 11mg m19FCPD CDCl3 (E:\bruk500adata\2015\Aug) ejt 43                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                      |                       |          |  |  |  |
| Date                   | 13 Aug 2015 14:32:48 |                      |                       | Date Stamp                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 13 Aug 2015 14:32:48 |                       |          |  |  |  |
| File Name              |                      |                      | k500adata\2015\Aug\da | ata\ejt\nmr\2015-08-13-ejt-4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 3\13\fid             | Frequency (MHz)       | 470.59   |  |  |  |
| Nucleus                | 19F                  | Number of Transients | 16                    | Origin                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | spect                | Original Points Count | 65536    |  |  |  |
| Owner                  | nmrsu                | Points Count         | 65536                 | Pulse Sequence                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | zgfhigan             | Receiver Gain         | 575.00   |  |  |  |
| SW(cyclical) (Hz)      | 113636.37            | Solvent              | CHLOROFORM-d          | Spectrum Offset (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | -47059.0234          | Spectrum Type         | STANDARD |  |  |  |
| Style) chean (172)     | 110000.01            | =                    | AE 000                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                      |                       |          |  |  |  |

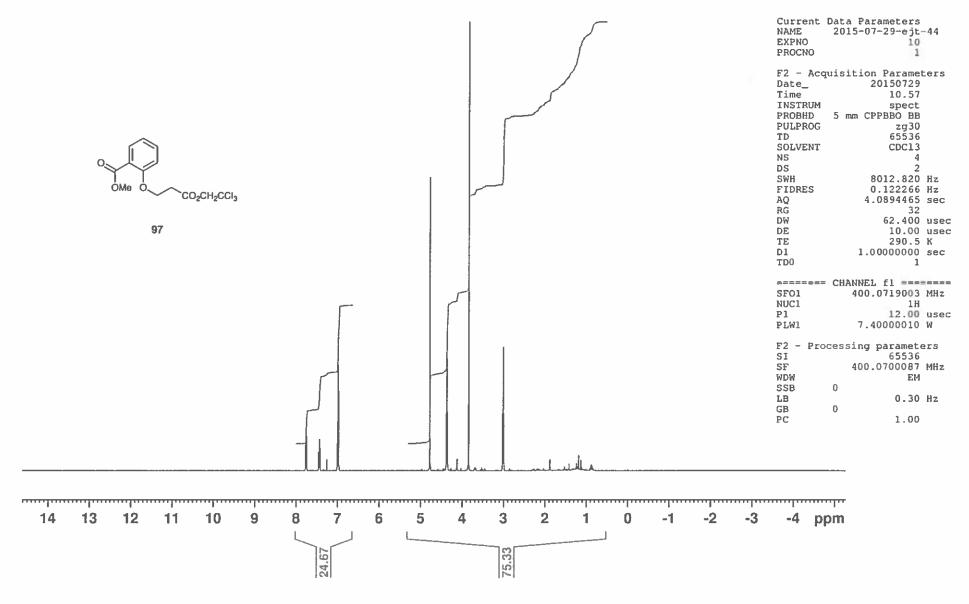


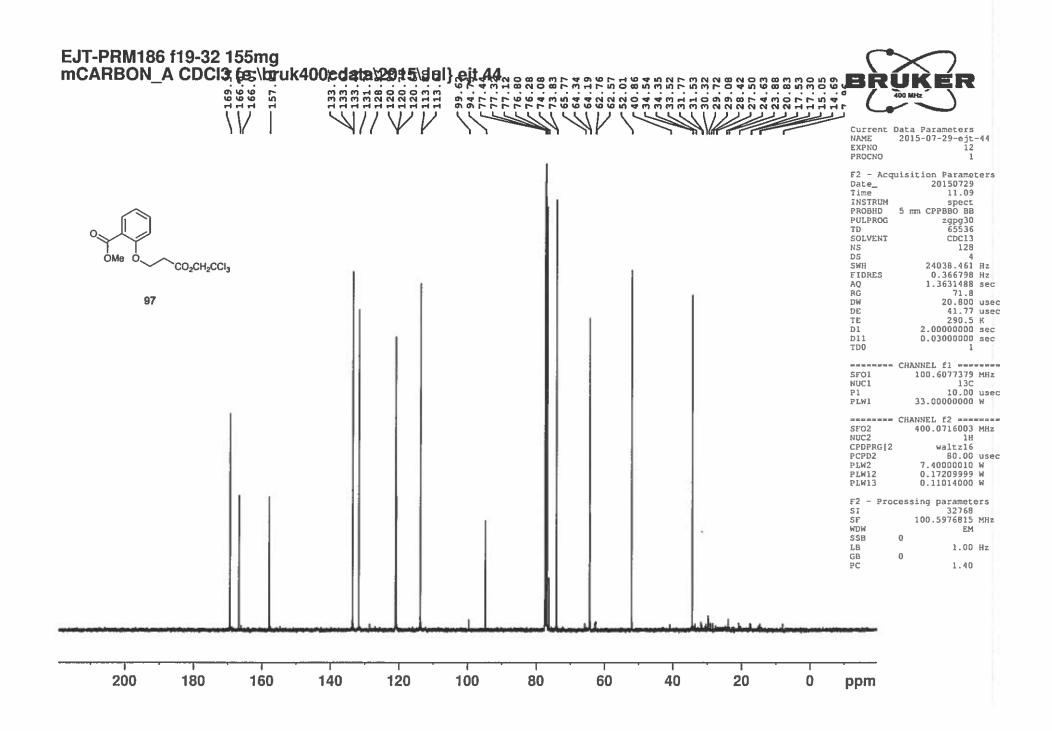
|                        | Tino topers mas of     |                             |                                                                                    | And the second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second s |               |                       | •        |  |
|------------------------|------------------------|-----------------------------|------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------|-----------------------|----------|--|
| Acquisition Time (sec) | 4.0894                 | Comment                     | EJT-PRM193 f11-18 5mg chloroform mPROTON_A CDCl3 {e:\bruk400cdata\2015\Aug} ejt 17 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |               |                       |          |  |
| Date                   | 21 Aug 2015 15:56:00   |                             | 21 Aug 2015 15:56:00                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |               |                       |          |  |
| File Name              | \\ss7a.ds.man.ac.uk\vo | l5\vol3\users\snmrdata\brul | (400cdata\2015\Aug\data                                                            | \ejt\nmr\2015-08-21-ejt-17\                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 10\PDATA\1\1r | Frequency (MHz)       | 400.07   |  |
| Nucleus                | 1H                     | Number of Transients        | 4                                                                                  | Origin                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | spect         | Original Points Count | 32768    |  |
| Owner                  | nmrsu                  | Points Count                | 65536                                                                              | Pulse Sequence                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | zg30          | Receiver Gain         | 203.00   |  |
| SW(cyclical) (Hz)      | 8012.82                | Solvent                     | CHLOROFORM-d                                                                       | Spectrum Offset (Hz)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1894.6188     | Spectrum Type         | STANDARD |  |
| 011,00,000             |                        |                             | 1 40 074                                                                           | N 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |               |                       |          |  |



## EJT-PRM186 f19-32 155mg mPROTON\_A CDCl3 {e:\bruk400cdata\2015\Jul} ejt 44







## EJT-PRM187 f22-29 14mg mPROTON\_A CDCl3 {e:\bruk400cdata\2015\Jul} ejt 21



