

## Supplementary Information-2

### Copies of $^1\text{H-NMR}$ , $^{13}\text{C-NMR}$ spectra and chiral HPLC chromatograms

#### Stereoselective synthesis of 1,3-disubstituted isoindolines via Rh(III)-catalyzed tandem oxidative olefination-cyclization of 4-aryl cyclic sulfamidates

Se-Mi Son<sup>a,+</sup>, Yeon Ji Seo<sup>a,b,+</sup>, and Hyeon-Kyu Lee<sup>a,b\*</sup>

a) Korea Chemical Bank, Korea Research Institute of Chemical Technology, PO Box 107, Yuseong, Daejeon 305-600, Korea.

b) Department of Medicinal Chemistry and Pharmacology, University of Science and Technology, 113 Gwahango, Yuseong, Daejeon 305-333, Korea.

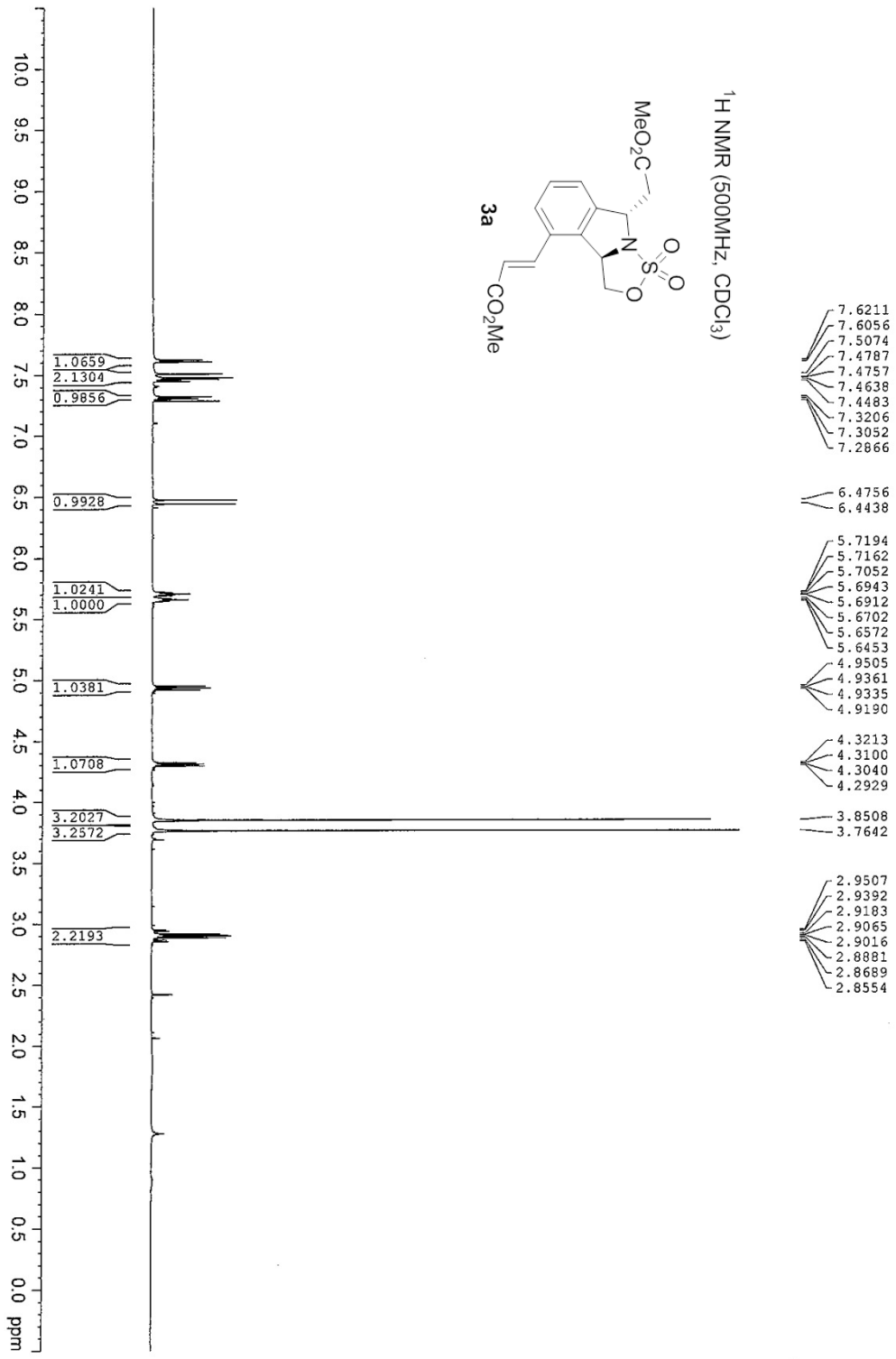
<sup>+</sup> These two authors contributed equally to this work

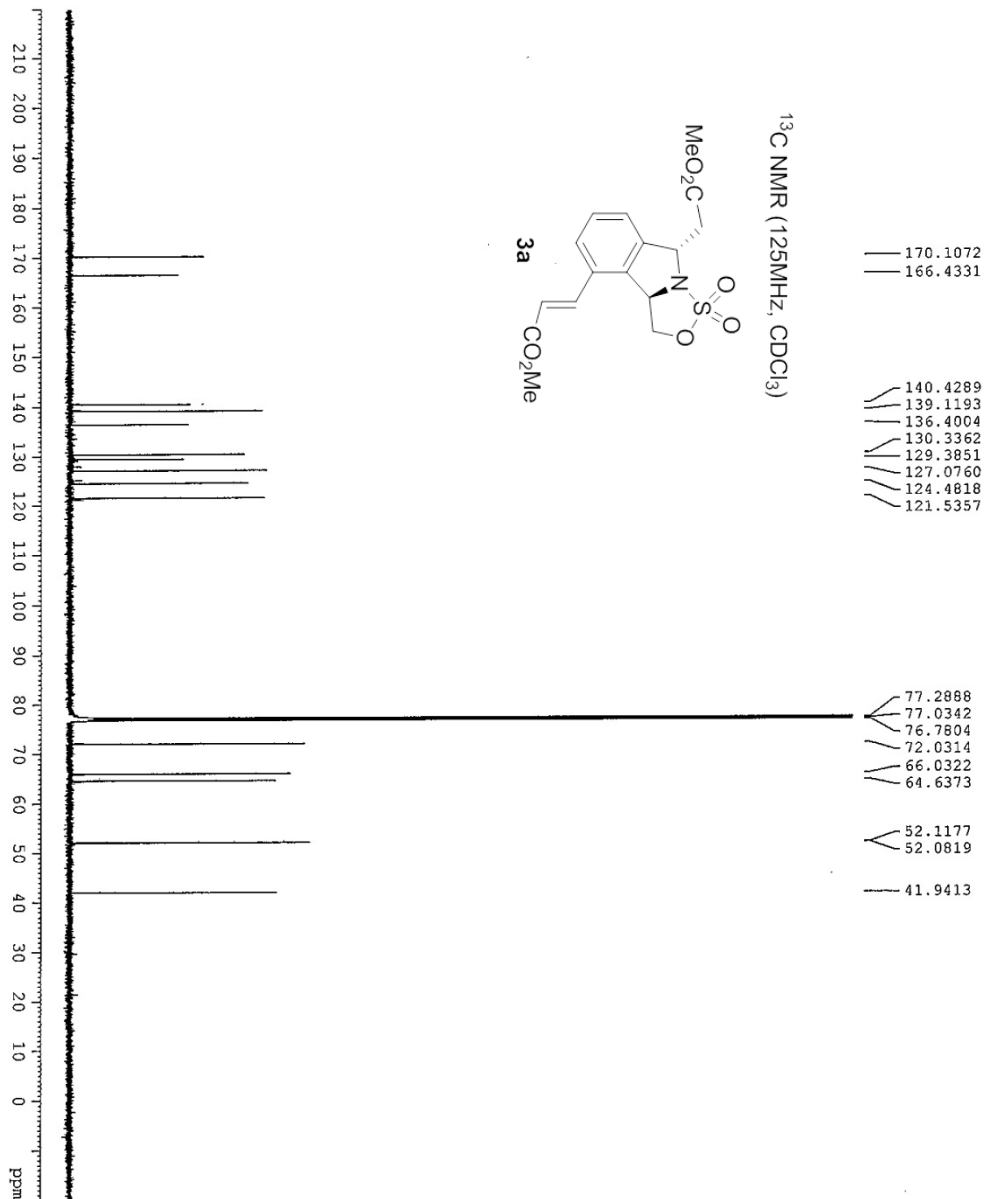
Tel: +82-42-860-7016; Fax: +82-42-860-7096

*e-mail: leehk@kRICT.re.kr*

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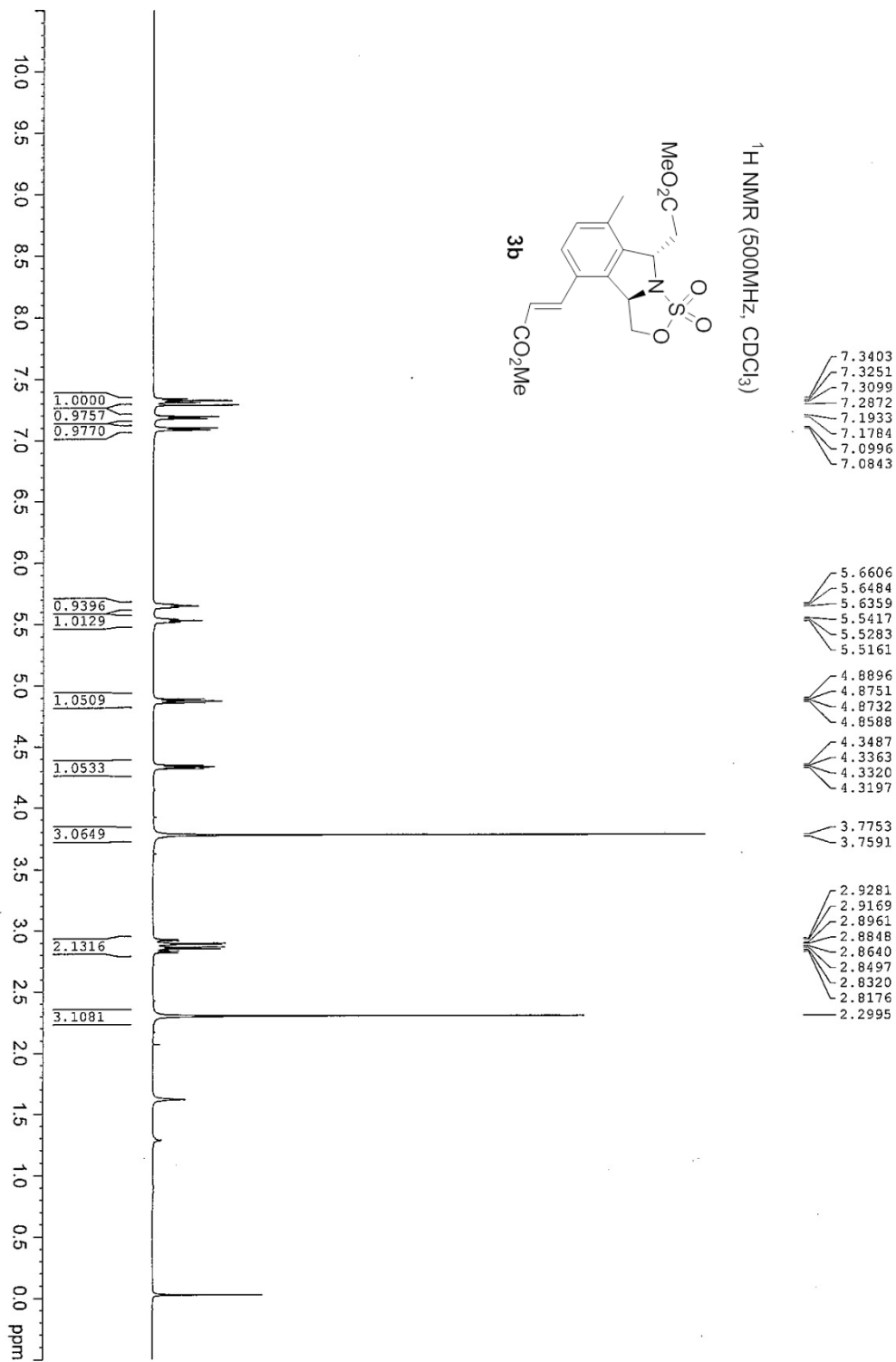
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TD 32768
SOLVENT CDCl3
NS 3000
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407385 sec
RG 4096
DW 16.500 usec
DE 6.00 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

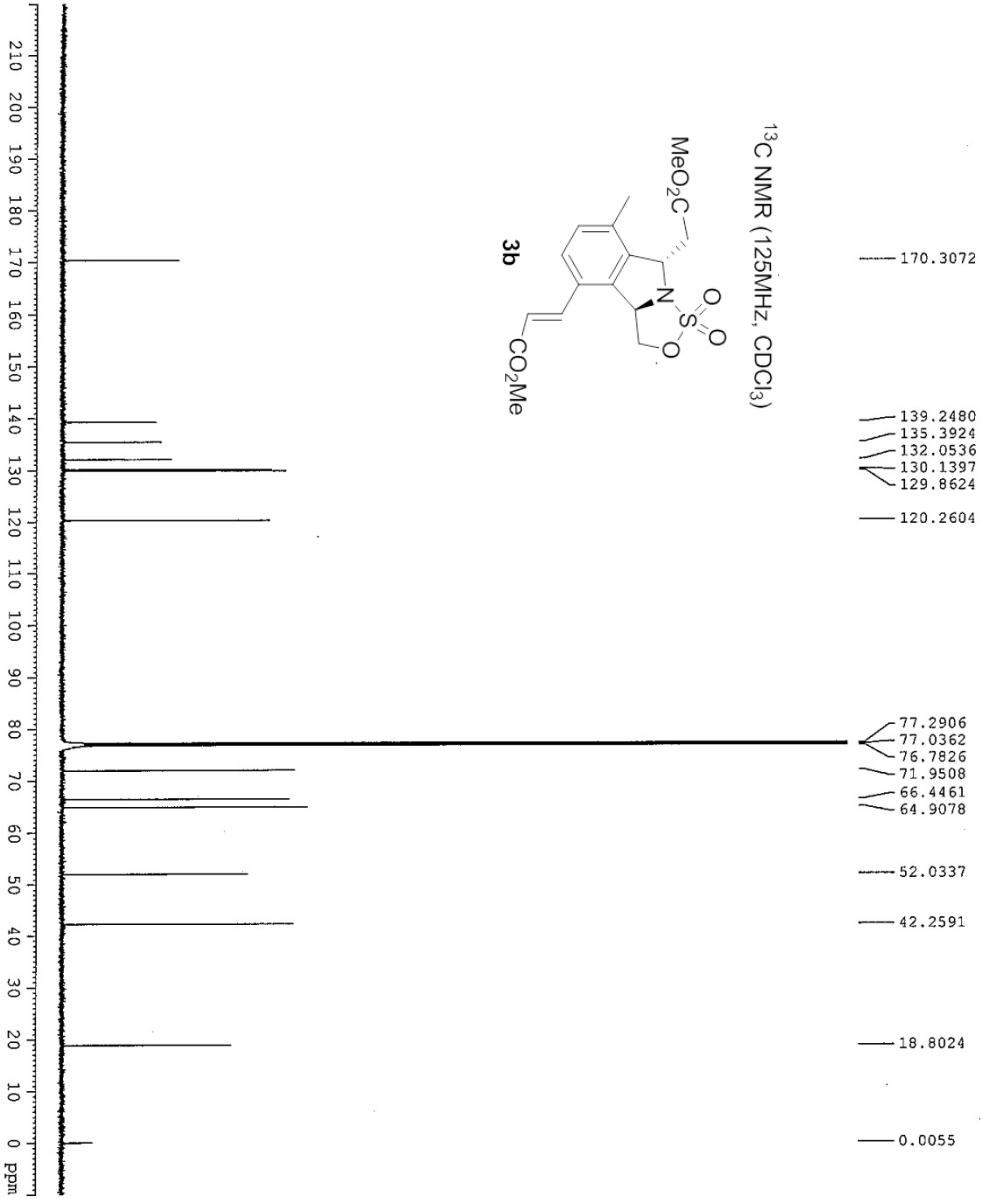
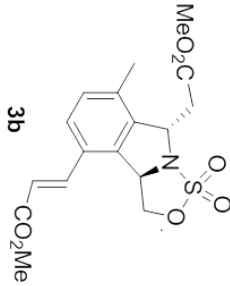
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NUC1 13C
P1 8.00 usec
PL1 1.40 dB
PL1W 70.60439301 W
SFO1 125.7703661 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPDZ 100.00 usec
FLZ 1.90 dB
PL12 16.00 dB
PL13 19.00 dB
PL1W 27.23316002 W
PL1Z 0.44167015 W
PL13W 0.22135943 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)

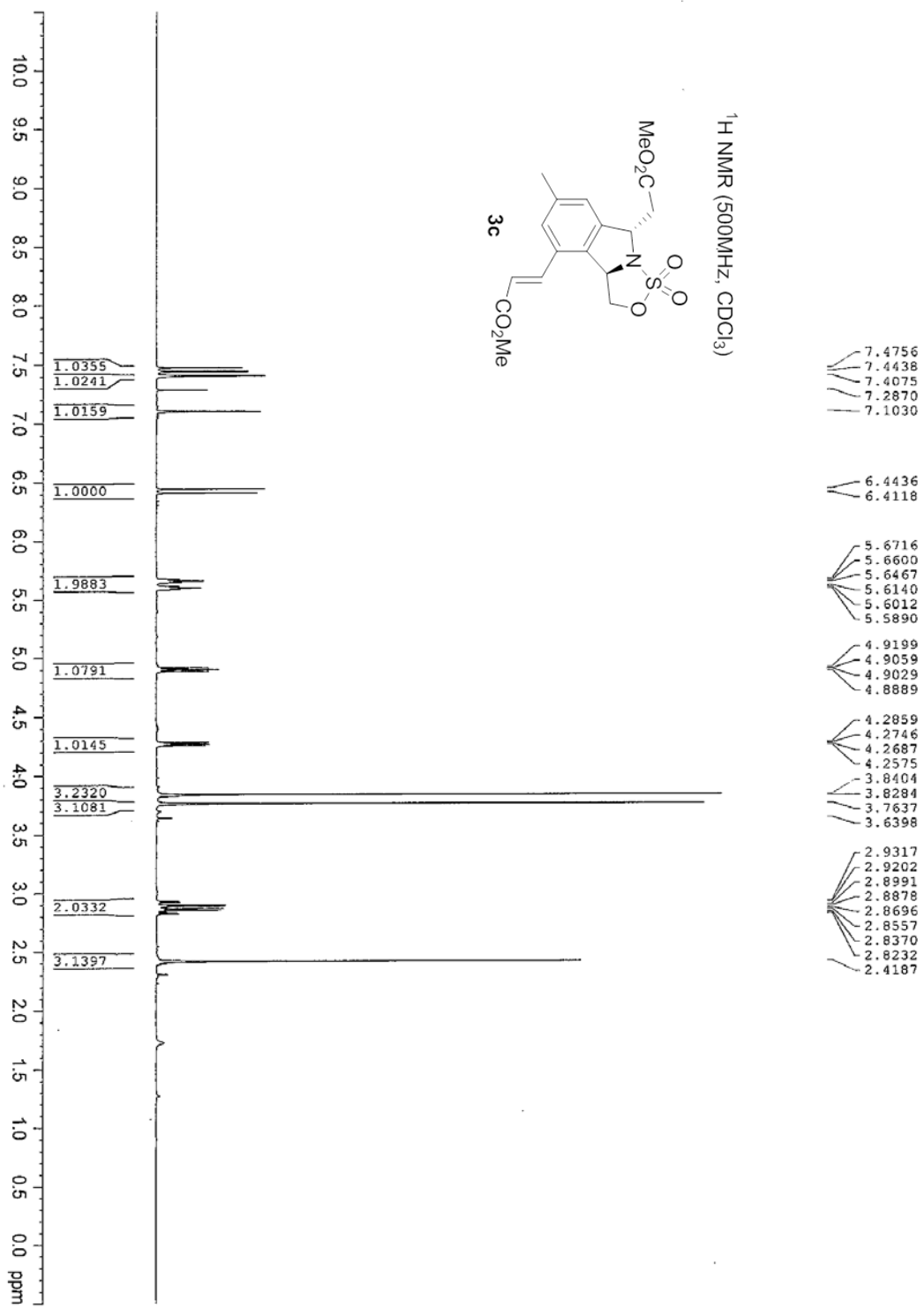


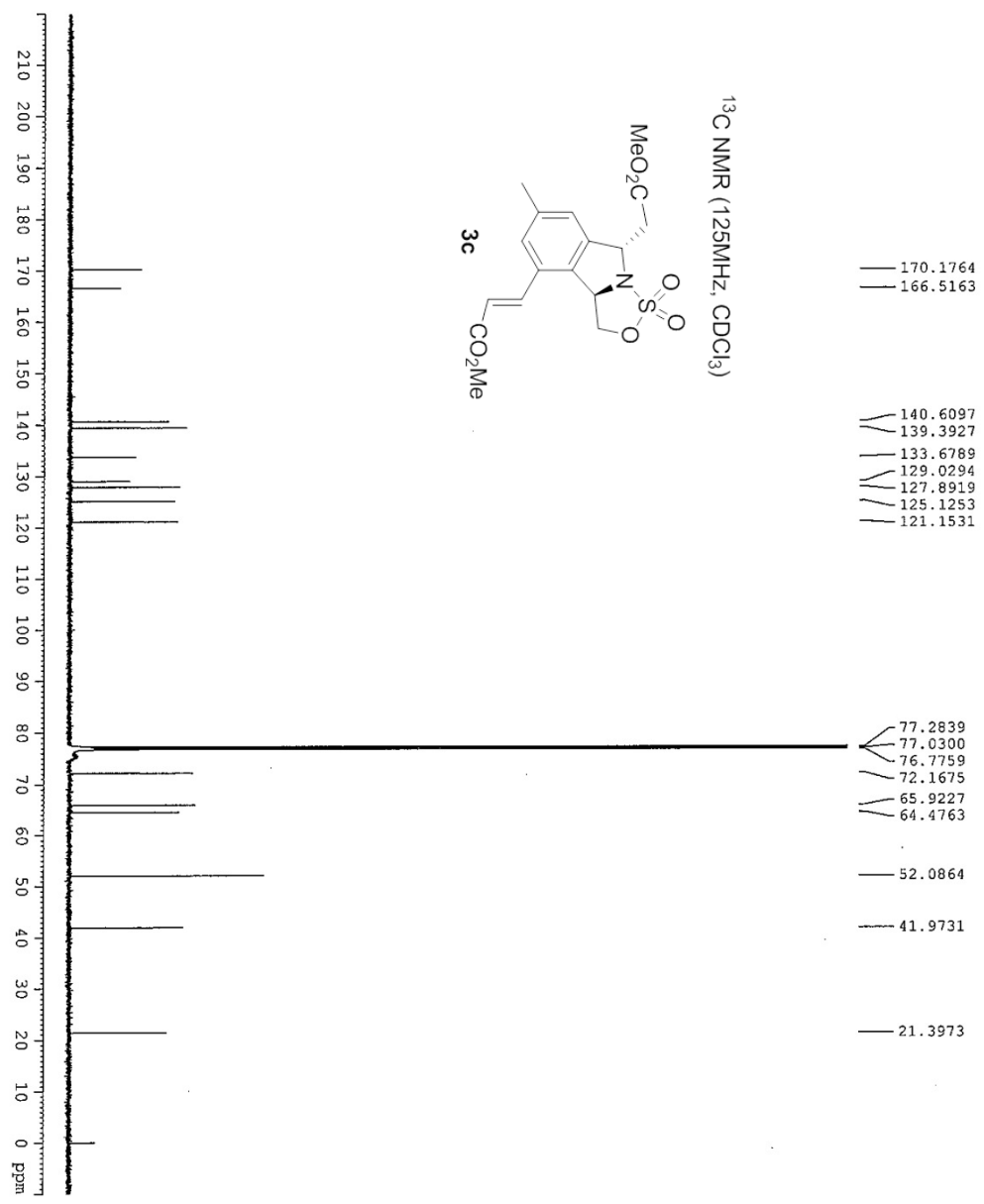
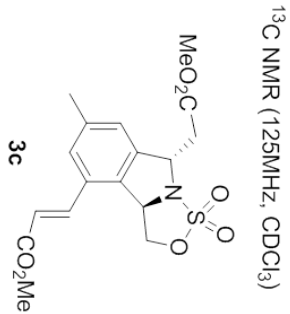
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PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            2912
DS            2
SWH           30303.031 Hz
FIDRES       0.924775 Hz
AQ           0.5407385 sec
RG           362
DE           16.500 usec
TE           296.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
EPL1         70.60438301 W
SFO1         129.7703661 MHz

===== CHANNEL f2 =====
CPDPRG2      walz16
NUC2          1H
PCPD2        100.00 usec
PL2           -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL14         27.23316002 W
PL15         0.44167015 W
PL16         0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
GB           0
PC           1.40
  
```



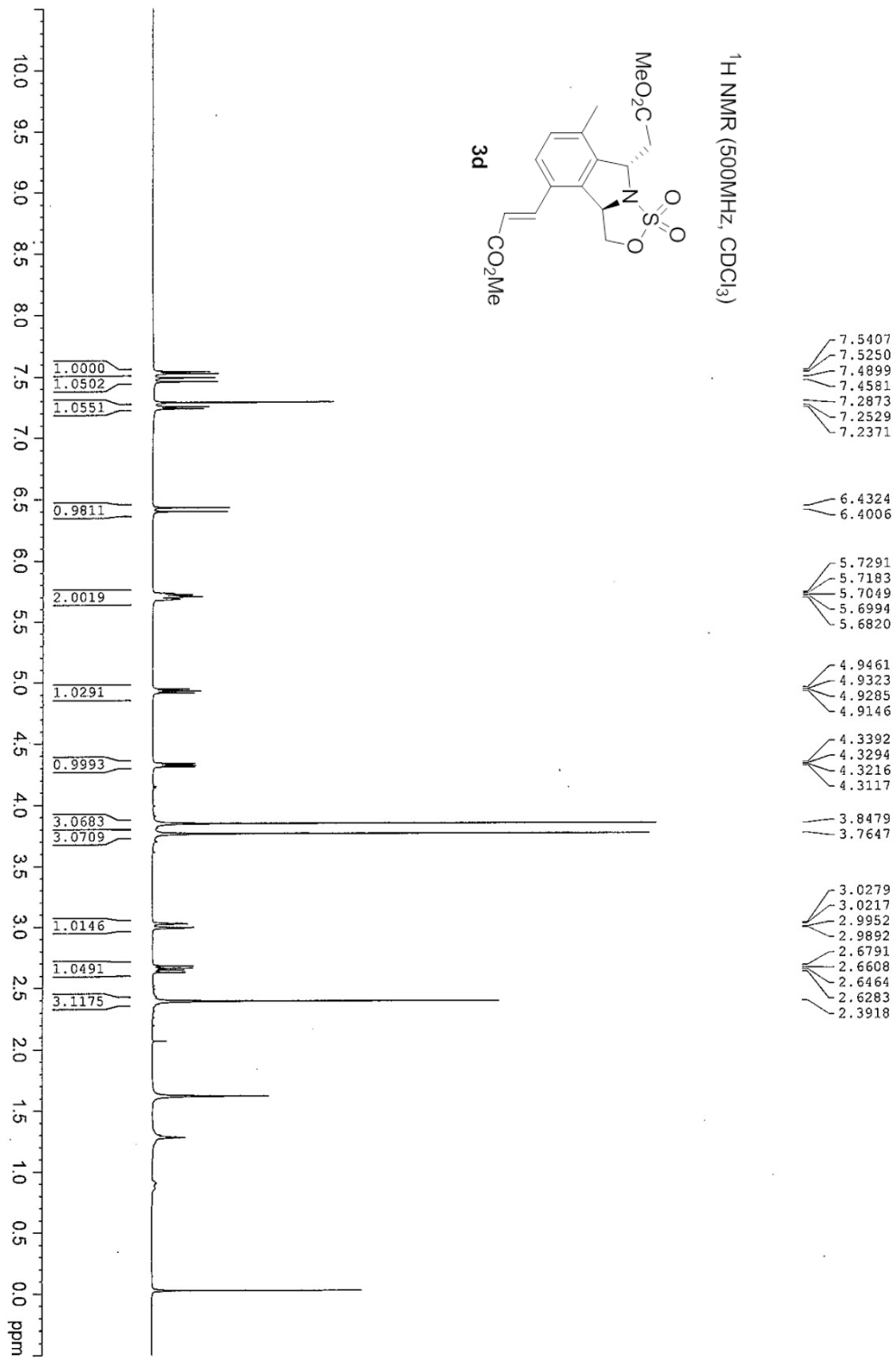


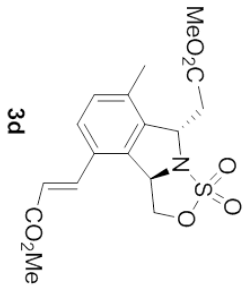
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PROBHD	specC
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	3000
DS	2
SWH	30303.031 Hz
FIDRES	0.924775 Hz
AQ	0.5407385 sec
RG	161.3
DW	16.500 usec
DE	6.00 usec
TE	296.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

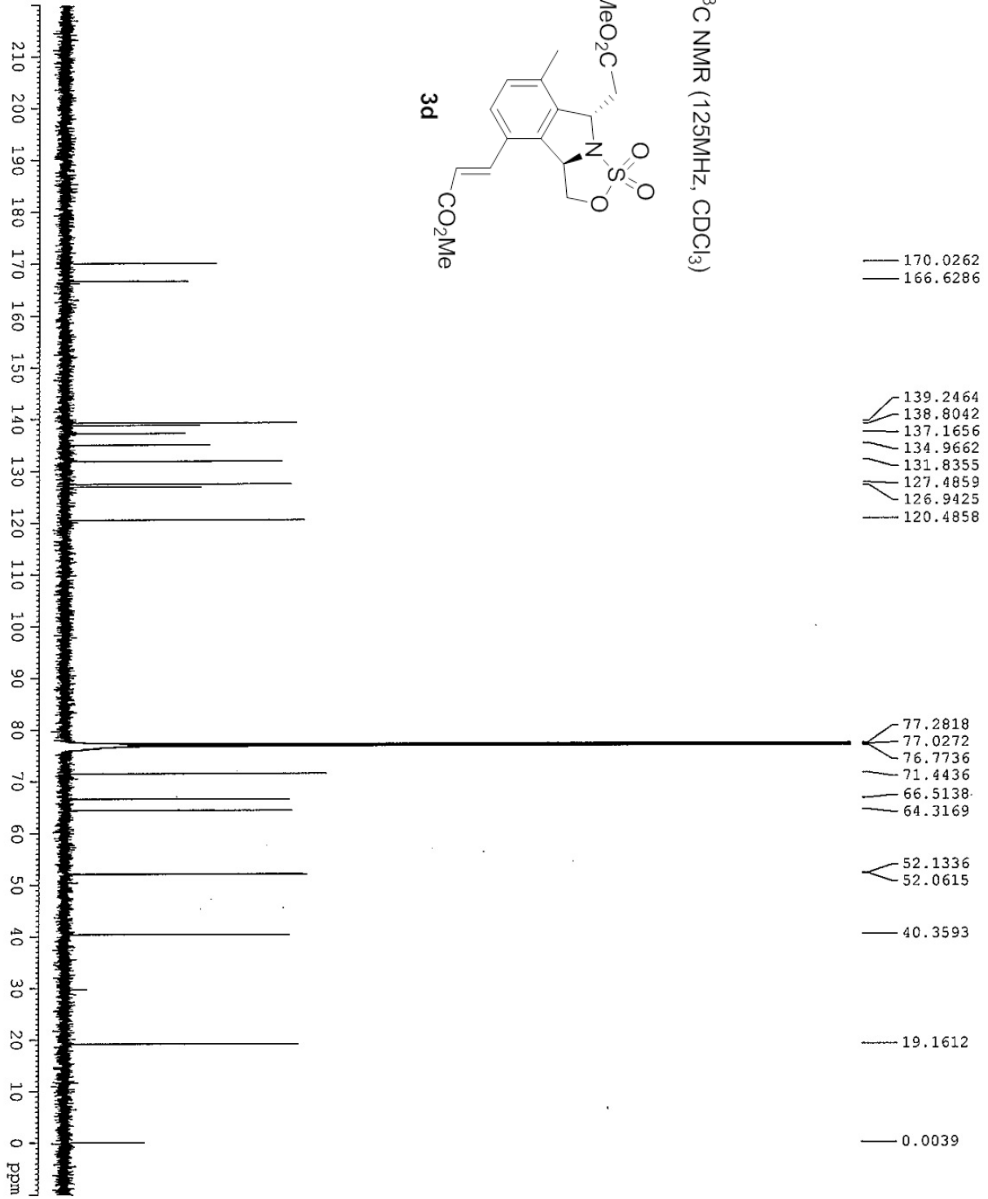
===== CHANNEL f1 =====	
NUC1	<sup>13</sup> C
P1	8.00 usec
P11	1.40 dB
P11W	70.60435301 W
SFO1	125.7703661 MHz
===== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	<sup>1</sup> H
PCPD2	100.00 usec
P12	-1.90 dB
P112	16.00 dB
P113	19.00 dB
P12W	27.23316002 W
P112W	0.44167015 W
P113W	0.22135943 W
SFO2	500.1328005 MHz
SI	32768
SP	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40







<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)



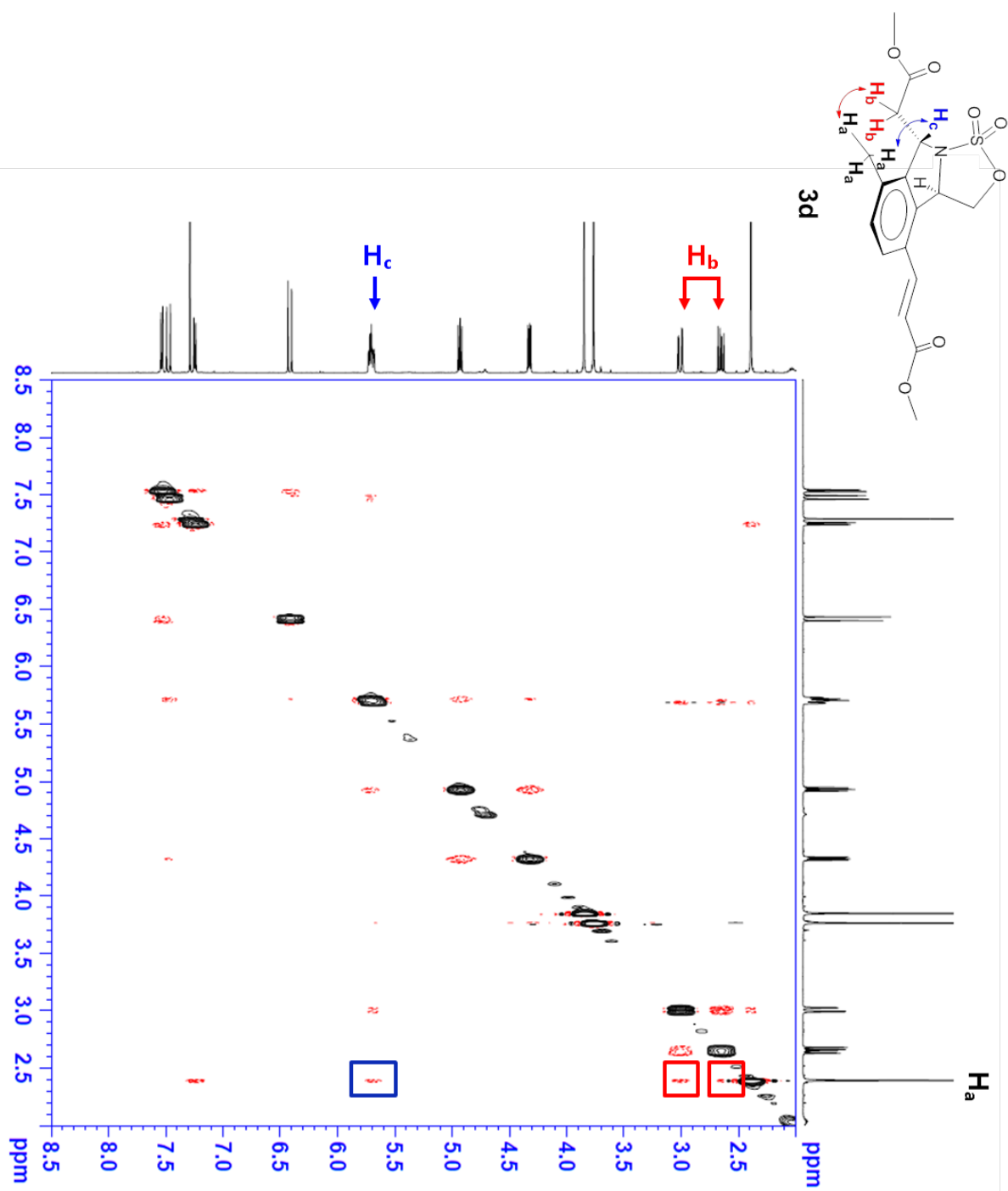
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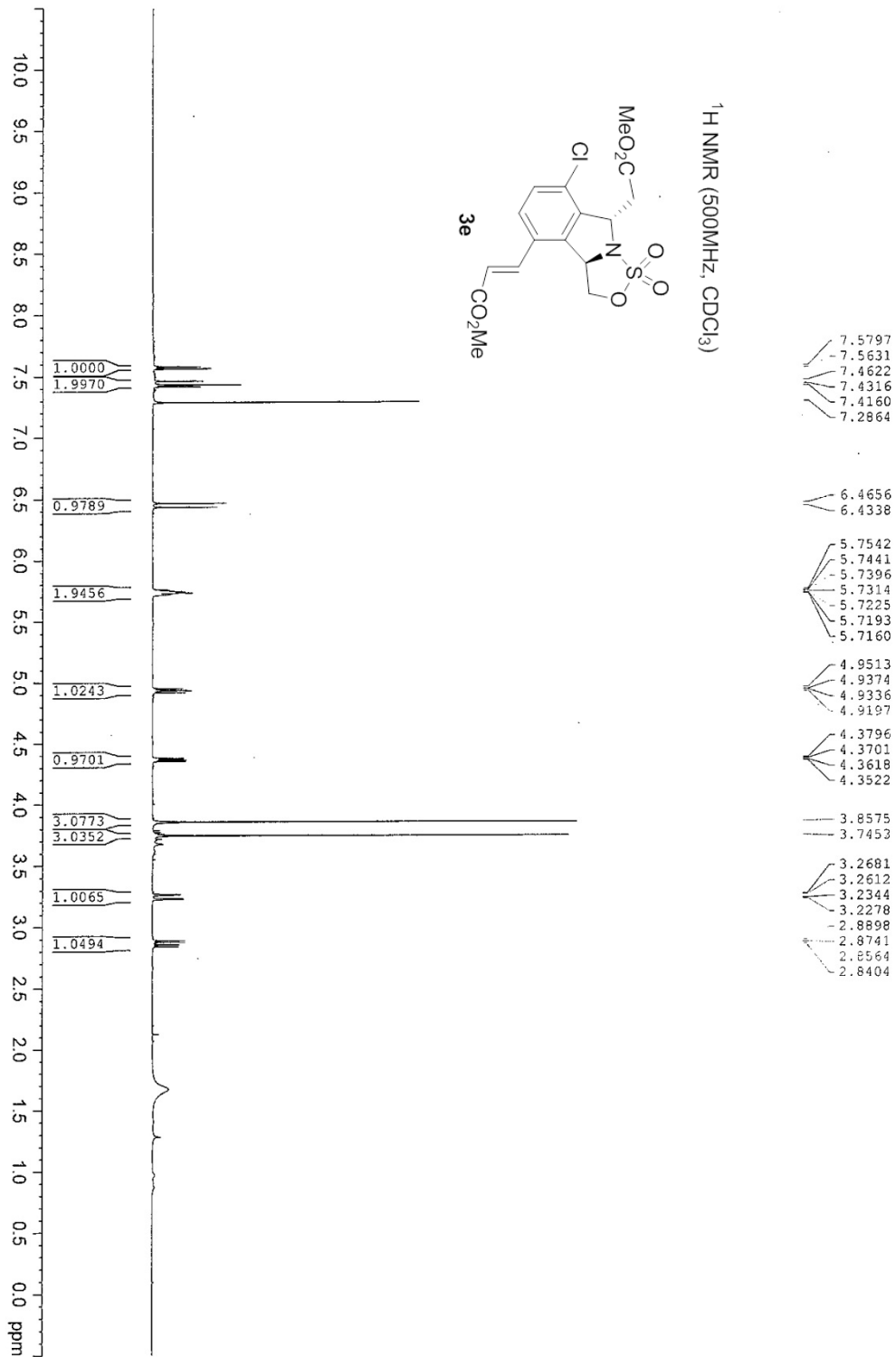
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PULPROG       zgpg30
TD            299768
SOLVENT       CDCl3
NS            3000
DS            2
SMH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407385 sec
RG            322.5
DM            16.500 usec
DE            6.00 usec
TE            300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1

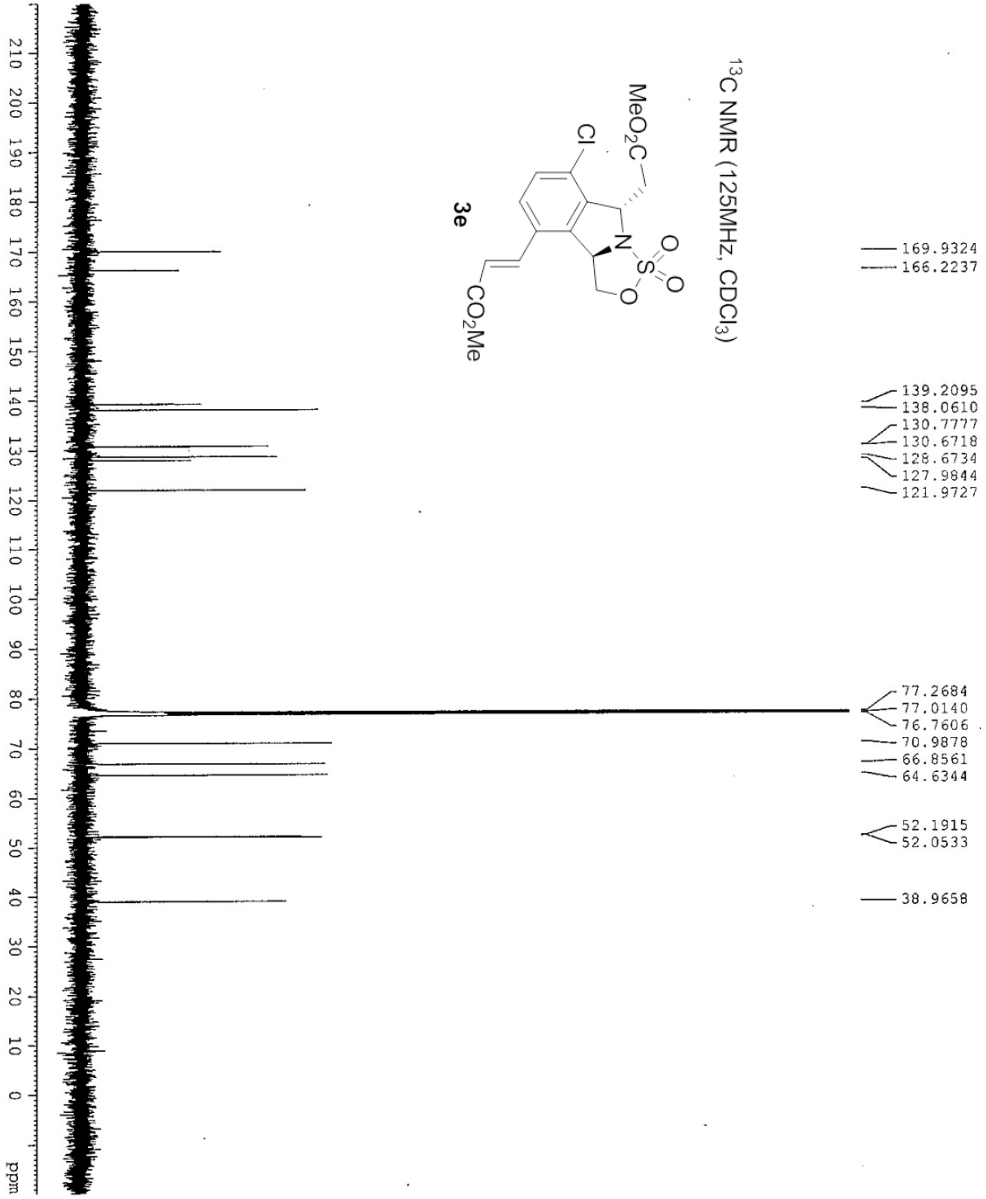
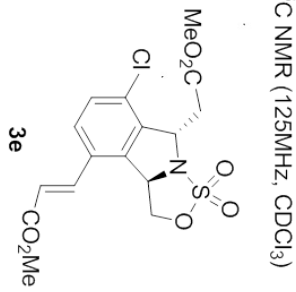
===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
PL1W         70.604393001 W
SFO1         125.7703661 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2          -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL1W         27.23316002 W
PL2W         0.44167015 W
PL13W        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

- 2D-NOESY of 3d







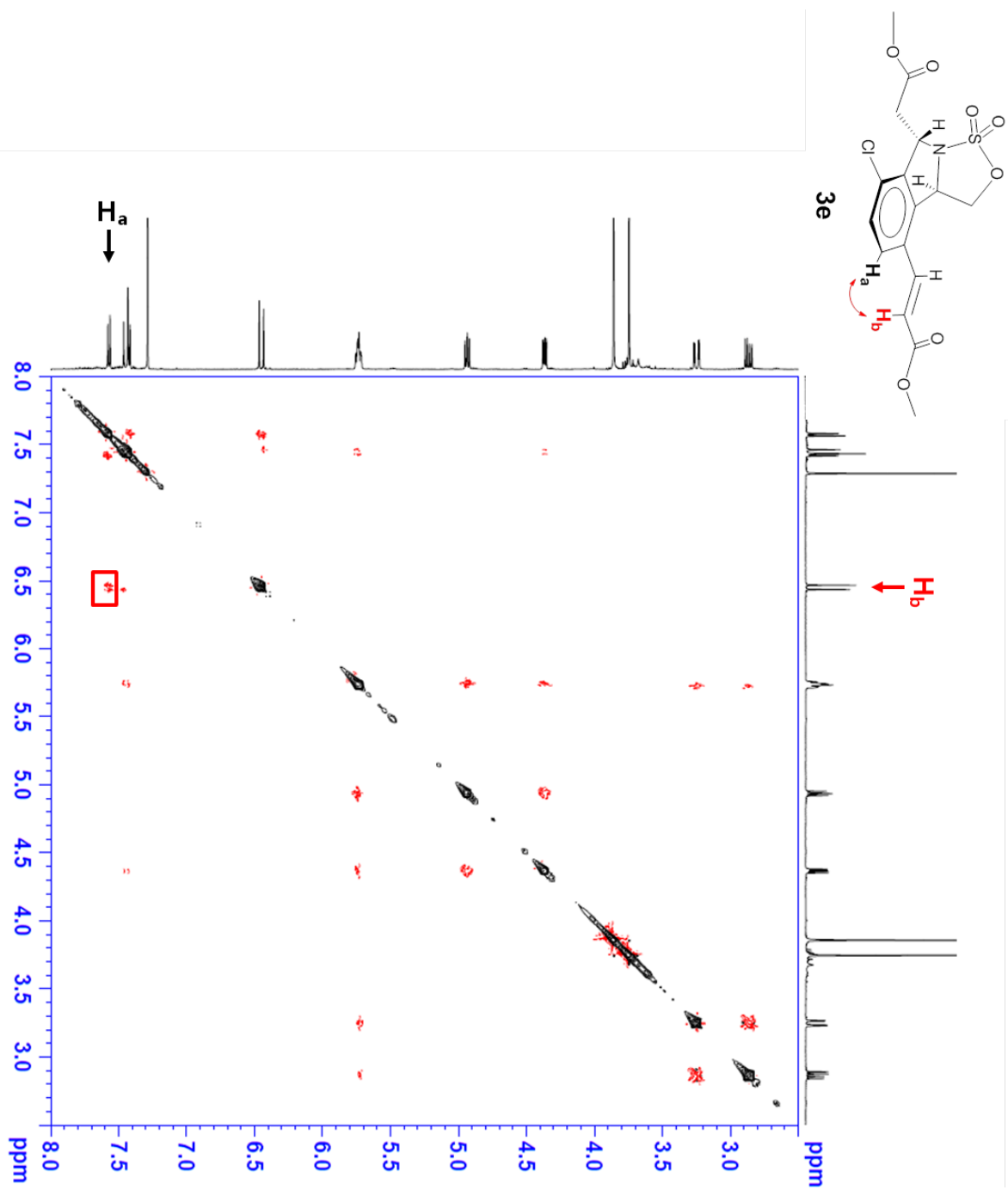
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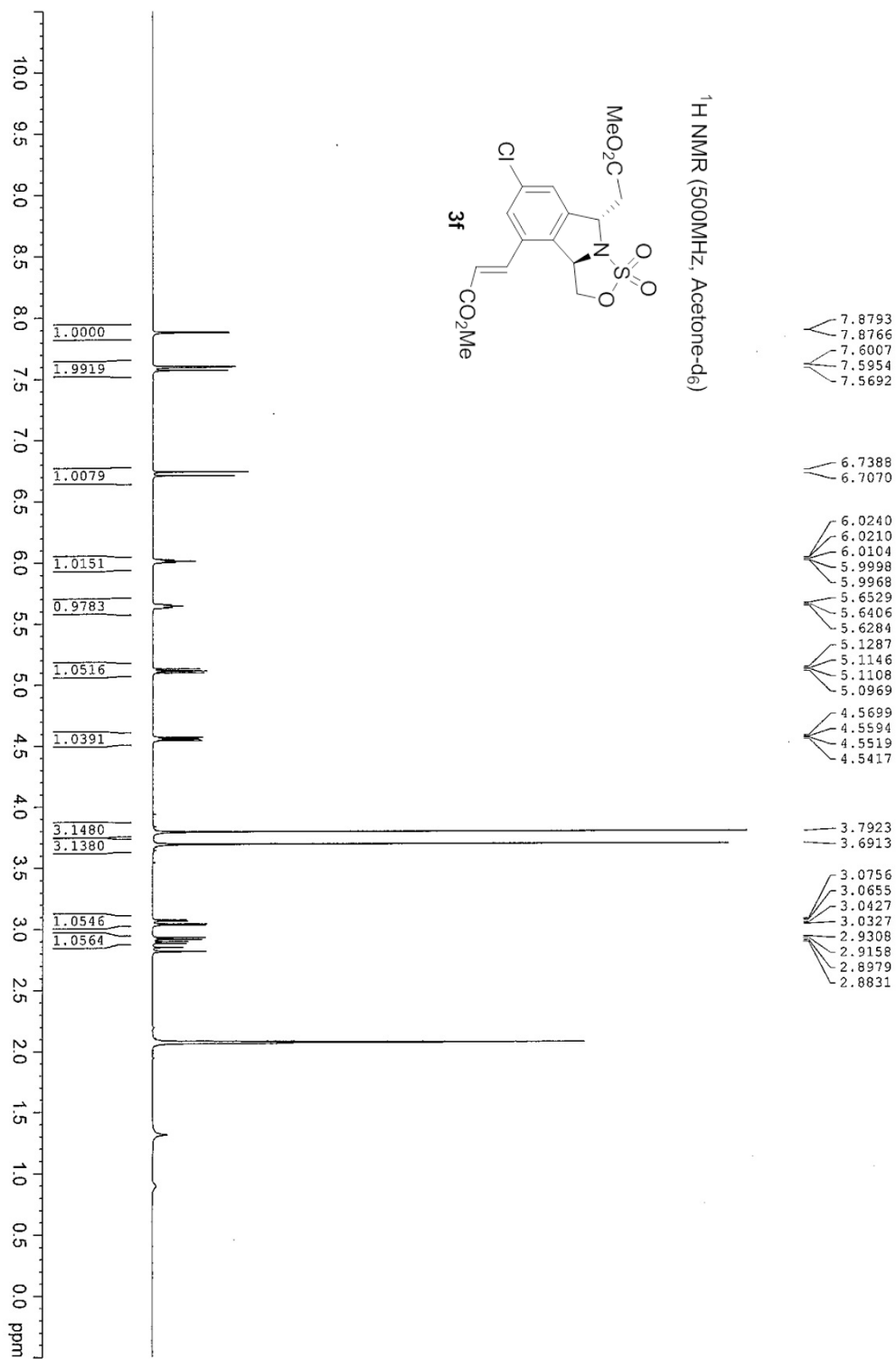
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 3000
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407385 sec
RG 161.3
DE 16.500 usec
DM 6.00 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 1.40 dB
PL1W 70.60439301 W
SFO1 125.7703661 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.80 dB
PL12 16.00 dB
PL13 19.00 dB
PL1W 27.23316002 W
PL2W 0.44167015 W
PL13W 0.22135943 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
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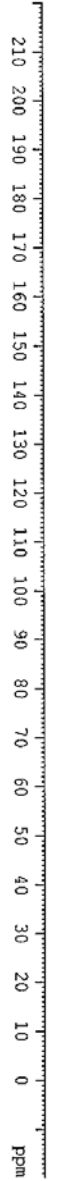
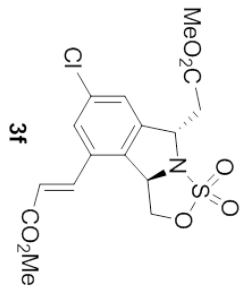
- 2D-NOESY of 3e





- 169.9151
- 166.0763
- 142.3050
- 137.7659
- 136.3548
- 134.9911
- 130.7247
- 126.9795
- 124.5636
- 122.8371
- 77.3234
- 77.0696
- 76.8147
- 71.8050
- 65.6023
- 64.2453
- 52.2480
- 52.1405
- 41.5359

<sup>13</sup>C NMR (125MHz, Acetone-d<sub>6</sub>)



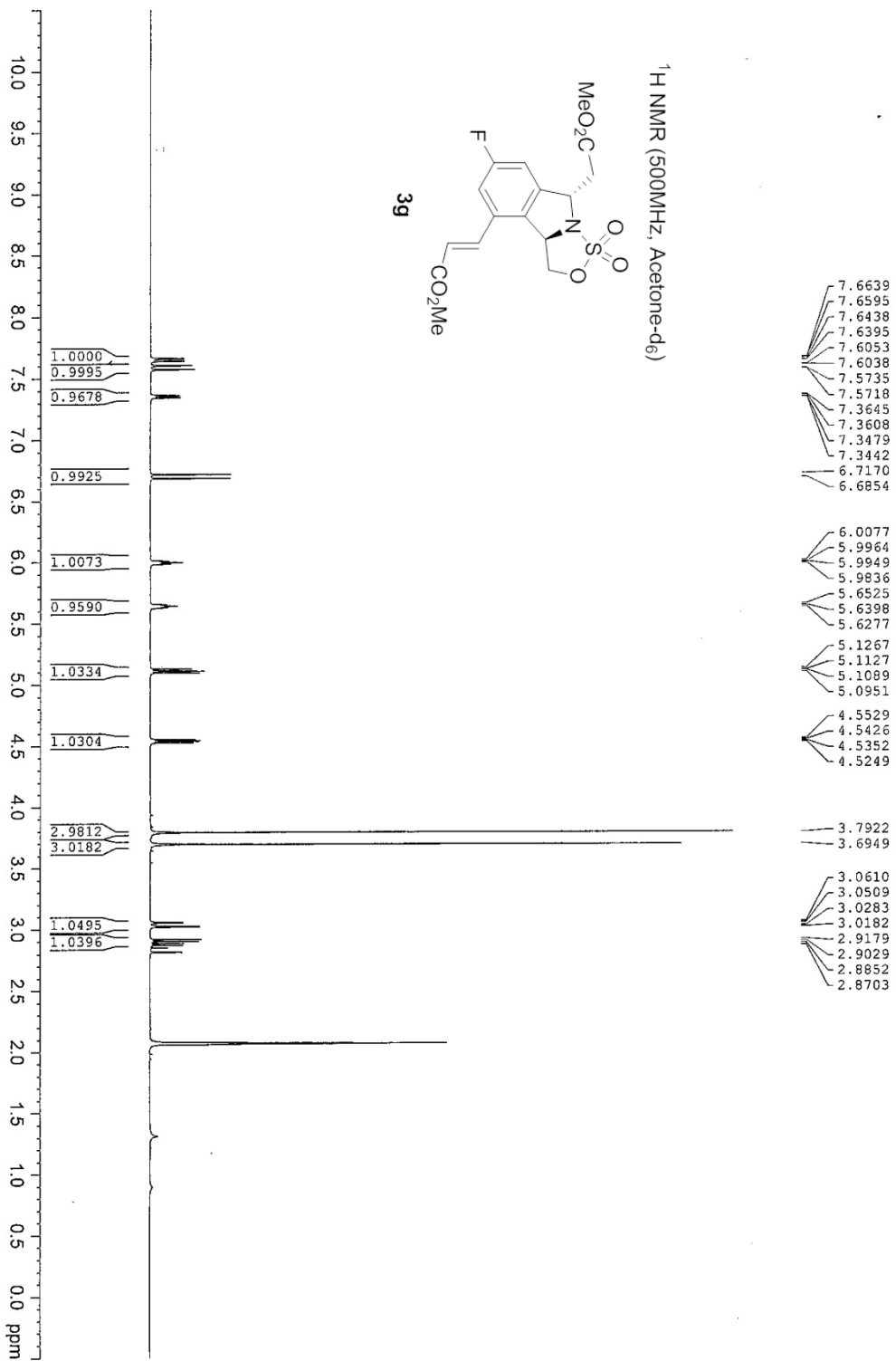
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Time          6.40
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PULPROG       32768
TD            CDC13
SOLVENT       5000
NS            2
DS            30303.031 Hz
SMH           0.924775 Hz
FIDRES        0.5407385 sec
AQ            161.3
RG            16.500 usec
DE            6.00 usec
TE            297.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
P1L1W        70.60439301 W
SFO1         125.7703661 MHz

===== CHANNEL f2 =====
CPOPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2          -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL2W         27.23316002 W
PL12W        0.44167015 W
PL13W        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
MDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

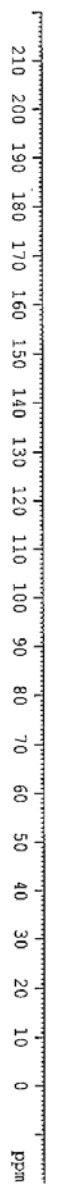
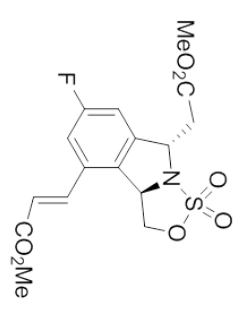




169.9198  
166.0623  
164.8127  
162.8261  
  
142.7781  
142.7088  
137.8782  
137.8634  
132.2302  
132.2138  
131.1039  
131.0347  
122.8023  
113.9274  
113.7365  
112.1242  
111.9293

72.0469  
65.4451  
64.2911  
64.2733  
  
52.2451  
52.1479  
  
41.5987

<sup>13</sup>C NMR (125MHz, Acetone-d<sub>6</sub>)

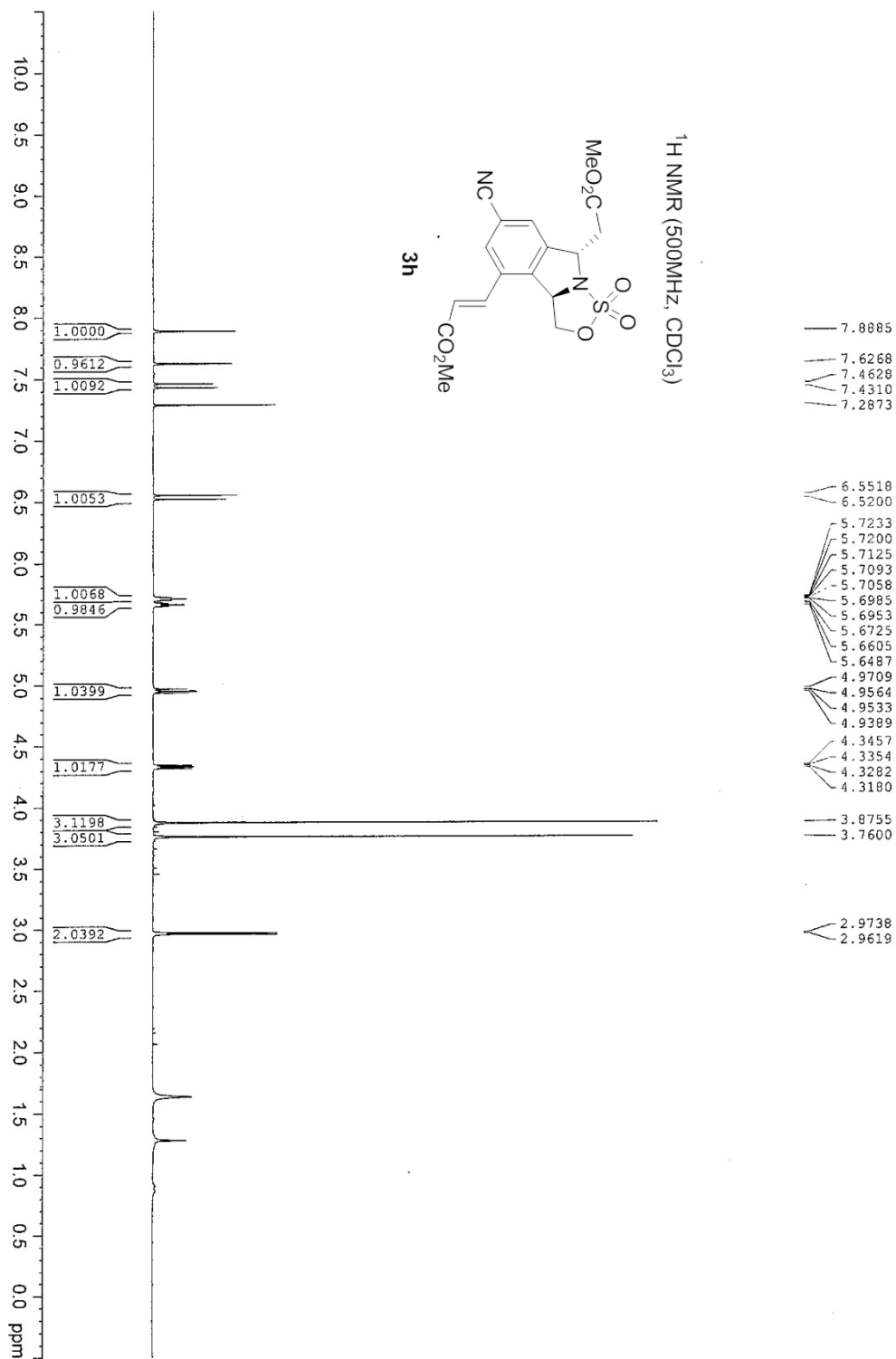


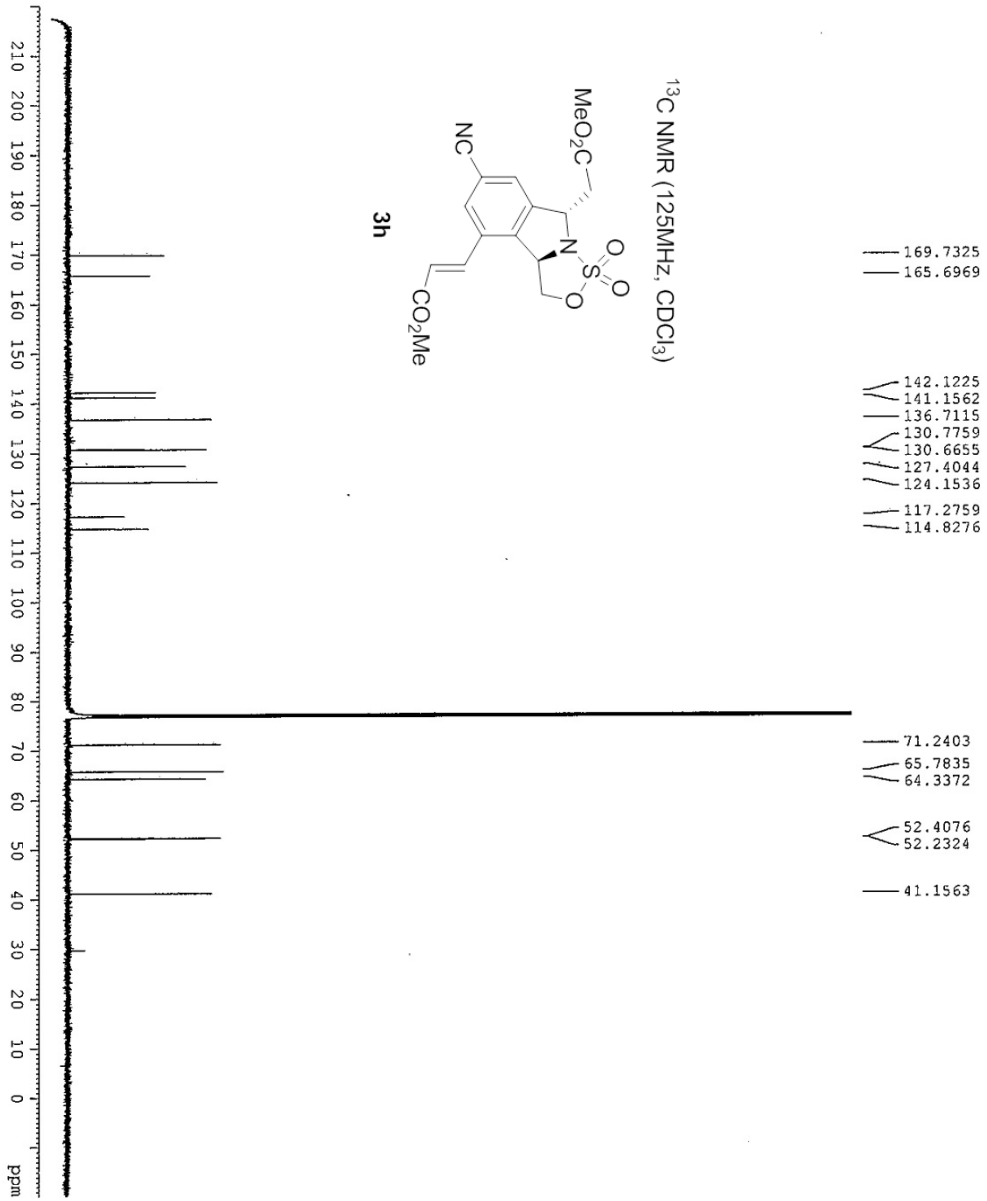
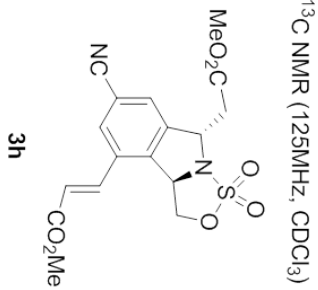
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PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            5000
DS            2
SWH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407385 sec
RG            161.3
DW            16.500 usec
DE            6.00 usec
TE            297.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL F1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
PL1W          70.60439301 W
SFO1          125.7703661 MHz

===== CHANNEL F2 =====
CDDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
P2           -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL1W         27.23316002 W
PL12W        0.44167015 W
PL13W        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
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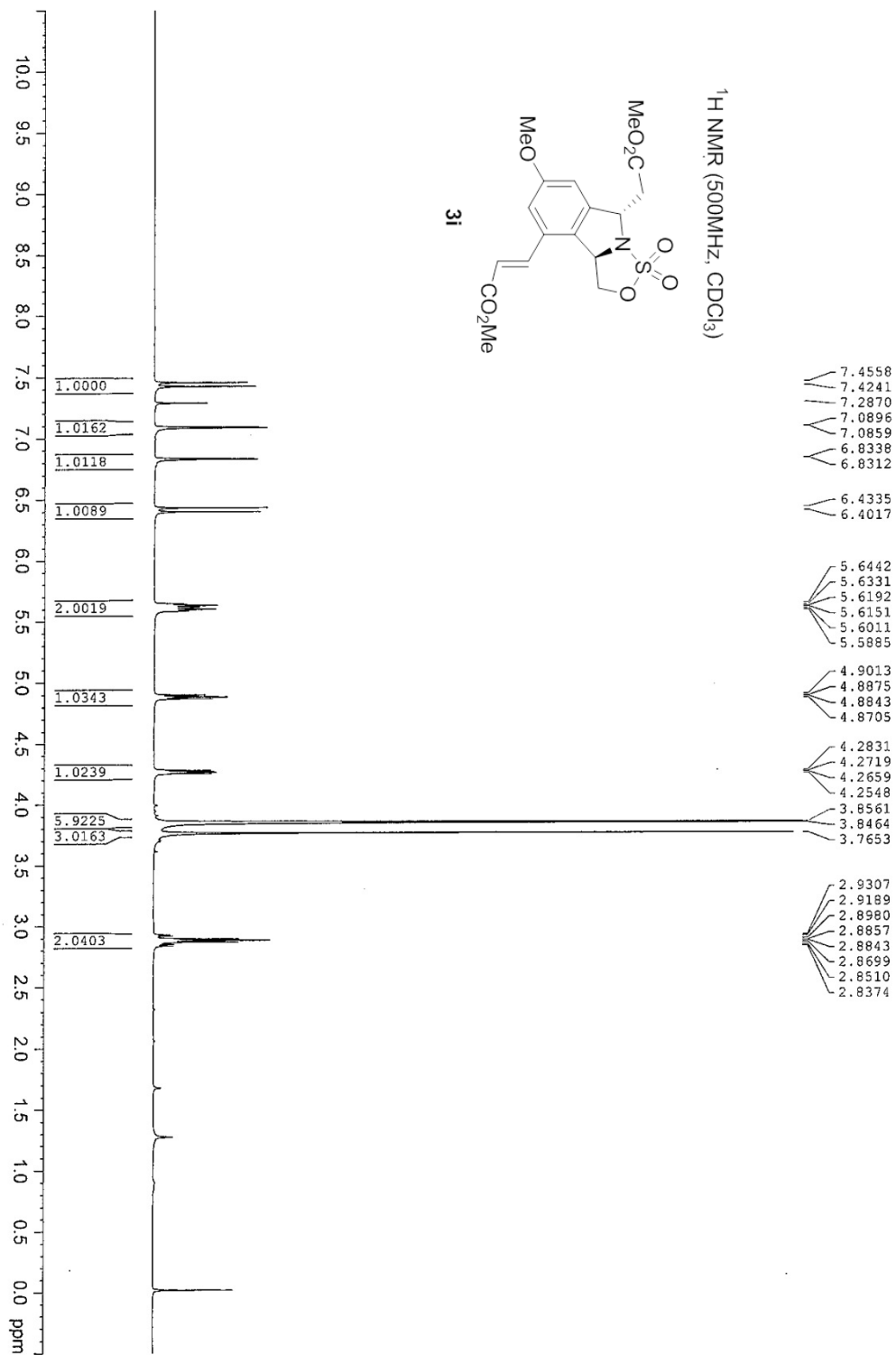


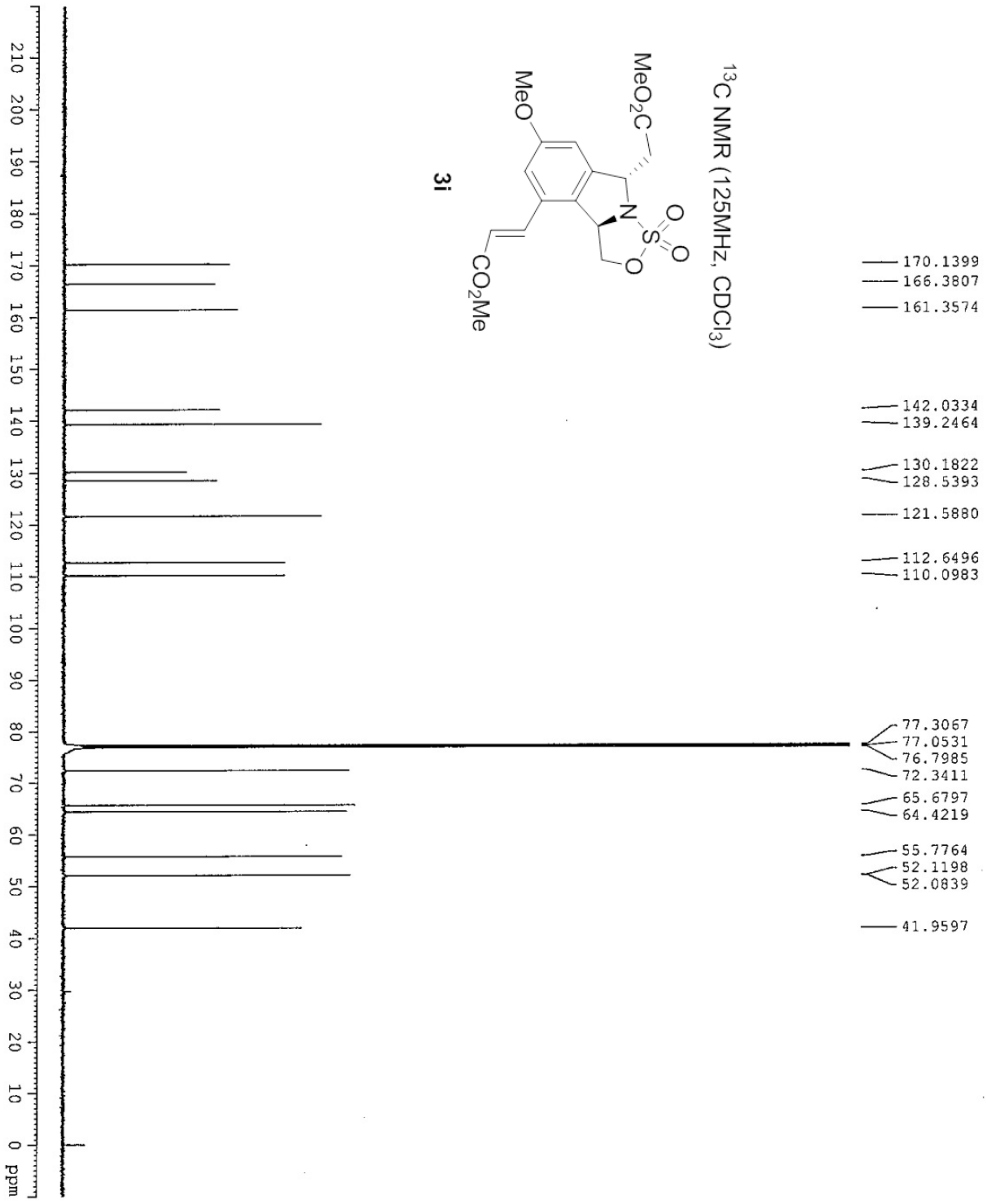
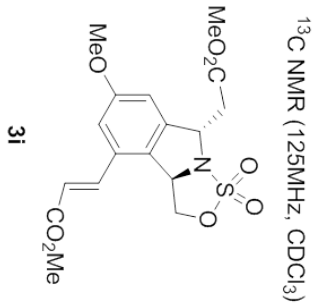
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TD            32768
SOLVENT       CDCl3
NS            3000
DS            2
SWH           30303.031 Hz
FIDRES       0.924775 Hz
AQ           0.5407385 sec
RG           161.3
DE           16.500 usec
TE           298.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1          13C
P1           8.00 usec
PL1          1.40 dB
EL1W         70.60439301 W
SFO1         125.7703661 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2          -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL14         27.23316002 W
PL15         0.44167015 W
PL16         0.22135943 W
PL17         500.1320005 MHz
SFO2         32768
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WDW          EM
SSB          0 Hz
GB          1.00 Hz
PC          0
  
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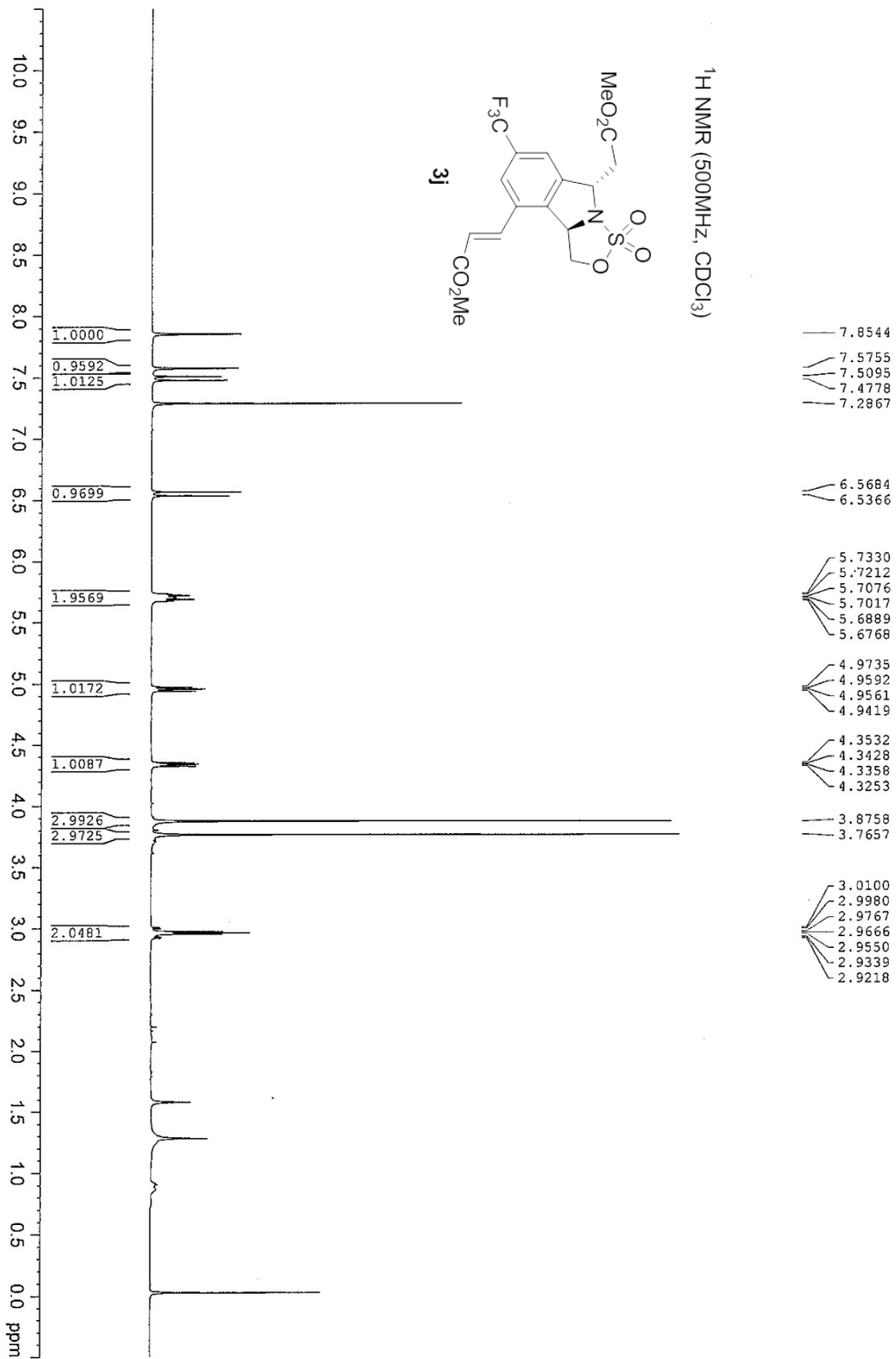


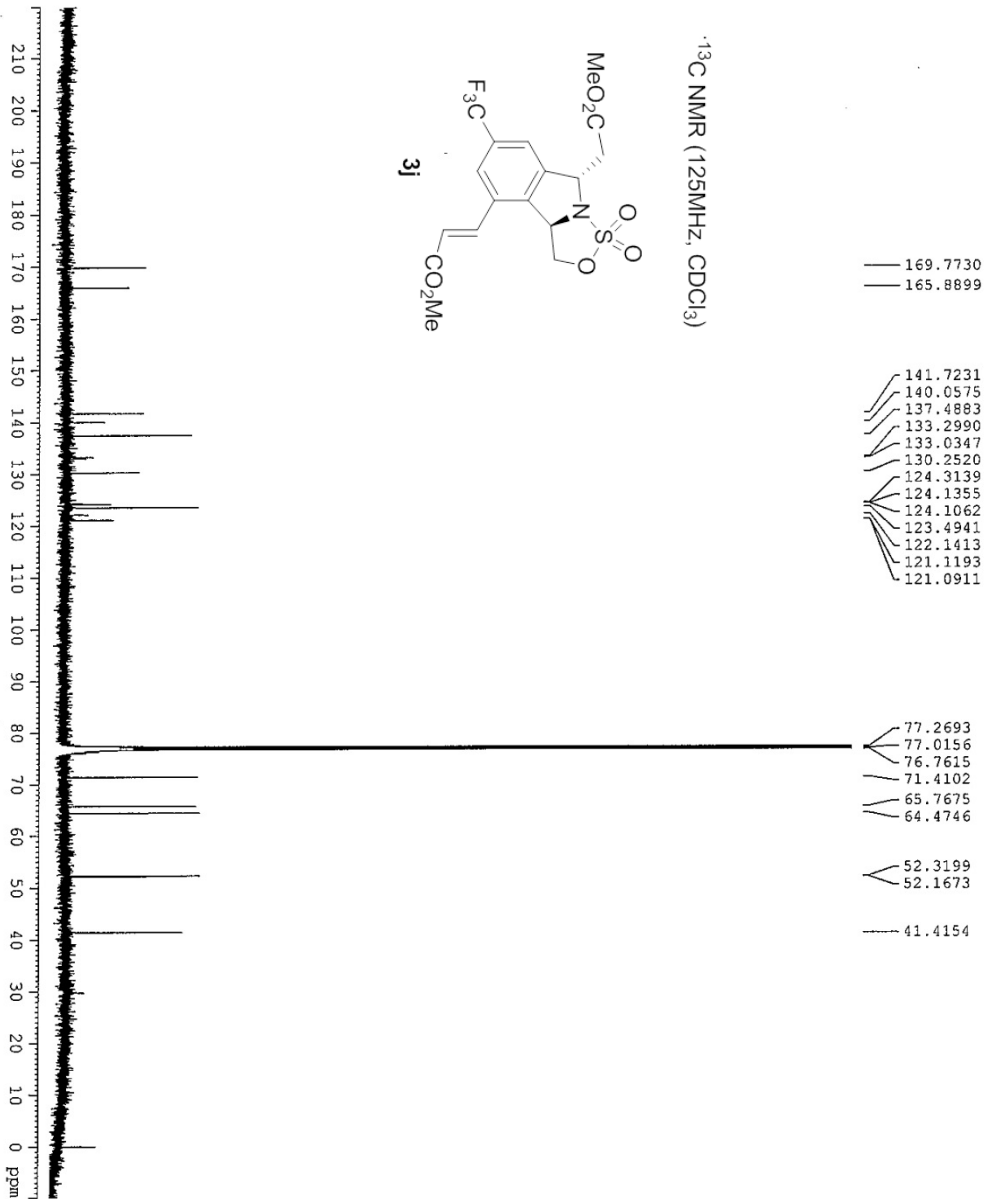
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PROCNO       20150413
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Time_
INSTRUM      spect
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PULPROG      zgpg30
TD           32768
SOLVENT      CDCl3
NS           3000
DS           2
SMH          30303.031 Hz
FIDRES      0.924775 Hz
AQ          0.5407385 sec
RG          322.5
DE          16.500 usec
TE          296.3 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1

===== CHANNEL F1 =====
NUC1         13C
P1          8.00 usec
PL1         1.40 dB
PL1W        70.60433901 W
SFO1        125.7703661 MHz

===== CHANNEL F2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2       100.00 usec
PL2         -1.90 dB
PL12        16.00 dB
PL13        19.00 dB
PL1W        27.233316002 W
PL2W        0.44167015 W
PL13W       0.22135943 W
SFO2        500.1320005 MHz
SI          32768
SF          125.7577890 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
  
```





```

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EXPNO         1
PROCNO        1
Date_         20150408
Time          5.57
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PROBHD        zppc30
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            3000
DS            2
SWH           30303.031 Hz
FIDRES       0.924775 Hz
AQ           0.5407385 sec
RG           161.3
DE           16.500 usec
TE           298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0          1

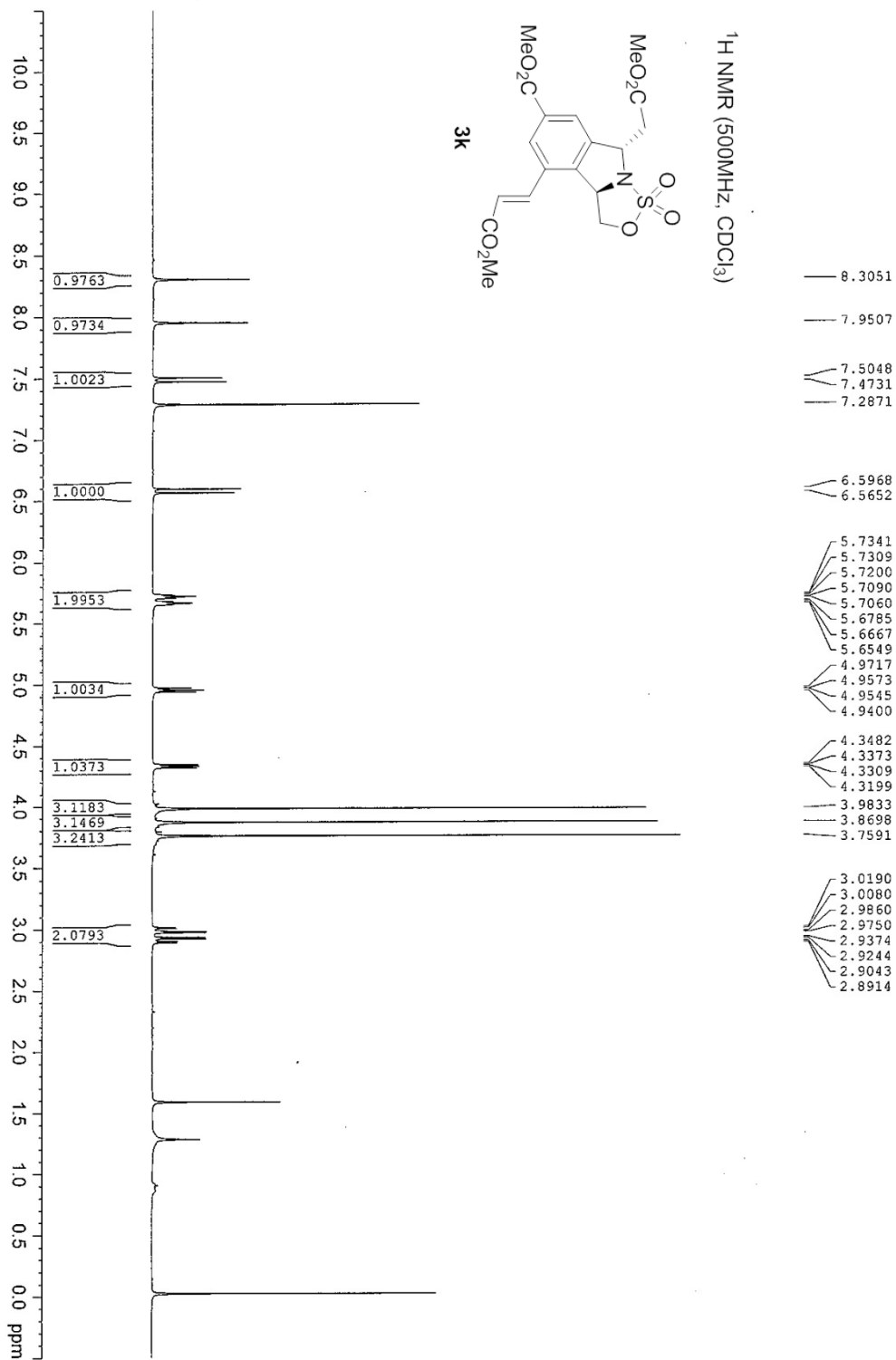
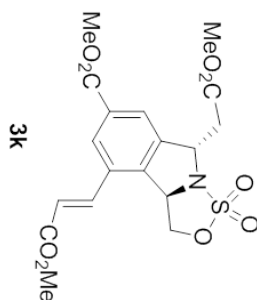
===== CHANNEL f1 =====
NUC1          13C
P1           8.00 usec
PL1          1.40 dB
PL1W         70.60439301 W
SFO1         125.7703661 MHz

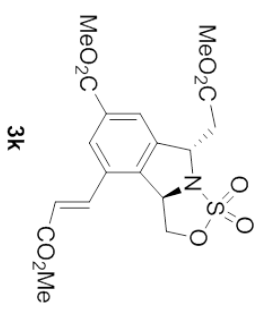
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2         1H
PCPD2        100.00 usec
PL2          -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL1W         27.23316002 W
PL12W        0.44167015 W
PL13W        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

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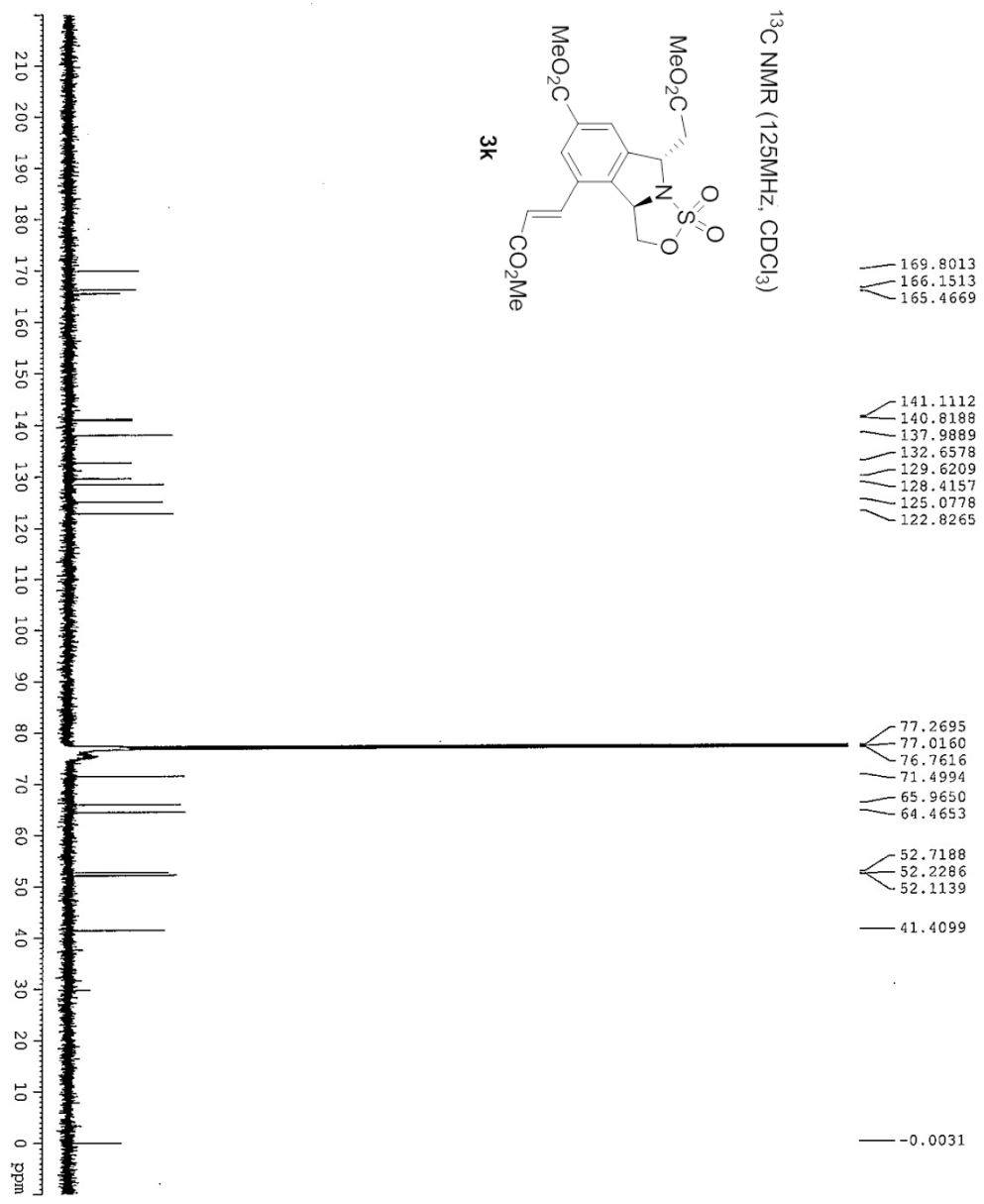


<sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>)





<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)



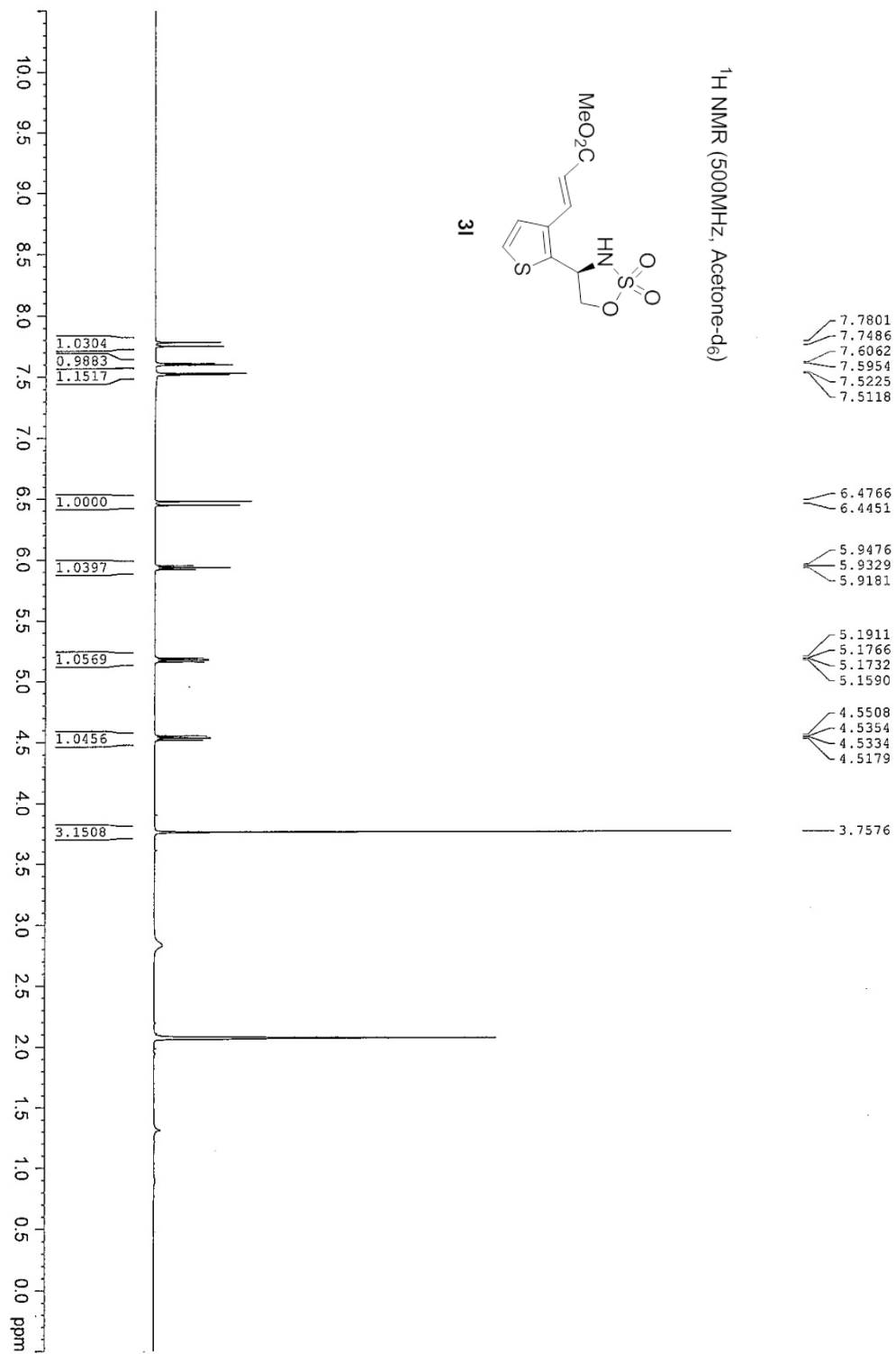
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- 166.1513
- 165.4669
- 141.1112
- 140.8188
- 137.9889
- 132.6578
- 129.6209
- 128.4157
- 125.0776
- 122.8265
- 77.2695
- 77.0160
- 76.7616
- 71.4994
- 65.9650
- 64.4653
- 52.7188
- 52.2286
- 52.1139
- 41.4099
- 0.0031

```

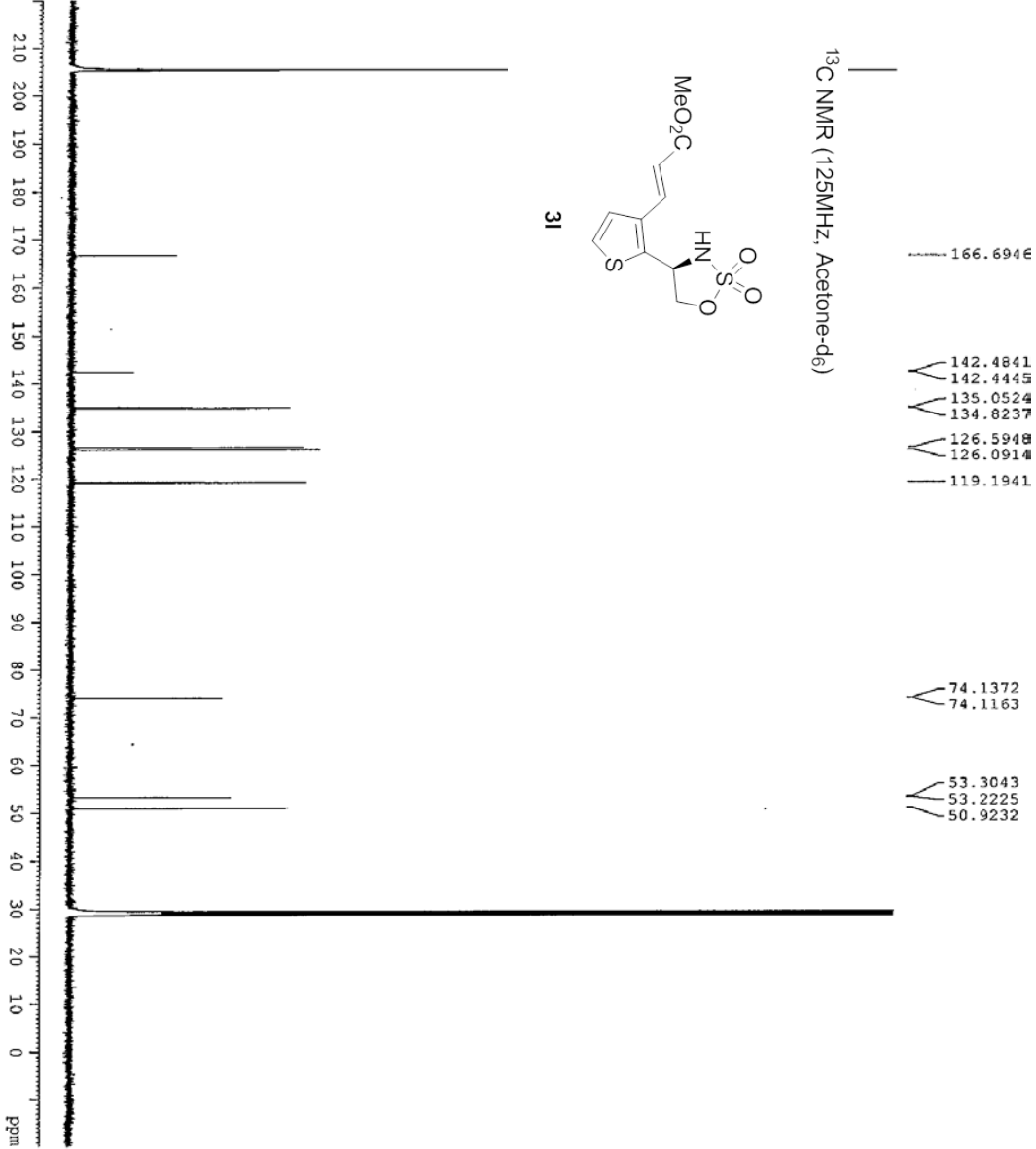
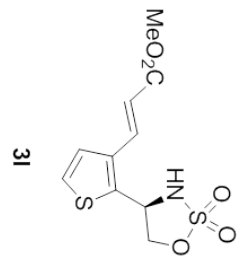
NAME          SSM_150407_CO2Me_CC
EXPNO         1
PROCNO        1
Date_         20150408
Time         3.41
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            3000
DS            2
SWH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407385 sec
RG            161.3
DE            16.500 usec
DM            6.00 usec
TE            298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.00 dB
P1M           70.6043301 W
SFO1          125.7703661 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2           -1.90 dB
PL12          16.00 dB
PL13          19.00 dB
PL1Z          27.23316002 W
PL2W          0.44167015 W
PL13W         0.22135943 W
SFO2          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



<sup>13</sup>C NMR (125MHz, Acetone-d<sub>6</sub>)



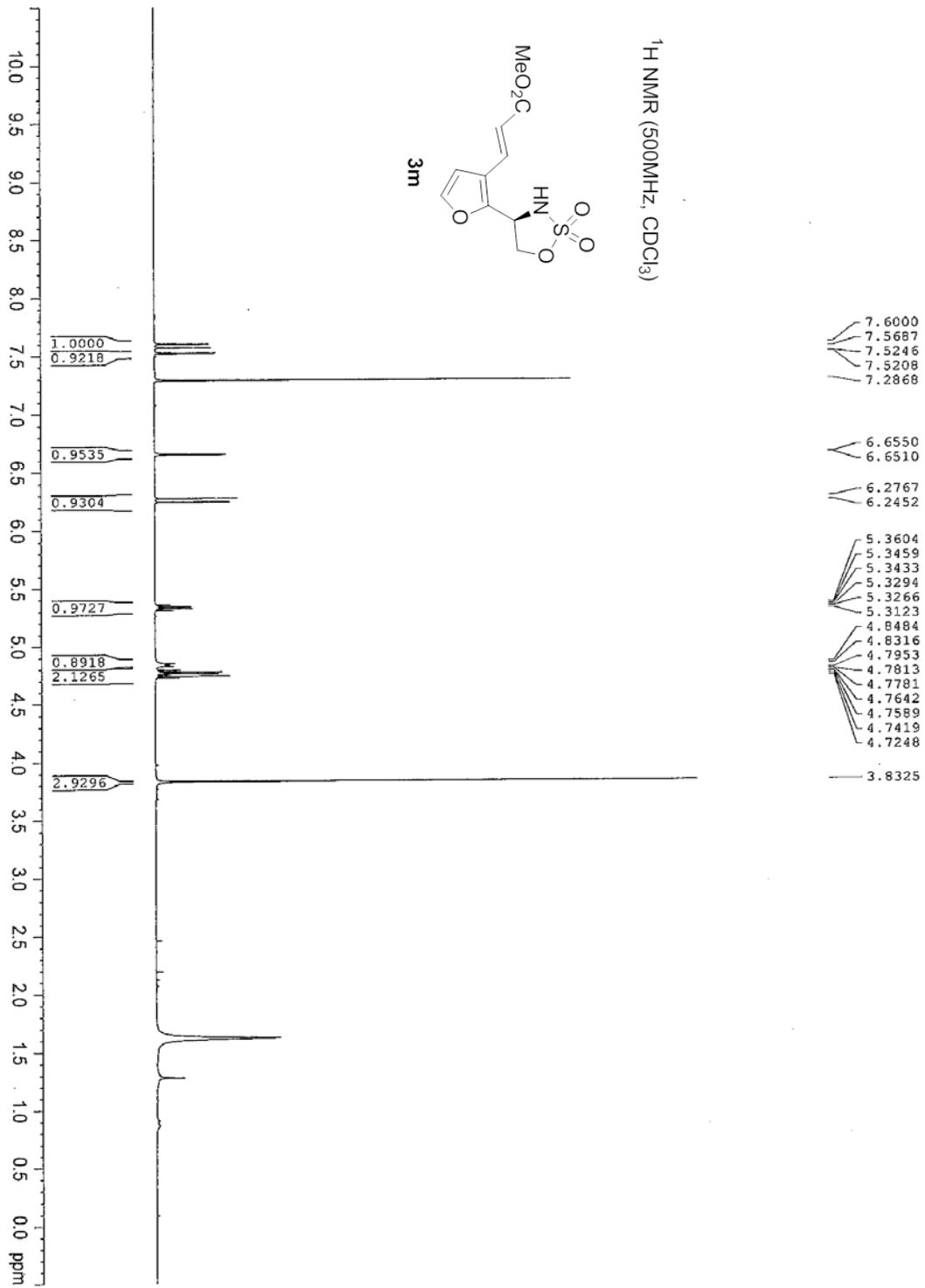
- 166.694
- 142.4841
- 142.4445
- 135.0524
- 134.8237
- 126.5948
- 126.0914
- 119.1941
- 74.1372
- 74.1163
- 53.3043
- 53.2225
- 50.9232

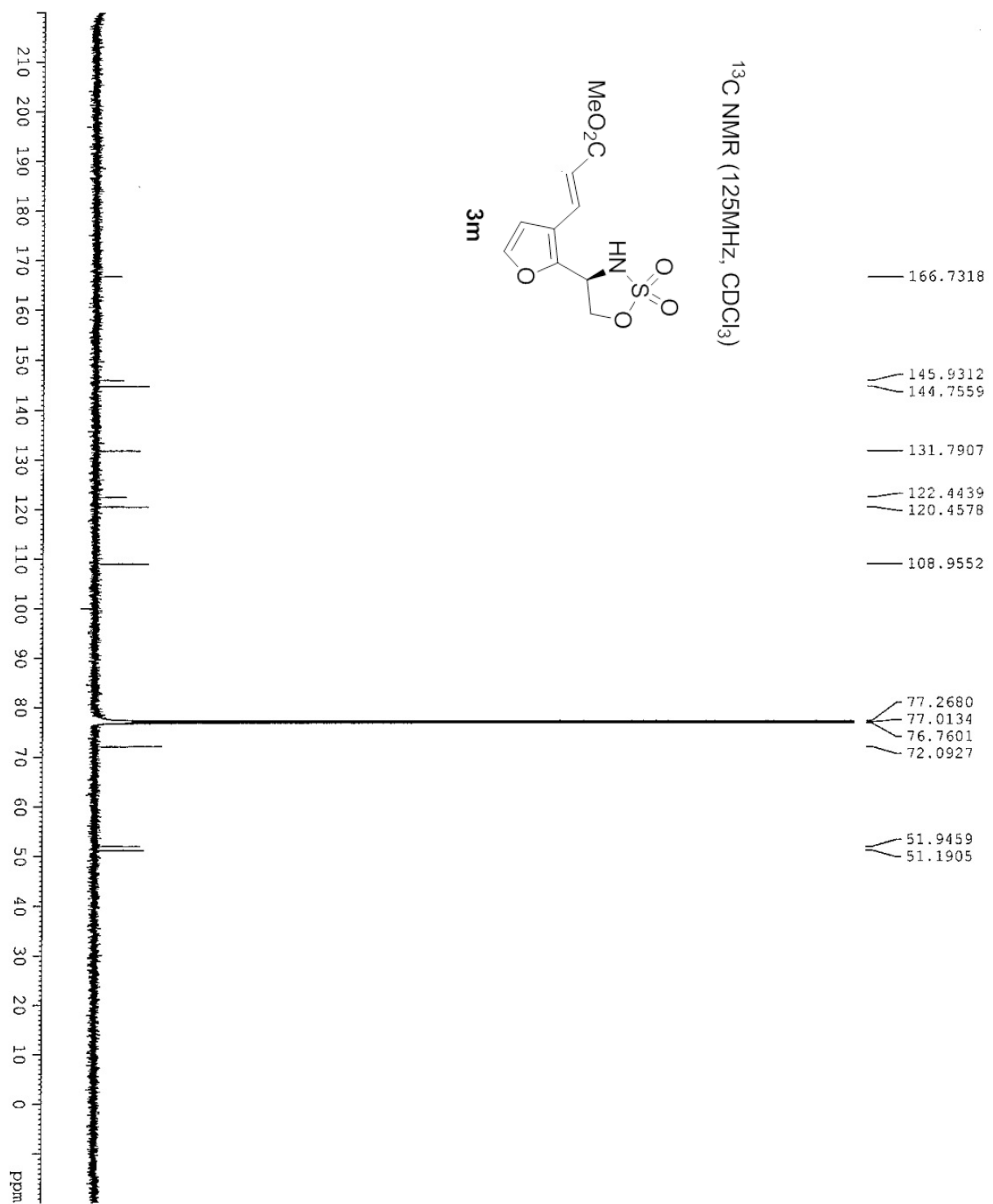
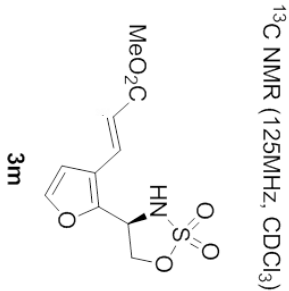
```

NAME: SSM_160113_S_cc
EXPNO: 1
PROCNO: 1
Date_ : 20160113
Time: 23.13
INSTRUM: spect
PROBHD: 5 mm DUL 13C-1
PULPROG: zgpg30
TD: 32768
SOLVENT: Acetone
NS: 5000
DS: 2
SWH: 30303.031 Hz
FIDRES: 0.924775 Hz
AQ: 0.5407385 sec
RG: 574.7
DM: 16.500 usec
DE: 6.00 usec
TE: 298.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TDO: 1

===== CHANNEL F1 =====
NUC1: 13C
P1: 8.00 usec
PL1: 1.40 dB
PL1W: 70.60439301 W
SFO1: 125.7703661 MHz

===== CHANNEL F2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 usec
PL2: -1.90 dB
PL12: 16.00 dB
PL13: 19.00 dB
PL2W: 27.23316002 W
PL12W: 0.44167013 W
PL13W: 0.22139443 W
SFO2: 500.1320005 MHz
SI: 32768
SF: 125.7577890 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.40
  
```





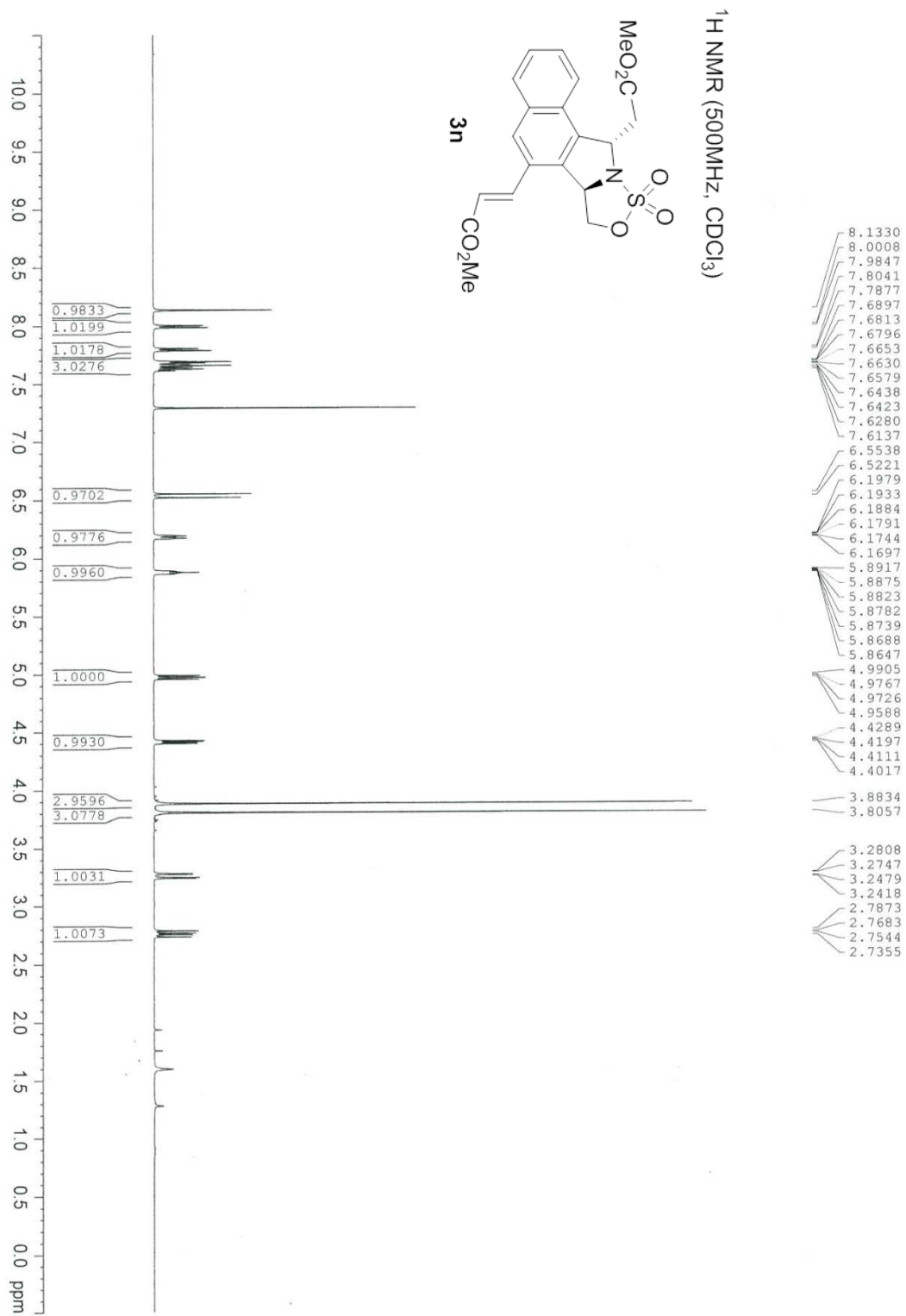
- 166.7318
- 145.9312
- 144.7559
- 131.7907
- 122.4439
- 120.4578
- 108.9552
- 77.2680
- 77.0134
- 76.7601
- 72.0927
- 51.9459
- 51.1905

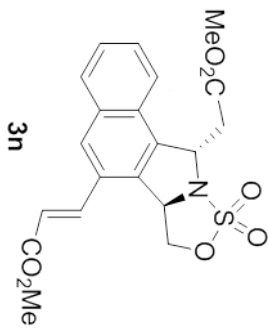
```

NAME          SSM_150723-0-CC_up_17
EXPNO         1
PROCNO        1
Date_         20150123
Time          22.12
INSTRUM      spect
PROBHD       5 mm DUL 125C1
PULPROG      zgpg30
TD           32768
SOLVENT      CDCl3
NS           3600
DS           4
SMH          30303.021 Hz
FIDRES       0.924175 Hz
AQ           0.5401385 sec
RG           5792.6
DM           16.500 usec
DE           6.00 usec
TE           298.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0          1

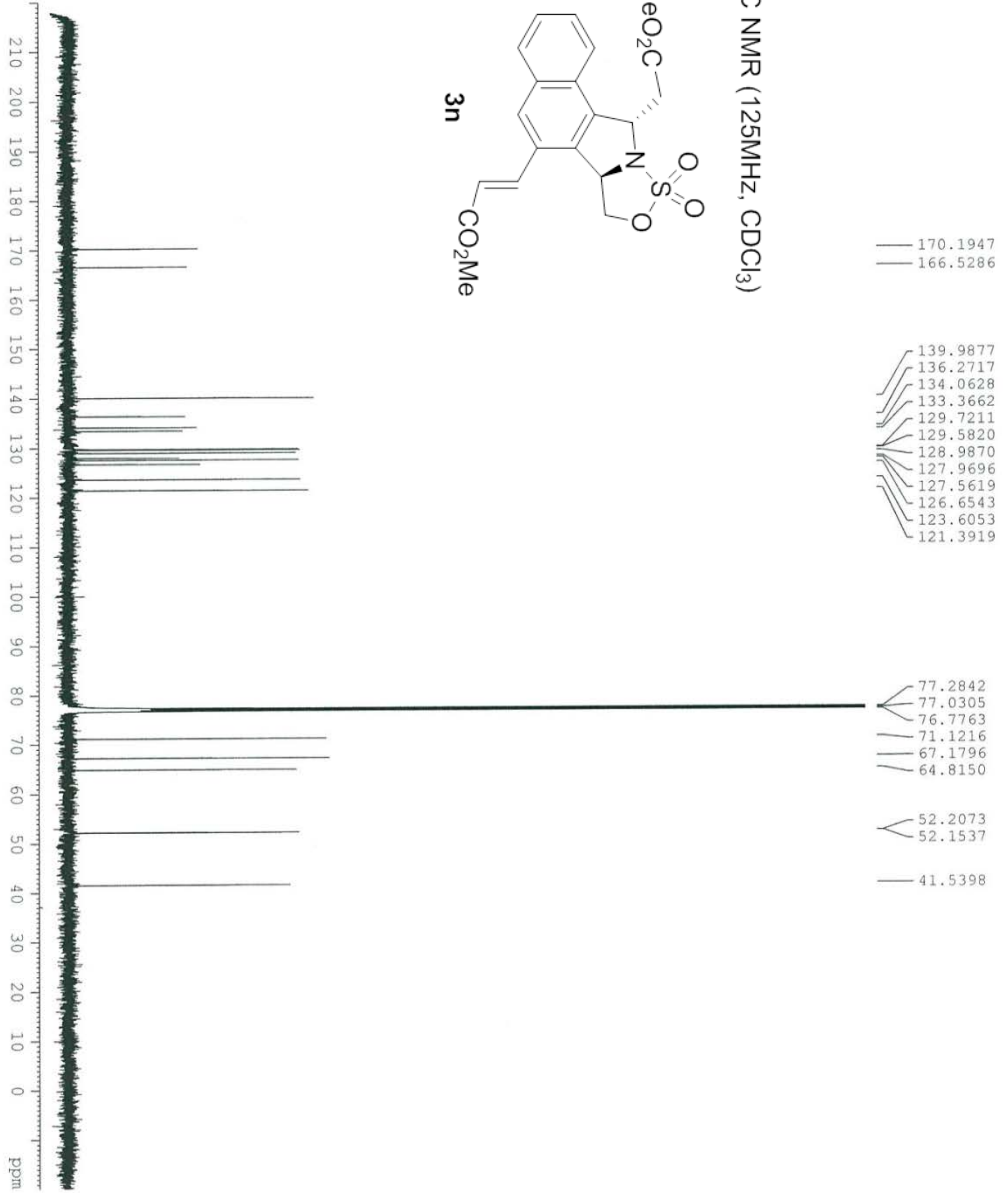
===== CHANNEL f1 =====
NUC1          13C
P1           8.00 usec
PL1          1.40 dB
PL1M         70.60438301 W
SFO1         125.7703661 MHz

===== CHANNEL f2 =====
CPOPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2          -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL2M         27.23318002 W
PL12M        0.44167015 W
PL13M        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```





<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)



```

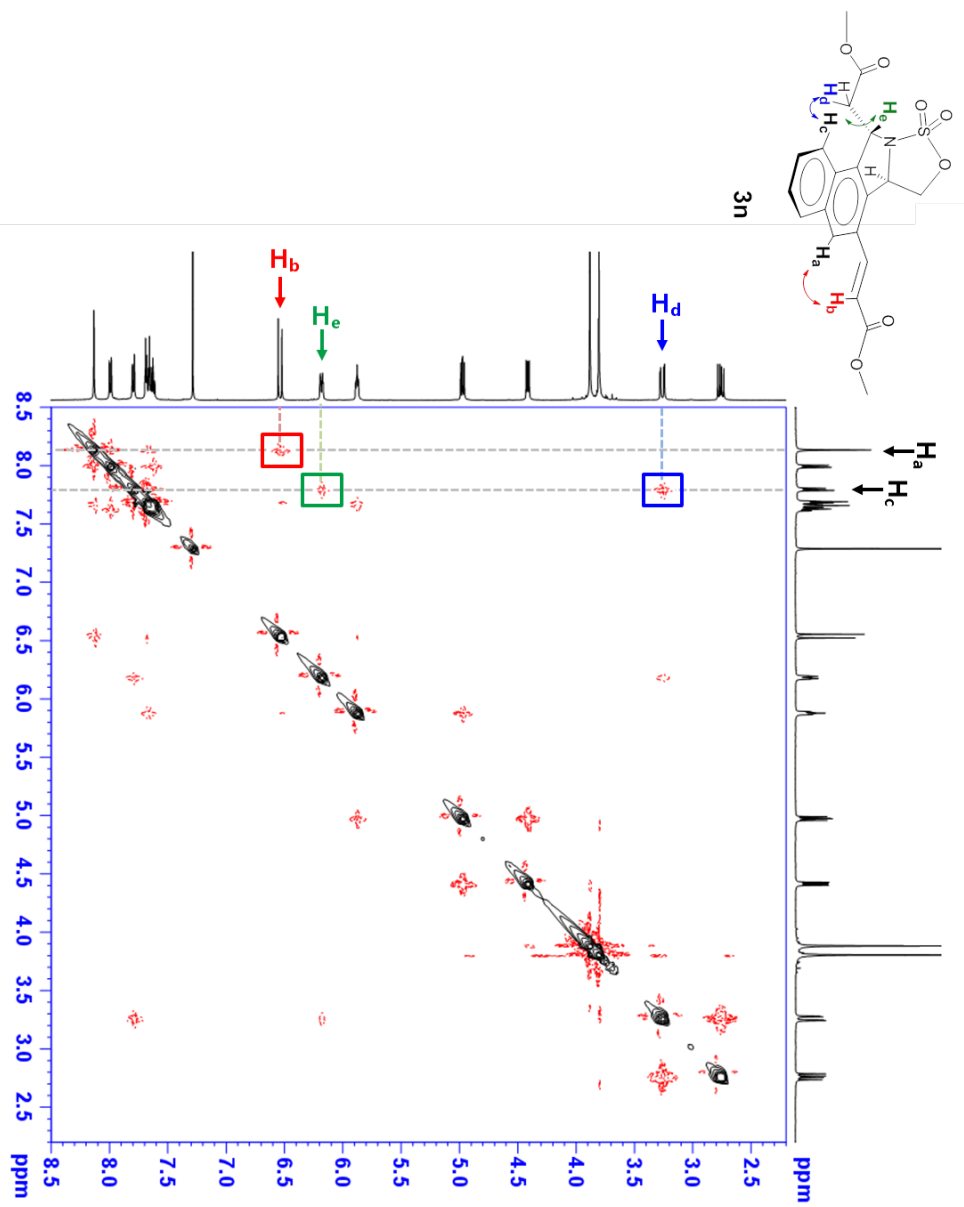
NAME          SSM_160122_naph_cc
EXPNO         1
PROCNO        1
Date_         20160125
Time_        11.12
INSTRUM       spect
PROBHD        13C-1
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            2640
DS            2
SWH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407385 sec
RG            256
DW            16.500 usec
DE            6.00 usec
TE            297.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

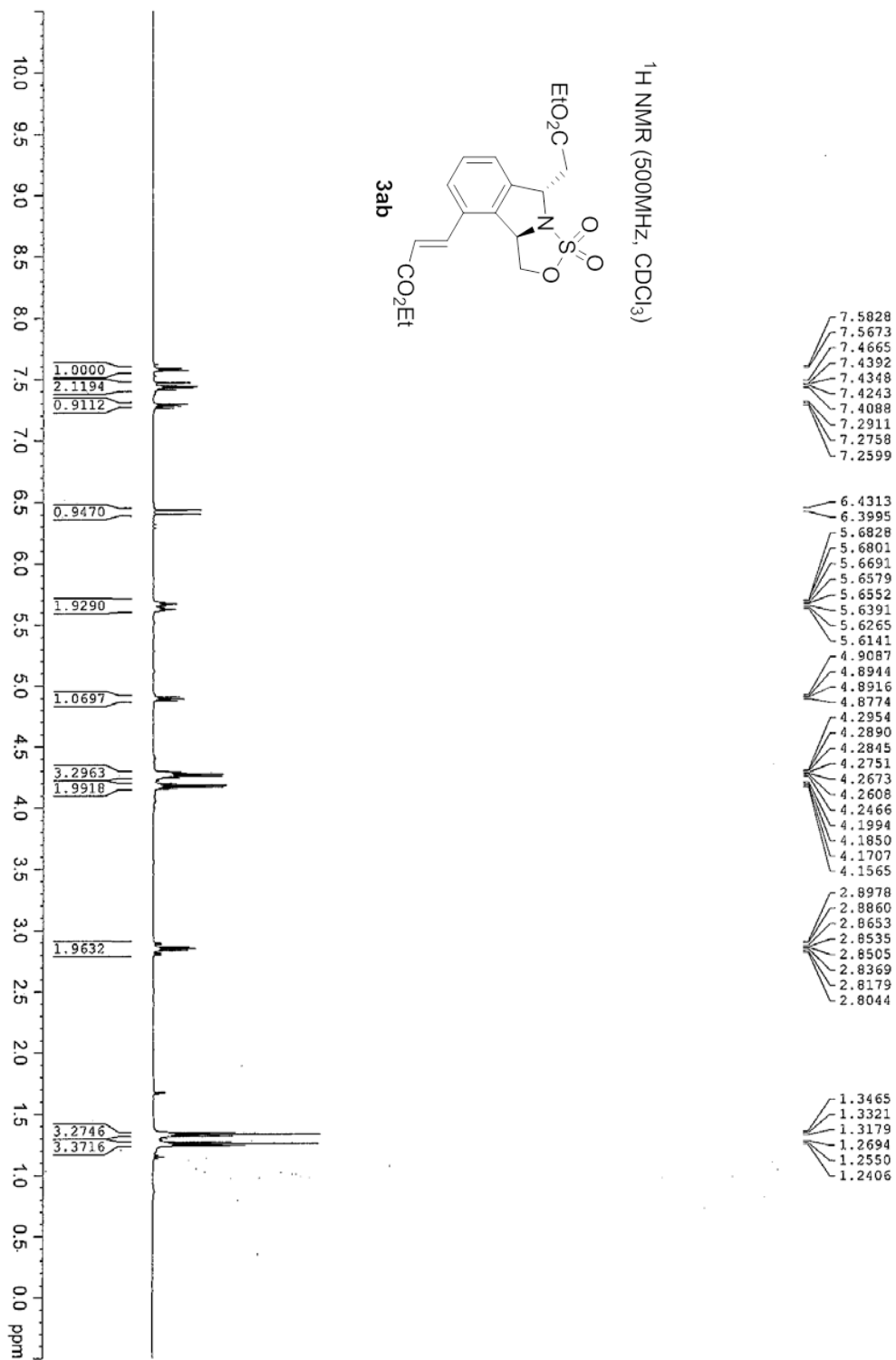
===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
PL1W          70.60439301 W
SFO1          125.7703661 MHz

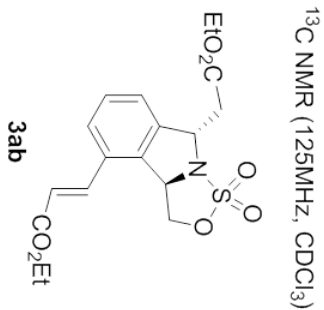
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2          -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL2W         27.23316002 W
PL12W        0.44167015 W
PL13W        0.22135943 W
SFO2          500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



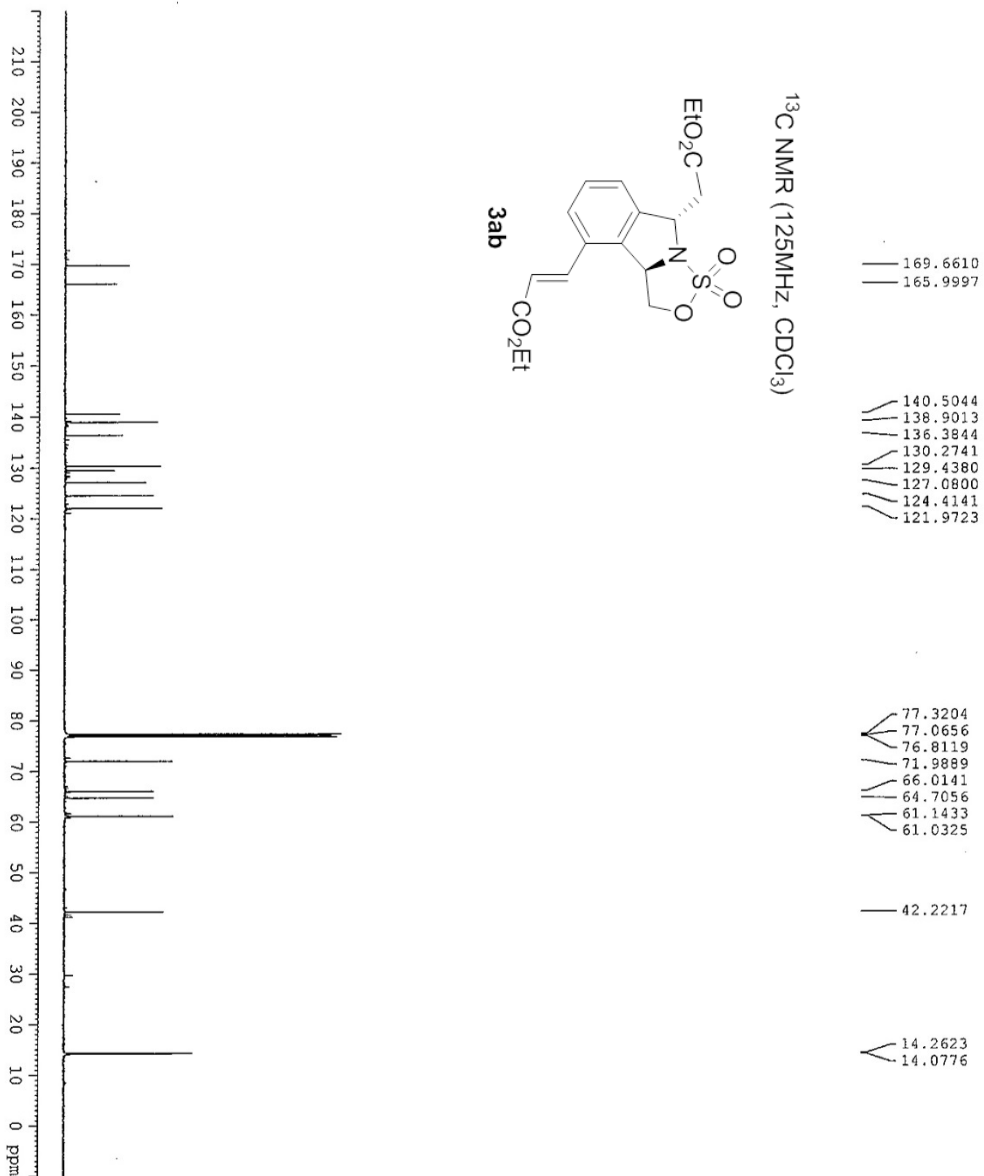
- 2D-NOESY of 3n







<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)

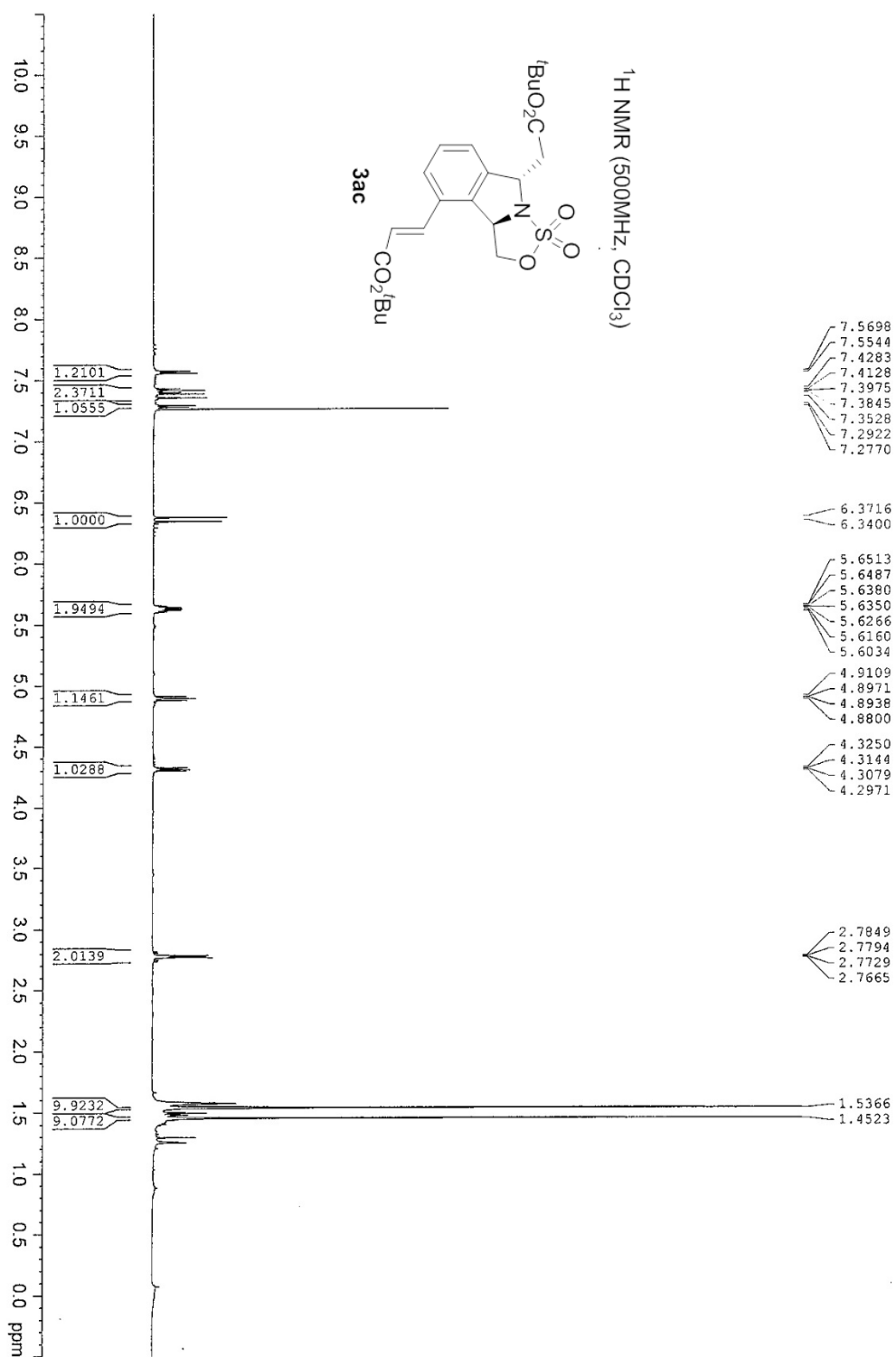


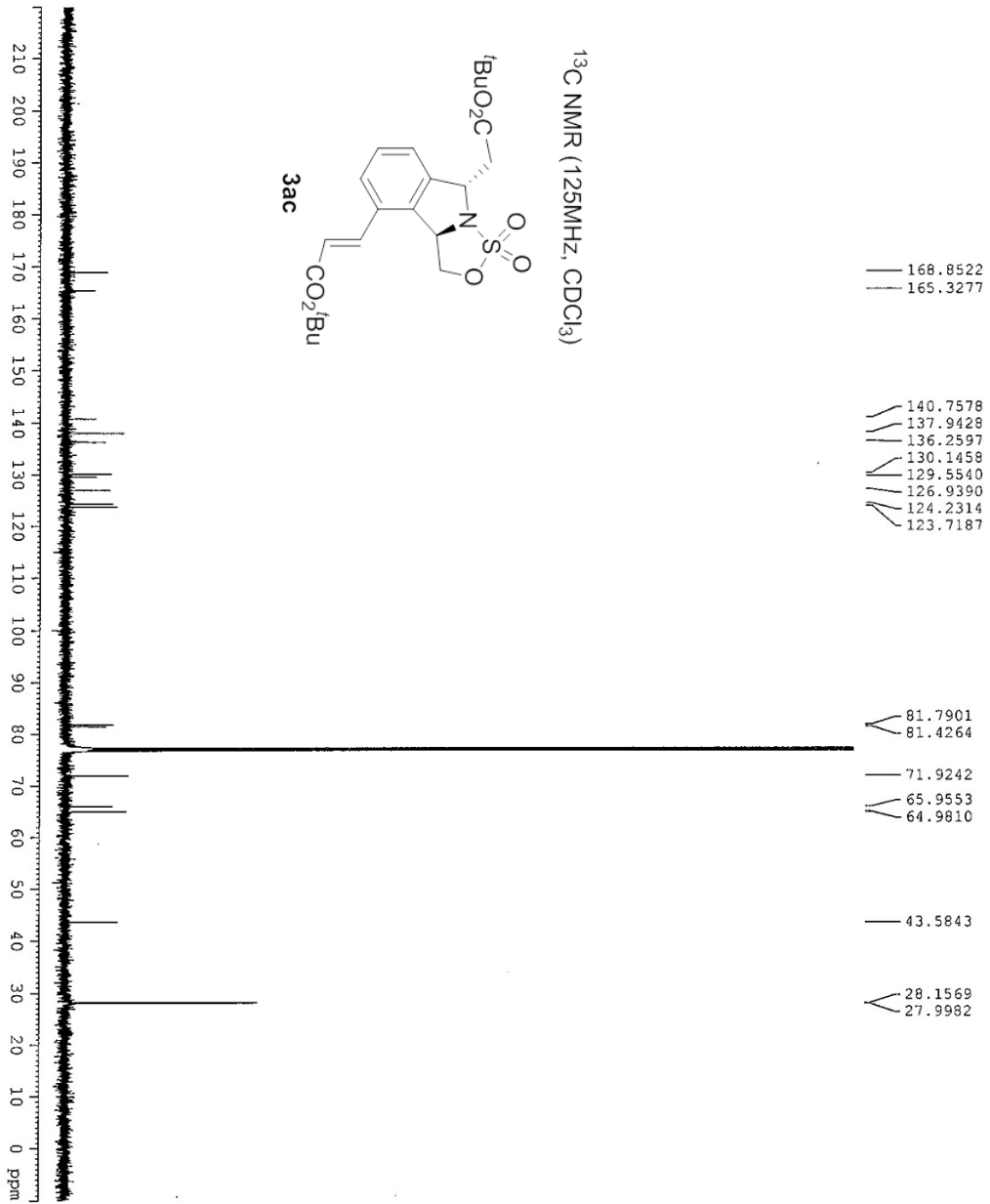
```

NAME          SYJ_Et_check_0619
EXPNO         1
PROCNO        1
Date_         20150619
Time          11:22
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            1000
DS            2
SFR          30303.031 Hz
FIDRES        0.324775 Hz
AQ            0.3407385 sec
RG            456.1
DW            16.500 usec
DE            6.00 usec
TE            298.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
PL1W          70.60433901 W
SFO1         125.7703661 MHz

===== CHANNEL f2 =====
CPRPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PI2           -1.90 dB
E1I2         16.00 dB
E1I3         19.00 dB
E1I2W        27.23316002 W
E1I3W        0.44167015 W
PL12W        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```





```

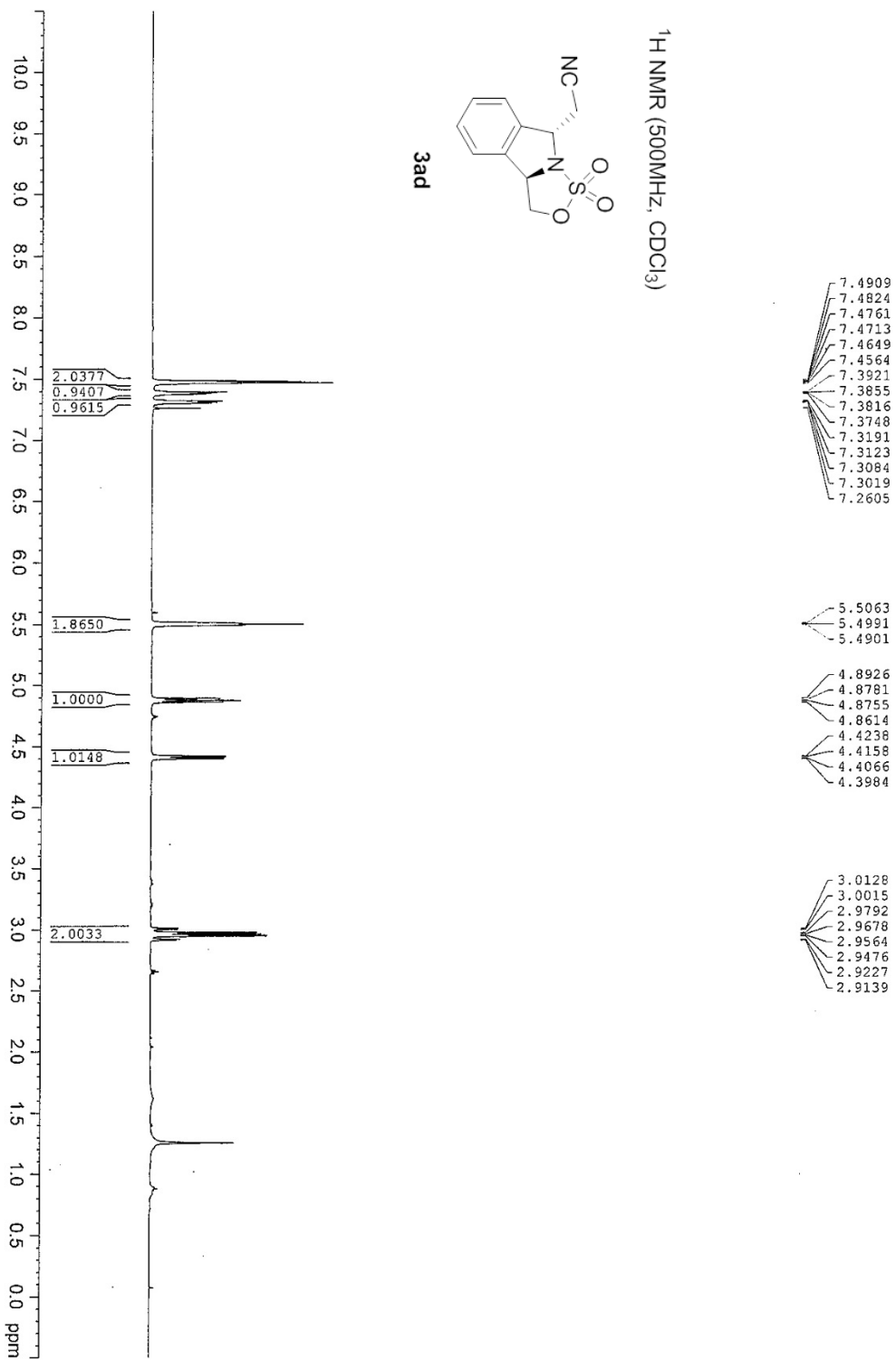
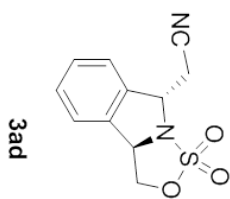
NAME          SVJ_f_bu_heck_ra_06:16_pure
EXPNO         2
PROCNO        1
Date_         20190626
Time          11:26
INSTRUM       spect
PROBHD        5 mm DUL 1Hc1
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            1000
DS            2
SWH           30303.031 Hz
FIDRES       0.924778 Hz
AQ           0.5407258 sec
RG           16.500 usec
DE           1.40 dB
TE           298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
T00          1

===== CHANNEL f1 =====
NUC1          13C
P1            8.40 usec
PL1           1.40 dB
PL1W          70.60439301 W
SFO1         125.7703661 MHz

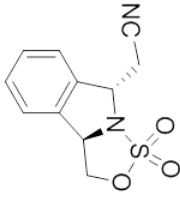
===== CHANNEL f2 =====
NAME         waltz16
NUC2         13C
PCPD2        100.00 usec
PL2          -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL14         27.23316002 W
PL15W        0.44167015 W
PL12W        0.22135043 W
SFO2         500.132009 MHz
SF           125.7578690 MHz
WDW          EM
SSB          0 Hz
LB           1.00 Hz
GB           0
FC           1.40

```

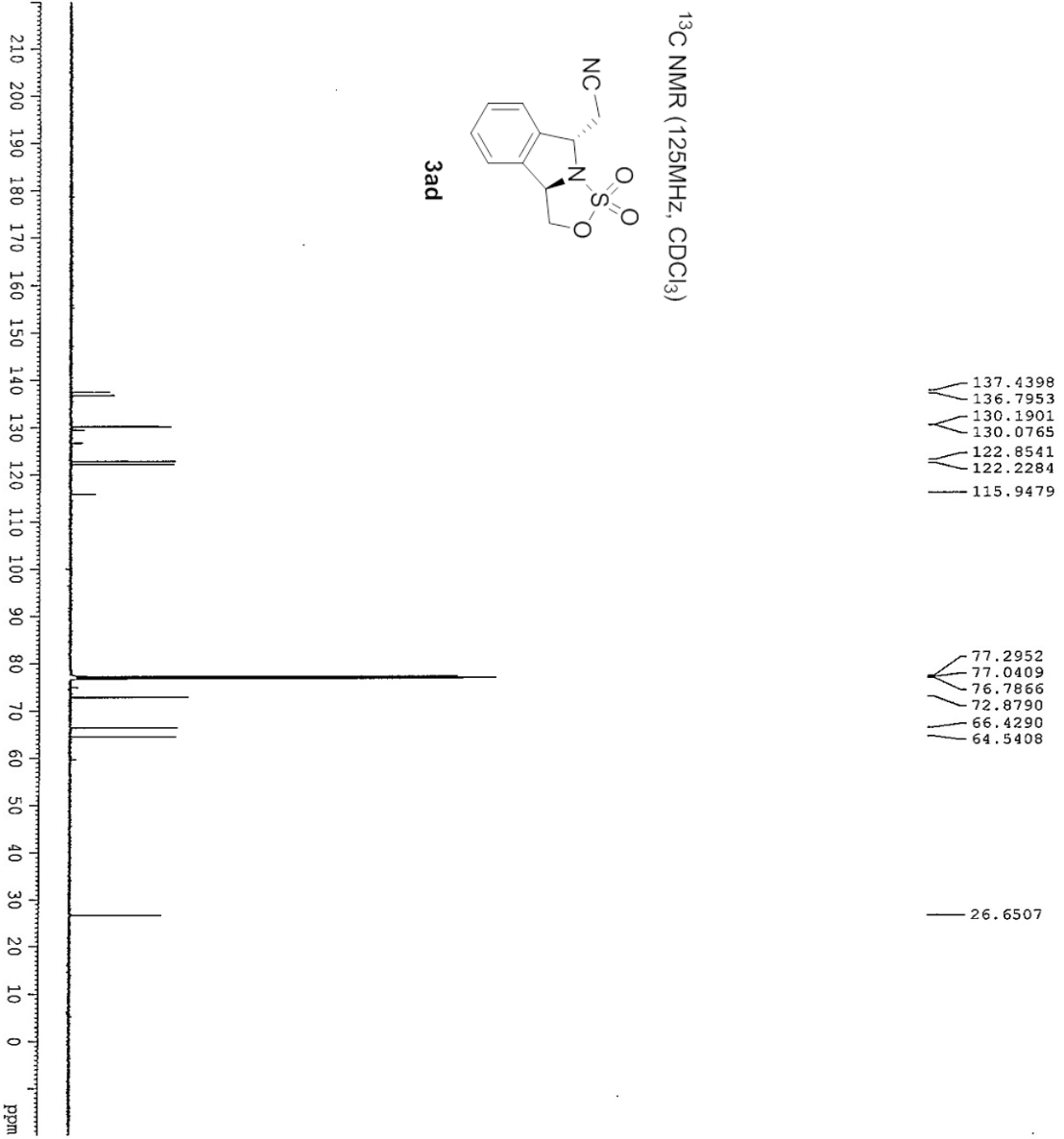
<sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)



3ad

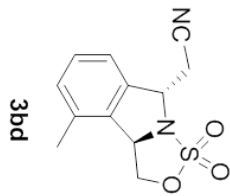


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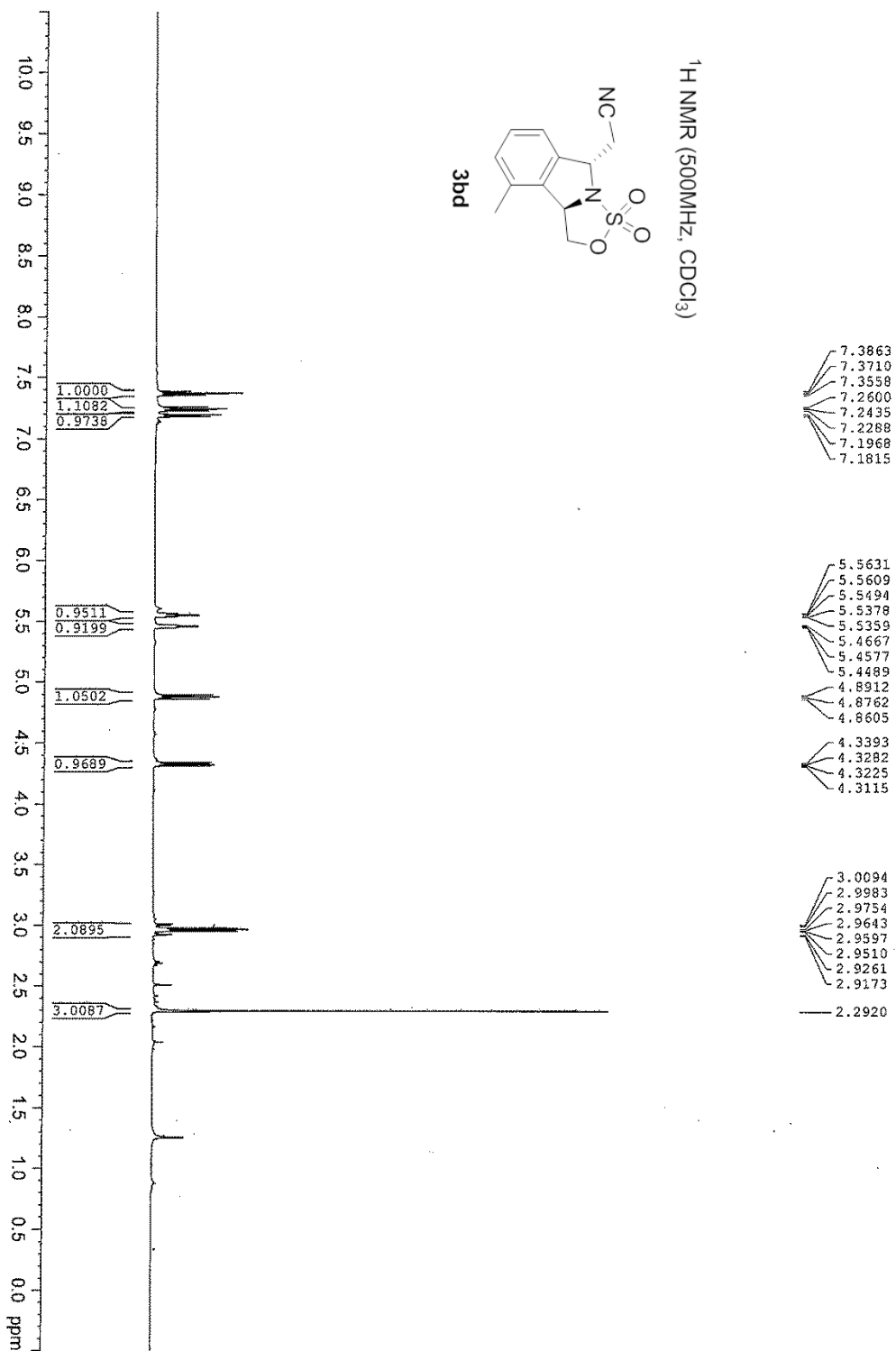
NAME          SYD_CNheck_0619
EXPNO         1
PROCNO        1
Date_         20150619
Time_         10.31
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            1000
DS            2
SWH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407385 sec
RG            161.3
DM            16.500 usec
DE            6.00 usec
TE            298.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL F1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
PL1W          70.60433301 W
SFO1          125.7703661 MHz

===== CHANNEL F2 =====
CPDPRG2      walcz16
NUC2          1H
PCPD2        100.00 usec
PL2          -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL2W         27.23316002 W
PL12W        0.44167015 W
PL13W        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

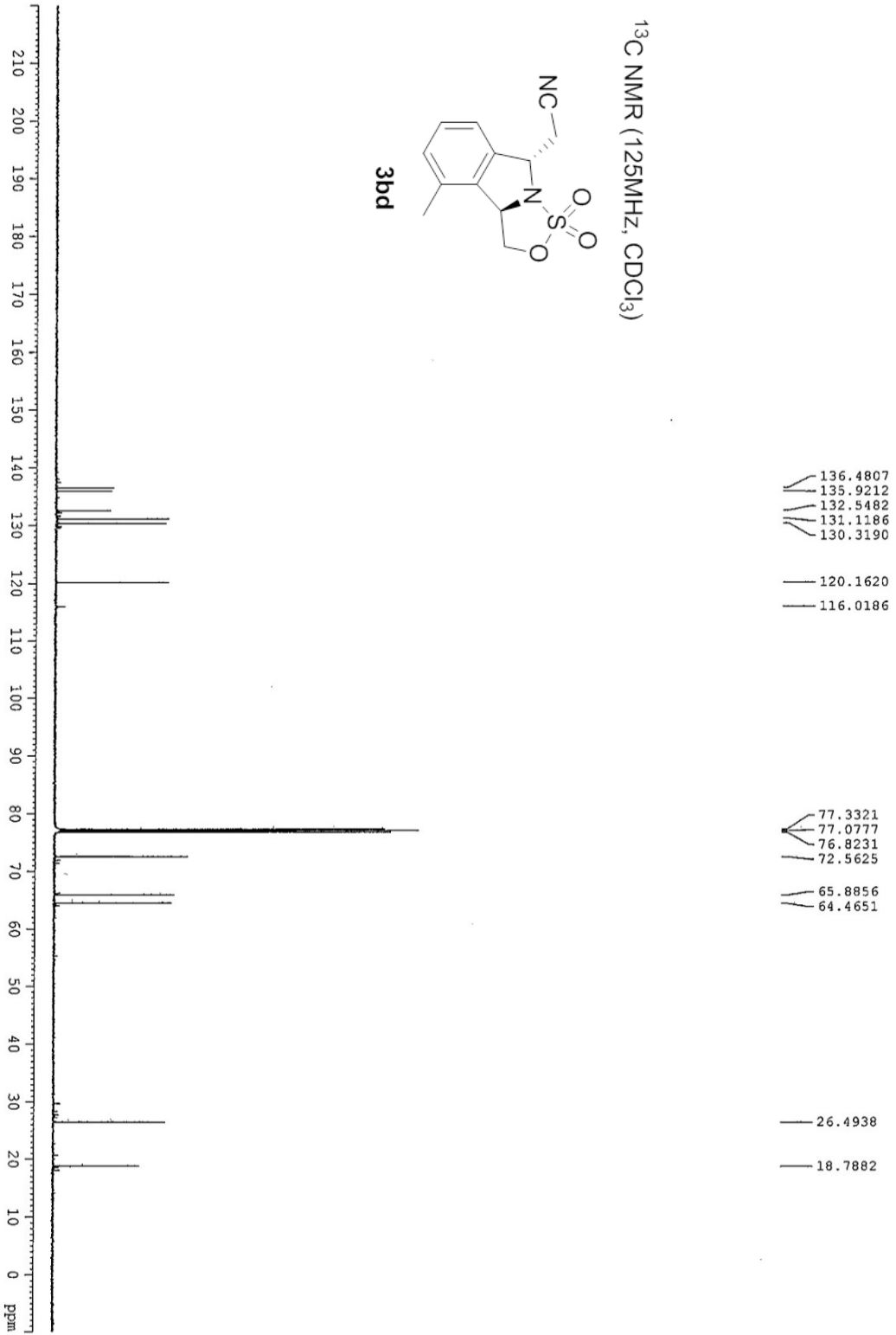
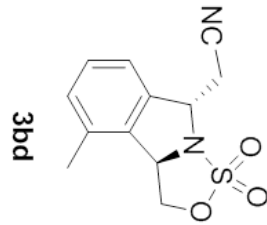


<sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>)



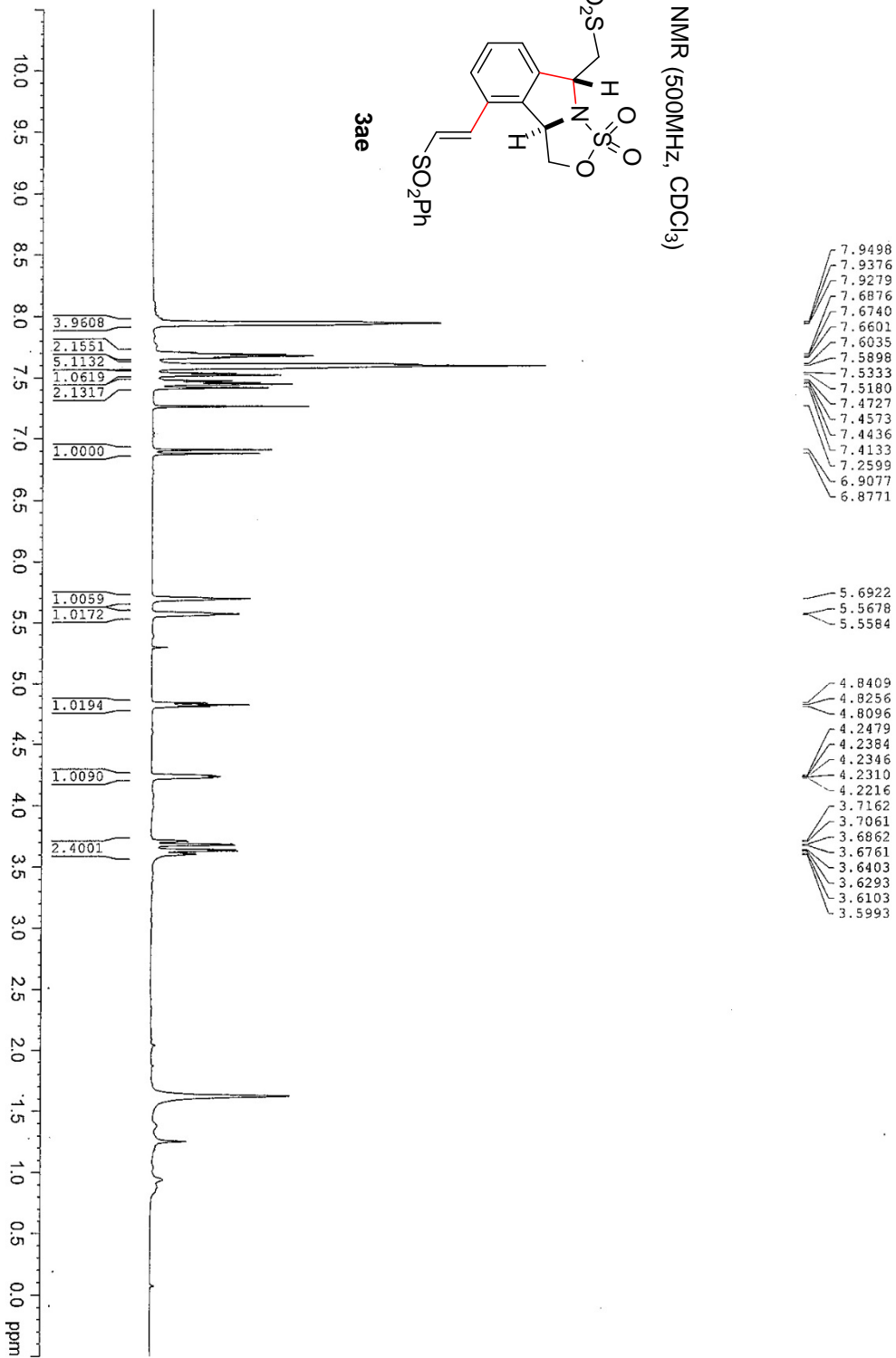
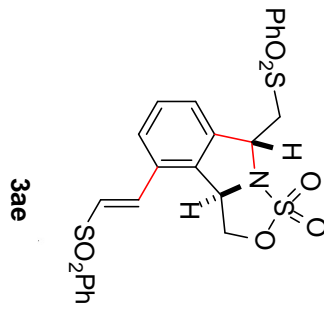


<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)



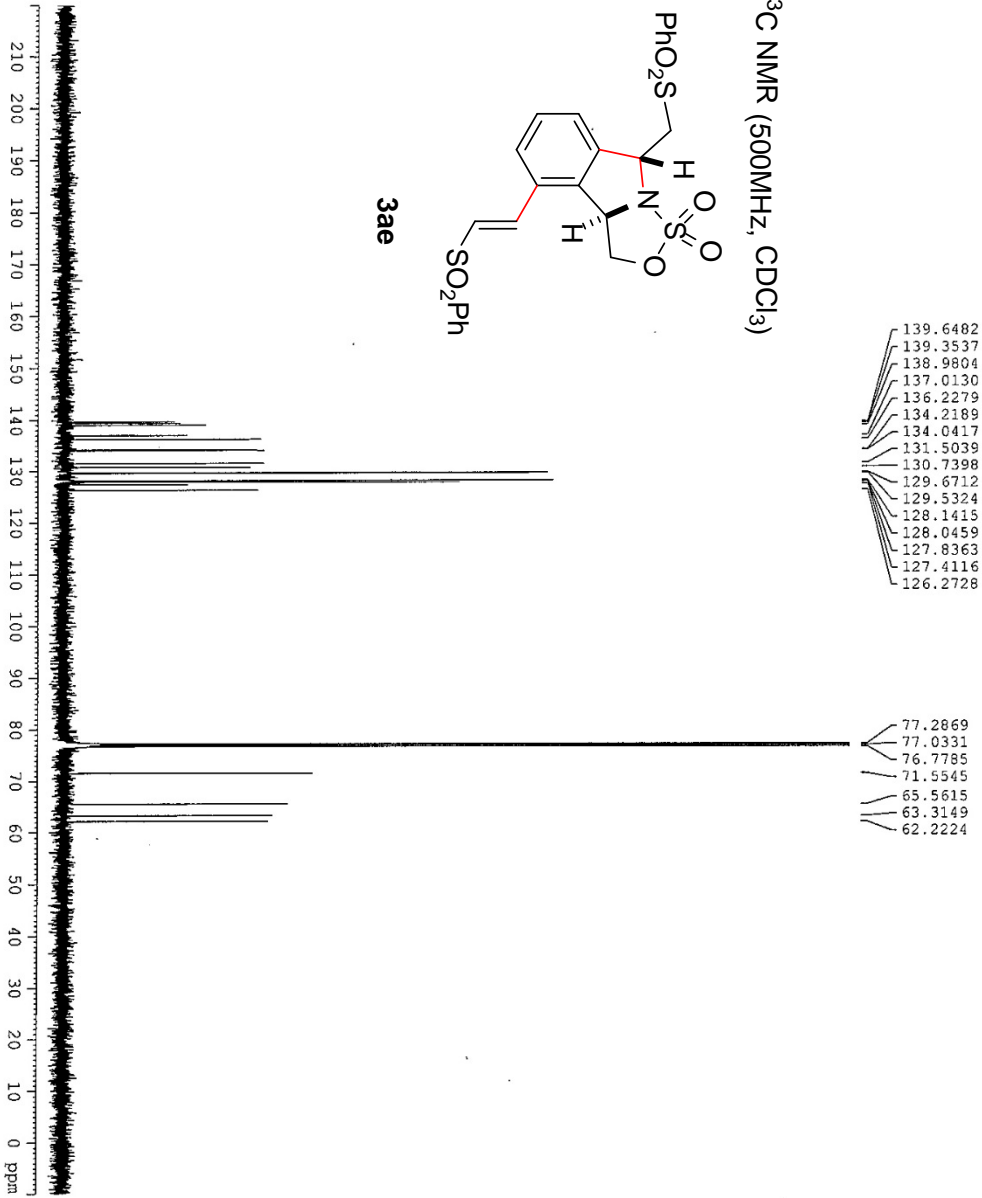
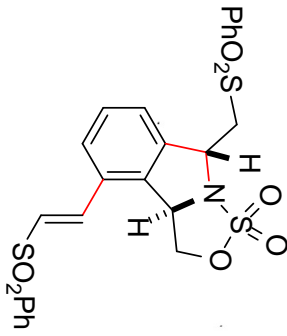
SYJ-sulfone-chiral-0713

<sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>)



SYJ\_sulfone\_chiral\_0713

<sup>13</sup>C NMR (500MHz, CDCl<sub>3</sub>)



139.6482  
139.3537  
138.9804  
137.0130  
136.2279  
134.2189  
134.0417  
131.5039  
130.7398  
129.6712  
129.5324  
128.1415  
128.0459  
127.8363  
127.4116  
126.2728

77.2869  
77.0331  
76.7785  
71.5545  
65.5615  
63.3149  
62.2224

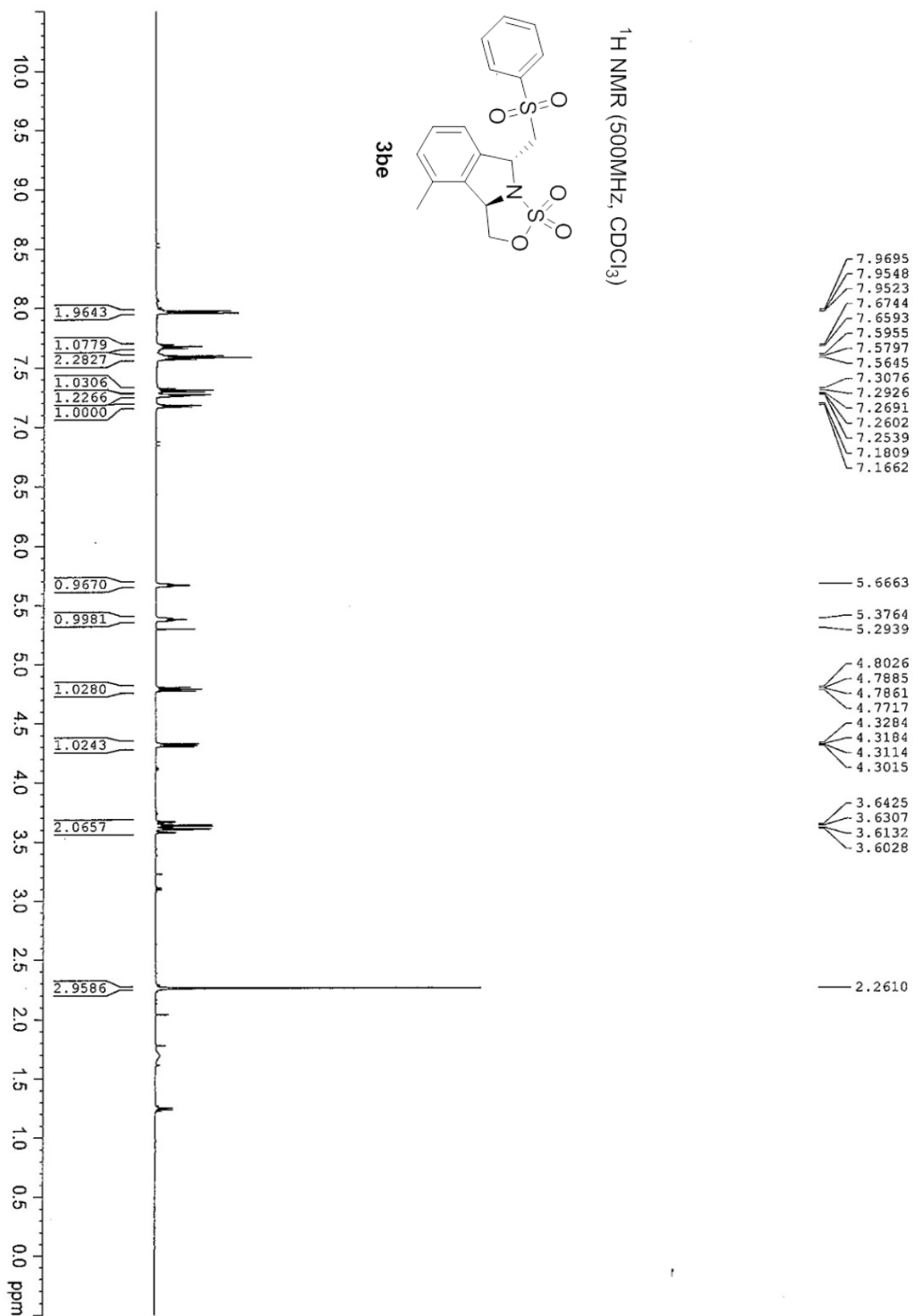
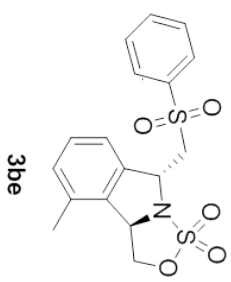
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NAME          SYJ_sulfone_chiral_0713
EXPNO         1
PROCNO        1
Date_         20150714
Time          10.13
INSTRUM      spect
PROBHD       5 mm DUL 13C-1
PULPROG      zgpg30
TD            32768
SOLVENT      CDCl3
DS            1000
SWH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407385 sec
RG            2298.8
DM            16.500 usec
DE            6.00 usec
TE            298.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

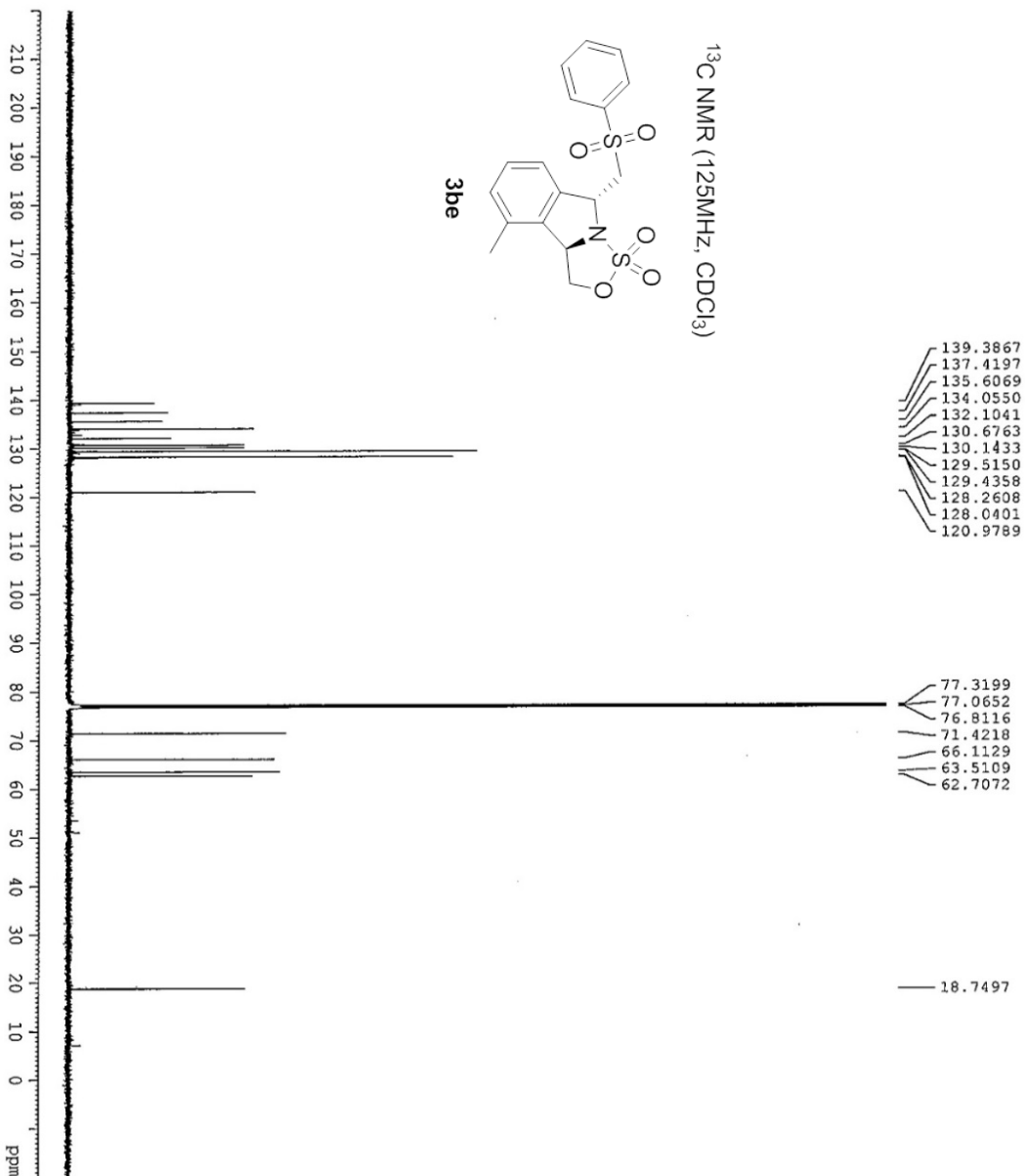
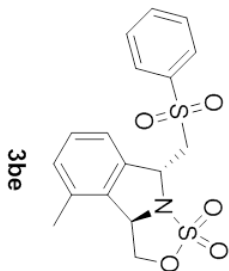
===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
F1M           70.6043301 W
SFO1          125.7703661 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2           -1.50 dB
PL12          16.00 dB
PL13          19.00 dB
PL2M          27.23316002 W
PL12M         0.44167015 W
PL13M         0.22135943 W
SFO2          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

<sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>)



<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)

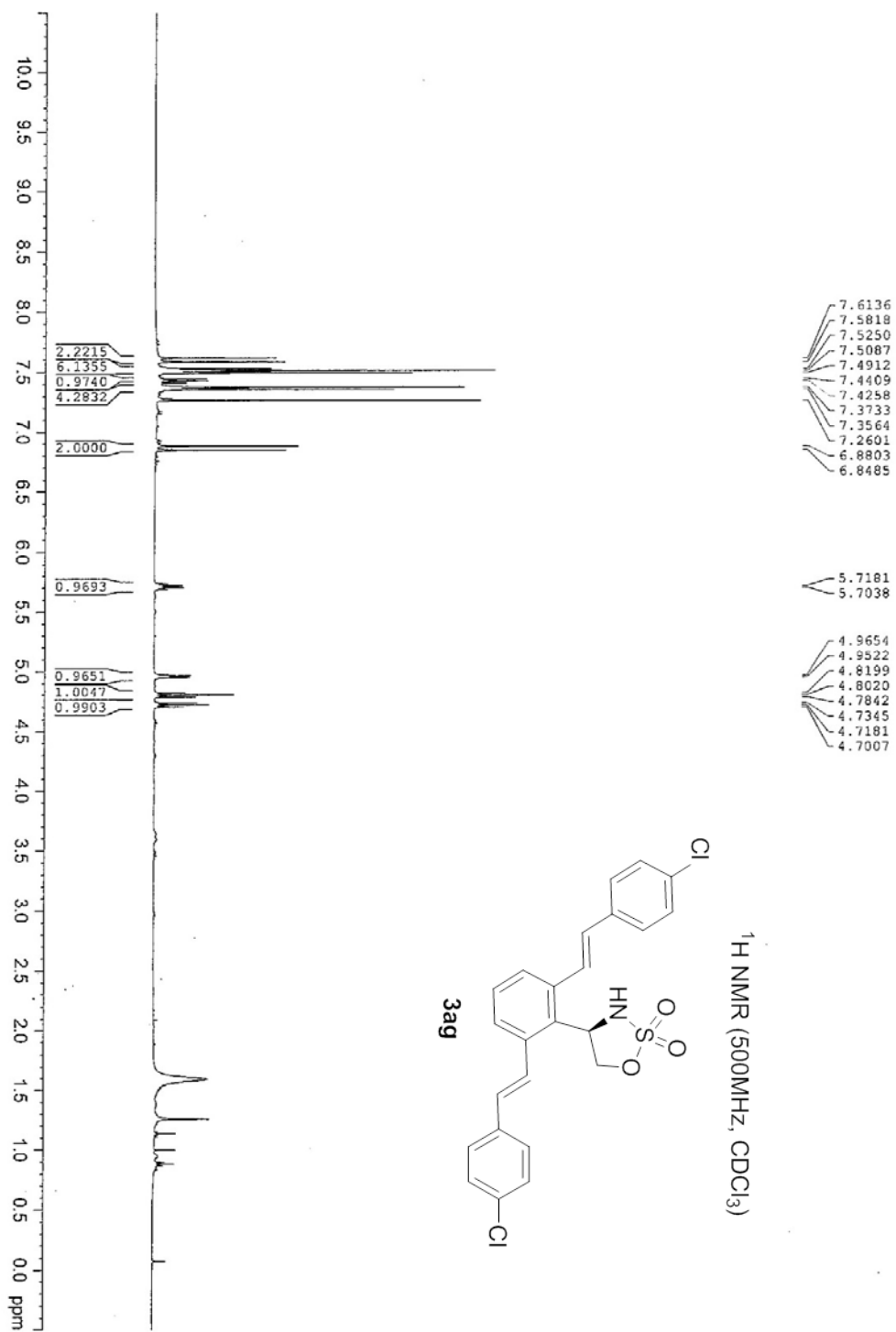


```

NAME          SYJ_2me_sulfone_1015
EXPNO         2
PROCNO        1
Date_         20151015
Time_         10.32
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            1000
DS            2
SWH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407385 sec
RG            3251
DM            16.500 usec
DE            6.00 usec
TE            295.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
PL1W          70.60439301 W
SFO1          125.7703661 MHz

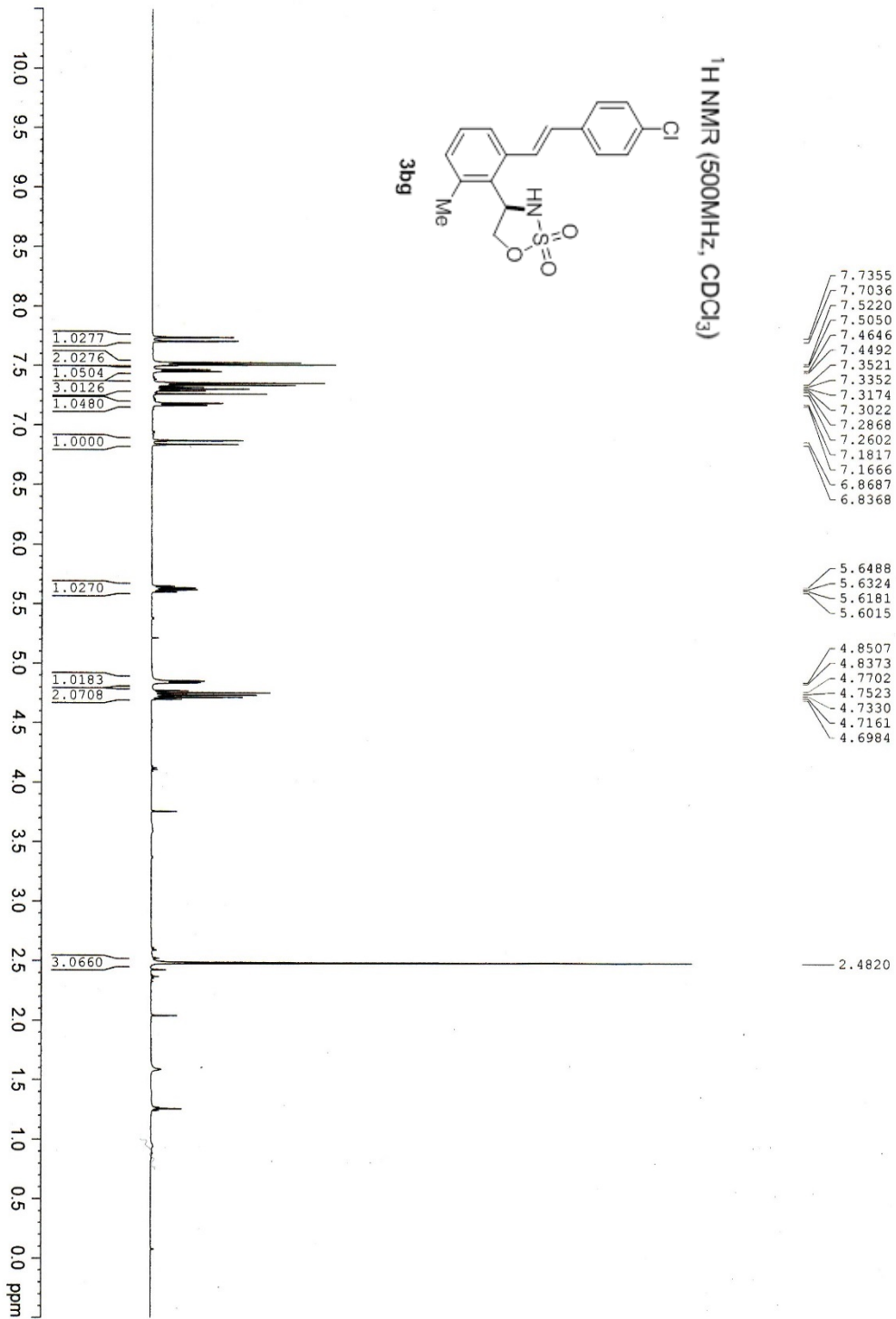
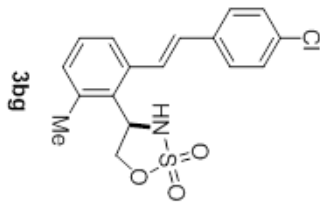
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2           -1.90 dB
PL12          16.00 dB
PL13          19.00 dB
PL2W          27.23316002 W
PL12W         0.44167015 W
PL13W         0.221358943 W
SE02          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



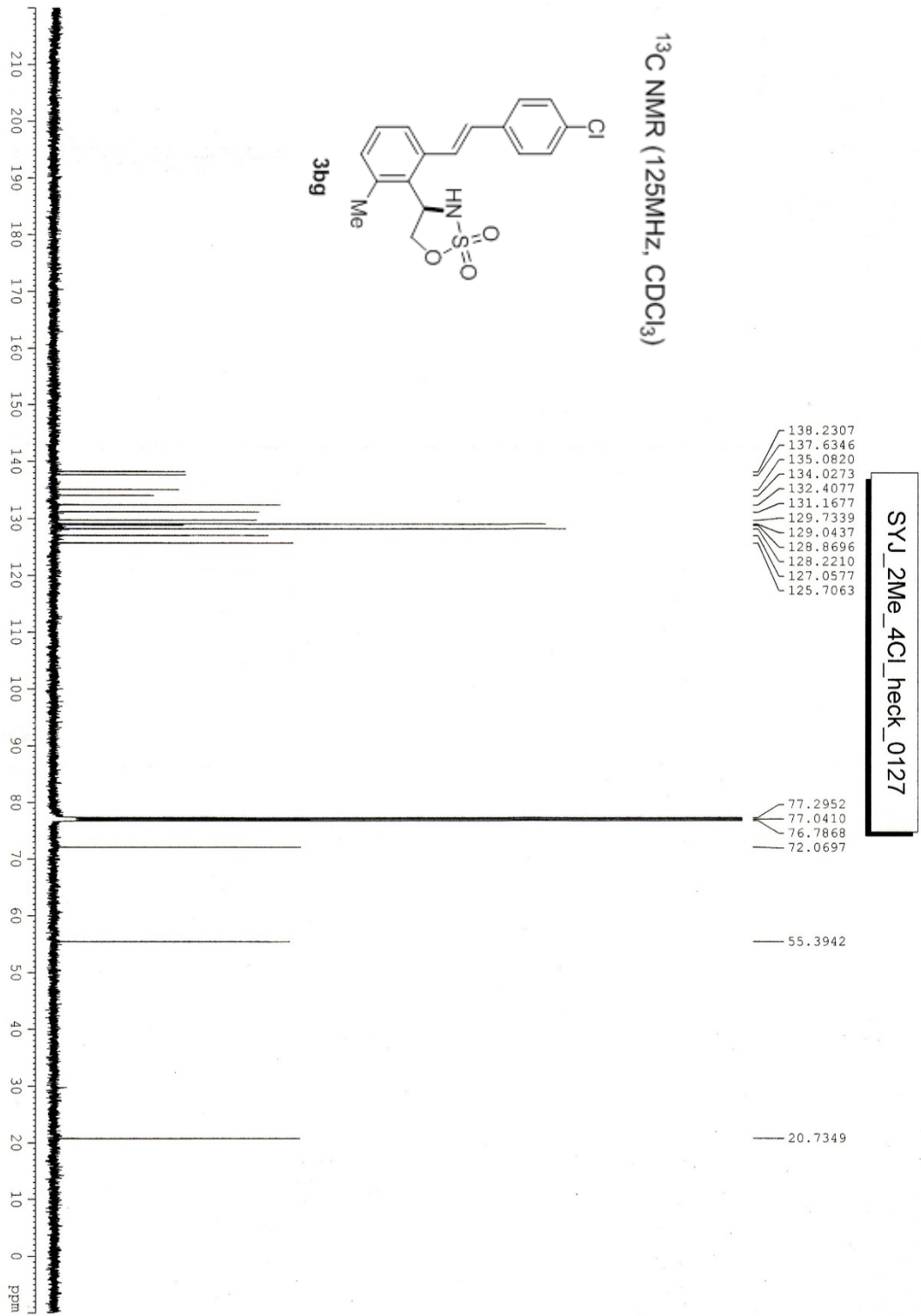


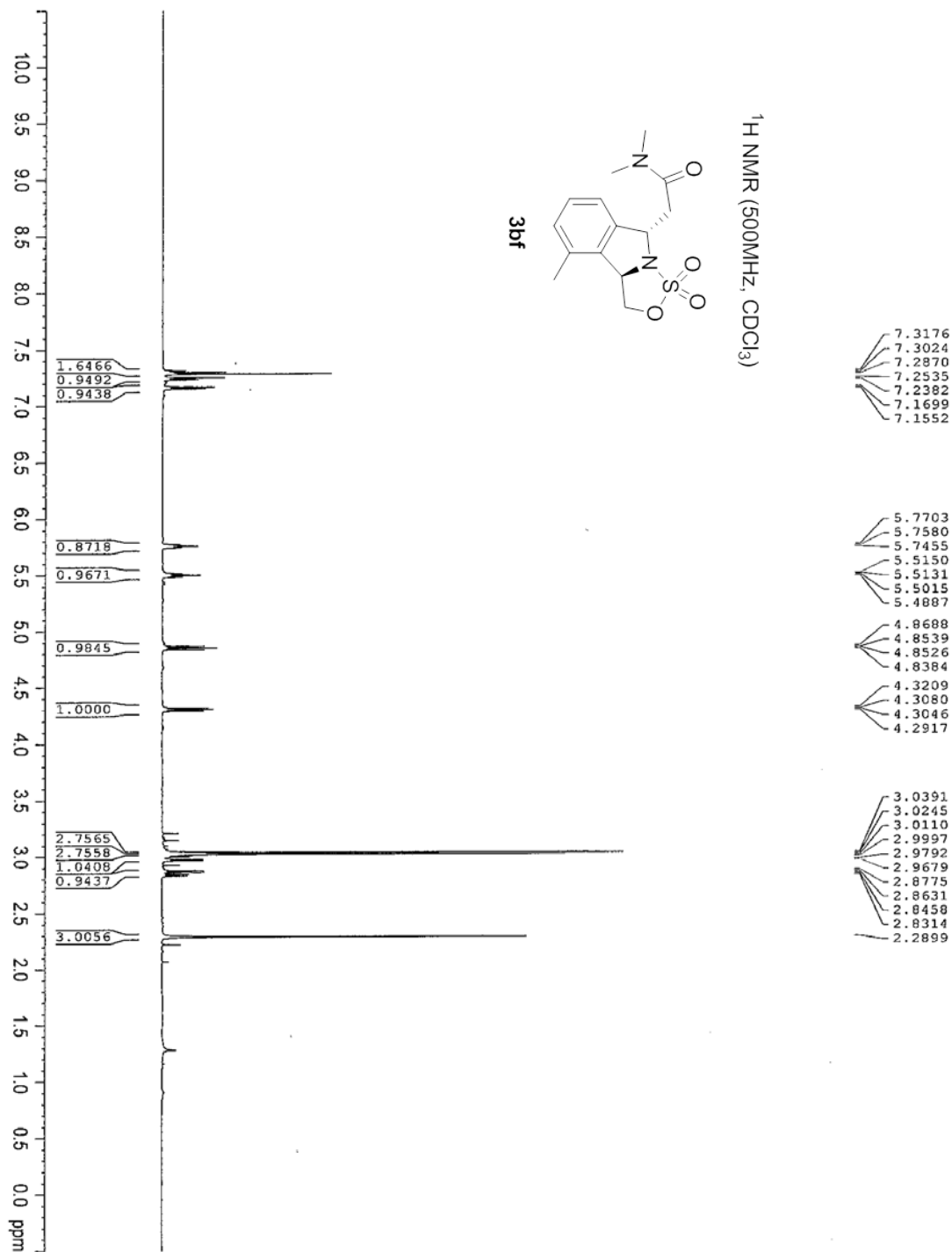
SYJ\_2Me\_4Cl\_heck\_0127

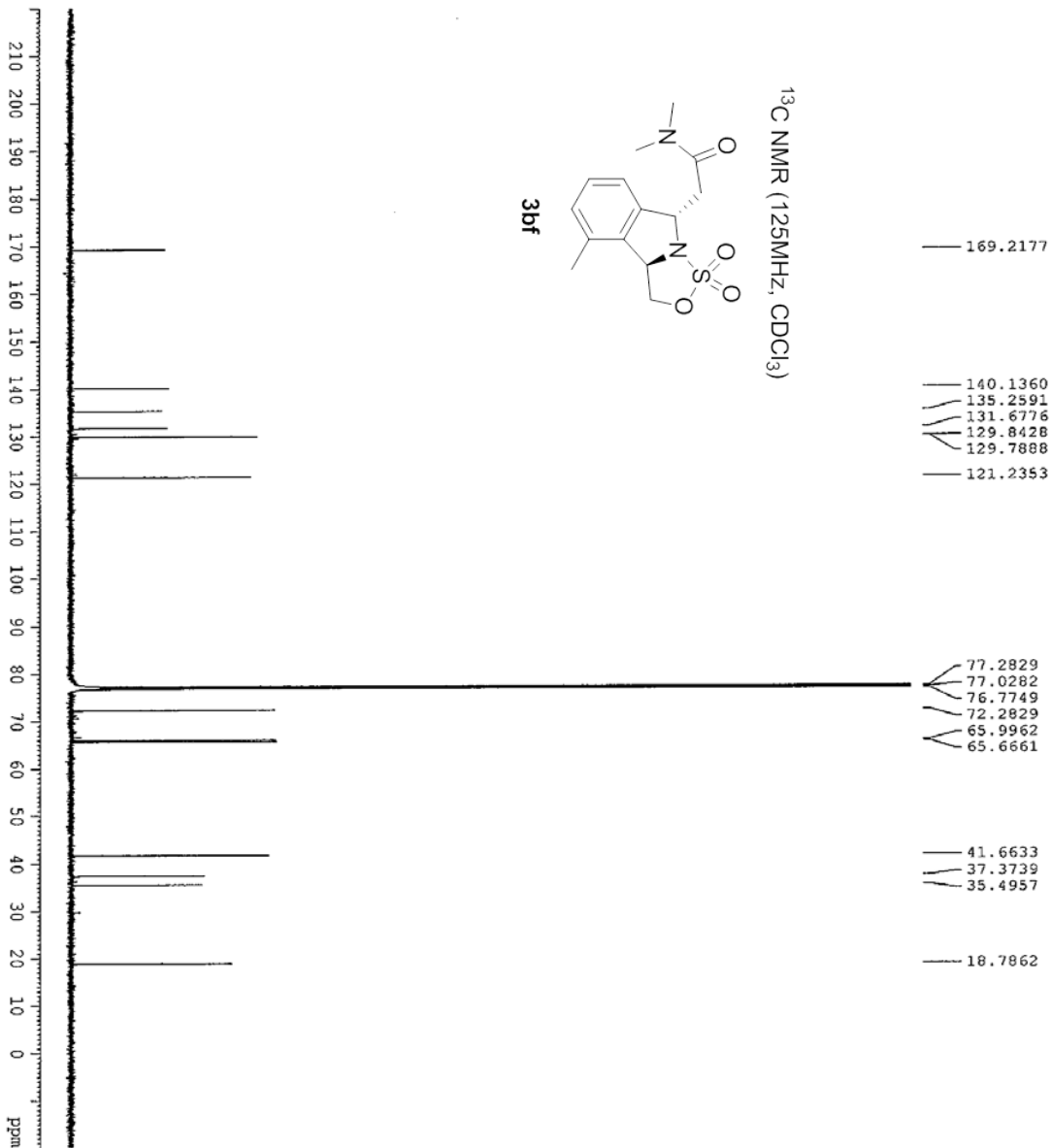
<sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>)







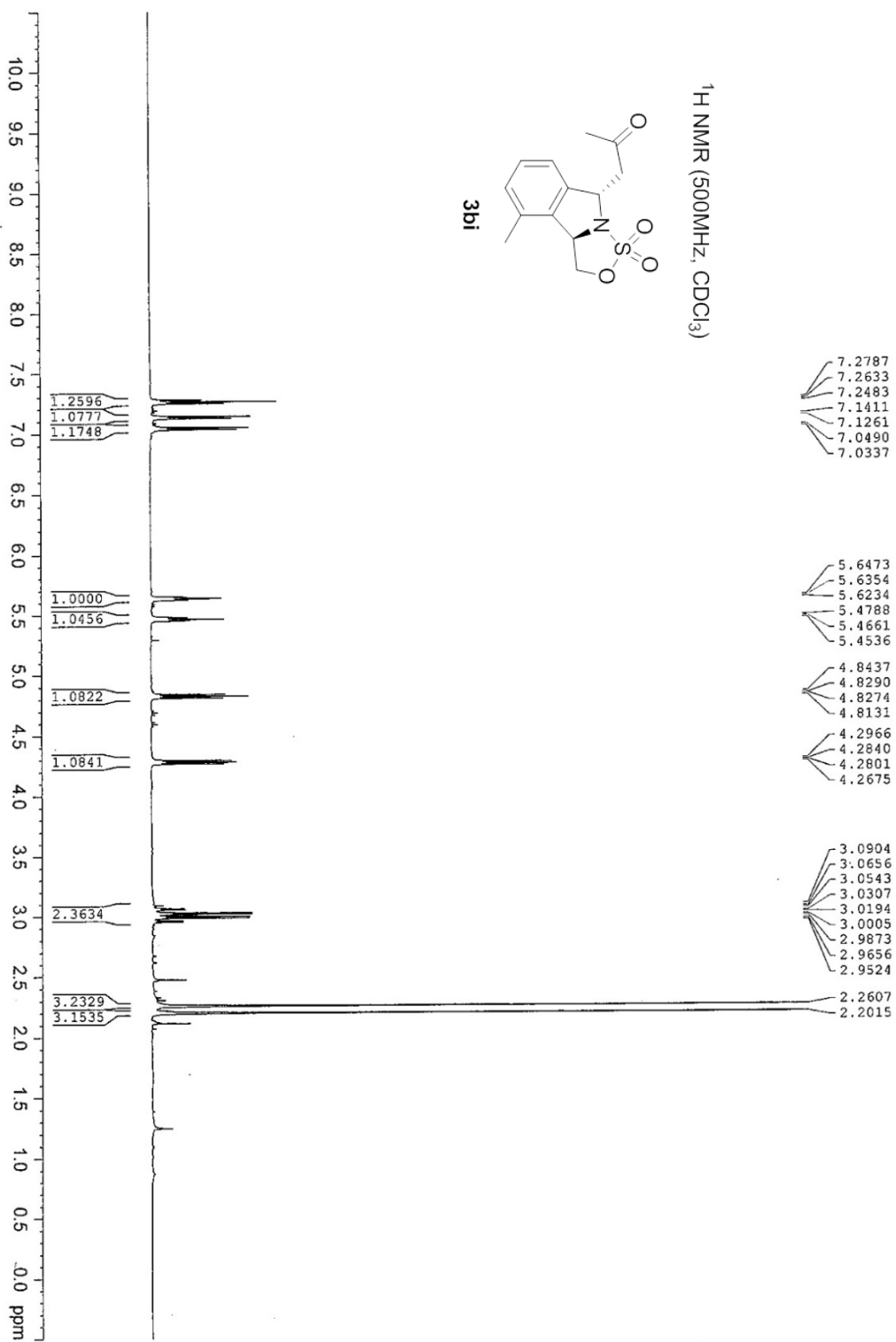


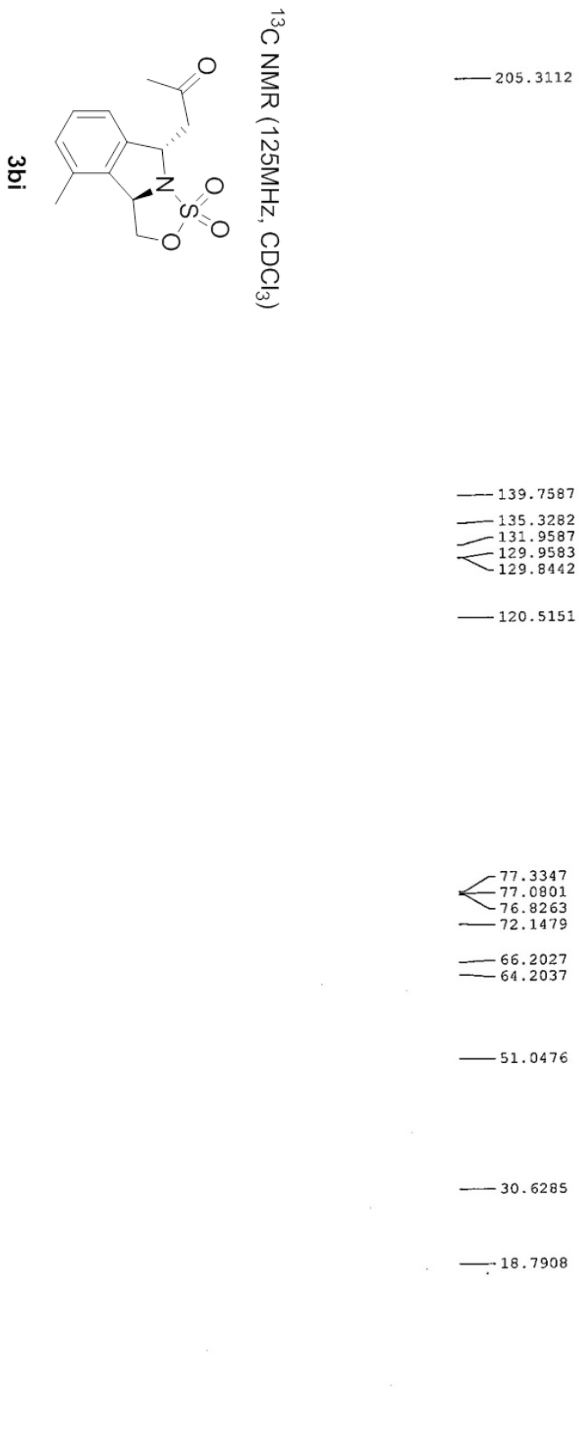


NAME SSM\_160118\_amide\_cc  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20160118  
 Time\_ 22.24  
 INSTRUM 5 mm DUL 13C-1  
 PROSHD spect  
 PULPROG zgpg30  
 TD 32768  
 CDCl3  
 SOLVENT CDCl3  
 NS 5000  
 DS 2  
 SWH 30303.031 Hz  
 FIDRES 0.924775 Hz  
 AQ 0.5407385 sec  
 RG 161.3  
 DW 16.500 usec  
 DE 6.00 usec  
 TE 297.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUCl 13C  
 P1 8.00 usec  
 PL1 1.40 dB  
 PL1W 70.60439301 W  
 SFO1 125.7703661 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waitz16  
 NUCl 1H  
 PCPD2 100.00 usec  
 PL2 -1.90 dB  
 PL12 16.00 dB  
 PL13 19.00 dB  
 EL2W 27.23316002 W  
 PL12W 0.44167015 W  
 PL13W 0.22135943 W  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

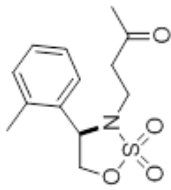




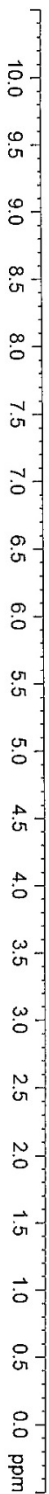
SYJ-2Me-MVK-II-pure-0120

- 7.2601
- 7.2147
- 7.1994
- 7.1842
- 7.0877
- 7.0722
- 7.0570
- 7.0438
- 7.0293
- 5.6080
- 5.5918
- 5.5760
- 5.5598
- 4.7116
- 4.6946
- 4.6779
- 4.6176
- 4.6007
- 4.5836
- 3.1561
- 3.1473
- 3.1365
- 3.1276
- 3.1206
- 3.0994
- 3.0782
- 3.0705
- 3.0582
- 3.0508
- 2.9521
- 2.9444
- 2.9333
- 2.9160
- 2.9053
- 2.8406
- 2.8297
- 2.8207
- 2.8100
- 2.8009
- 2.4856
- 2.1228

<sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>)



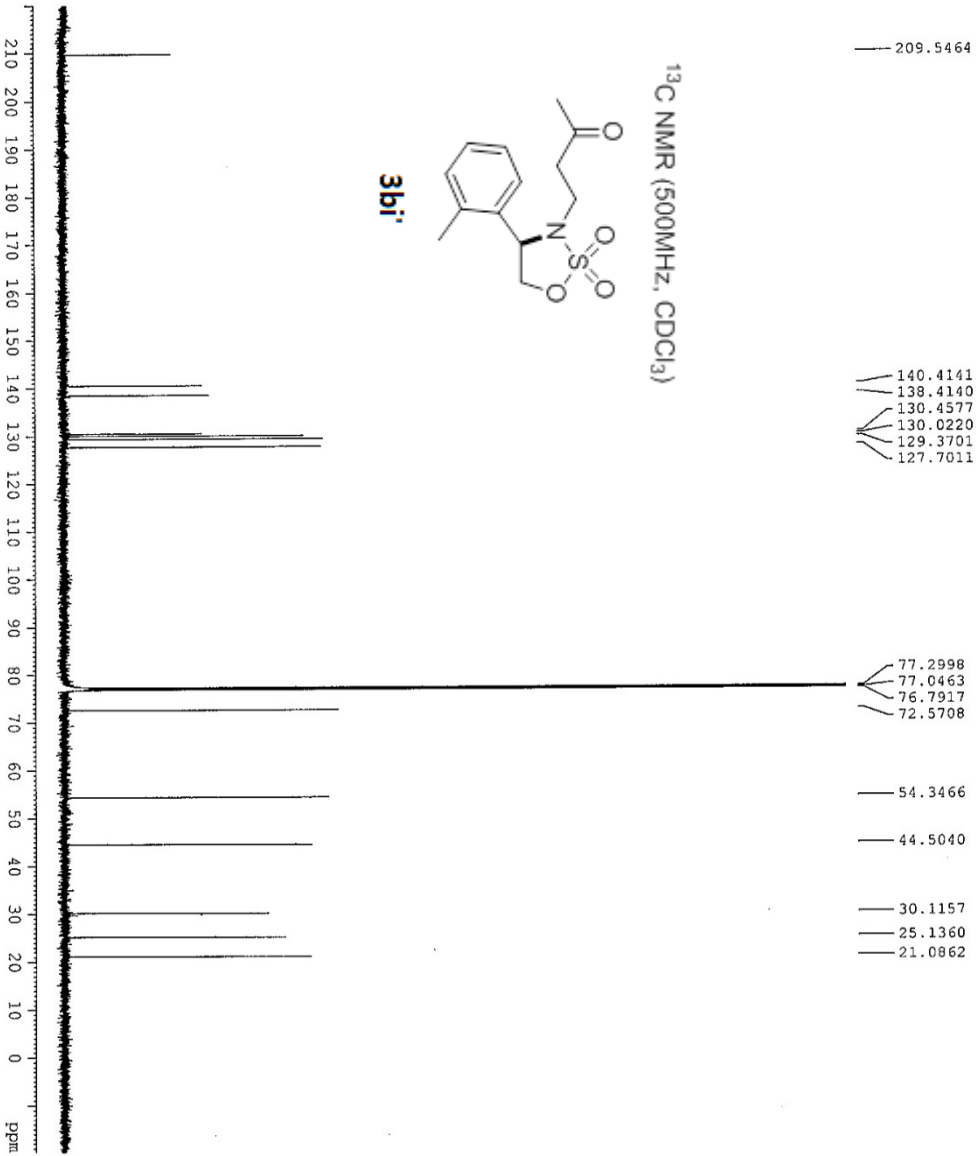
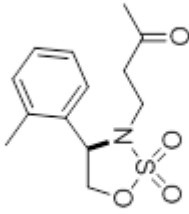
3bi'



SYJ\_2Me\_MVK\_II\_pure\_0119

<sup>13</sup>C NMR (500MHz, CDCl<sub>3</sub>)

3bi



209.5464  
140.4141  
138.4140  
130.4577  
130.0220  
129.3701  
127.7011

77.2998  
77.0463  
76.7917  
72.5708

54.3466

44.5040

30.1157

25.1360

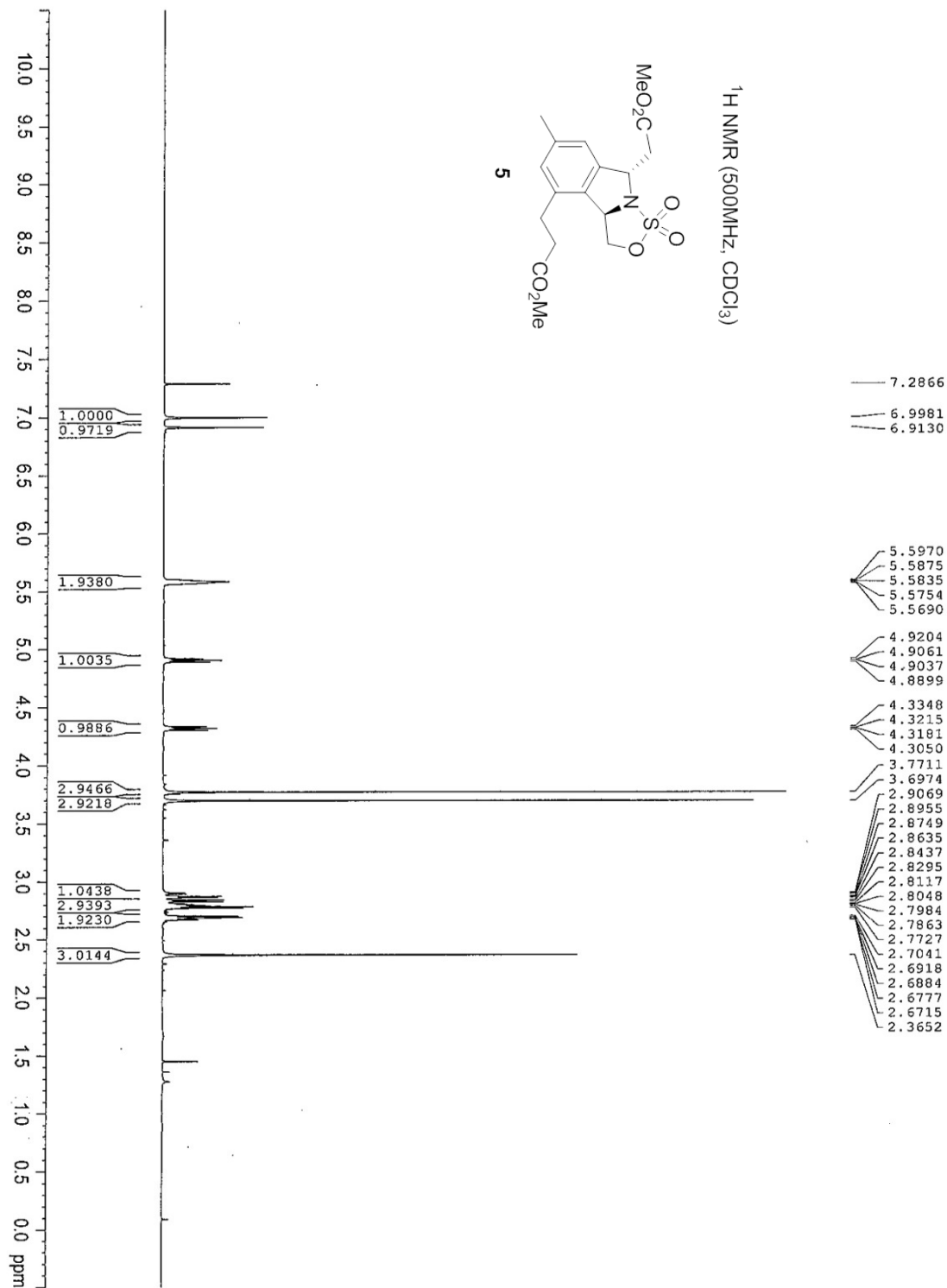
21.0862

```

NAME          SYJ_2Me_MVK_II_pure_0119
EXPNO         1
PROCNO        1
Date_         20160120
Time          10.12
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            1000
DS            1
SWH           30303.031 Hz
FIDRES       0.924775 Hz
AQ           0.5407385 sec
RG           574.7
NR           16.500 usec
DE           6.00 usec
TE           295.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1          1.40 dB
PL1W         70.60439301 W
SFO1         125.7703661 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
P2            100.00 usec
PL2          19.00 dB
PL2W         16.300
PL13         19.00 dB
PL14         27.23316012 W
PL15W        0.44167015 W
PL16W        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
FC           1.40
    
```

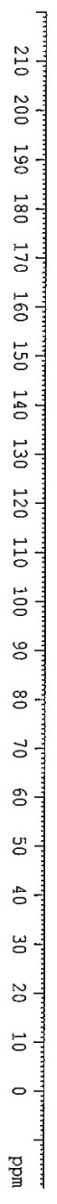
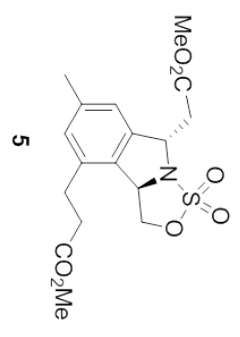




172.6205  
170.3327  
140.3284  
139.8555  
134.5685  
132.4969  
129.1549  
121.5168

72.7420  
66.1557  
64.4857  
52.0047  
51.9278  
42.2844  
34.0076  
27.4565  
21.4328

<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)



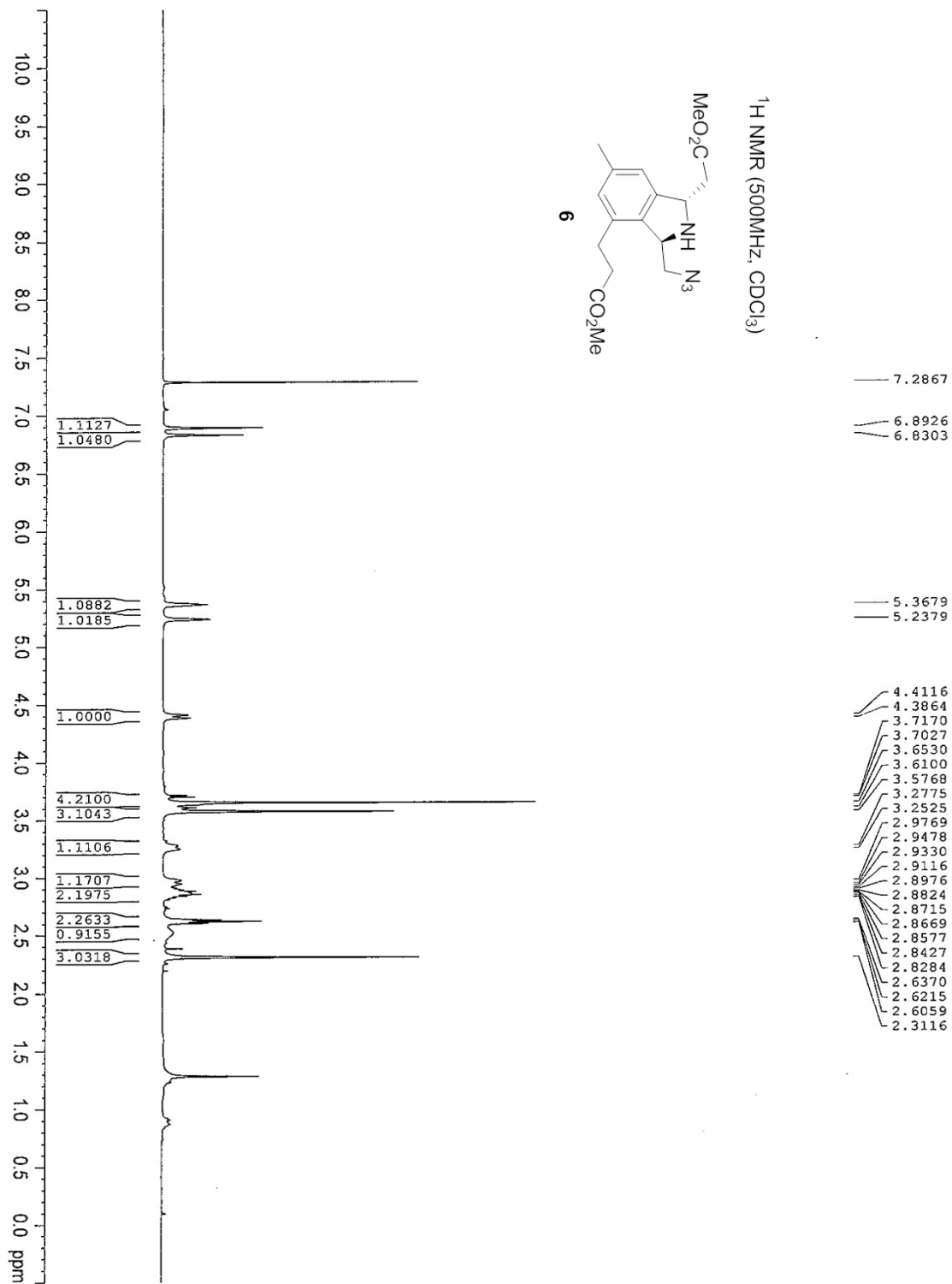
```

NAME SSM_151030_Hydrogenation
EXPNO 2
PROCNO 1
Date_ 20151030
Time_ 19:55
INSTRUM spect
PROBHD 5 mm DUL 13C-Q1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 3000
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407385 sec
RG 3251
DE 16.500 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 1.40 dB
PL1W 70.60439301 W
SFO1 125.7703661 MHz

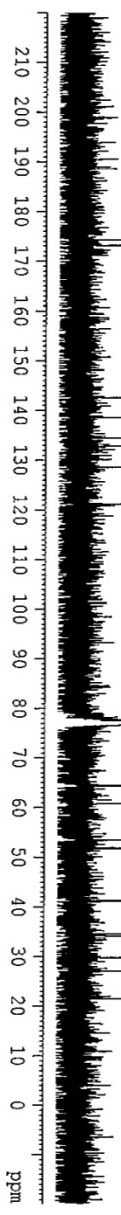
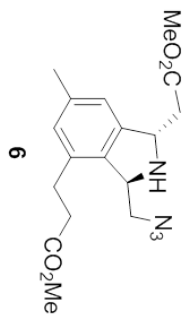
===== CHANNEL f2 =====
MAGIz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.90 dB
PL12 18.00 dB
PL13 19.00 dB
PL2W 27.23316002 W
PL12W 0.44167015 W
PL13W 0.22135943 W
SFO2 500.1320005 MHz
SI 32768
SF 125.757890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



174.2041  
173.0619  
142.5533  
138.5201  
134.4075  
132.7794  
128.4685  
121.1615  
77.2679  
77.0133  
76.7600  
64.3456  
60.7042  
53.4484  
51.7647  
51.6688  
41.2247  
34.4991  
27.0680  
21.4404

<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)

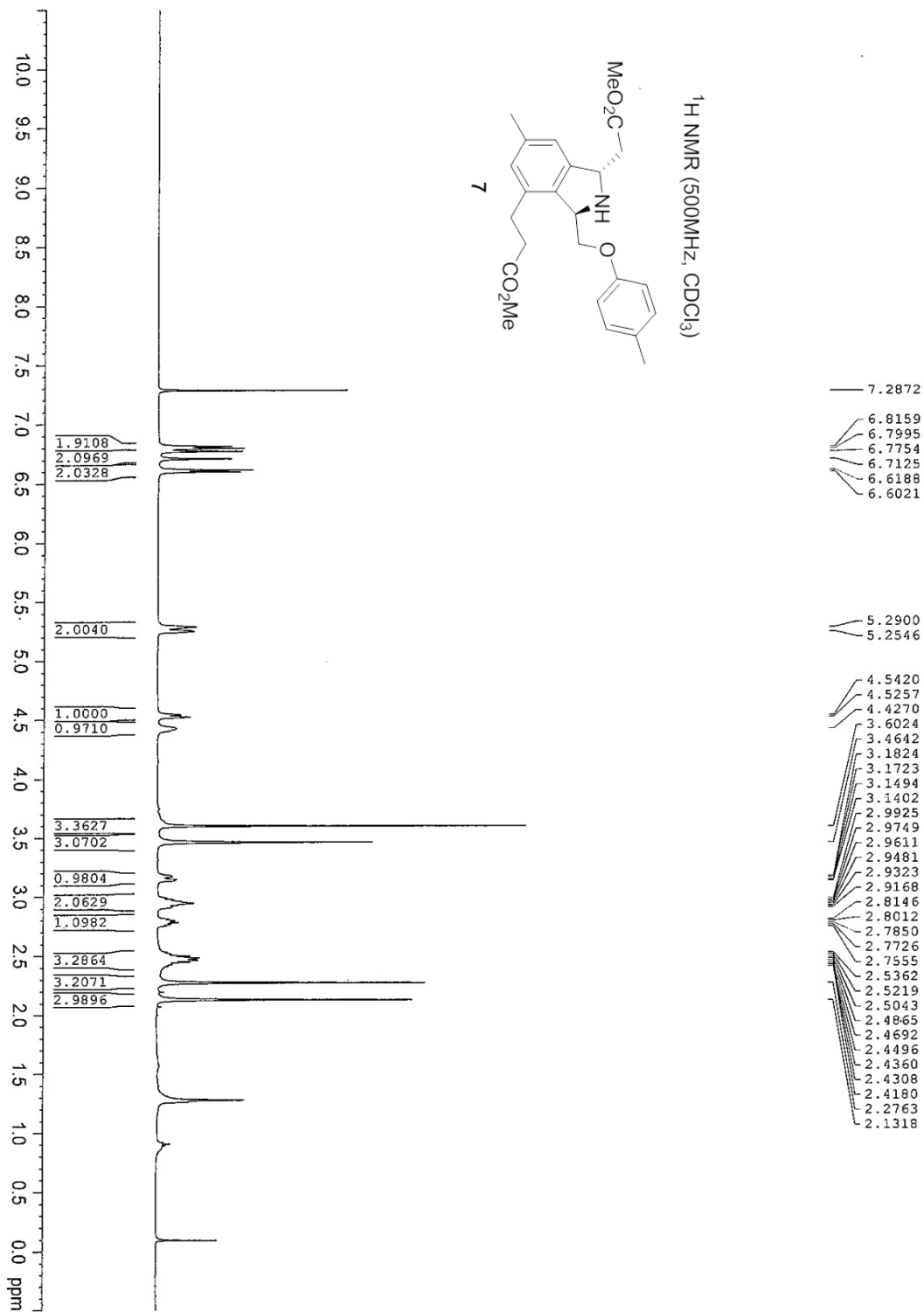


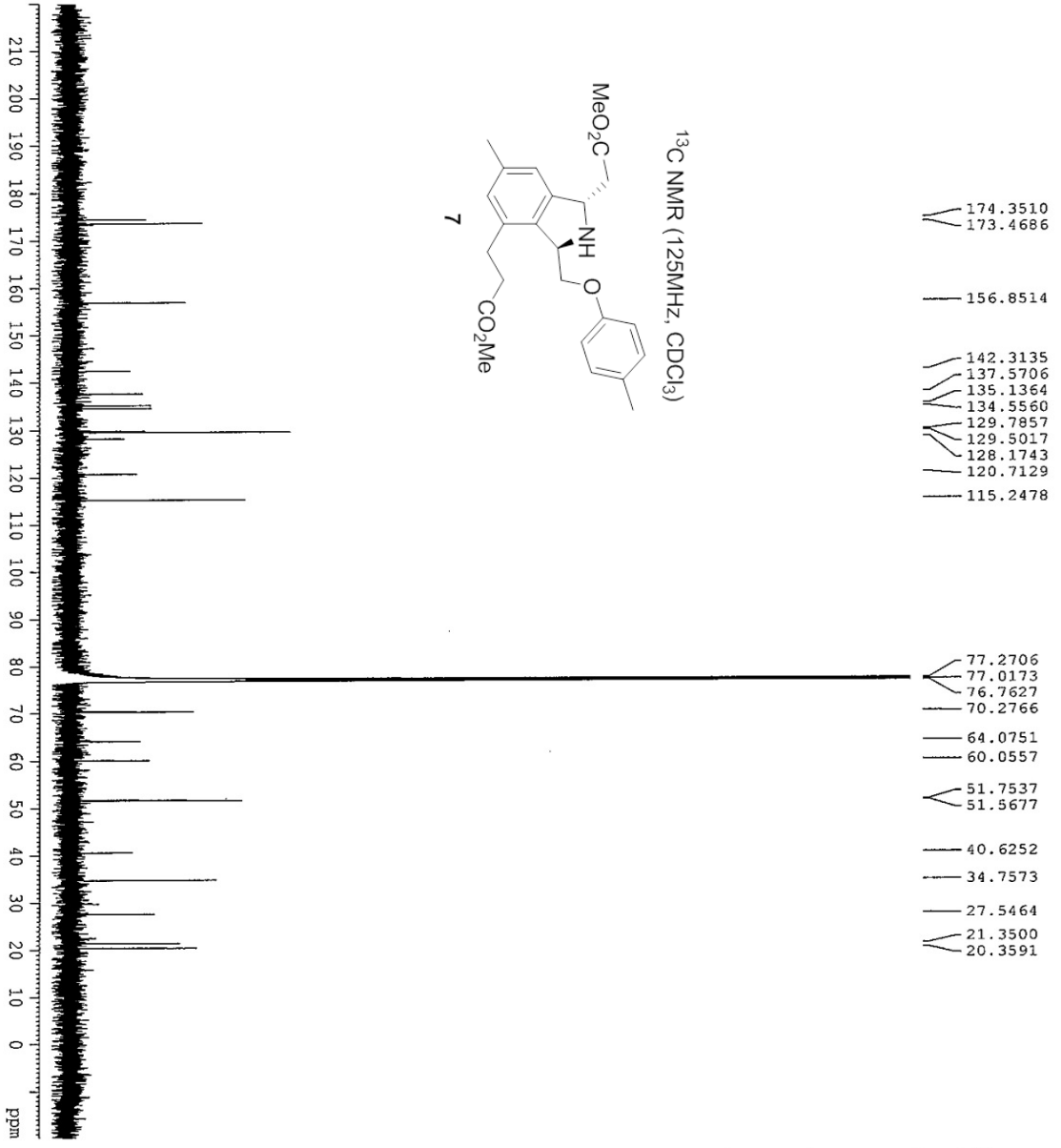
```

NAME          SSN_151102_hy_N3_P
EXPNO         1
PROCNO        1
Date_         20151102
Time          21.07
INSTRUM       spect
PROBHD        5 mm DUE 13C-1
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            3000
DS            2
SMH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407385 sec
RG            5792.6
DM            16.500 usec
DE            6.00 usec
TE            300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
PL1W          70.60439301 W
SFO1          125.7703661 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2           -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL1W         27.23318002 W
PL12W        0.44167015 W
PL13W        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```





- 174.3510
- 173.4686
- 156.8514
- 142.3135
- 137.5706
- 135.1364
- 134.5560
- 129.7857
- 129.5017
- 128.1743
- 120.7129
- 115.2478
- 77.2706
- 77.0173
- 76.7627
- 70.2766
- 64.0751
- 60.0557
- 51.7537
- 51.5677
- 40.6252
- 34.7573
- 27.5464
- 21.3500
- 20.3591

```

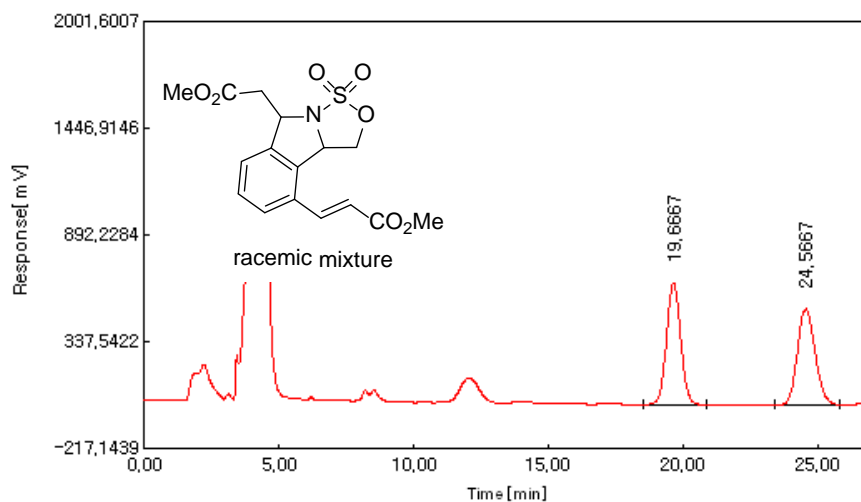
NAME          SSM_151120_cresol_D
EXPNO         1
PROCNO        1
Date_         20151121
Time          1.05
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            10000
DS            2
SWH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407385 sec
RG            2298.8
DE            16.500 usec
TE            298.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
PL1           1.40 dB
PL1W          70.60439301 W
SFO1          125.7703661 MHz

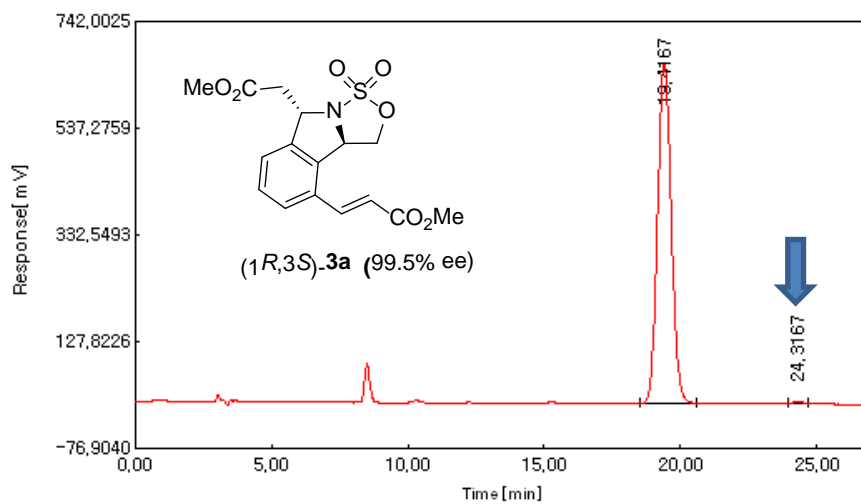
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2          -1.90 dB
PL12         16.00 dB
PL13         19.00 dB
PL1W         27.23316002 W
PL1Z         0.44167015 W
PL13W        0.22135943 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW           EM
SSB           0
LB           1.00 Hz
GB           0
PC           1.40
  
```

► **Sample name: 3a**

► **Analysis condition: Chiralpak IC, 40%EtOH/n-hexane, 1.0ml/min, 215nm**



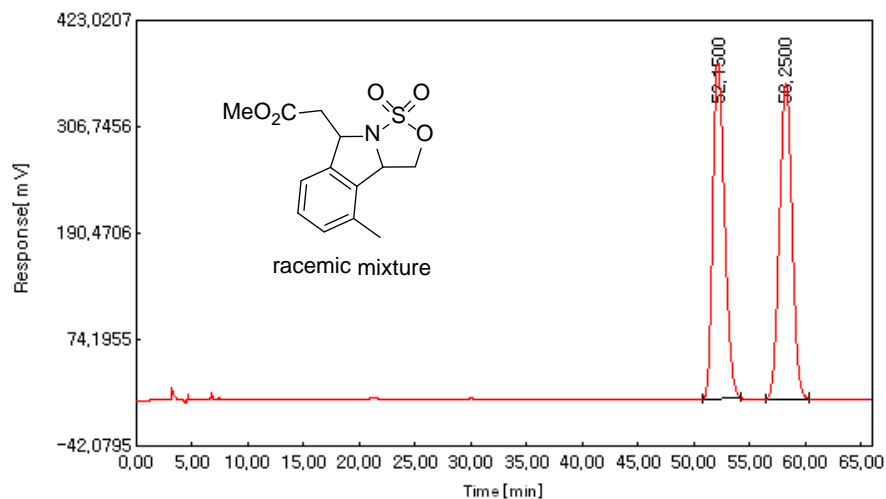
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	19.6667	24104.2025	BB	141.0000	50.5815
2	24.5667	23549.9903	BB	145.0000	49.4185
Total		47654.1953			



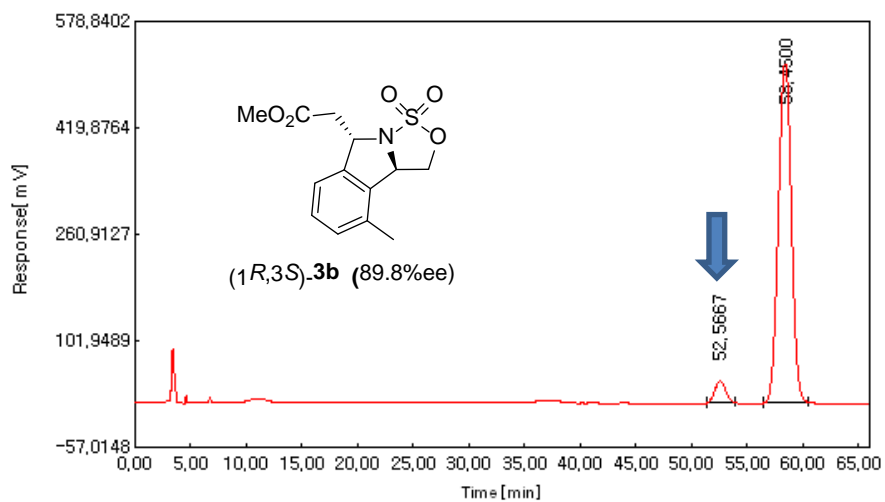
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	19.4167	23580.0859	BB	122.0000	99.7423
2	24.3167	60.9137	FF	47.0000	0.2577
Total		23641.0000			

► **Sample name: 3b**

► **Analysis condition:** Chiralpak IC, 10%EtOH/n-hexane, 1.0ml/min, 215nm



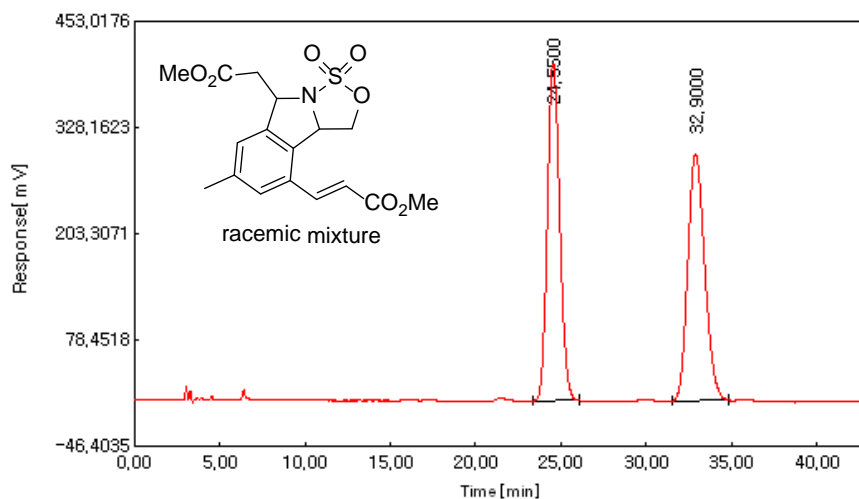
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	52.1500	27616.7729	BB	210.0000	49.9167
2	58.2500	27708.9791	BB	228.0000	50.0833
Total		55325.7539			



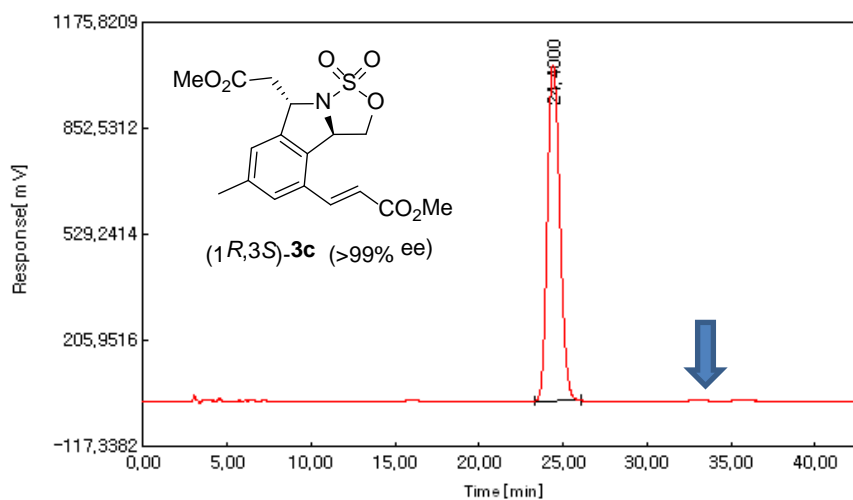
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	52.5667	2251.4052	BB	155.0000	5.1048
2	58.4500	41852.0271	BB	241.0000	94.8952
Total		44103.4336			

► **Sample name: 3c**

► **Analysis condition:** Chiralpak IC, 40%EtOH/n-hexane, 1.0ml/min, 215nm



Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	24.5500	20700.4727	BB	158.0000	50.0223
2	32.9000	20682.0239	BB	198.0000	49.9777
Total		41382.4961			

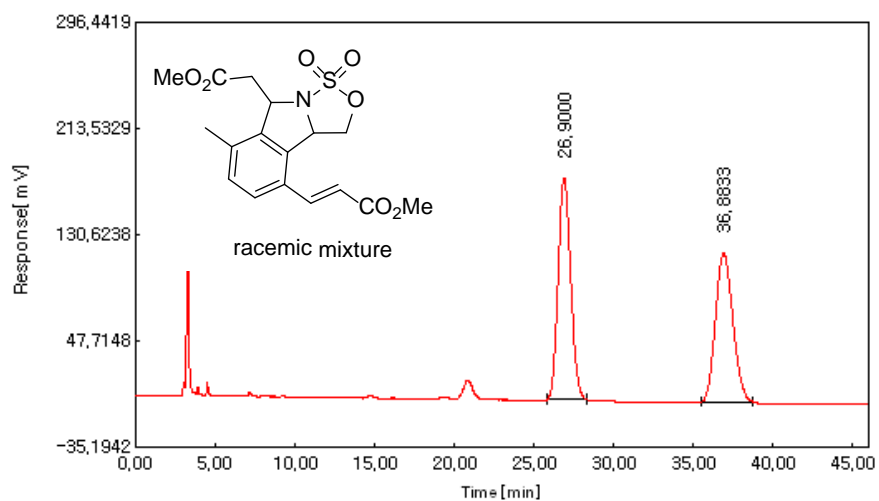


Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	24.4000	54905.2761	BB	165.0000	100.0000
Total		54905.2773			

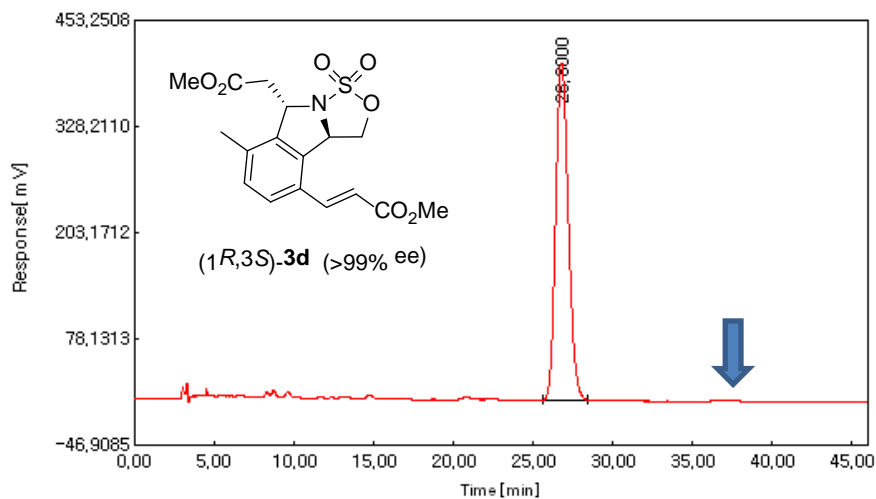


► **Sample name: 3d**

► **Analysis condition: Chiralpak IC, 20%EtOH/n-hexane, 1.0ml/min, 215nm**



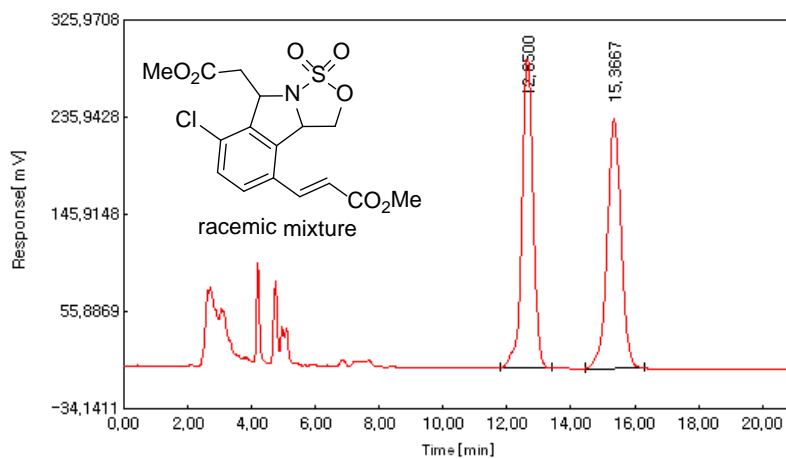
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	26.9000	9798.4882	BB	152.0000	51.8215
2	36.8833	9109.6646	BB	196.0000	48.1785
Total		18908.1523			



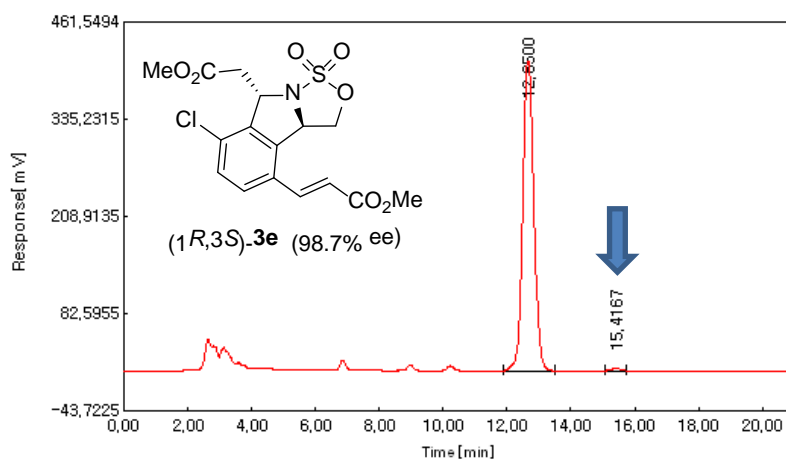
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	26.8000	22634.8903	BB	169.0000	100.0000
Total		22634.8906			

► **Sample name: 3e**

► **Analysis condition: Chiralpak IC, 50%EtOH/n-hexane, 1.1ml/min, 215nm**



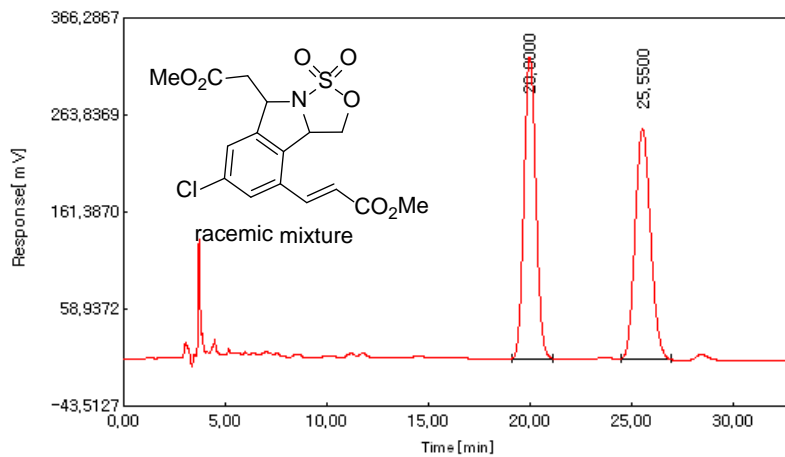
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	12.6500	7235.8937	BB	96.0000	50.0116
2	15.3667	7232.5439	BB	112.0000	49.9884
Total		14468.4375			



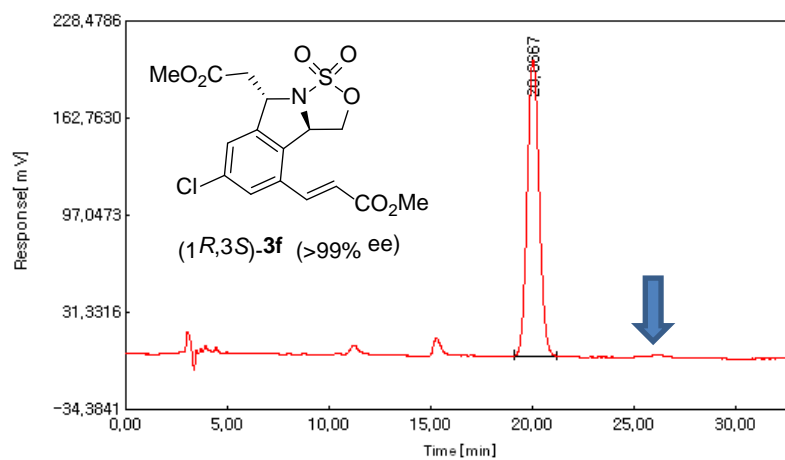
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	12.6500	9995.0123	BB	98.0000	99.3443
2	15.4167	65.9705	FF	41.0000	0.6557
Total		10060.9834			

► **Sample name: 3f**

► **Analysis condition: Chiralpak IC, 40%EtOH/n-hexane, 1.0ml/min, 215nm**



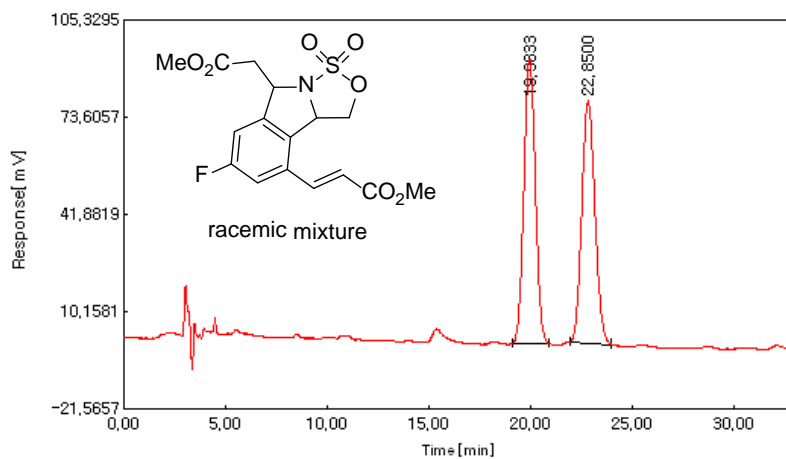
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	20.0000	13372.2393	BB	125.0000	50.1590
2	25.5500	13287.4718	BB	150.0000	49.8410
Total		26659.7109			



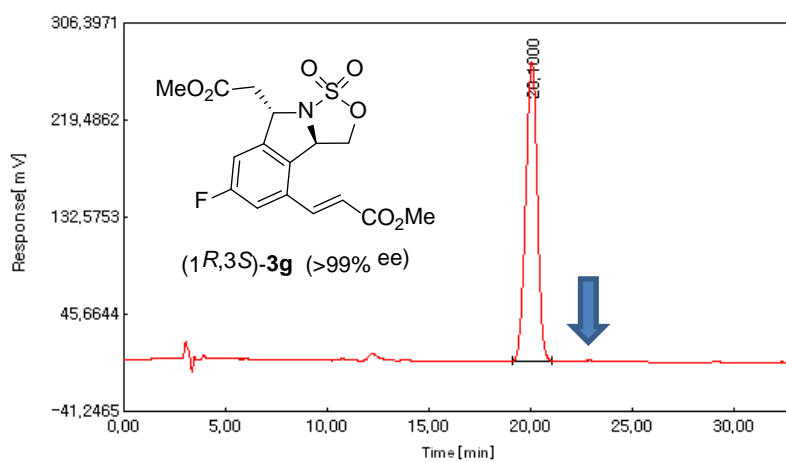
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	20.0667	8406.7910	BB	124.0000	100.0000
Total		8406.7910			

► **Sample name: 3g**

► **Analysis condition: Chiralpak IC, 40%EtOH/n-hexane, 1.0ml/min, 215nm**



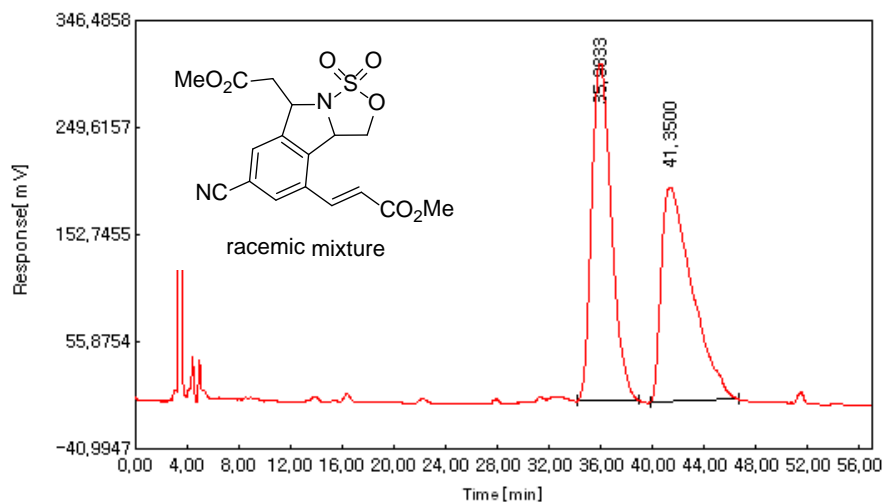
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	19.9833	3742.1226	BB	108.0000	50.4885
2	22.8500	3669.7148	BB	120.0000	49.5115
Total		7411.8374			



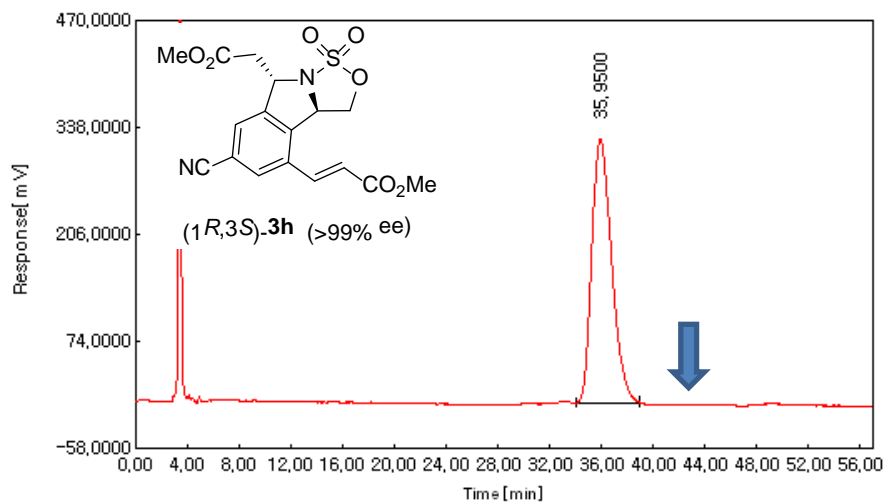
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	20.1000	10941.0685	BB	119.0000	100.0000
Total		10941.0684			

► **Sample name: 3h**

► **Analysis condition: Chiralcel OD-H, 30%IPA/n-hexane, 1.0ml/min, 215nm**



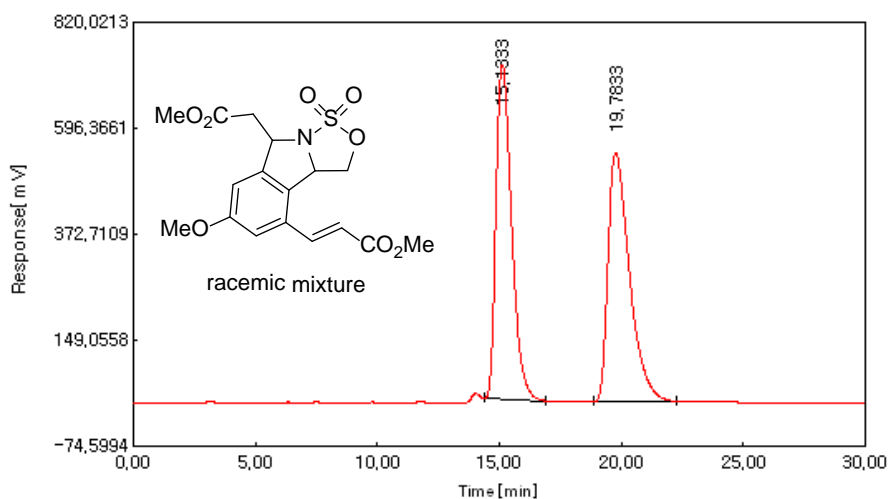
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	35.9833	33458.7592	BB	283.0000	50.0785
2	41.3500	33353.9121	FF	410.0000	49.9215
Total		66812.6719			



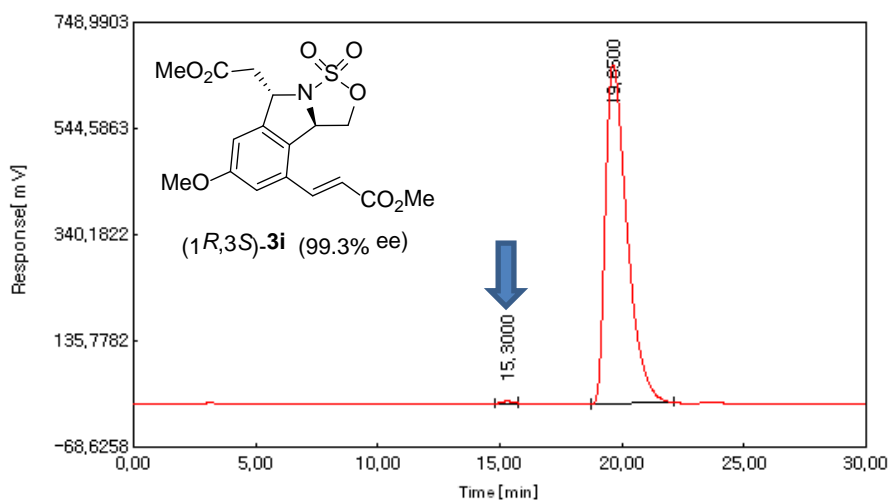
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	359500	34126.1394	BB	291.0000	100.0000
Total		34126.1394			

► **Sample name: 3i**

► **Analysis condition:** Chiralcel OD-H, 30% IPA/n-hexane, 1.0ml/min, 215nm



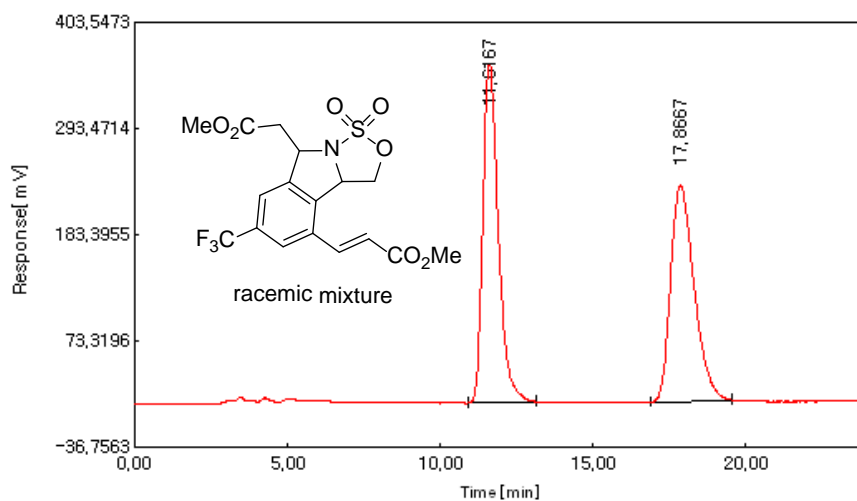
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	15.1333	32514.1144	BB	151.0000	49.4101
2	19.7833	33290.4902	BB	203.0000	50.5899
Total		65804.6016			



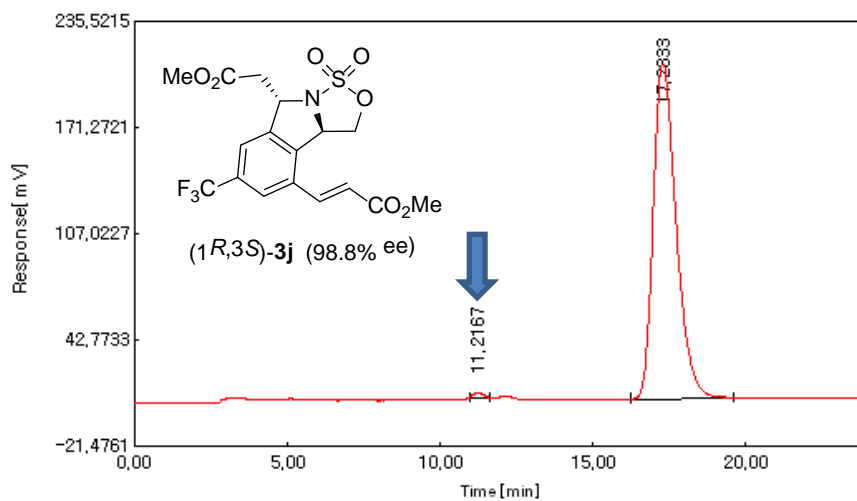
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	15.3000	156.6294	FF	59.0000	0.3719
2	19.6500	41961.5187	BB	205.0000	99.6281
Total		42118.1484			

► **Sample name: 3j**

► **Analysis condition:** Chiralcel OD-H, 30%IPA/n-hexane, 1.0ml/min, 215nm



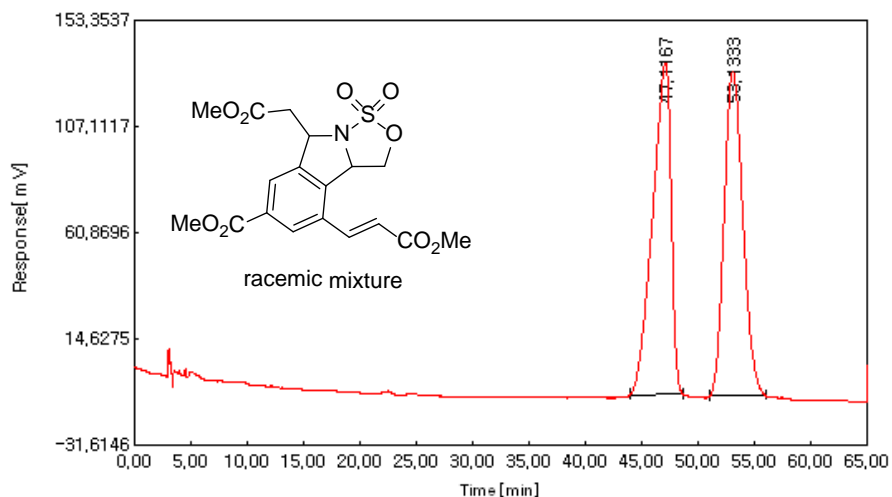
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	11.6167	12864.4116	BB	132.0000	50.9475
2	17.8667	12385.9046	BB	158.0000	49.0525
Total		25250.3164			



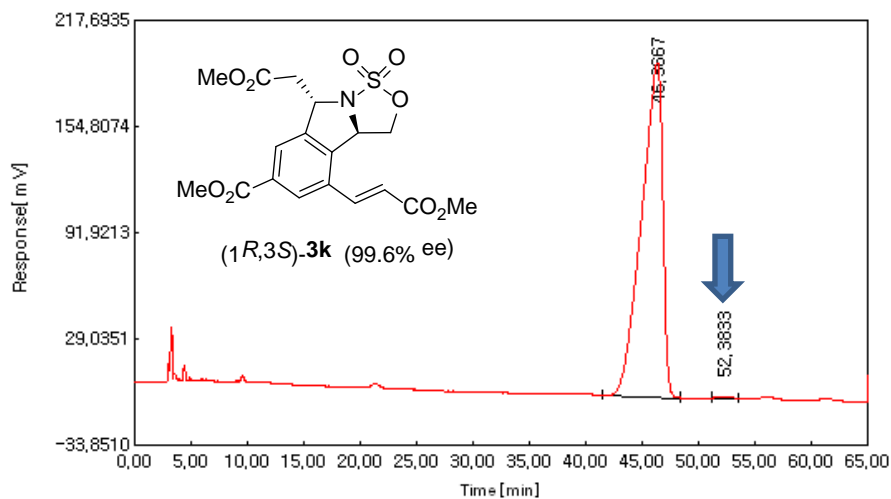
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	11.2167	63.5482	FF	39.0000	0.5776
2	17.2833	10937.9071	FF	202.0000	99.4224
Total		11001.4551			

► **Sample name: 3k**

► **Analysis condition: Chiralpak IC, 40%EtOH/n-hexane, 1.0ml/min, 215nm**



Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	47.1167	16919.6976	BB	281.0000	50.1719
2	53.1333	16803.7854	BB	297.0000	49.8281
Total		33723.4844			

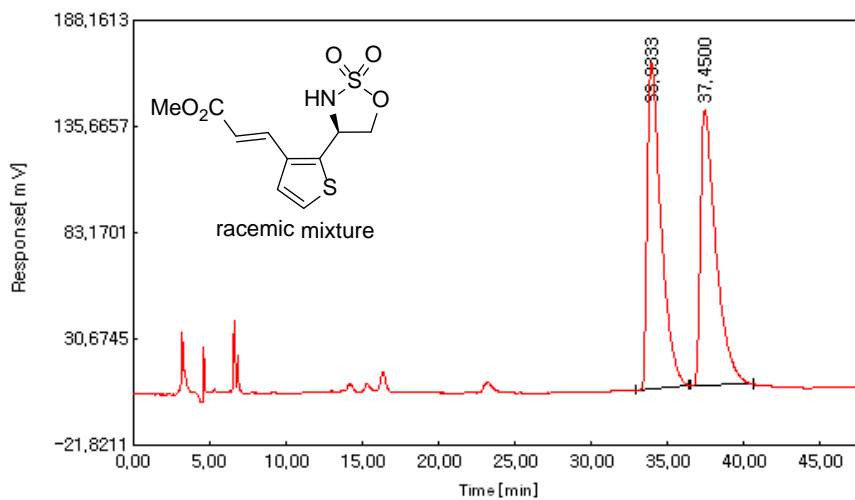


Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	46.3667	26445.8875	FF	411.0000	99.7901
2	52.3833	55.6255	FF	137.0000	0.2099
Total		26501.5117			

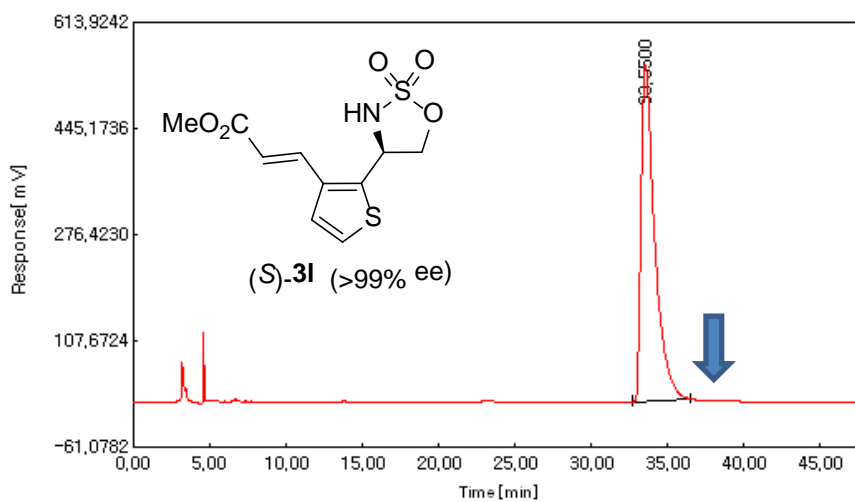


► **Sample name: 3I**

► **Analysis condition:** Chiralpak IC, 10%EtOH/n-hexane, 1.0ml/min, 215nm



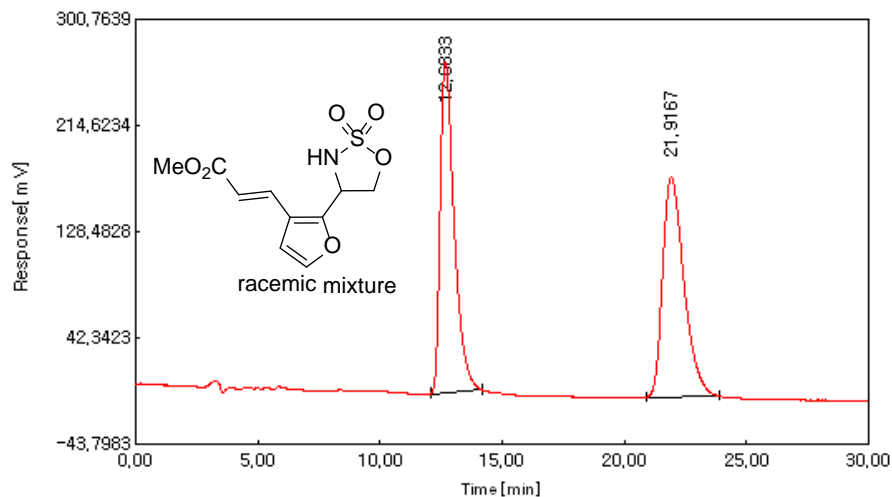
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	33.9333	10353.5611	FF	211.0000	51.2288
2	37.4500	9856.8699	FF	248.0000	48.7712
Total		20210.4316			



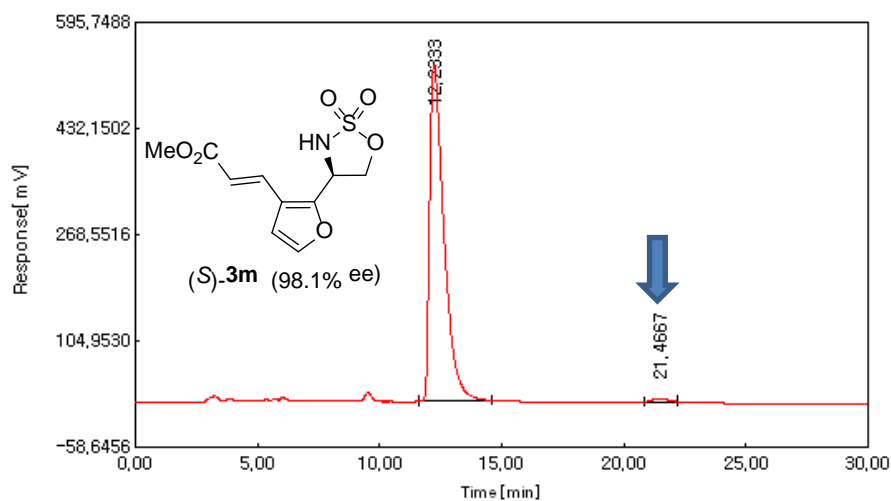
Peak #	RT[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	33.5500	33879.5617	BB	223.0000	100.0000
Total		33879.5625			

► **Sample name: 3m**

► **Analysis condition: Chiralcel OD-H, 30%IPA/n-hexane, 1.0ml/min, 215nm**



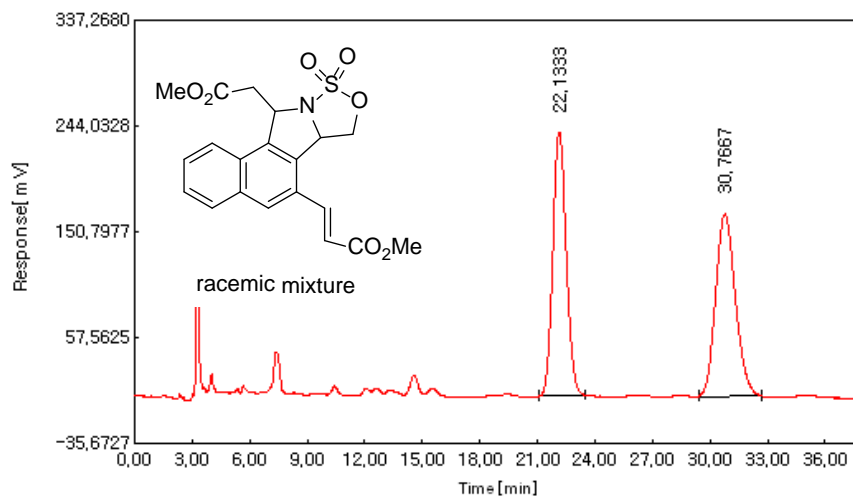
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	12.6833	11124.0456	BB	127.0000	49.8113
2	21.9167	11208.3124	BB	179.0000	50.1887
Total		22332.3574			



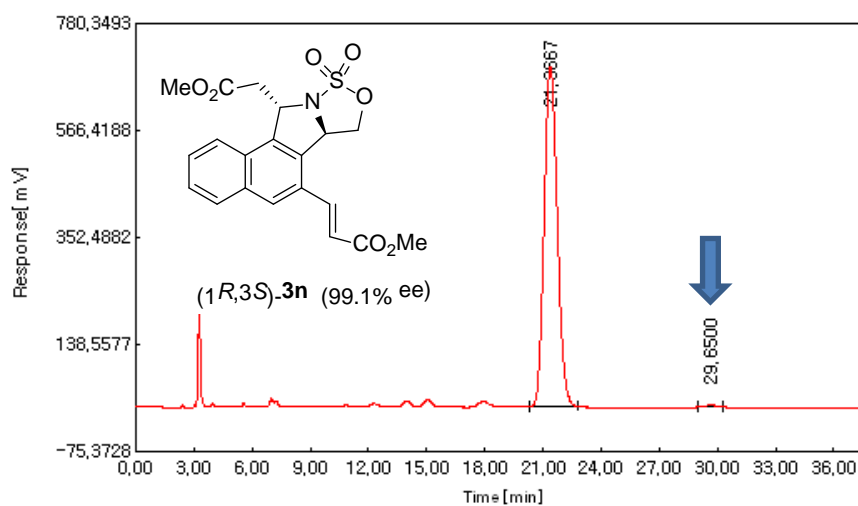
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	12.2333	21673.1318	FF	182.0000	99.0270
2	21.4667	212.9511	FF	79.0000	0.9730
Total		21886.0820			

► **Sample name: 3n**

► **Analysis condition: Chiralpak IC, 50%EtOH/n-hexane, 1.0ml/min, 215nm**



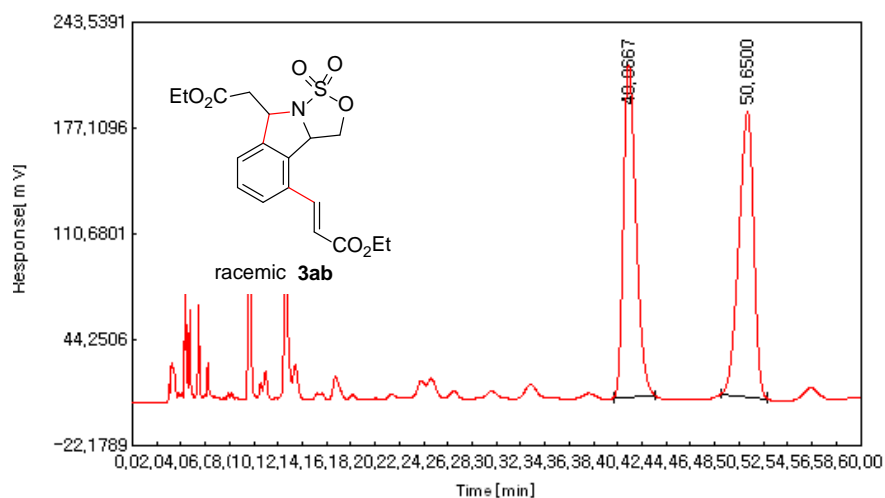
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	22.1333	11687.1699	BB	145.0000	49.5586
2	30.7667	11895.3693	BB	199.0000	50.4414
Total		23582.5391			



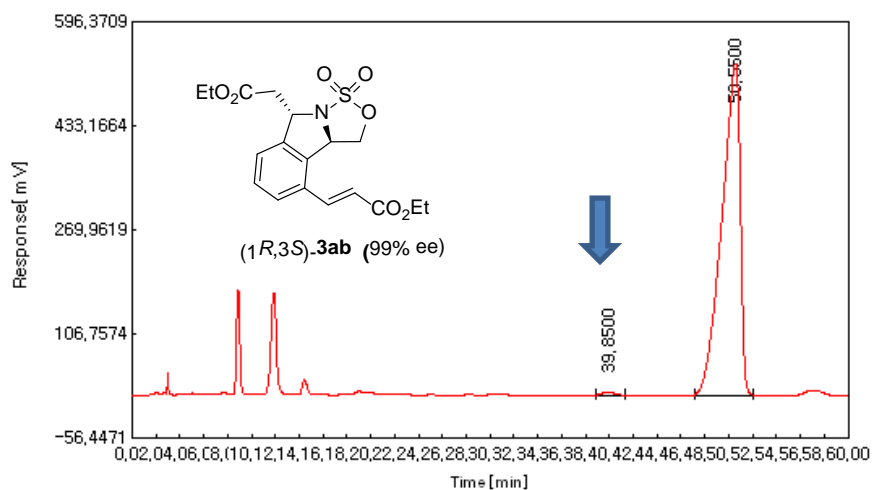
Peak #	RT [min]	Area [mV*s]	BL	Wide [sec]	Area%
1	21.3667	33141.9075	BB	152.0000	99.5443
2	29.6500	151.7227	FF	77.0000	0.4557
Total		33293.6289			

► **Sample name:** (1*R*,3*S*)-**3ab**

► **Analysis condition:** Chiralpak IC, 20% EtOH/n-hexane, 1.0 ml/min, 254nm



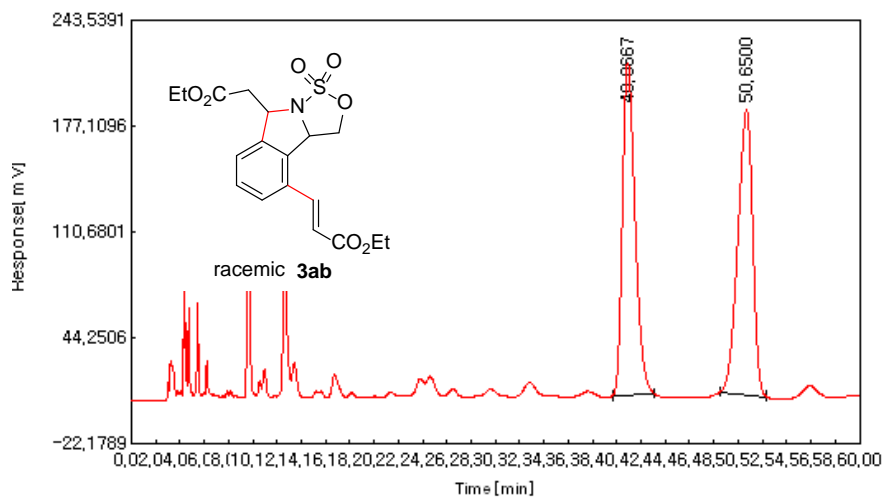
Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	40.8667	15577.1004	BB	211.0000	49.7761
2	50.6500	15717.2431	BB	230.0000	50.2239
Total		31294.3438			



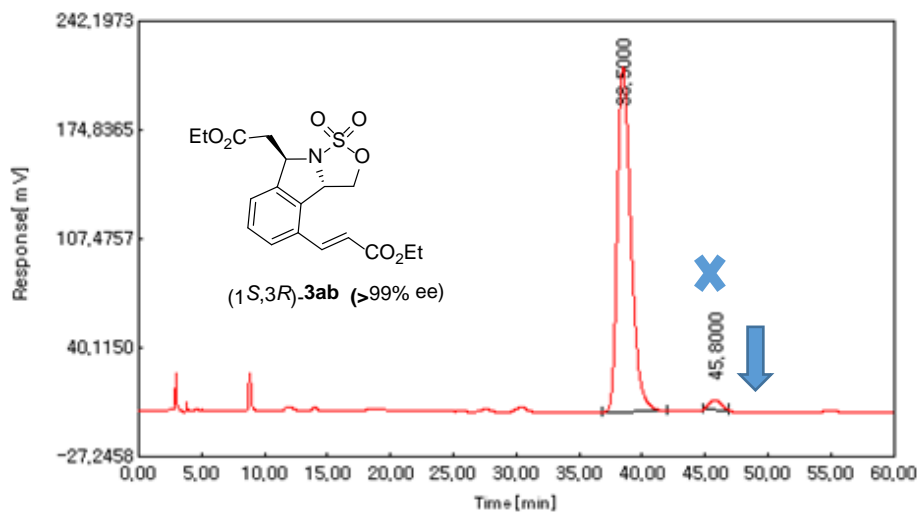
Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	39.8500	322.4641	FF	143.0000	0.5585
2	50.5500	57419.2212	BB	293.0000	99.4415
Total		57741.6836			

► **Sample name: (1*S*,3*R*)-3ab**

► **Analysis condition: Chiralpak IC, 20% EtOH/n-hexane, 1.0 ml/min, 254nm**



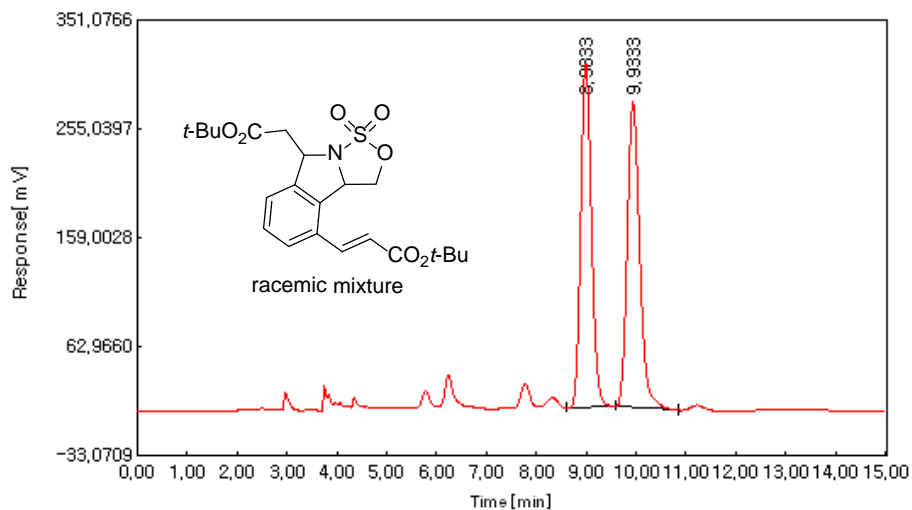
Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	40.8667	15577.1004	BB	211.0000	49.7761
2	50.6500	15717.2431	BB	230.0000	50.2239
Total		31294.3438			



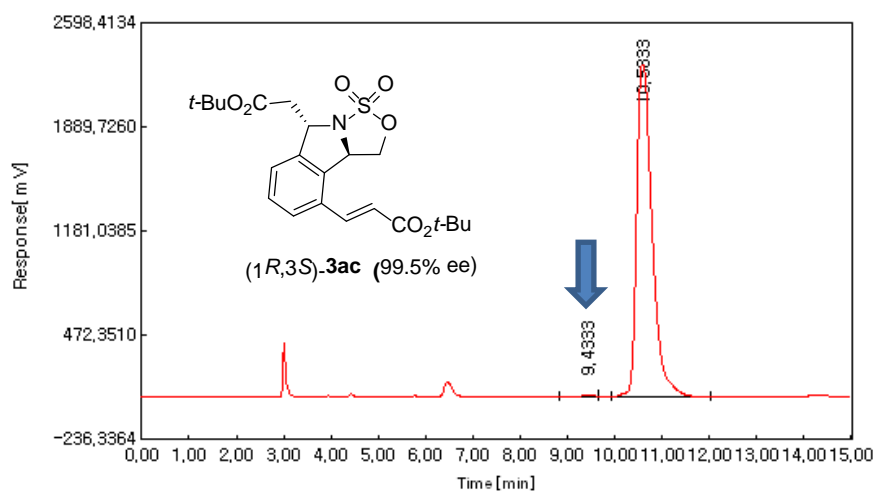
Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	38.5000	16291.3085	FF	306.0000	100.0000
Total		16291.3085			

► **Sample name: 3ac**

► **Analysis condition: Chiralpak IC, 20% EtOH/n-hexane, 1.0 ml/min, 254nm**



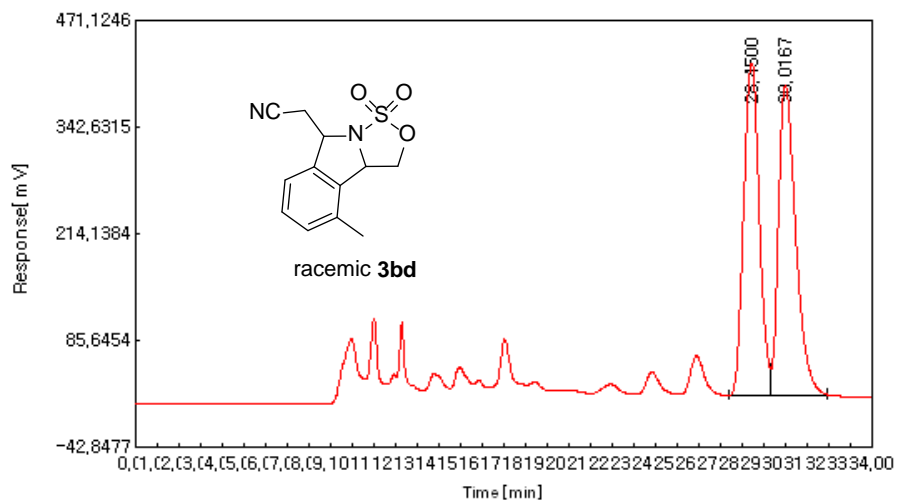
Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	8.9833	4605.5190	BB	58.0000	49.3164
2	9.9333	4733.2019	BB	76.0000	50.6836
Total		9338.7207			



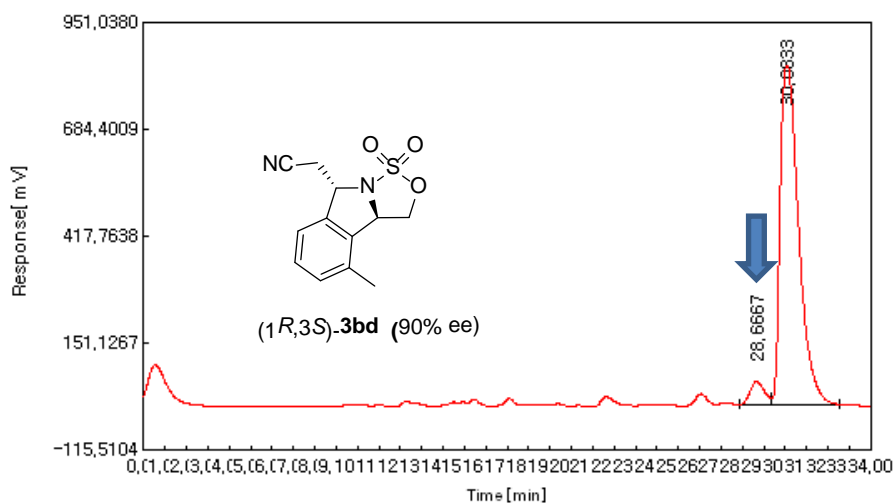
Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	9.4333	130.6417	FF	51.0000	0.2413
2	10.5833	54002.7480	BB	127.0000	99.7587
Total		54133.3906			

► **Sample name: 3bd**

► **Analysis condition: Chiralpak AD-H, 30% IPA/n-hexane, 0.7 ml/min, 215nm**



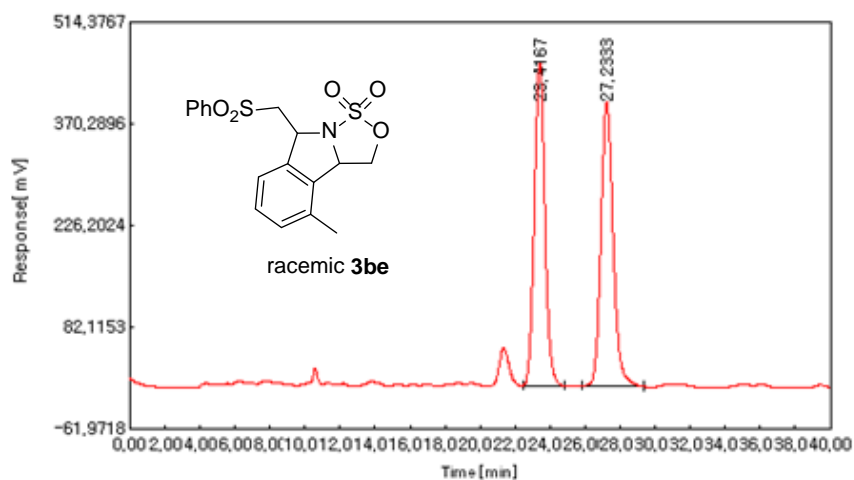
Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	28.4500	20793.8758	BB	116.0000	49.2533
2	30.0167	21424.3463	BB	157.0000	50.7467
Total		42218.2227			



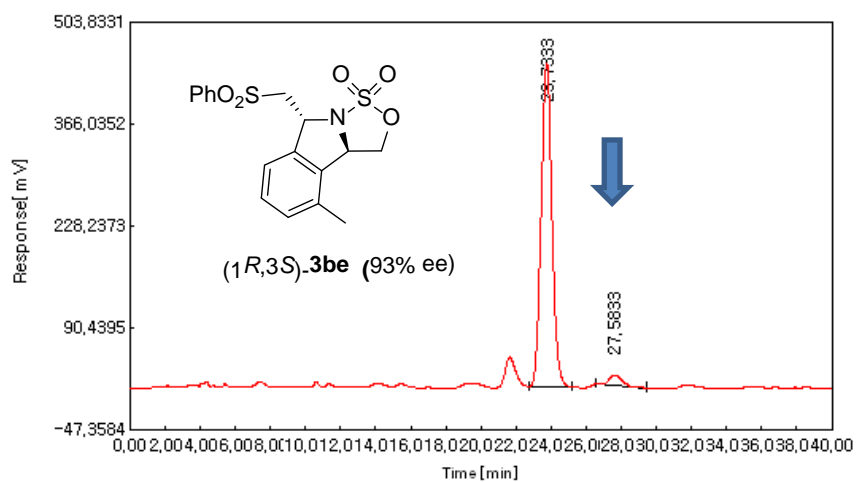
Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	28.6667	2774.2129	BB	90.0000	5.0040
2	30.0833	52665.8729	BB	192.0000	94.9960
Total		55440.0859			

► **Sample name: 3be**

► **Analysis condition: Chiralpak AD-H, 30% IPA/n-hexane, 0.7 ml/min, 215nm**



Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	23.4167	20009.8324	BB	143.0000	49.5343
2	27.2333	20386.0624	BB	209.0000	50.4657
Total		40395.8945			



Peak #	Time[min]	Area[mV*s]	BL	Wide[sec]	Area%
1	23.7333	19337.7291	BB	143.0000	96.5832
2	27.5833	684.1124	FF	169.0000	3.4168
Total		20021.8418			