

SUPPLEMENTARY INFORMATION

A Microwave-Assisted Highly Practical Chemoselective Esterification and Amidation of Carboxylic Acids

GunindraPathak, Diparjun Das and Samuel LalthazualaRokhum*

^aDepartment of Chemistry, National Institute of Technology Silchar, Silchar-10, Assam, India

* Corresponding author. Tel.: +91 3842 242915; fax: +91 3842-224797; email address: rokhum@che.nits.ac.in

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General Remarks

IR spectra were recorded on a Perkin–Elmer Spectrum One FTIR spectrometer. ^1H and ^{13}C NMR spectra were recorded on a Bruker (500 MHz, 400 MHz and 300 MHz) spectrometer using TMS as internal reference. Chemical shifts for ^1H NMR spectra are reported (in parts per million) relative to internal tetramethylsilane (Me_4Si $\delta = 0.0$ ppm) with CDCl_3 as solvents. ^{13}C NMR spectra were recorded at 125 MHz and 100 MHz. Chemical shifts for ^{13}C NMR spectra are reported (in parts per million) relative to internal tetramethylsilane (Me_4Si $\delta = 0.0$ ppm) with CDCl_3 as solvent. ^1H NMR data are reported in the order of chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublet, and m = multiplet), number of protons, and coupling constant in hertz (Hz). Mass spectra were obtained from Waters ZQ 4000 mass spectrometer by the ESI method, while the elemental analyses of the complexes were performed on a Perkin–Elmer-2400 CHN/S analyzer. TLC plates were visualized by exposing in iodine chamber, UV-lamp or spraying with KMnO_4 and heating.

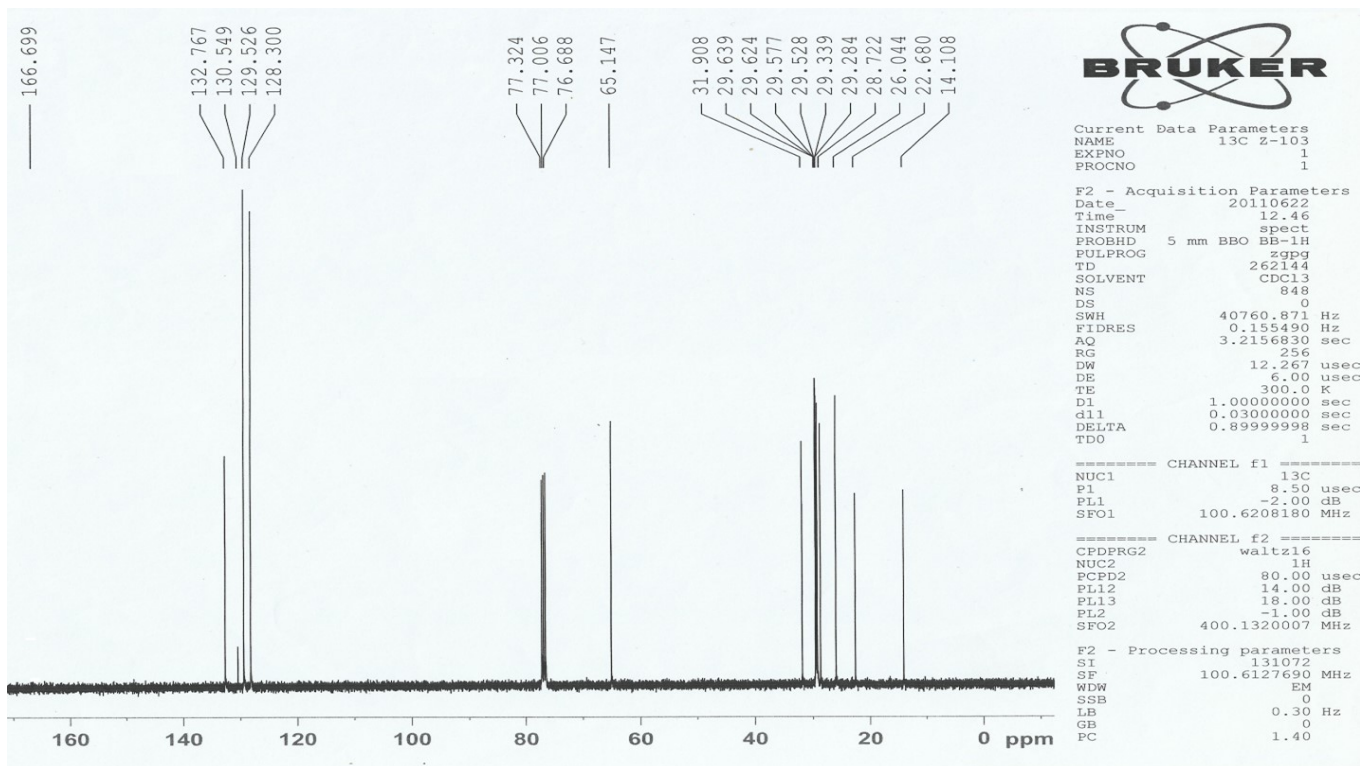
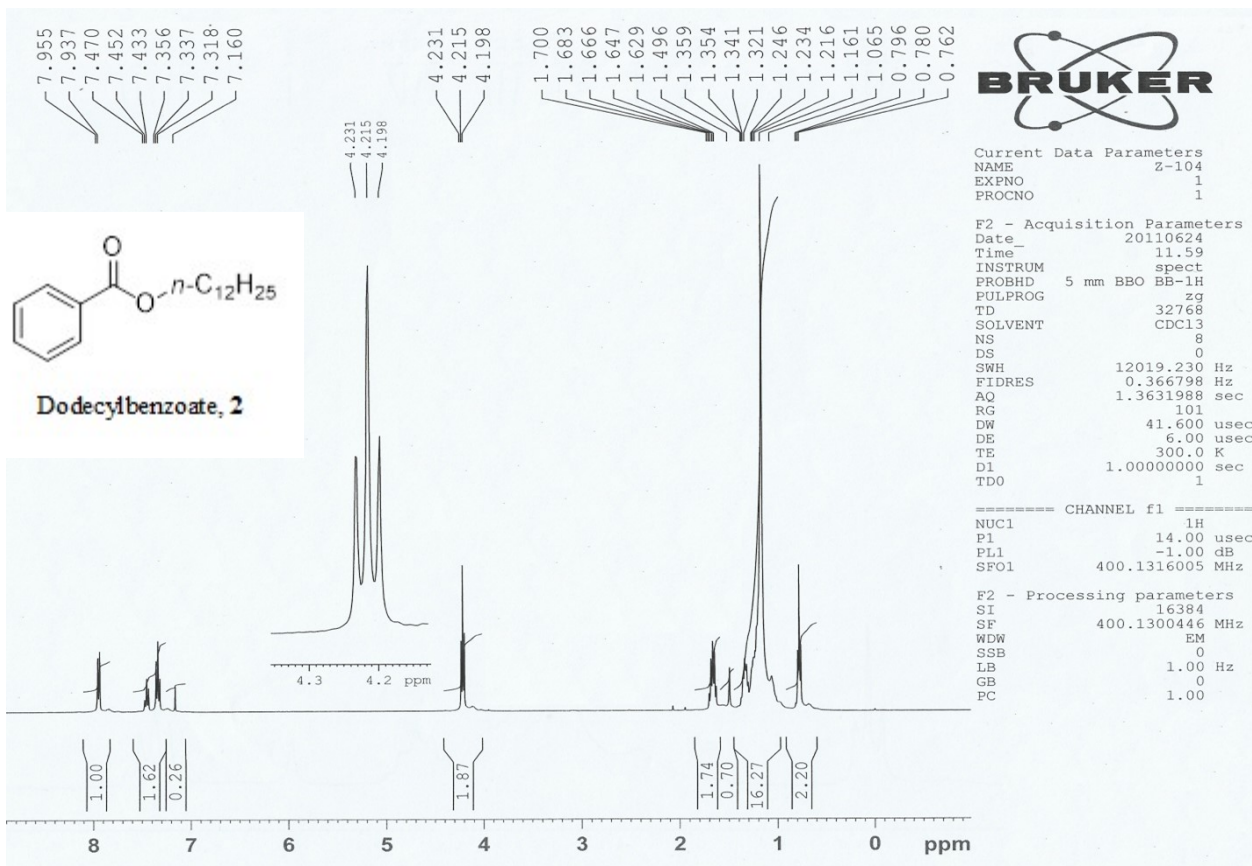
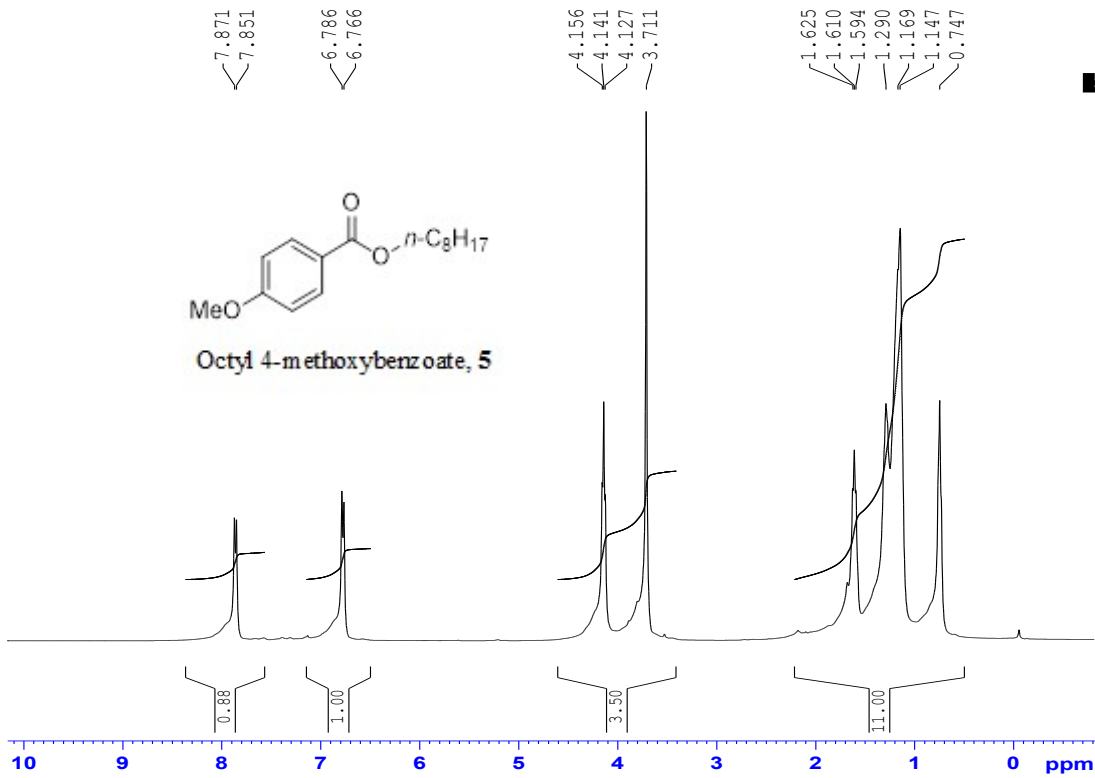


Fig: ¹H & ¹³C NMR of Dodecylbenzoate, 2

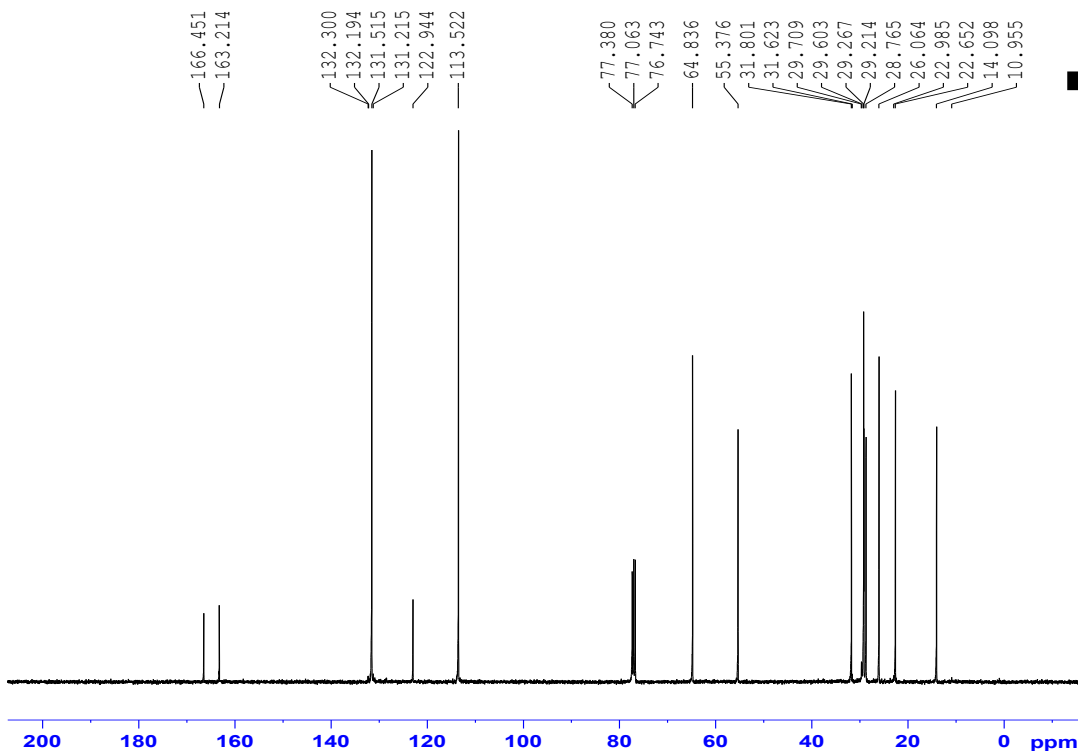
1H EN1, CDCl3, 28/05/15, SAIF, NEHU



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FIDRES 0.610352 Hz
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RG 28.5
DW 25.000 usec
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TE 300.0 K
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TDO 1
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13C EN1, CDCl3, 28/05/15, SAIF, NEHU



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SOLVENT CDCl3
NS 940
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SWH 40760.871 Hz
FIDRES 0.612393 Hz
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TDO 1
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PL1 0.00 dB
SFO1 100.6208180 MHz

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PL12 16.00 dB
PL13 20.00 dB
SFO2 400.1320007 MHz
SI 32768
SF 100.6127690 MHz
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Fig: ¹H & ¹³C NMR of Octyl 4-methoxybenzoate . 5

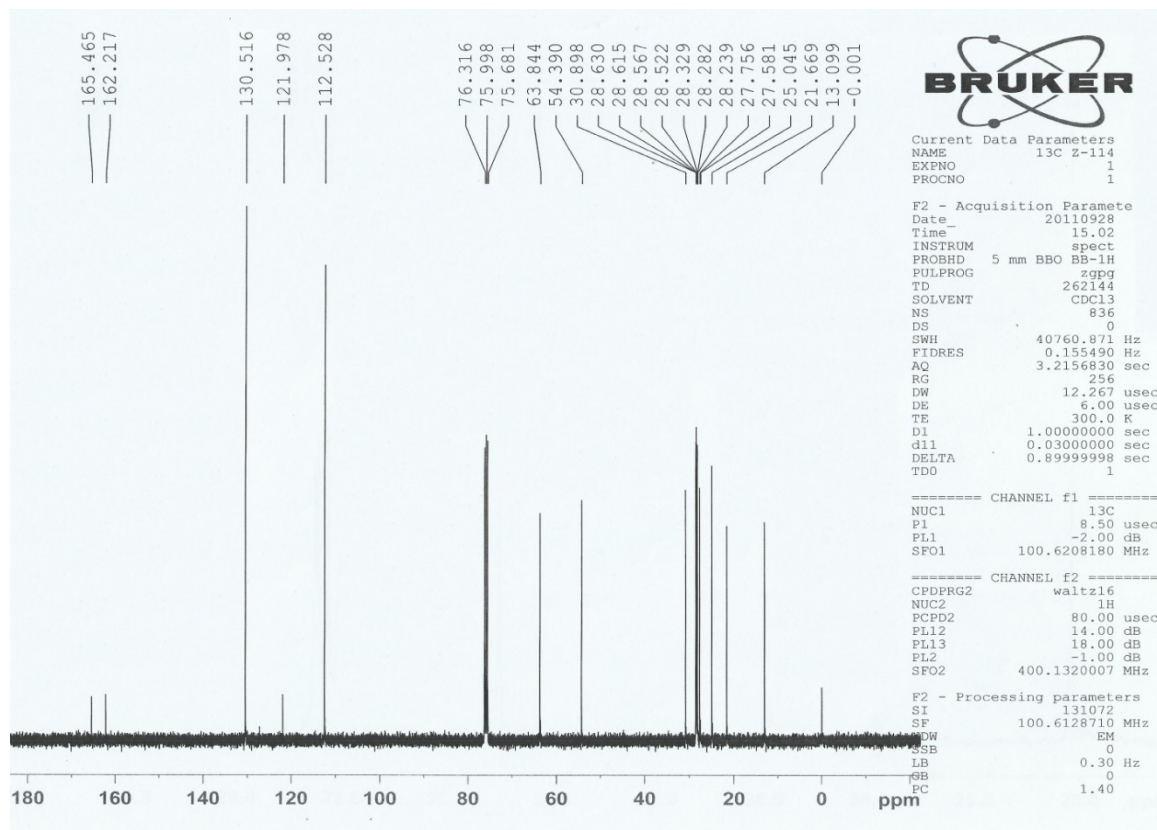
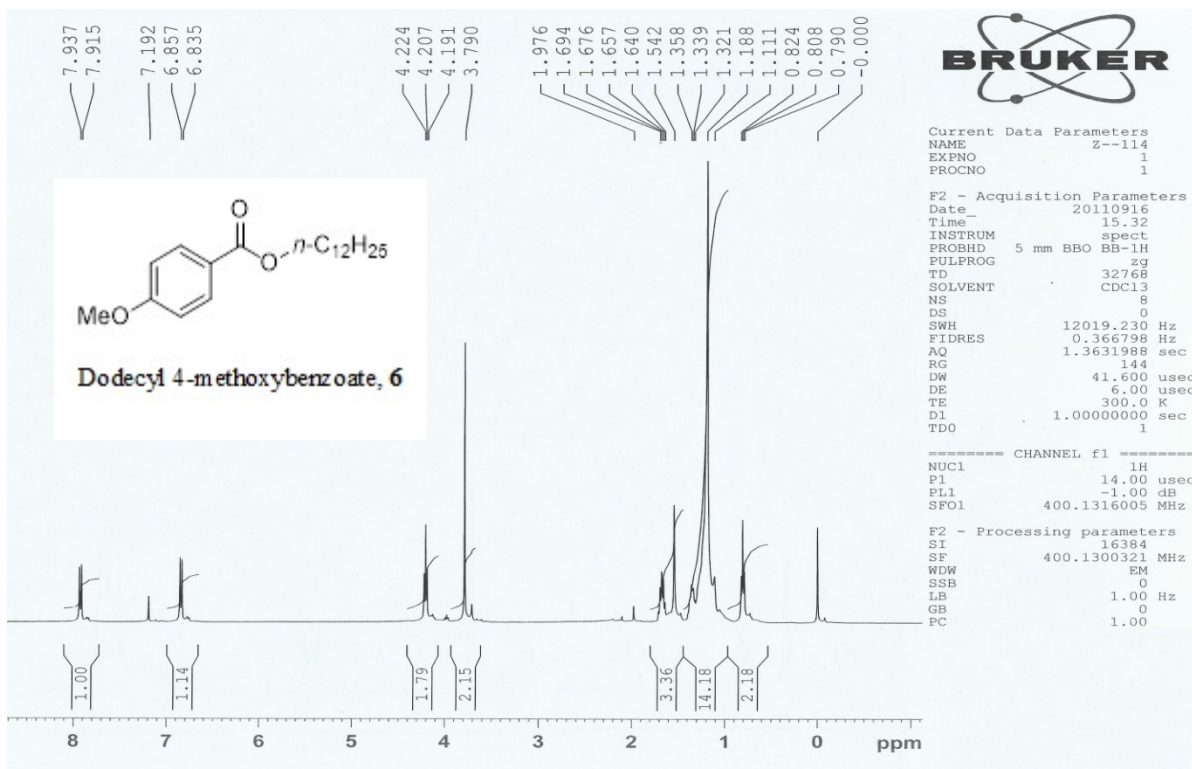


Fig: ¹H & ¹³C NMR of Dodecyl 4-methoxybenzoate, 6

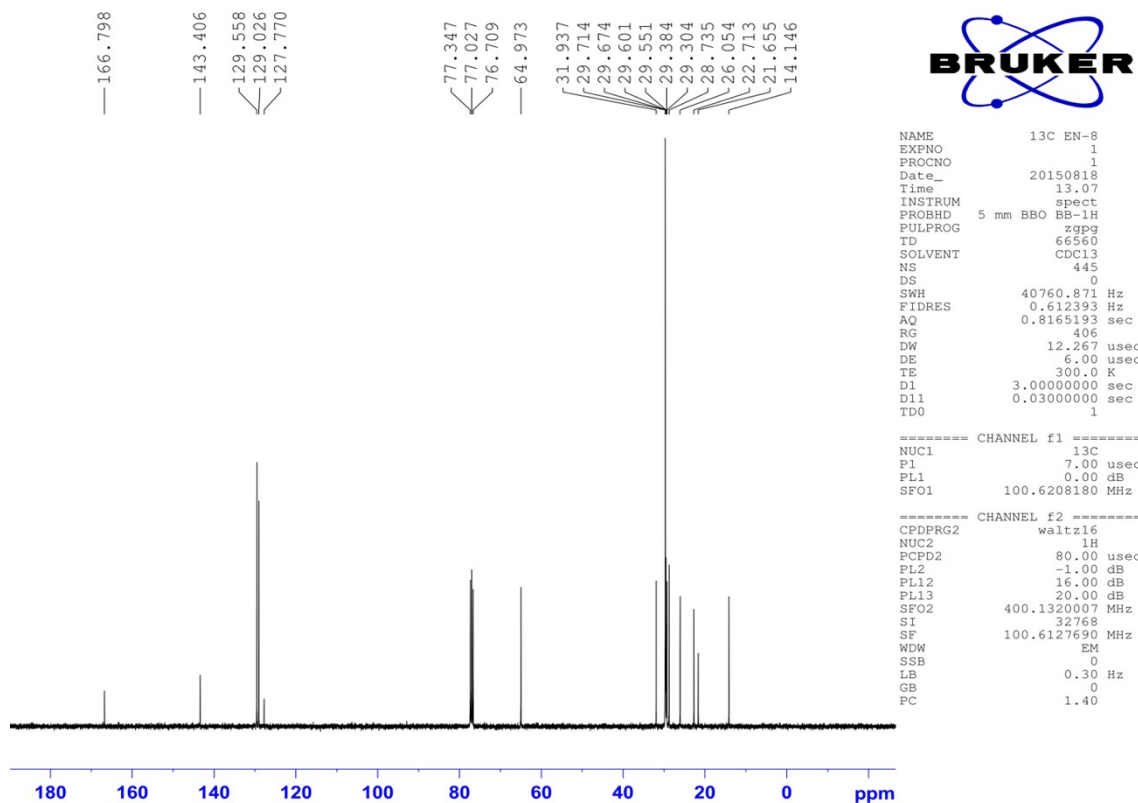
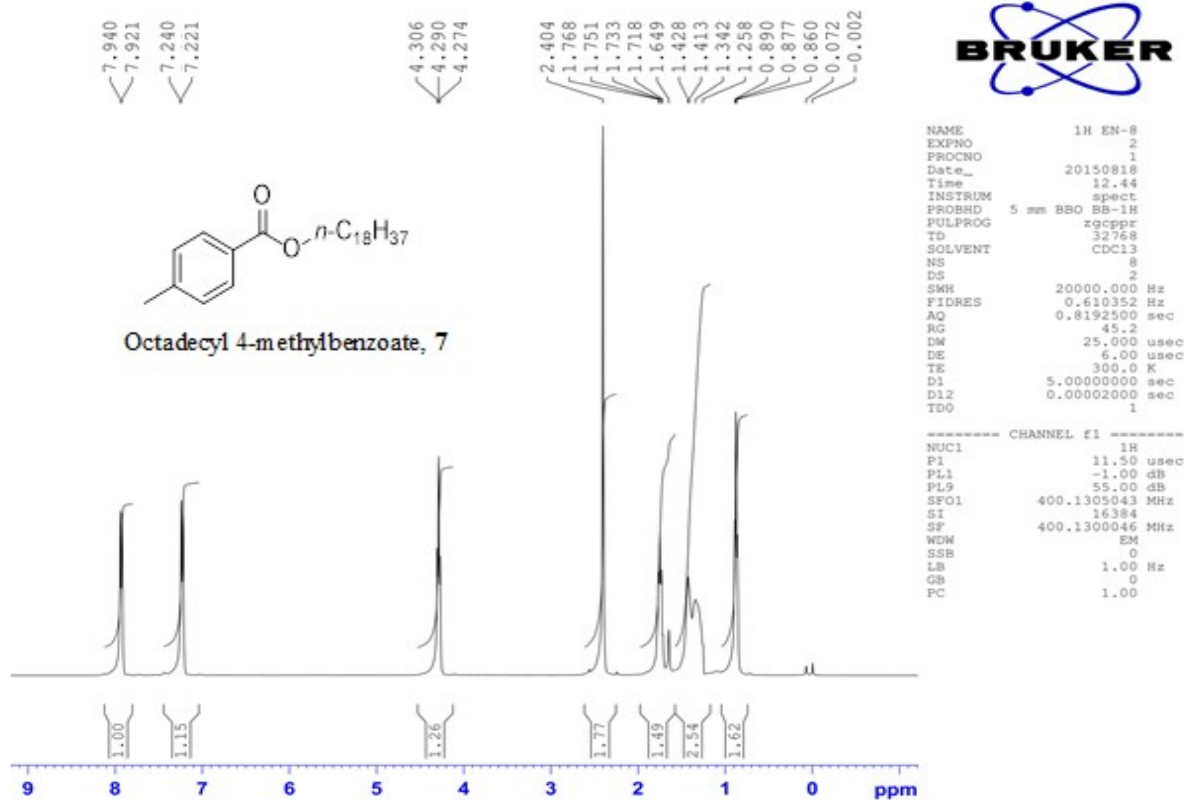


Fig: ¹H & ¹³C NMR of Octadecyl 4-methylbenzoate, 7

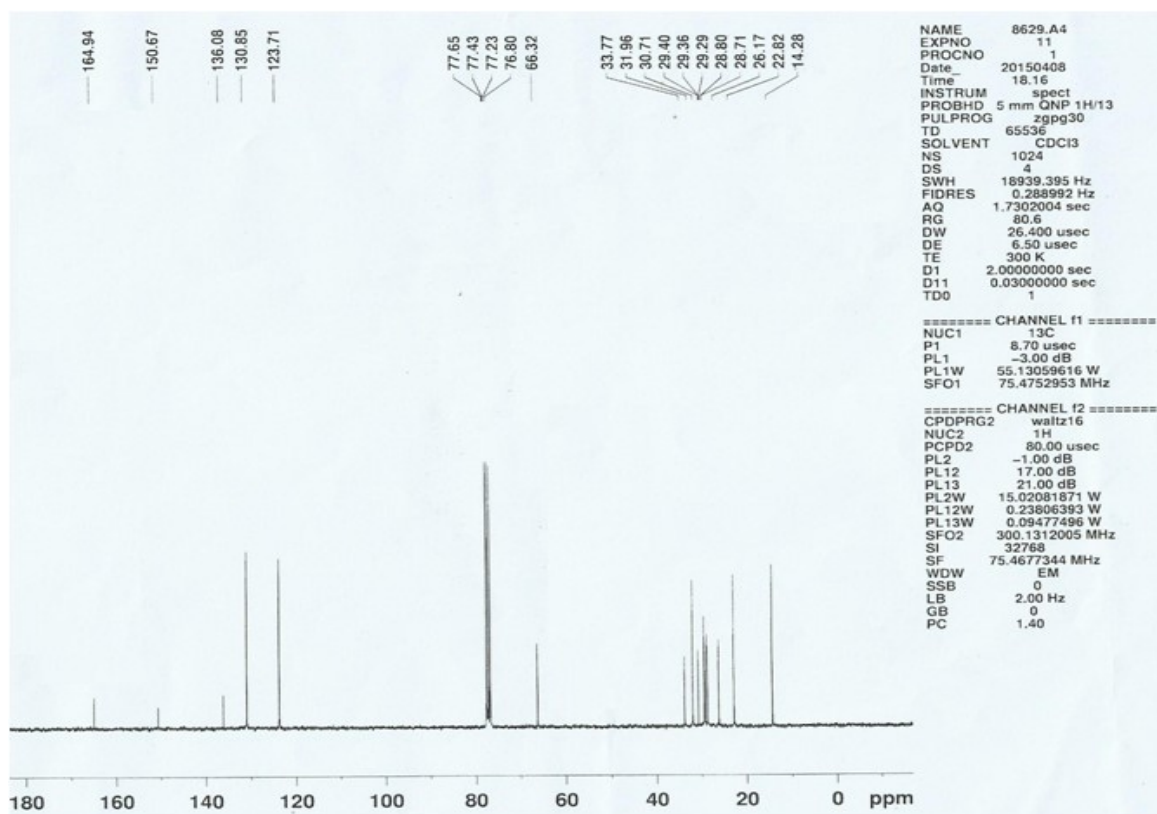
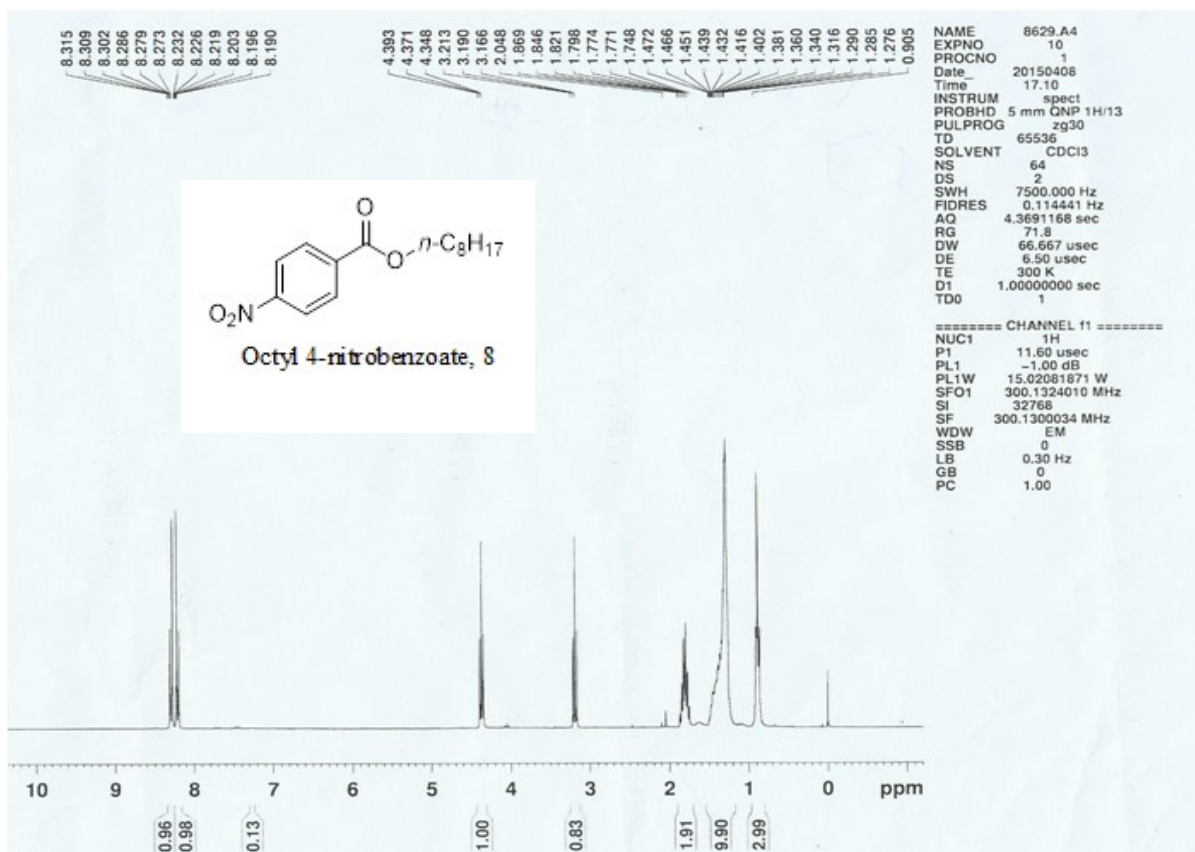
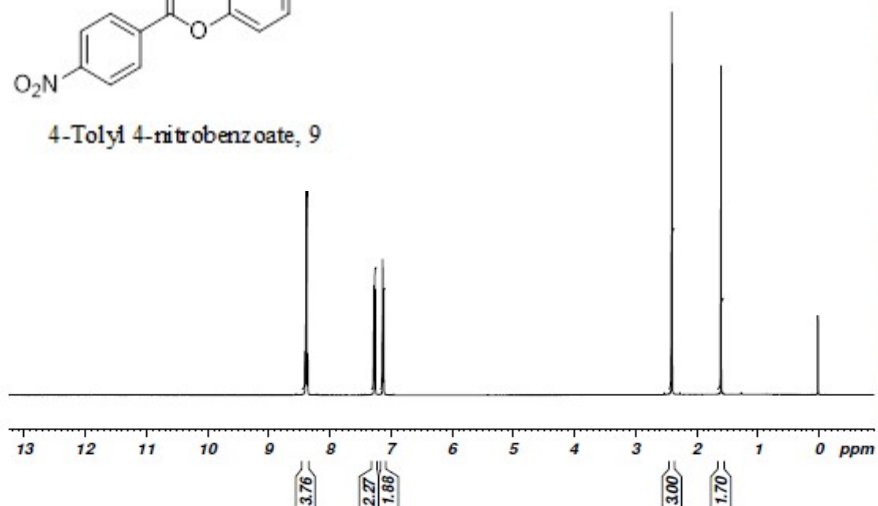
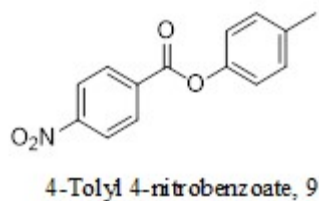


Fig: ^1H & ^{13}C NMR of Octyl 4-nitrobenzoate, **8**



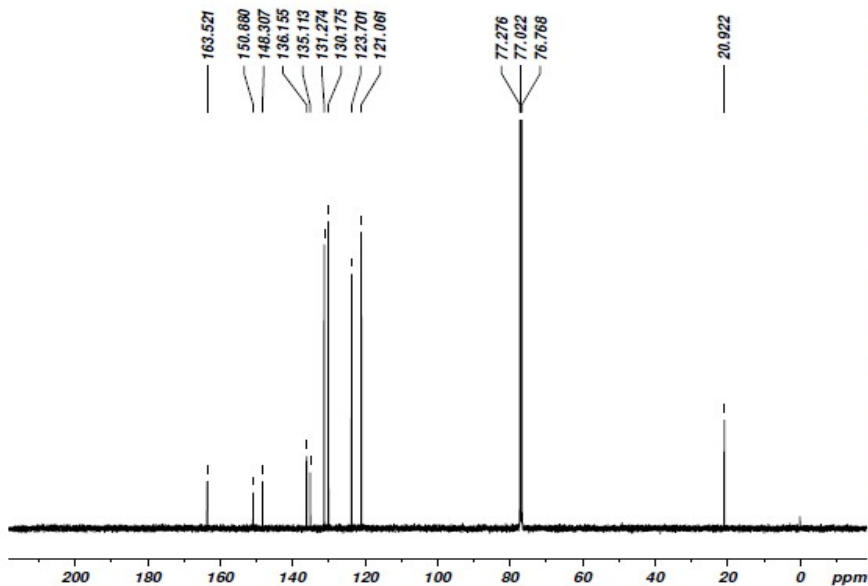
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PROCNO   1

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PL12     17.51 dB
PL13     18.00 dB
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PL12W    0.41757989 W
PL13W    0.37302643 W
SFO2     500.1320005 MHz

F2 - Processing parameters
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Fig: ^1H & ^{13}C NMR of 4-Tolyl 4-nitrobenzoate, 9

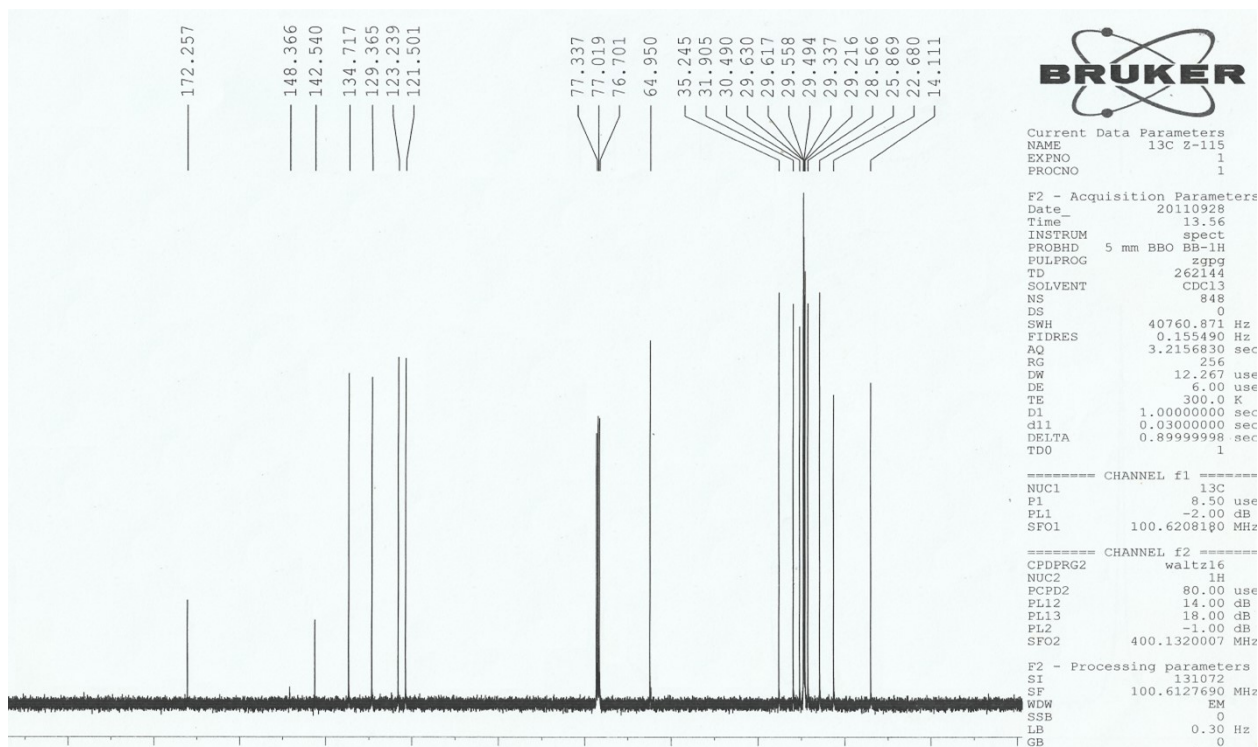
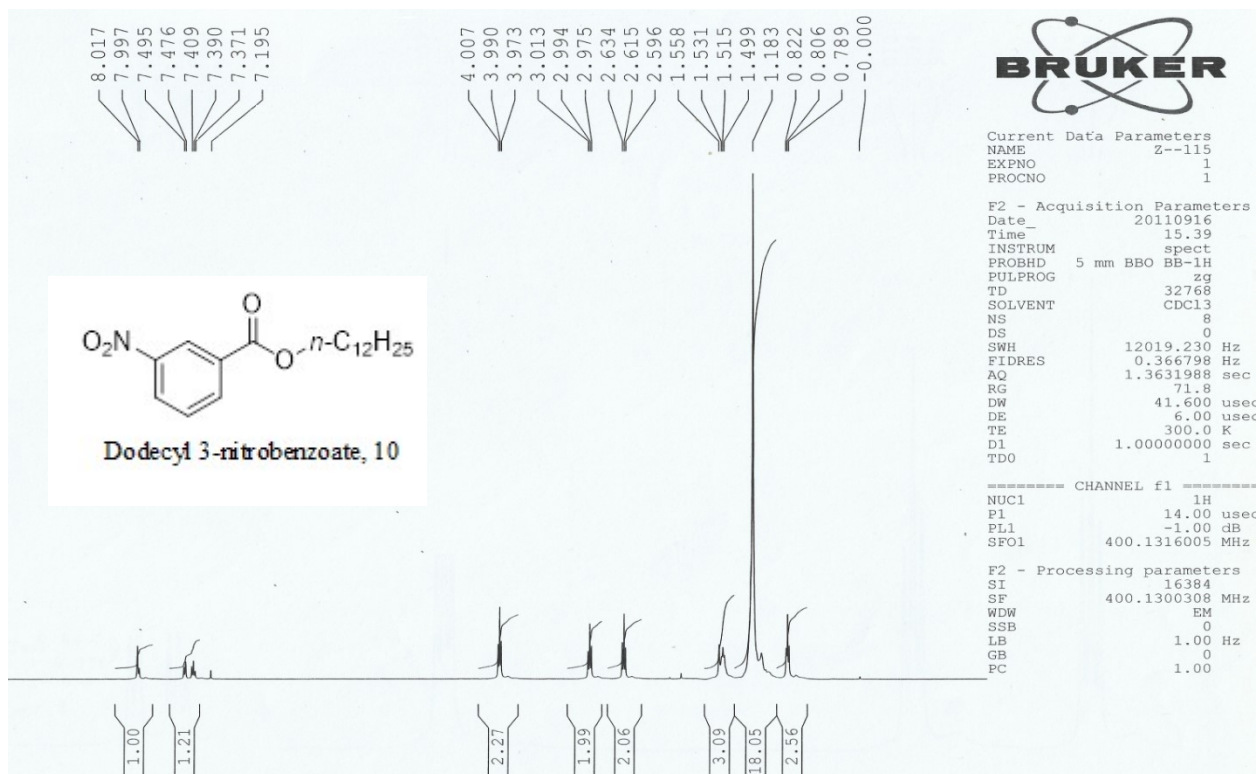


Fig: ¹H & ¹³C NMR of Dodecyl 3-nitrobenzoate, 10

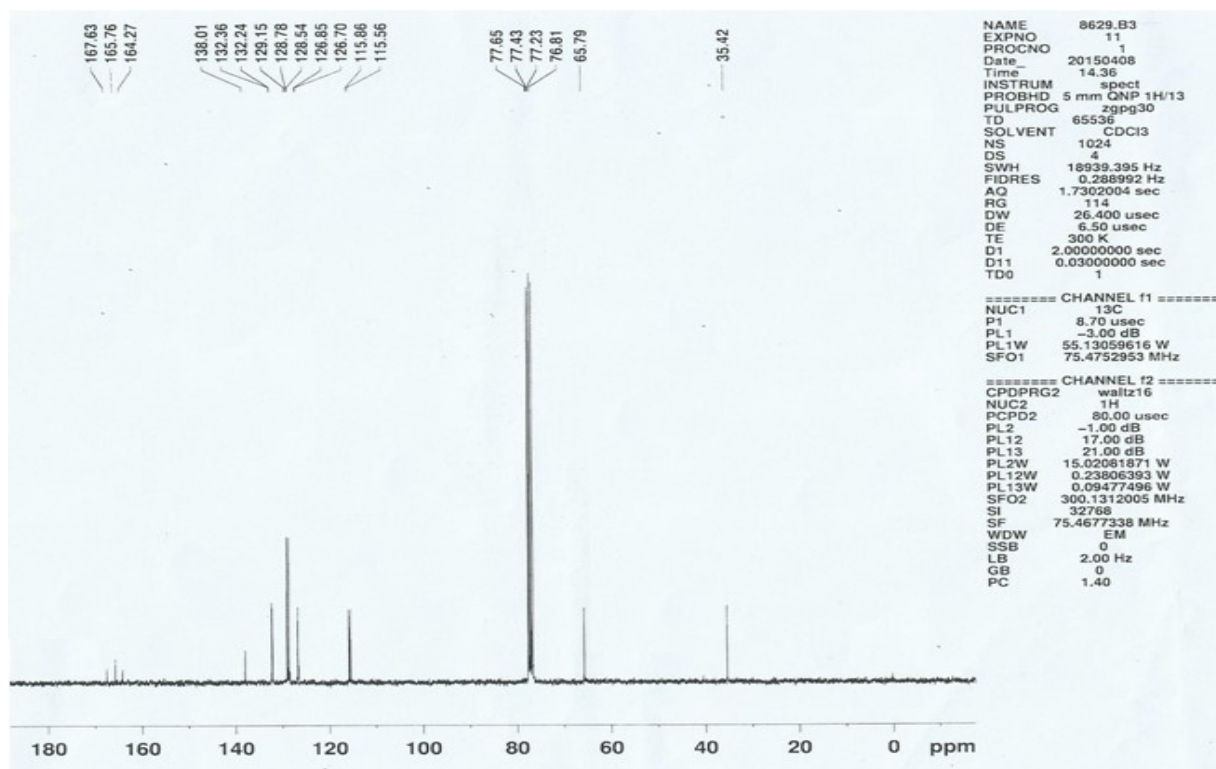
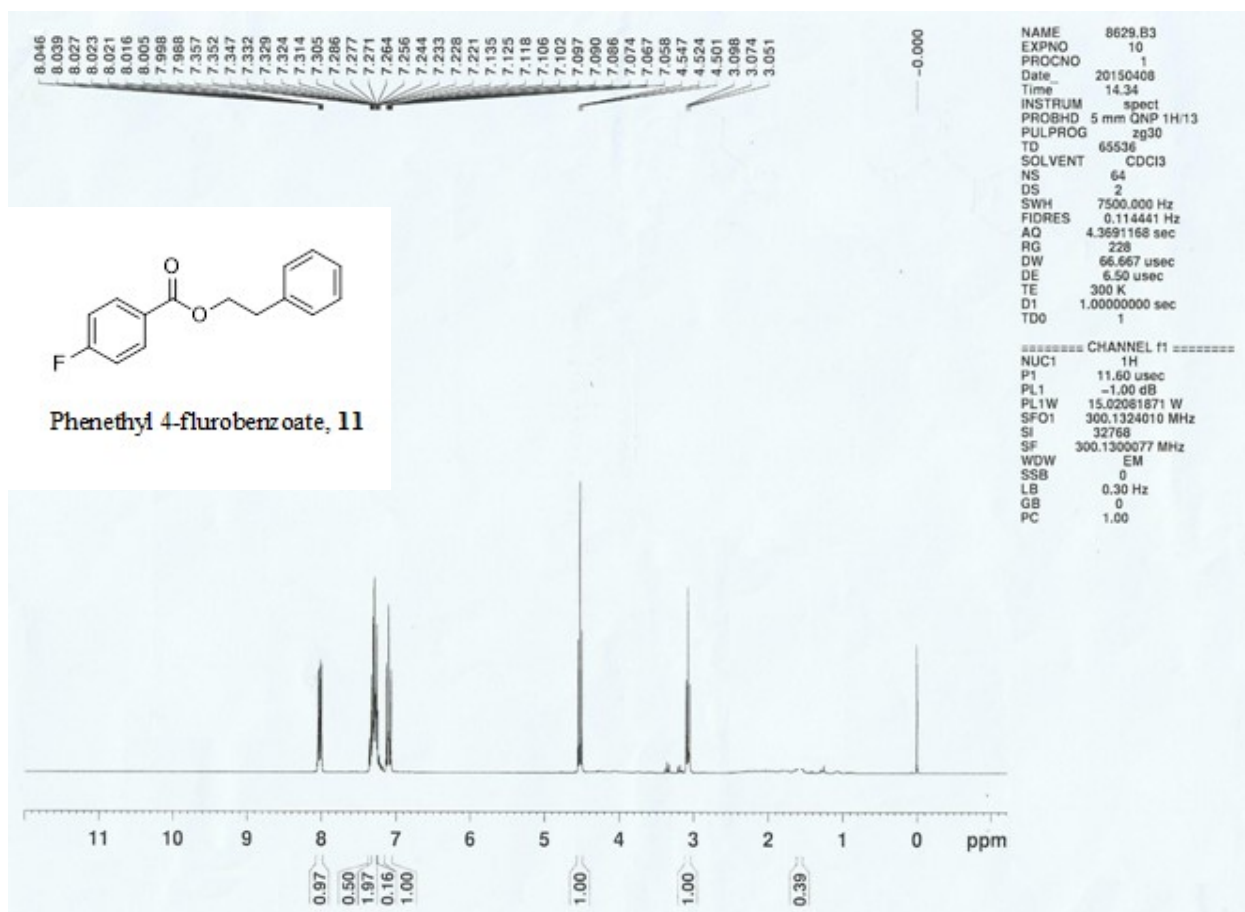


Fig: ¹H & ¹³C NMR of Phenethyl 4-fluorobenzoate, 11

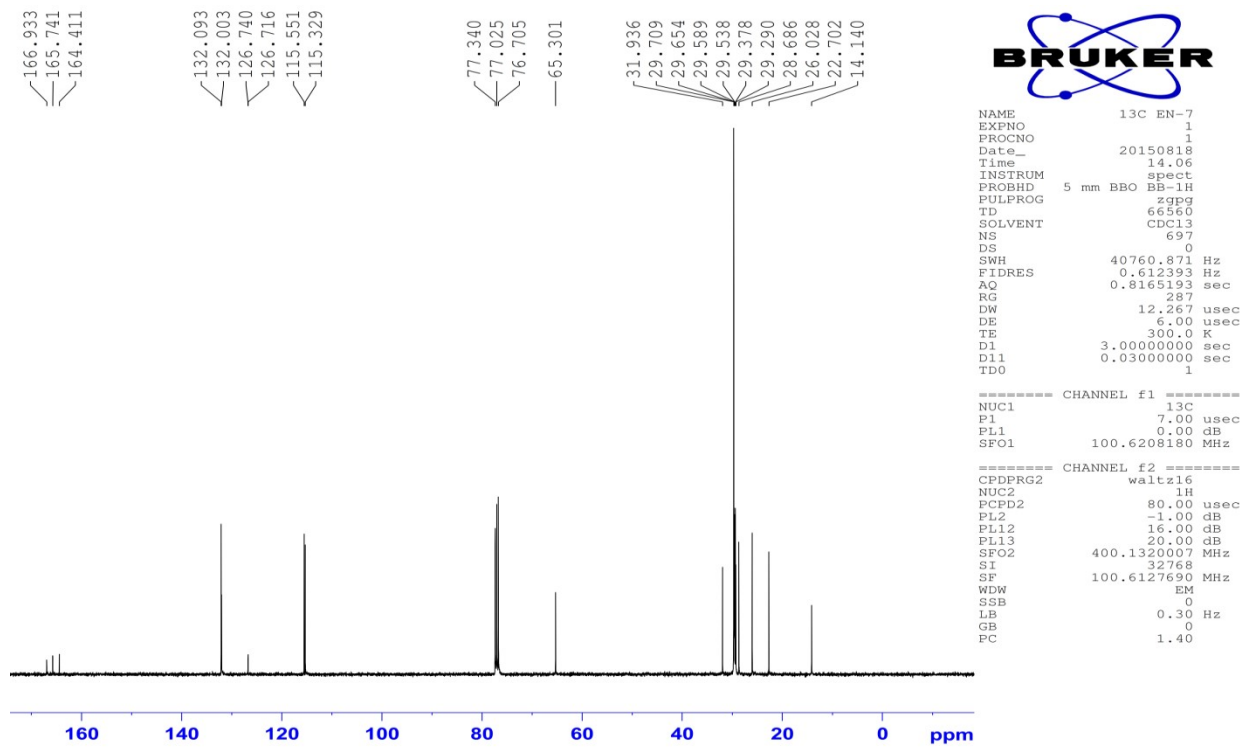
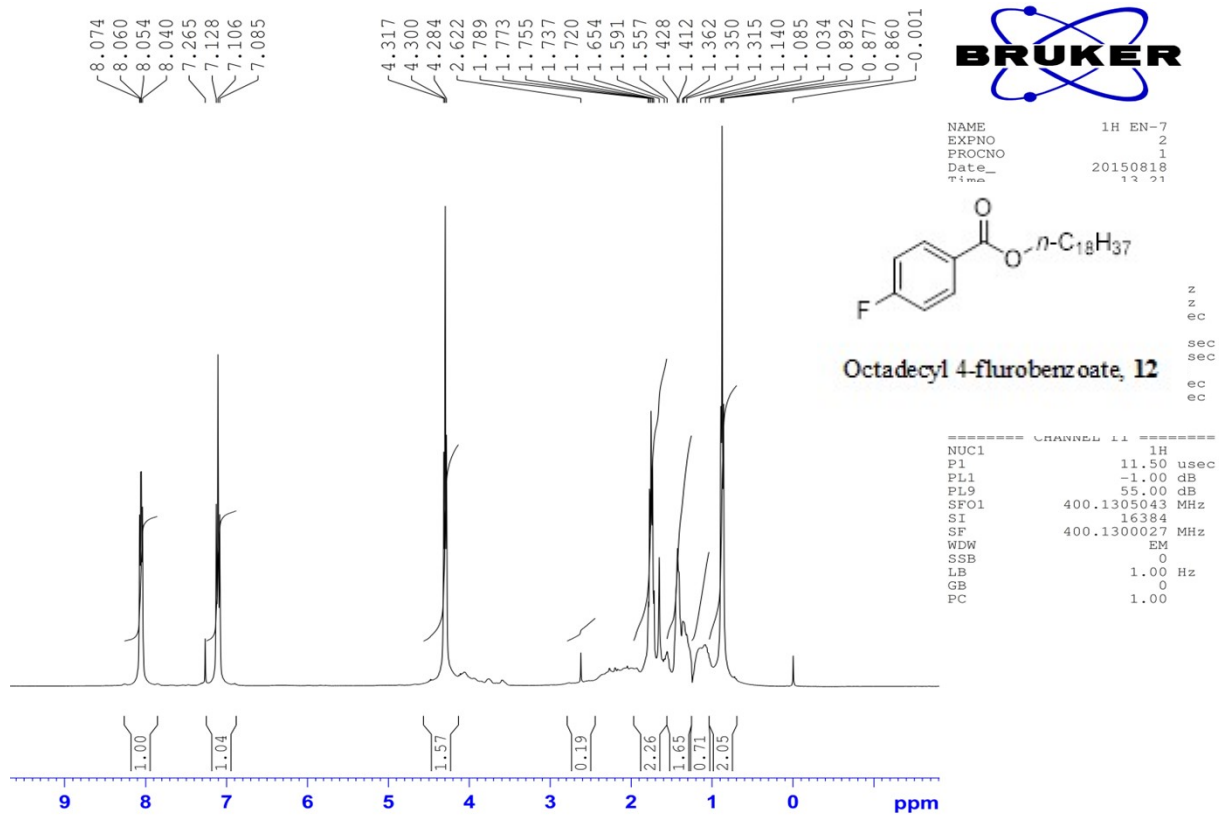


Fig: ¹H & ¹³C NMR of Octadecyl 4- fluorobenzoate, **12**

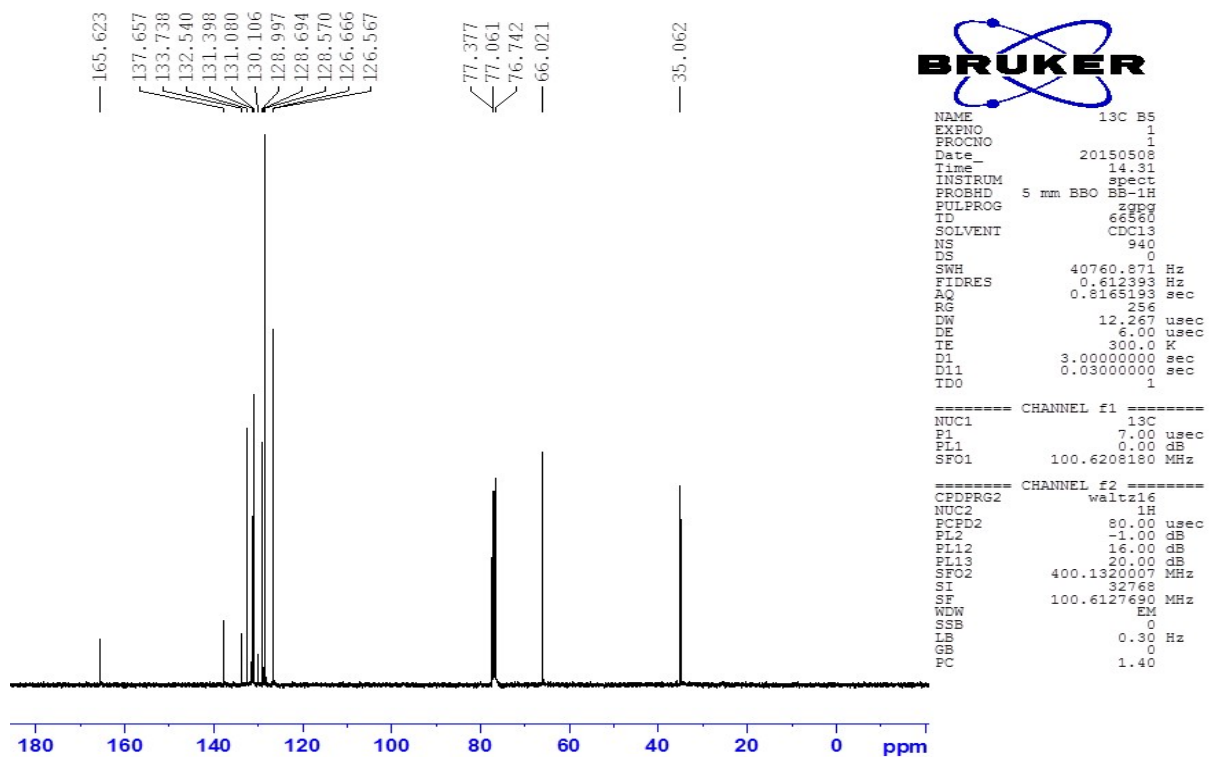
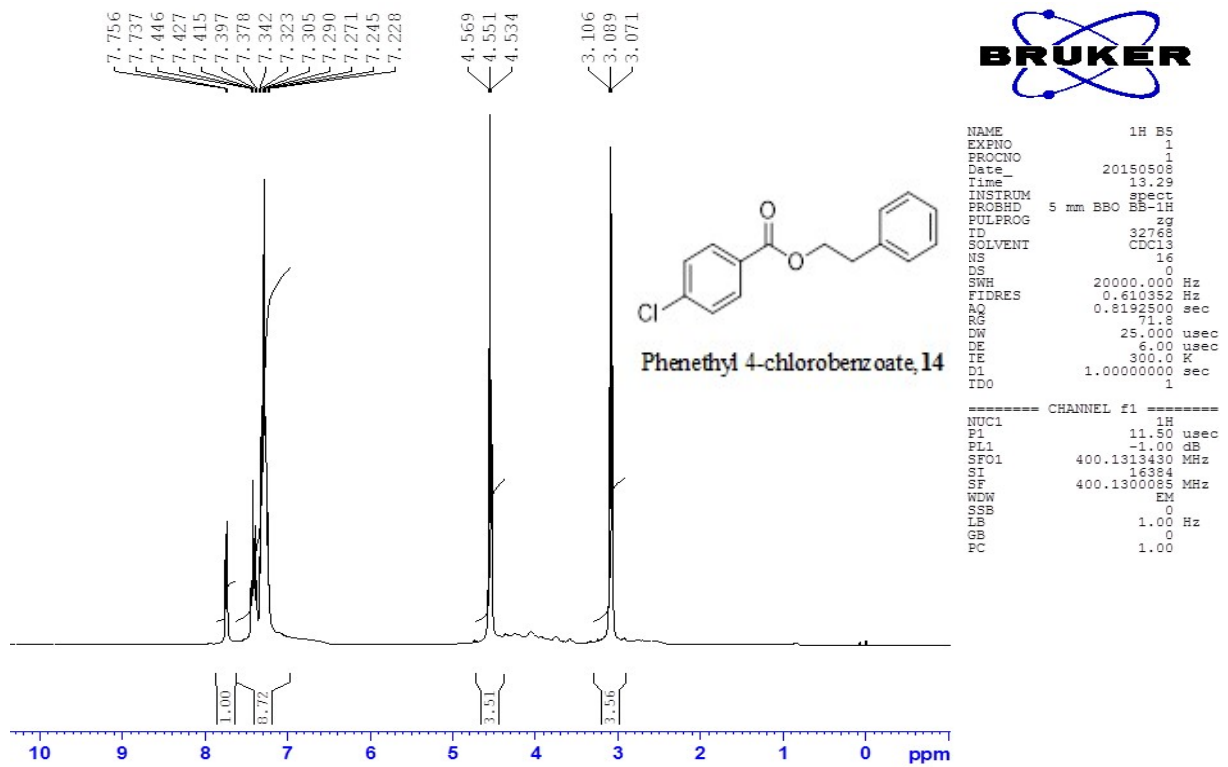


Fig: ¹H & ¹³C NMR of Phenethyl 4-chlorobenzoate, 14

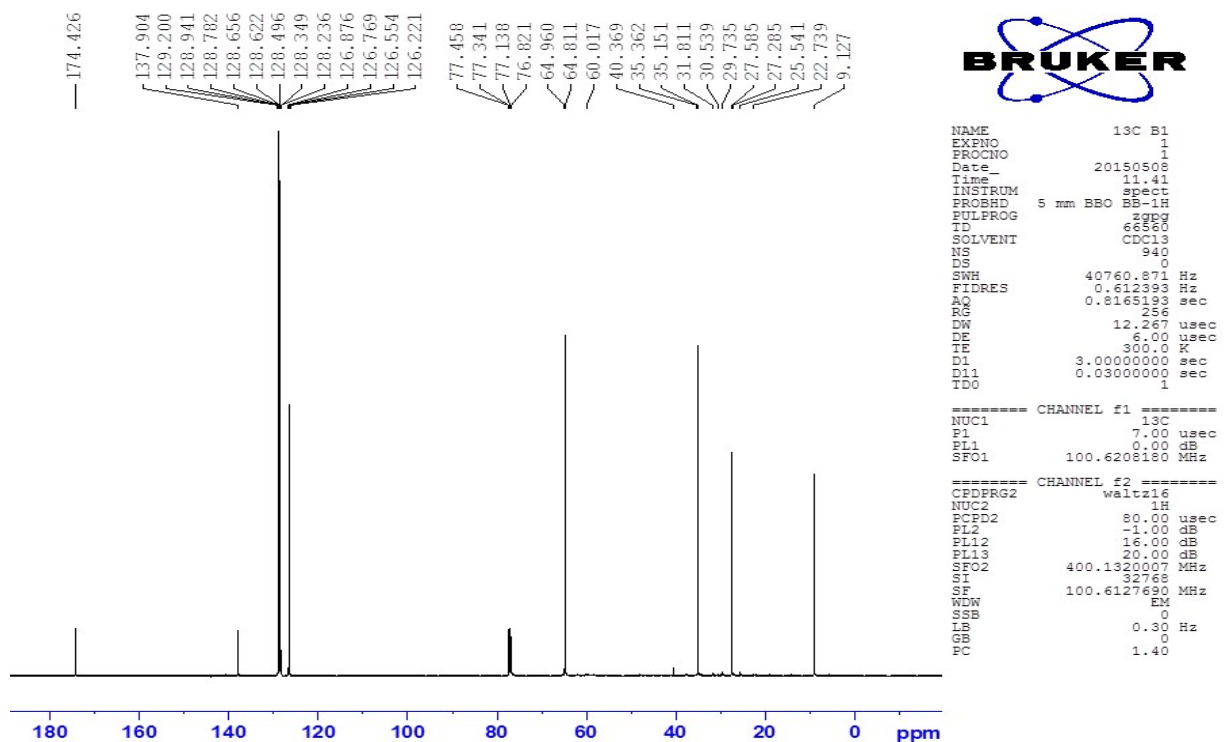
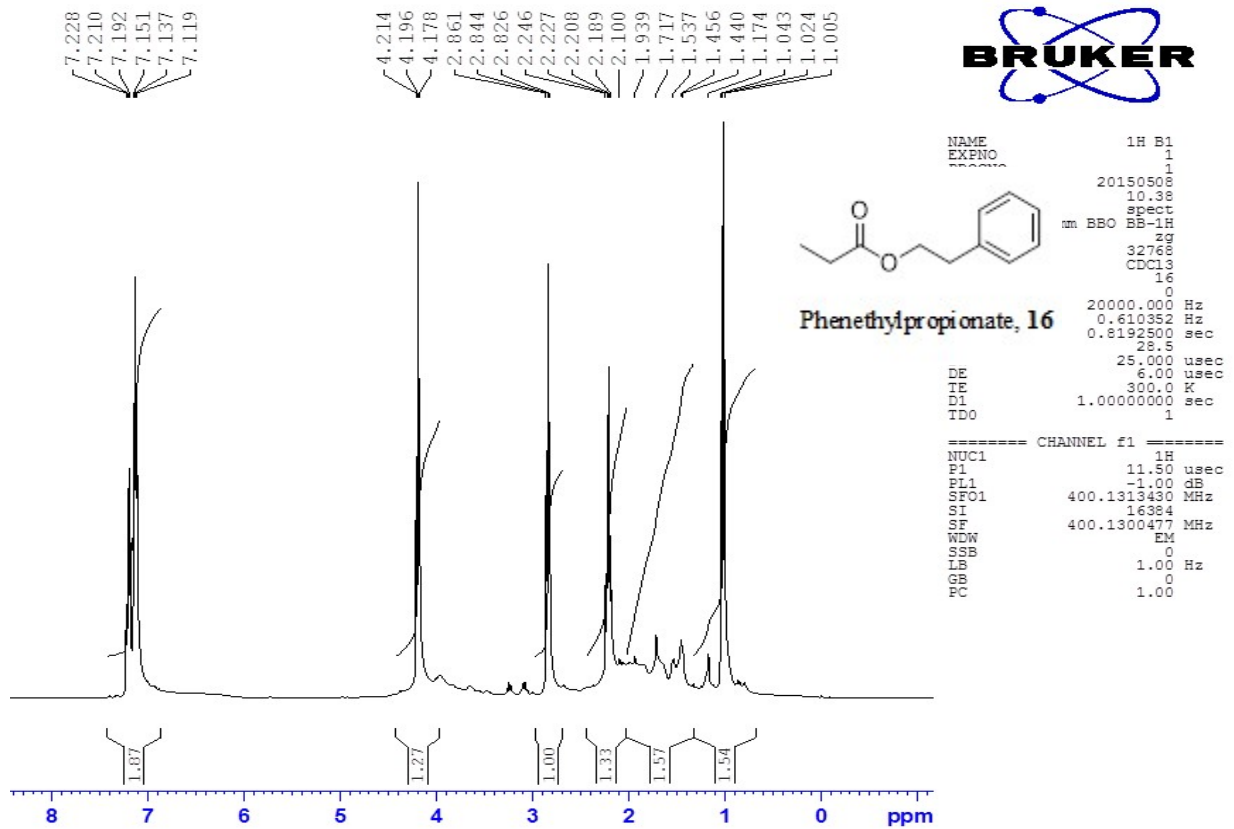
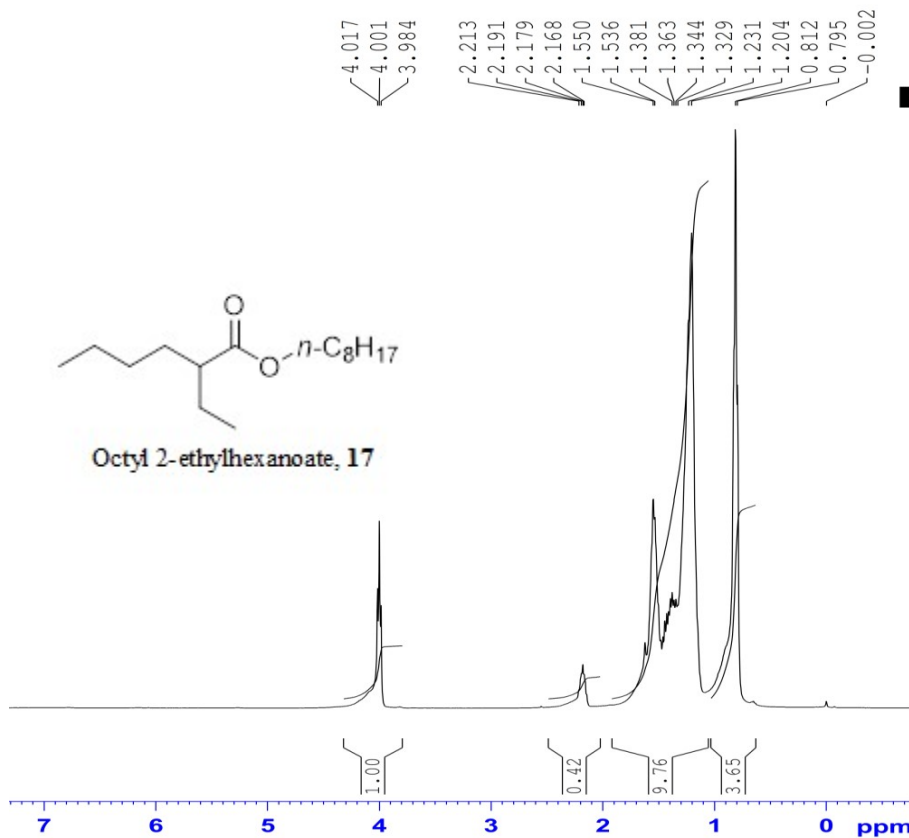


Fig: ¹H & ¹³C NMR of Phenethylpropionate, 16



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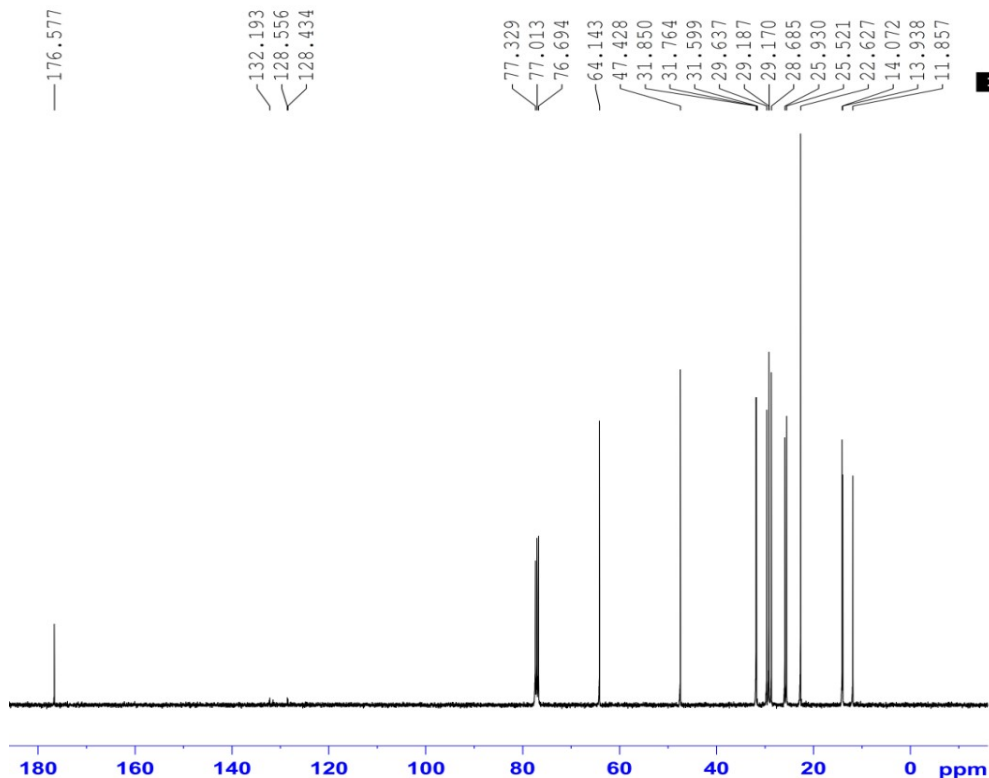
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FIDRES        0.610352 Hz
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RG            23.5
DW            25.000 usec
DE            6.00 usec
TE            300.0 K
D1            1.00000000 sec
D11           1
TD0           1

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```

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SSB           0
LB            1.00 Hz
GB            0
PC            1.00

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```

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PROCNO        1
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PULPROG       zgpg
TD            66560
SOLVENT       CDCl3
NS            940
DS            0
SWH           40760.871 Hz
FIDRES        0.612393 Hz
AQ            0.8165193 sec
RG            256
DW            12.267 usec
DE            6.00 usec
TE            300.0 K
D1            4.00000000 sec
D11           0.03000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
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P1            7.00 usec
PL1           0.00 dB
SFO1          100.6208180 MHz

```

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===== CHANNEL f2 =====
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PCPD2         80.00 usec
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PL12          16.00 dB
PL13          20.00 dB
SFO2          400.1320007 MHz
SI            32768
SF            100.6127690 MHz
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SSB           0
LB            0.30 Hz
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PC            1.40

```

Fig: ¹H & ¹³C NMR of Octyl 2-ethylhexanoate, 17

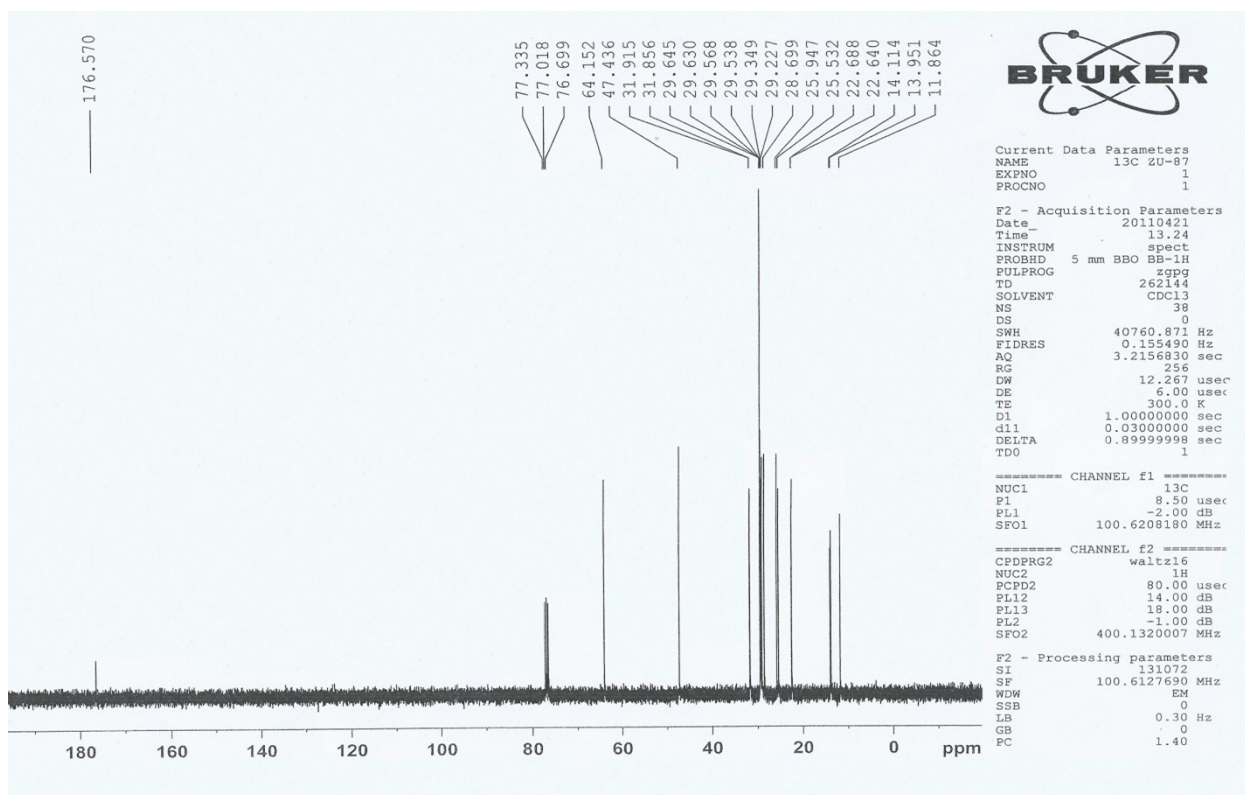
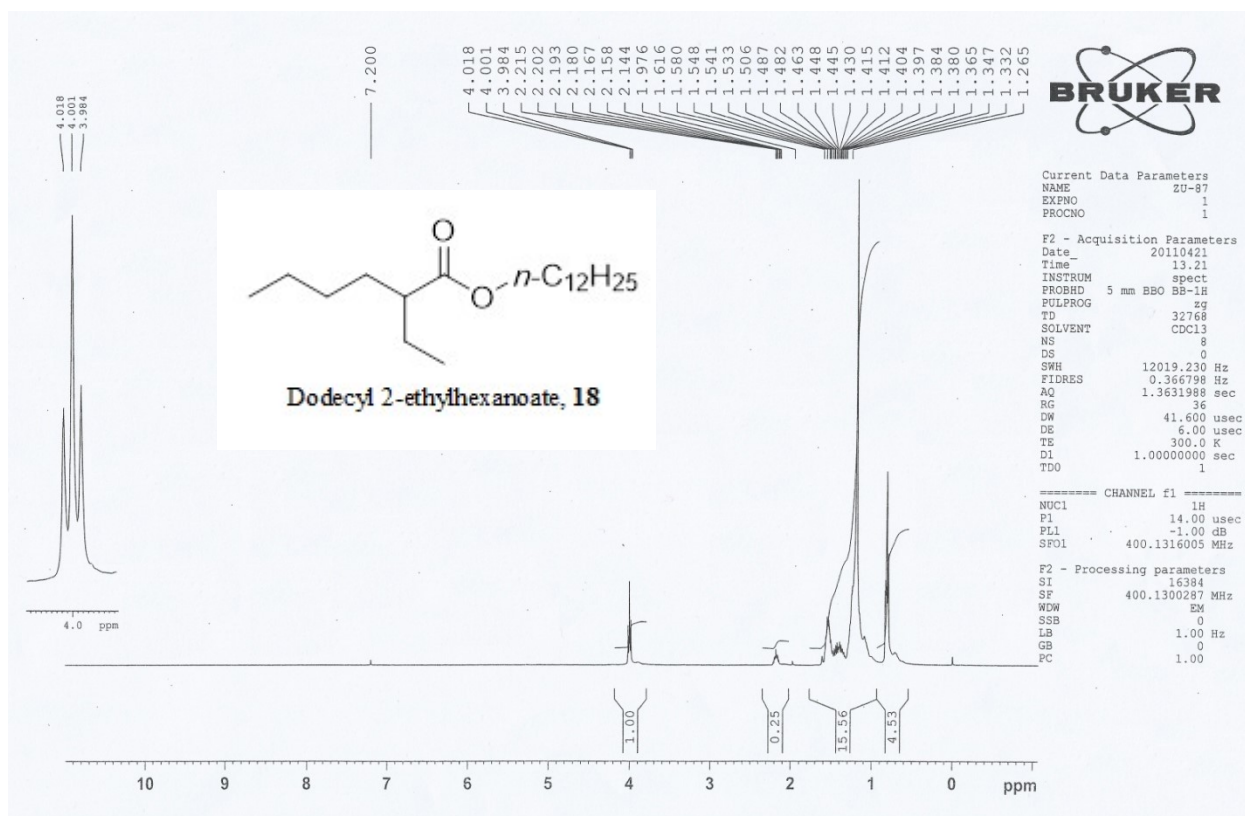
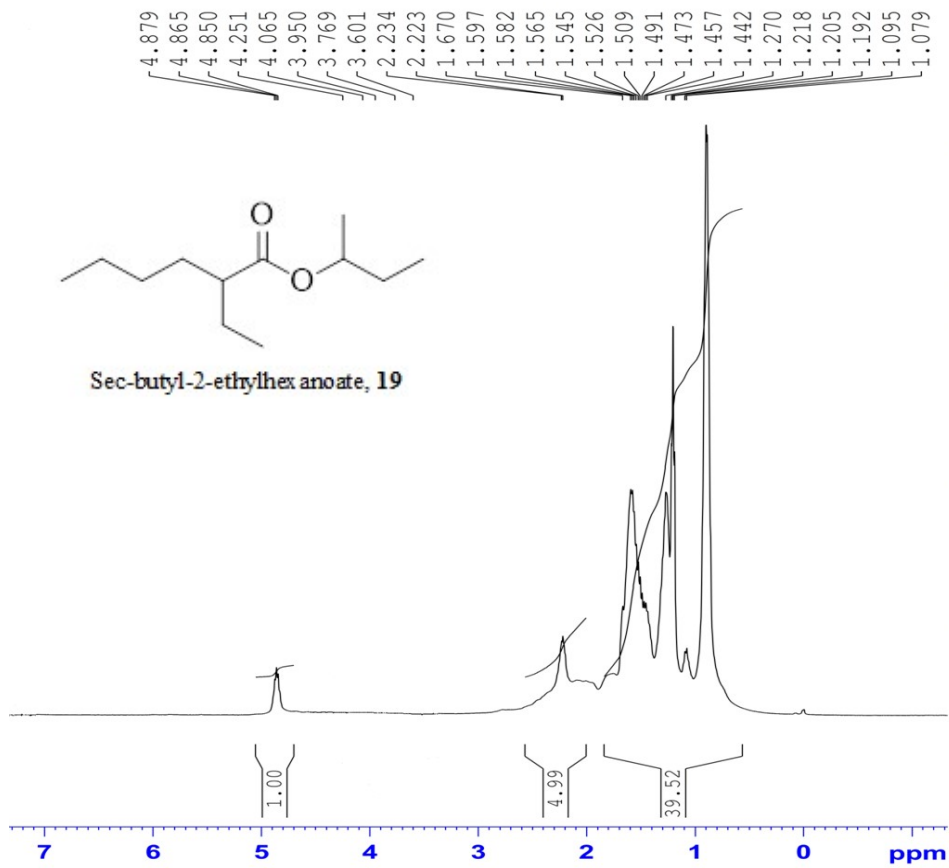


Fig: ^1H & ^{13}C NMR of Dodecyl 2-ethylhexanoate, 18

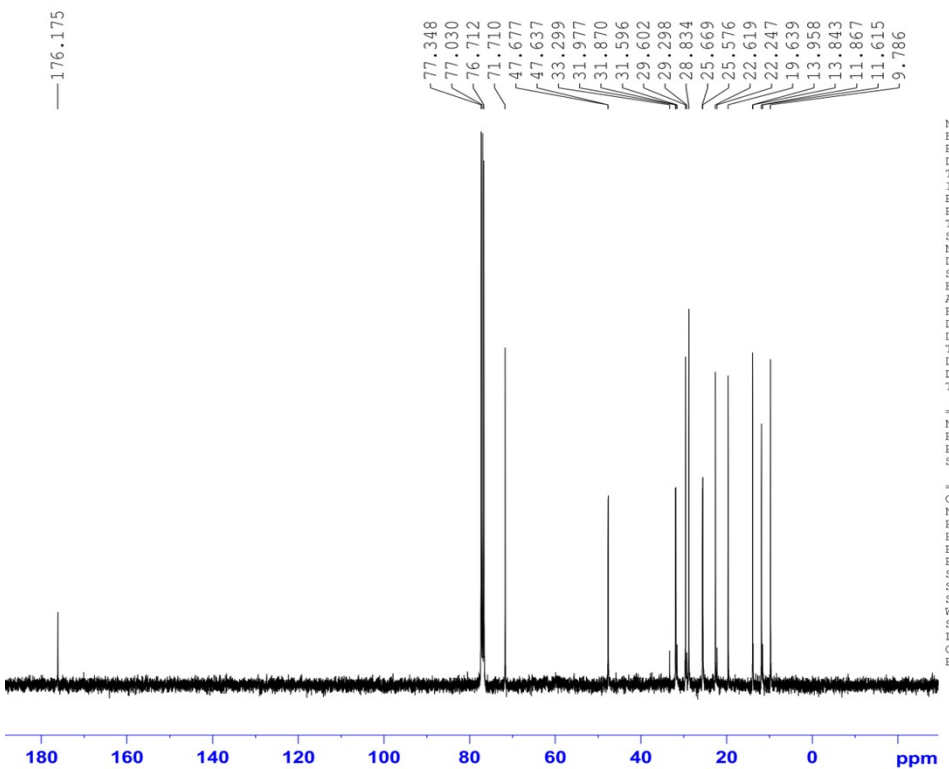


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TE            300.0 K
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D11           1
TDO           1
  
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```

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PL1           -1.00 dB
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PROCNO        1
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Time_         16.24
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SOLVENT       CDCl3
NS            940
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SWH           40760.871 Hz
FIDRES        0.612393 Hz
AQ            0.8165193 sec
RG            287
DW            12.267 usec
DE            6.00 usec
TE            300.0 K
D1            3.00000000 sec
D11           0.03000000 sec
TDO           1
  
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P1            7.00 usec
PL1           0.00 dB
SFO1         100.6208180 MHz

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NUC2          1H
PCPD2         80.00 usec
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PL12          16.00 dB
PL13          20.00 dB
SFO2         400.1320007 MHz
SI           32768
SF           100.6127690 MHz
WDW           EM
SSB           0
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Fig: ¹H & ¹³C NMR of Sec-butyl-2-ethylhexanoate, 19

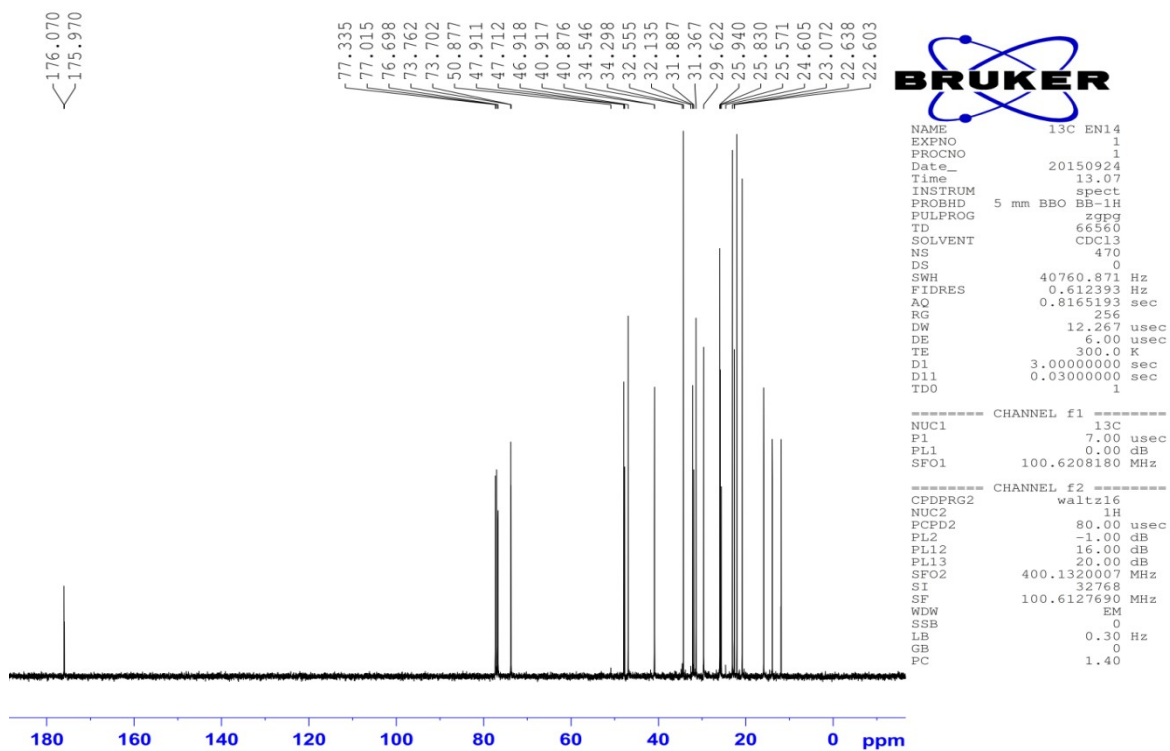
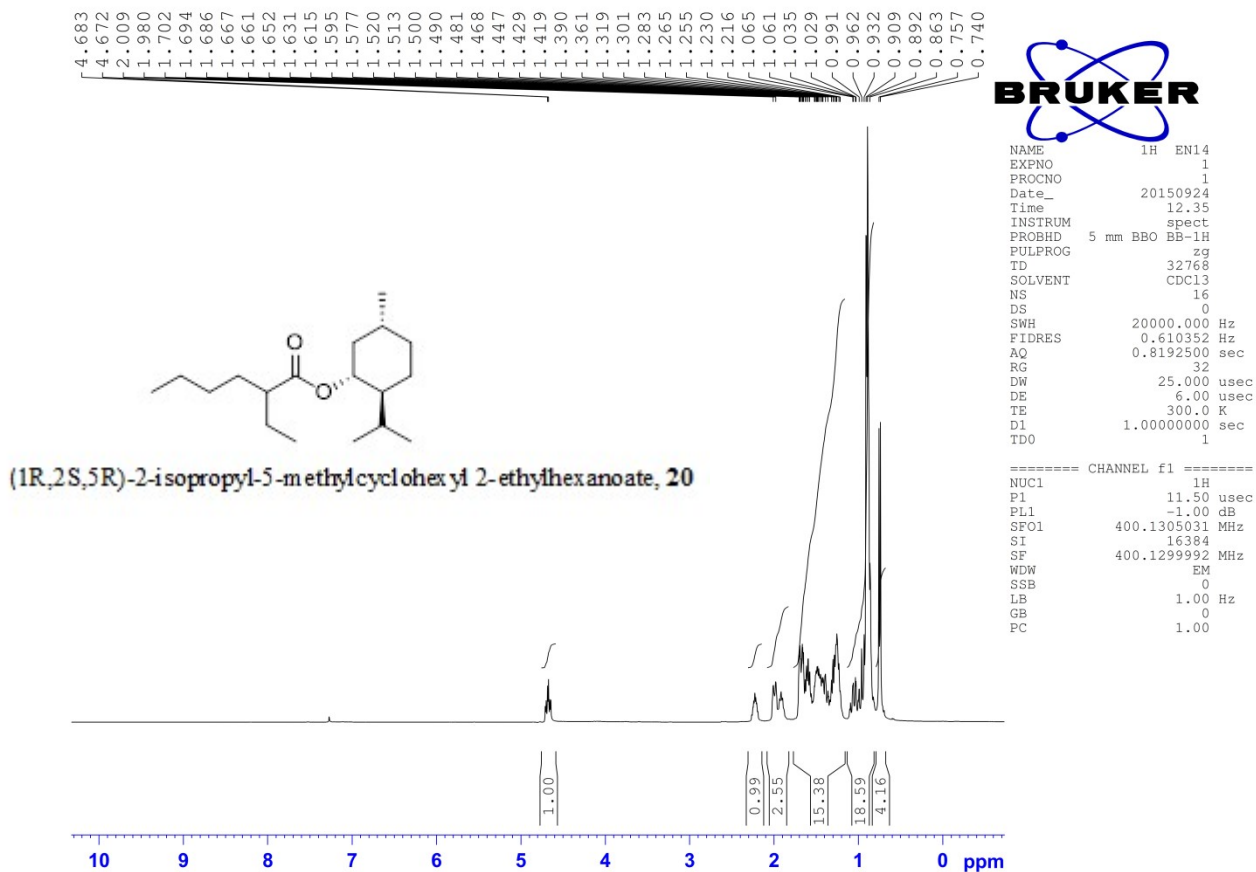
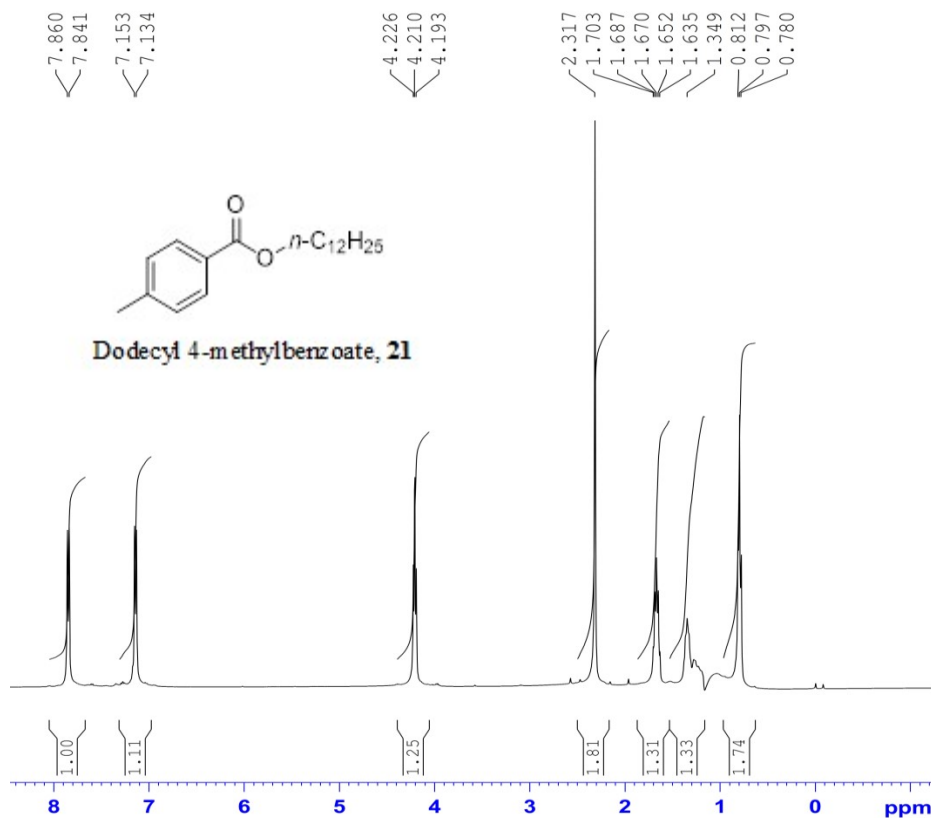


Fig: ^1H & ^{13}C NMR of (1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 2-ethylhexanoate, **20**

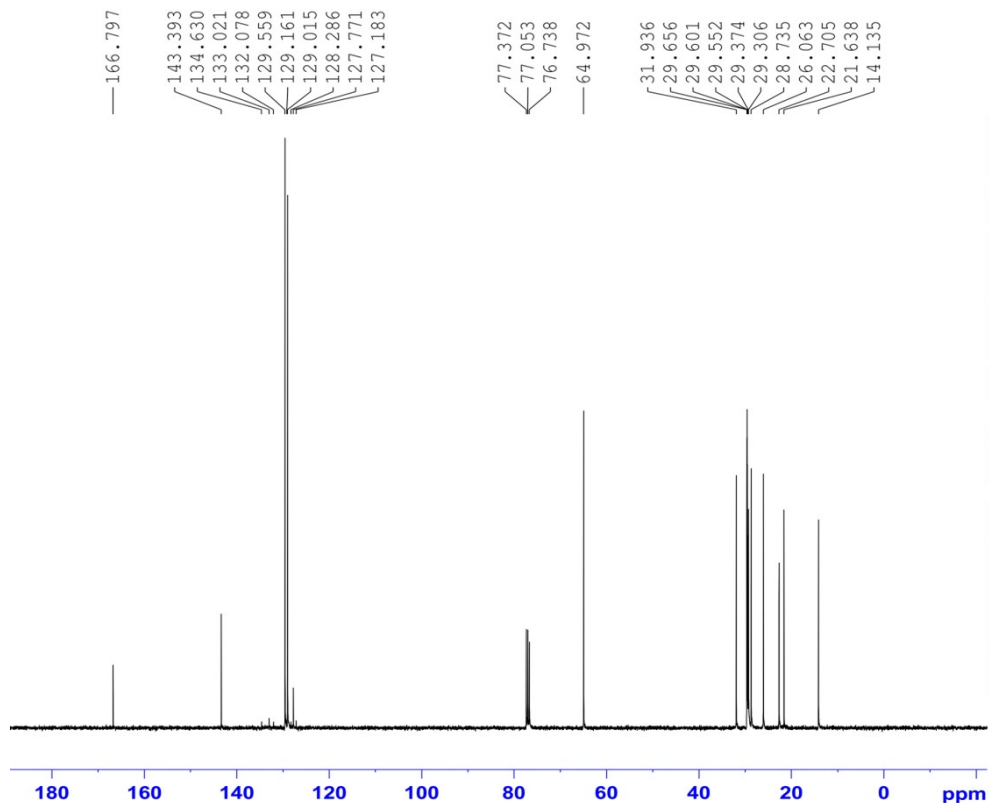


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SOLVENT       CDCl3
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SWH           20000.000 Hz
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TE            300.0 K
D1            5.00000000 sec
D12           0.00002000 sec
TDO           1
  
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```

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SI            16384
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SSB           0
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GB            0
PC            1.00
  
```



```

NAME          13C EN-4
EXPNO         1
PROCNO        1
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Time          15.16
INSTRUM       spect
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PULPROG       zgpg
TD            66560
SOLVENT       CDCl3
NS            453
DS            0
SWH           40760.871 Hz
FIDRES        0.612393 Hz
AQ            0.8165193 sec
RG            287
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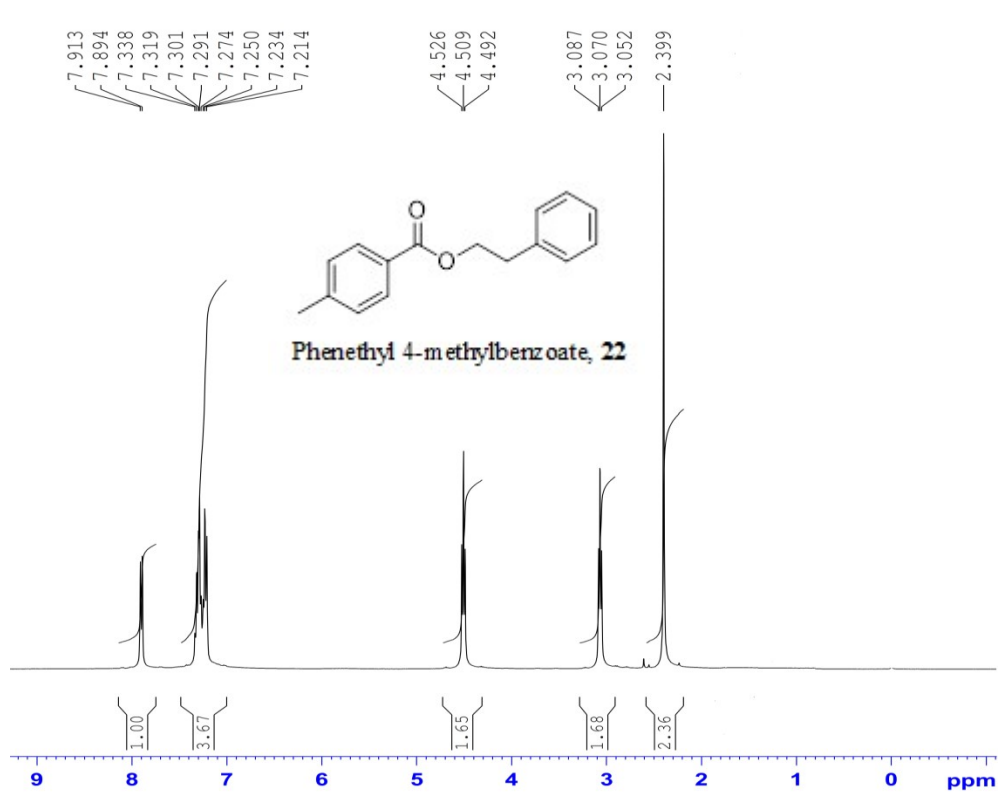
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NUC2          1H
PCPD2         80.00 usec
PL2           -1.00 dB
PL12          16.00 dB
PL13          20.00 dB
SFO2          400.1320007 MHz
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.40
  
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Fig: ¹H & ¹³C NMR of Dodecyl 4-methylbenzoate, 21

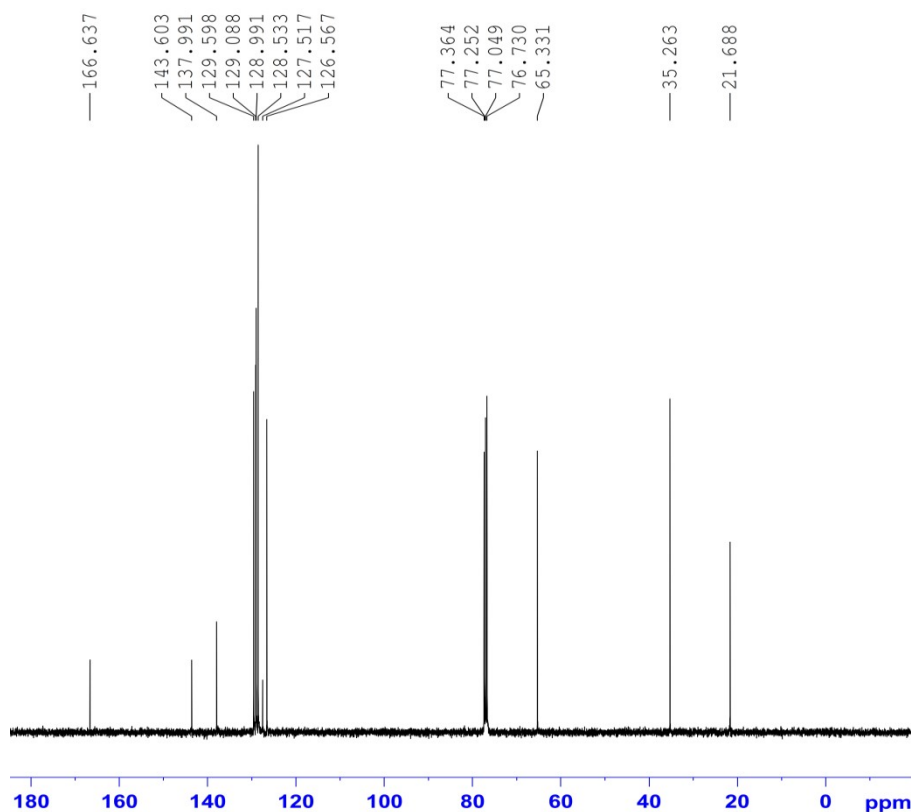


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RG             114
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DE             6.00 usec
TE             300.0 K
D1             1.00000000 sec
TDO           1
  
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PC             1.00
  
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PROCNO        1
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TD             66560
SOLVENT       CDC13
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DS             0
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FIDRES        0.612393 Hz
AQ             0.8165193 sec
RG             406
DW             12.267 usec
DE             6.00 usec
TE             300.0 K
D1             3.00000000 sec
D11            0.03000000 sec
TDO           1
  
```

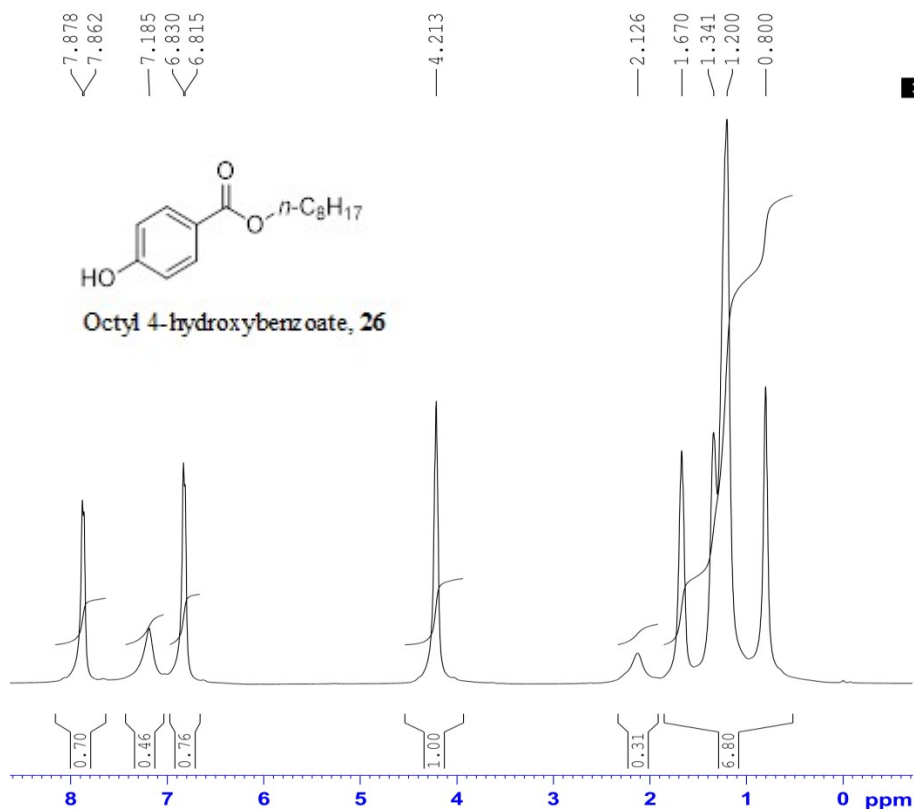
```

----- CHANNEL f1 -----
NUC1          13C
P1             7.00 usec
PL1            0.00 dB
SFO1          100.6208180 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2            -1.00 dB
PL12          16.00 dB
PL13          20.00 dB
SFO2          400.1320007 MHz
SI             32768
SF            100.6127690 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB             0
PC             1.40
  
```

Fig: ¹H & ¹³C NMR of Phenethyl 4-methylbenzoate, 22



```

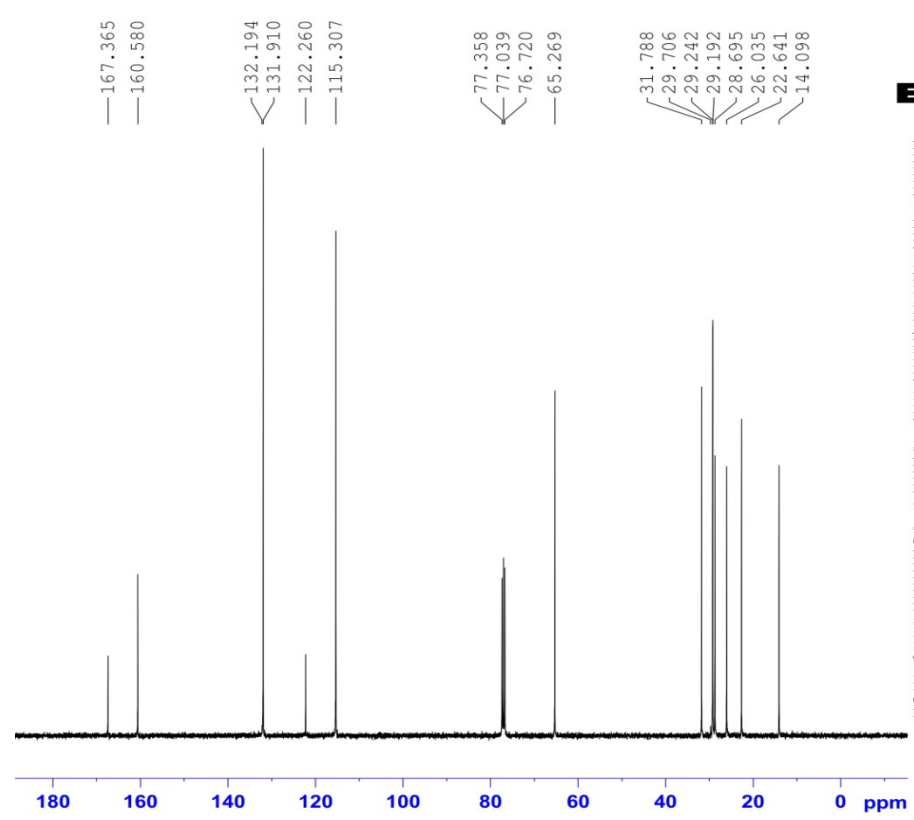
NAME 1H EN3
EXPNO 1
PROCNO 1
Date_ 20150528
Time 11.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 28.5
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

```

```

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1310341 MHz
SI 16394
SF 400.1300338 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

```



```

NAME 13C EN3
EXPNO 1
PROCNO 1
Date_ 20150528
Time 13.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 66560
SOLVENT CDC13
NS 940
DS 0
SWH 40760.871 Hz
FIDRES 0.612393 Hz
AQ 0.8165193 sec
RG 256
DW 12.267 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
D11 0.03000000 sec
TDO 1

```

```

===== CHANNEL f1 =====
NUC1 13C
P1 7.00 usec
PL1 0.00 dB
SFO1 100.6208180 MHz

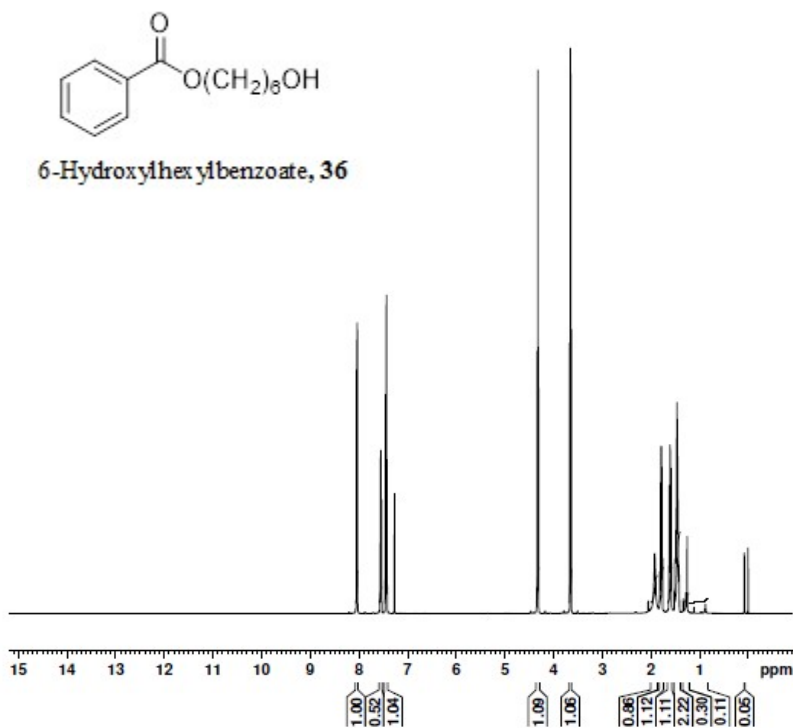
```

```

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.00 dB
PL13 20.00 dB
SFO2 400.1320007 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

```

Fig: ¹H & ¹³C NMR of Octyl 4-hydroxybenzoate, 26

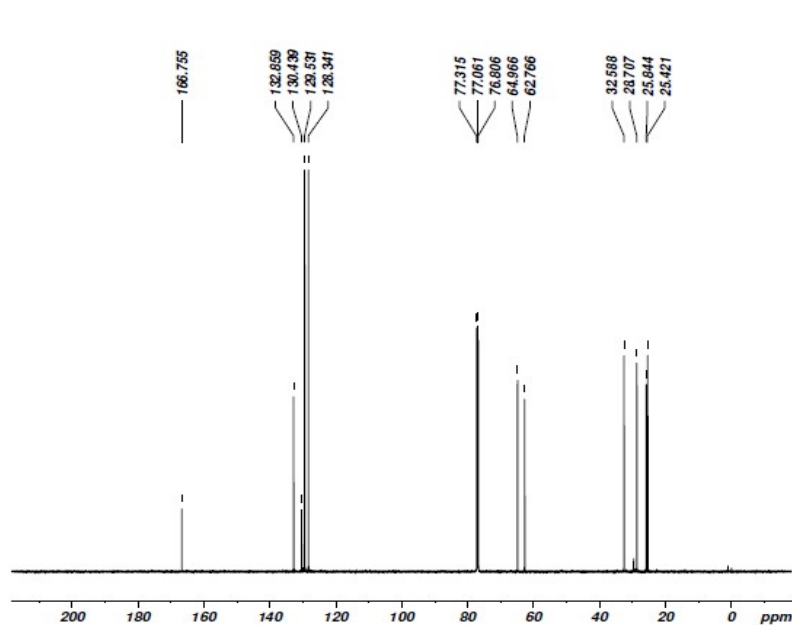


Current Data Parameters
 NAME Dec26-2014
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141225
 Time 23.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860212 sec
 RG 80.6
 DW 48.400 usec
 DE 6.50 usec
 TE 297.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.65 usec
 PL1 0.00 dB
 PL1W 23.53637505 W
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



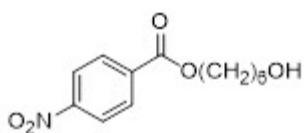
Current Data Parameters
 NAME Dec26-2014
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141225
 Time 0.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505524 sec
 RG 203
 DW 16.800 usec
 DE 6.50 usec
 TE 298.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

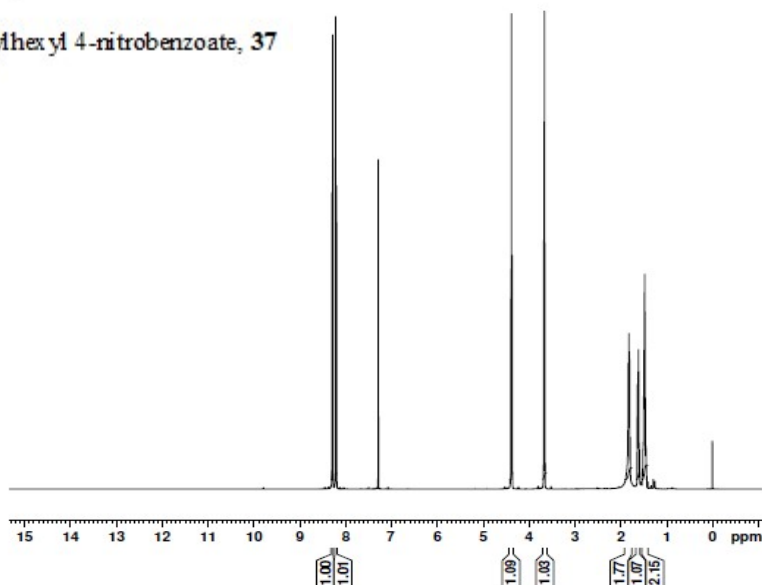
===== CHANNEL f1 =====
 NUC1 13C
 P1 7.80 usec
 PL1 0.00 dB
 PL1W 70.83519745 W
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.51 dB
 PL13 18.00 dB
 PL2W 23.53637505 W
 PL12W 0.41757989 W
 PL13W 0.37302643 W
 SFO2 500.1320065 MHz

Fig: ¹H & ¹³C NMR of 6-Hydroxyhexylbenzoate, **36**



6-Hydroxyhexyl 4-nitrobenzoate, 37

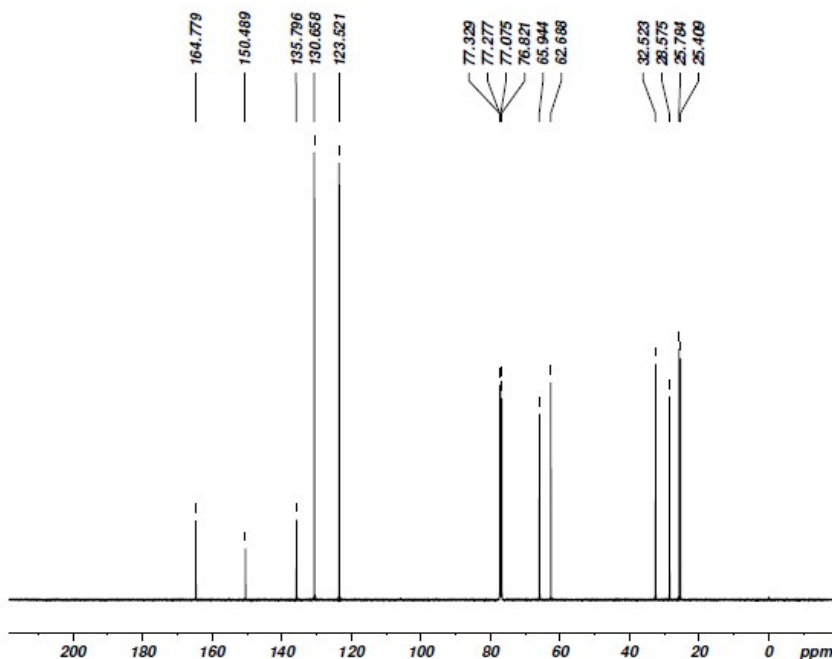


Current Data Parameters
 NAME Dec26-2014
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141226
 Time 0.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860212 sec
 RG 71.8
 DW 48.400 usec
 DE 6.50 usec
 TE 297.4 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.65 usec
 PL1 0.00 dB
 PL1W 23.53637505 W
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1299959 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



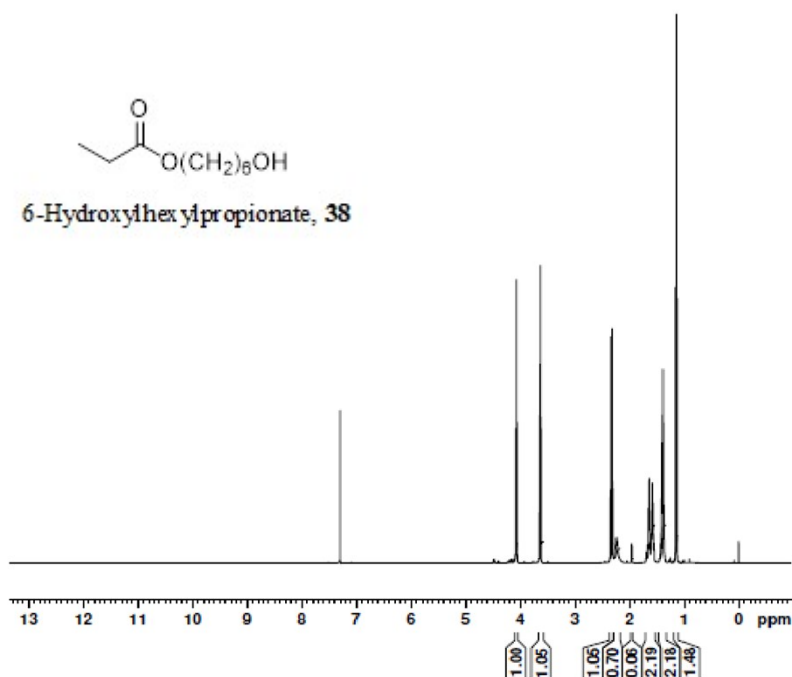
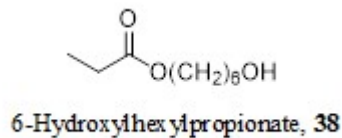
Current Data Parameters
 NAME Dec26-2014
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141226
 Time 0.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505524 sec
 RG 203
 DW 16.800 usec
 DE 8.50 usec
 TE 298.7 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.80 usec
 PL1 0.00 dB
 PL1W 70.83519745 W
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.51 dB
 PL13 18.00 dB
 PL2W 23.53637505 W
 PL12W 0.41757989 W
 PL13W 0.37302643 W
 SFO2 500.1320005 MHz

Fig: ¹H & ¹³C NMR of 6-Hydroxyhexyl 4-nitrobenzoate, 37

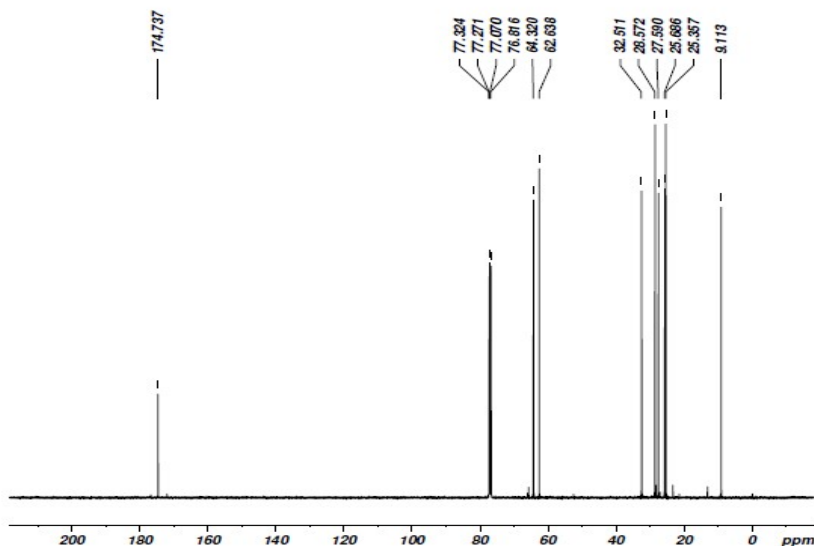


Current Data Parameters
 NAME Dec26-2014
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141226
 Time 1.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860212 sec
 RG 57
 DW 48.400 usec
 DE 6.50 usec
 TE 296.9 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.65 usec
 PL1 0.00 dB
 PL1W 23.53637505 W
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1299912 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



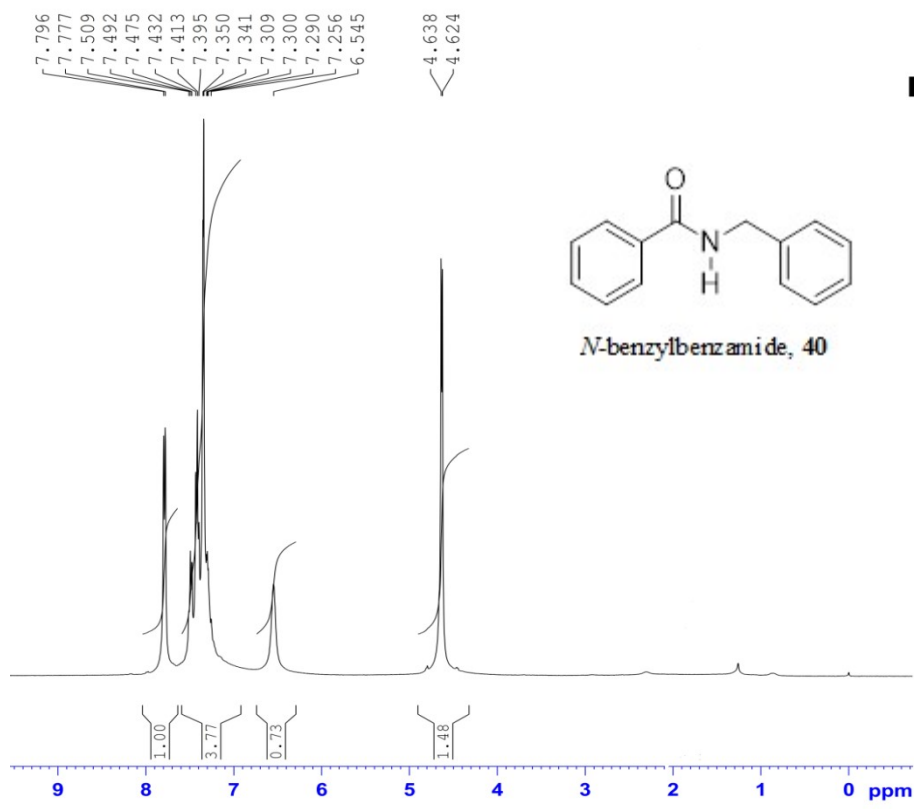
Current Data Parameters
 NAME Dec26-2014
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141226
 Time 1.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505524 sec
 RG 203
 DW 16.800 usec
 DE 6.50 usec
 TE 298.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.80 usec
 PL1 0.00 dB
 PL1W 70.83519745 W
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2 walz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.51 dB
 PL13 18.00 dB
 PL2W 23.53637505 W
 PL12W 0.41757989 W
 PL13W 0.37302643 W
 SFO2 500.1320005 MHz

Fig: ¹H & ¹³C NMR of 6-Hydroxyhexylpropionate, **38**

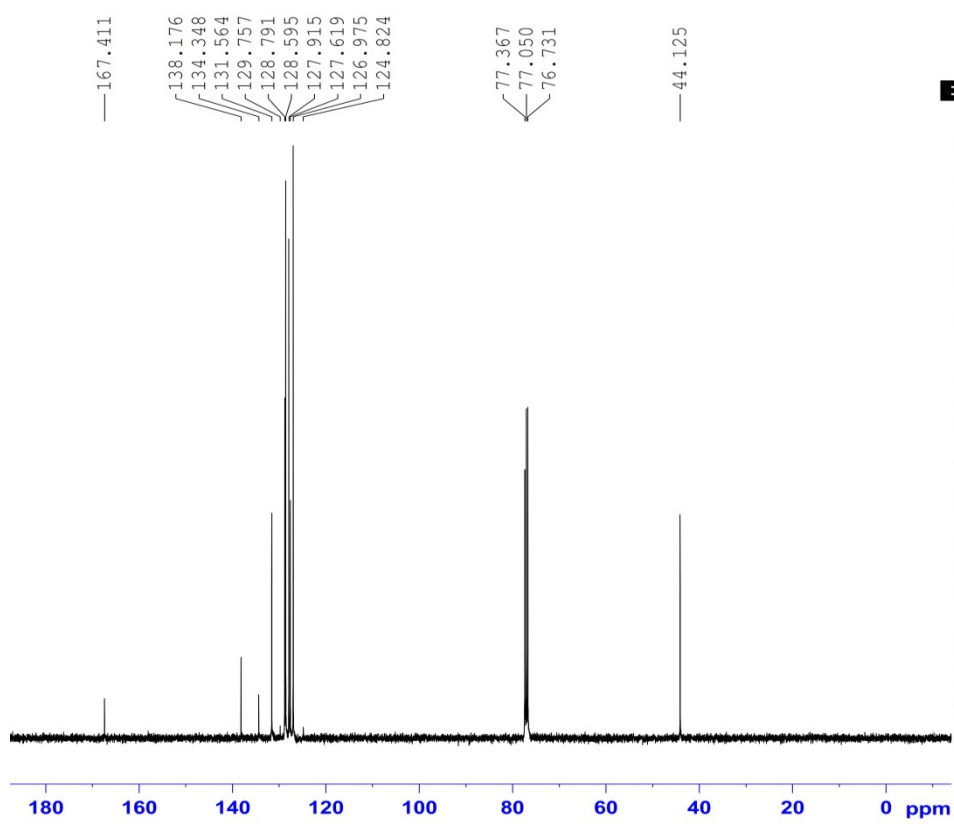


```

NAME 1H AN1
EXPNO 1
PROCNO 1
Date_ 20150611
Time_ 10.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 101
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1306386 MHz
SI 16384
SF 400.1300061 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

```



```

NAME 13C AN1
EXPNO 1
PROCNO 1
Date_ 20150611
Time_ 11.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 872
DS 0
SWH 40760.871 Hz
FIDRES 0.612393 Hz
AQ 0.8165193 sec
RG 256
DW 12.267 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.00 usec
PL1 0.00 dB
SFO1 100.6208180 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.00 dB
PL13 20.00 dB
SFO2 400.1320007 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

```

Fig: ¹H & ¹³C NMR of *N*-benzylbenzamide, 40

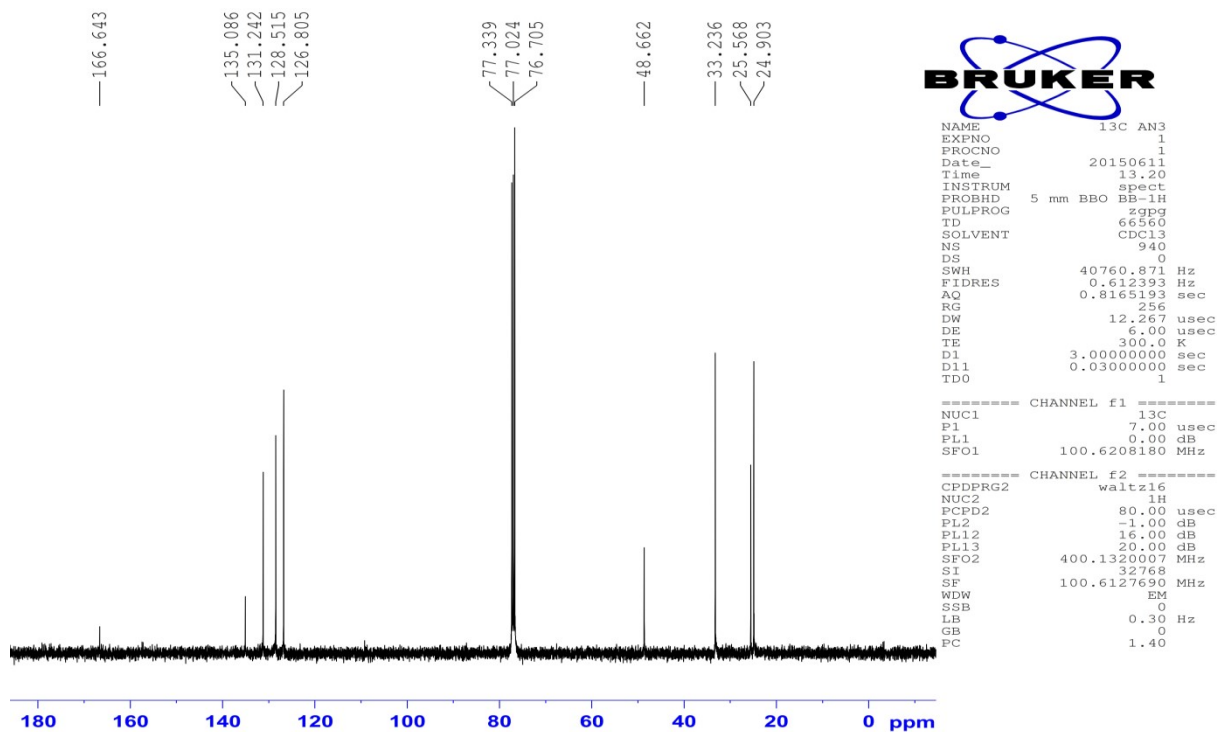
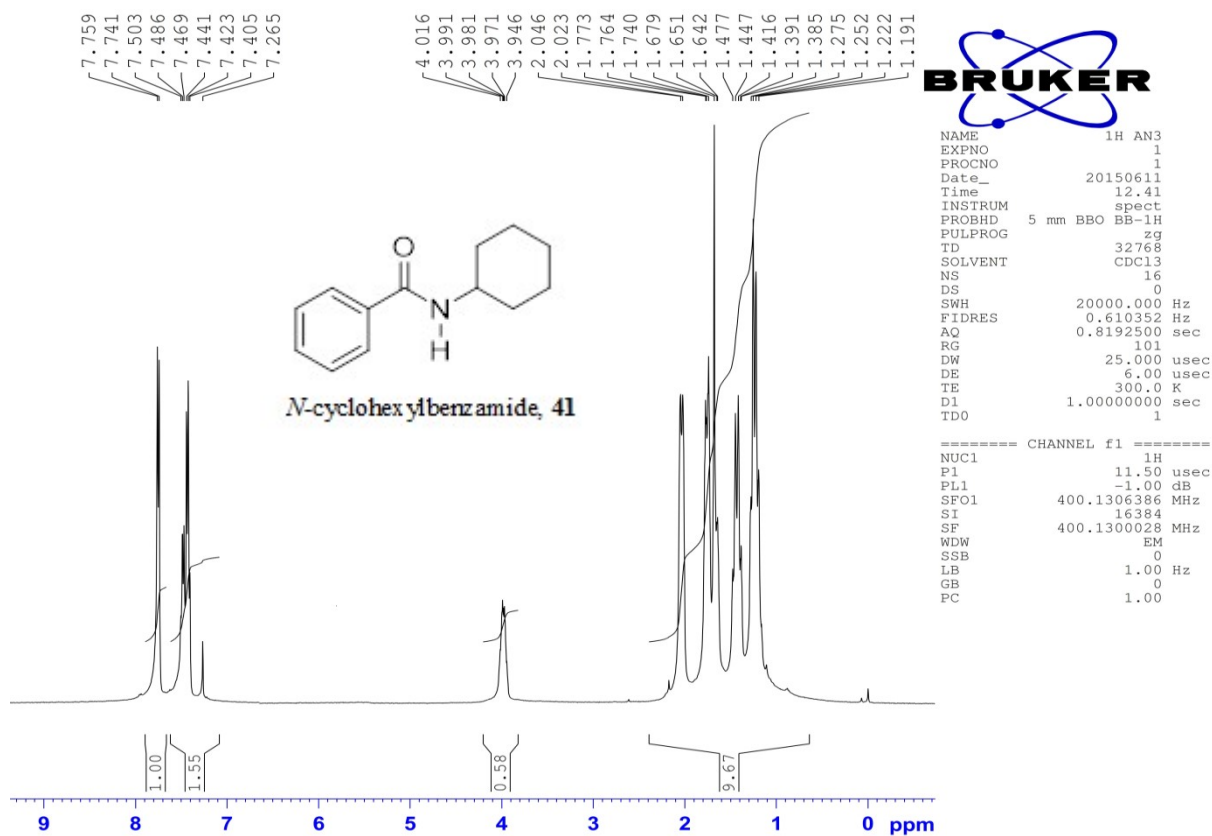
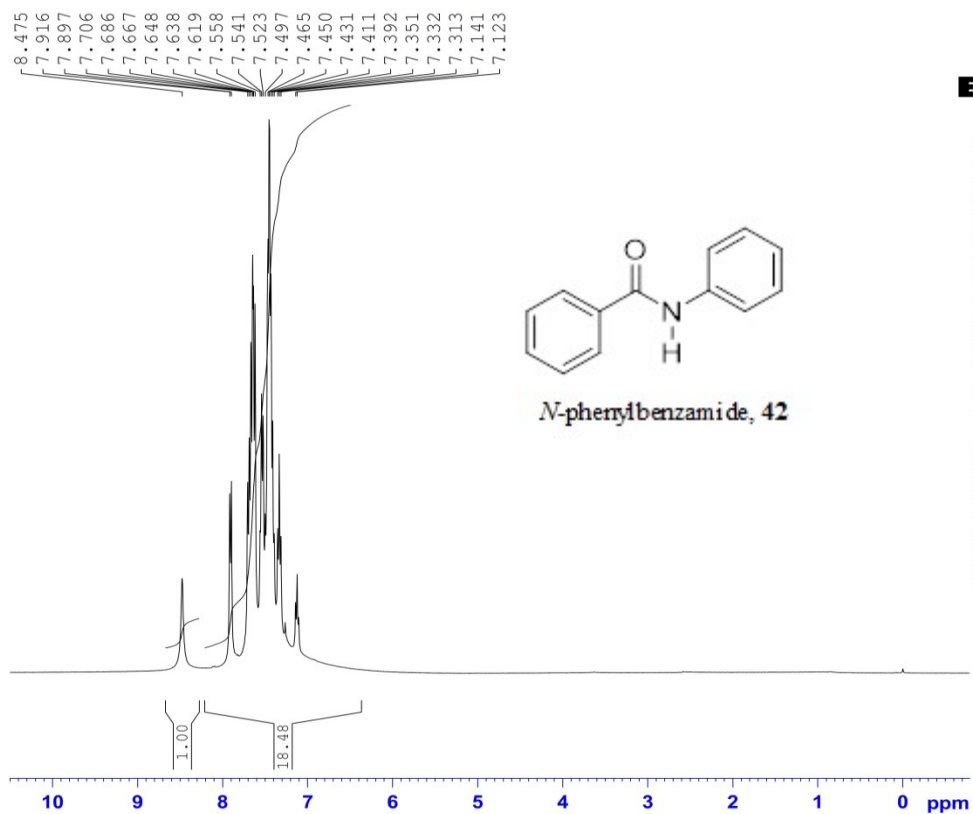


Fig: ^1H & ^{13}C NMR of *N*-cyclohexylbenzamide, 41

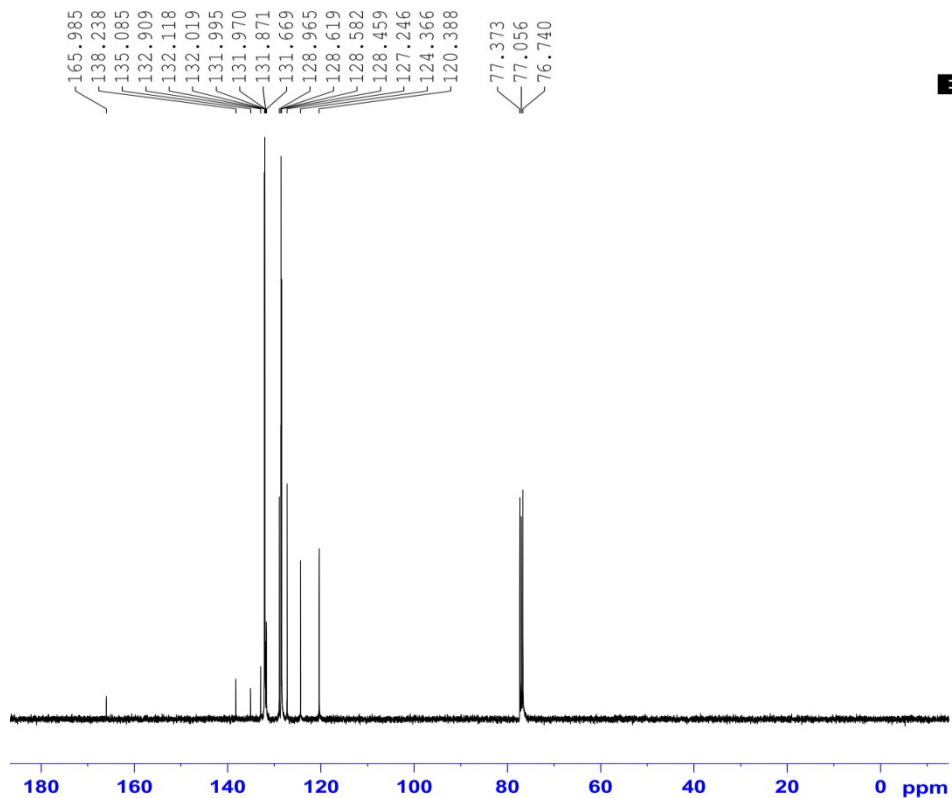


```

NAME          1H AN2
EXPNO         1
PROCNO        1
Date_         20150611
Time_         11.47
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpgg
TD            32768
SOLVENT       CDC13
NS            16
DS            0
SWH           20000.000 Hz
FIDRES        0.610352 Hz
AQ            0.8192500 sec
RG            101
DW            25.000 usec
DE            6.00 usec
TE            300.0 K
D1            1.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            11.50 usec
PL1           -1.00 dB
SFO1          400.1306386 MHz
SI            16384
SF            400.1300038 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.00
  
```



```

NAME          13C AN2
EXPNO         1
PROCNO        1
Date_         20150611
Time_         12.35
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpgg
TD            66560
SOLVENT       CDC13
NS            731
DS            0
SWH           40760.871 Hz
FIDRES        0.612393 Hz
AQ            0.8165193 sec
RG            256
DW            12.267 usec
DE            6.00 usec
TE            300.0 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1           0.00 dB
SFO1          100.6208180 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.00 dB
PL12          16.00 dB
PL13          20.00 dB
SFO2          400.1320007 MHz
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.40
  
```

Fig: ¹H & ¹³C NMR of *N*-phenylbenzamide, 42

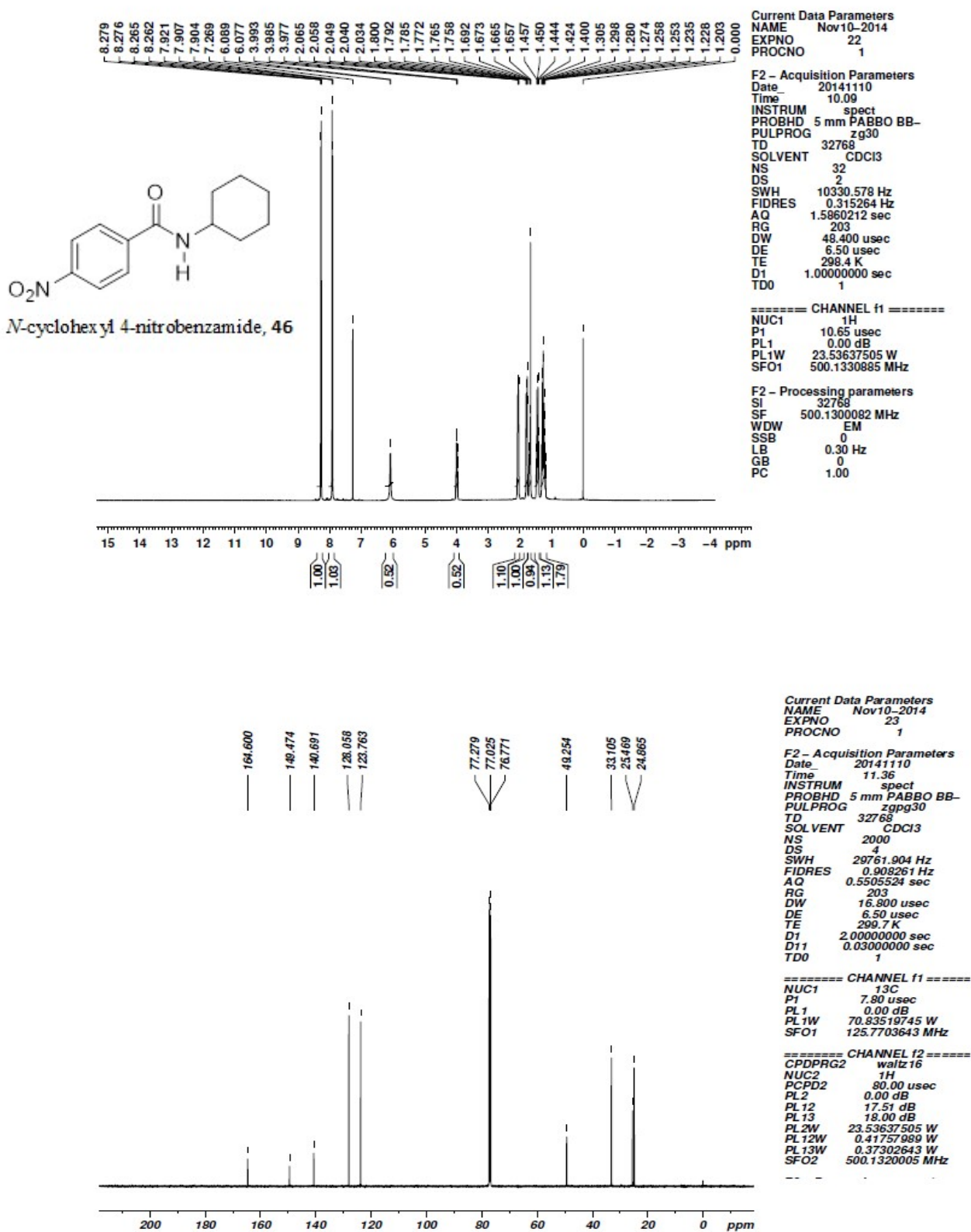


Fig: ¹H & ¹³C NMR of *N*-cyclohexyl 4-nitrobenzamide, 46