

Supplementary Information for

A Novel Neutral Organic Electron Donor with Record Half-Wave Potential

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Computational results

S2-S7

NMR spectra

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Optimised geometry (M05-2X/cc-pVTZ) of donor 26

6	2.775096000	-0.724035000	0.677223000
1	3.553441000	-1.166210000	1.267815000
6	2.775096000	-0.724035000	-0.677223000
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6	1.526658000	-0.192208000	-1.159673000
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1	-0.055252000	1.930146000	0.878744000
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6	0.902228000	-0.181972000	2.379691000
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1	-4.295405000	-0.376879000	-4.784845000
6	-3.288124000	0.382917000	-2.478983000
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6	1.807009000	2.545779000	0.000000000
1	2.404821000	2.336203000	-0.883964000
1	2.404821000	2.336203000	0.883964000
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E = -1130.9445492

Optimised geometry (M05-2X/cc-pVTZ) of donor **26**, in DMF

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6	-2.794520000	0.675458000	-0.678102000
1	-3.589145000	1.088091000	-1.268545000
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6	-1.532999000	0.174263000	-1.162372000
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1	0.084753000	-1.924079000	0.877069000
6	-0.906940000	0.178828000	-2.384432000
6	-0.906940000	0.178828000	2.384432000
7	-1.573212000	0.345362000	-3.610749000
7	-1.573212000	0.345362000	3.610749000
6	-3.018844000	0.419724000	-3.663206000
1	-3.381076000	1.388407000	-3.329348000
1	-3.442530000	-0.355829000	-3.029360000
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6	-3.018844000	0.419724000	3.663206000
1	-3.339680000	0.260895000	4.685607000
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6	-0.883518000	0.311927000	4.780217000
1	-1.491559000	0.404525000	5.665103000
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1	0.904127000	0.090504000	5.841418000
6	1.207613000	0.017832000	3.649481000
6	0.525959000	0.022516000	2.472280000
1	1.042235000	-0.025836000	1.532471000
7	2.583451000	-0.155517000	3.728380000
6	3.288468000	-0.343554000	2.477702000
1	3.261595000	0.552390000	1.847115000
1	2.853795000	-1.171540000	1.925044000
1	4.325035000	-0.577805000	2.699040000

6	3.314596000	0.715869000	4.638979000
1	4.307065000	0.304507000	4.797136000
1	2.817222000	0.784899000	5.597007000
1	3.416786000	1.724286000	4.225784000
6	0.525959000	0.022516000	-2.472280000
1	1.042235000	-0.025836000	-1.532471000
6	1.207613000	0.017832000	-3.649481000
6	0.450598000	0.157625000	-4.870326000
1	0.904127000	0.090504000	-5.841418000
6	-0.883518000	0.311927000	-4.780217000
1	-1.491559000	0.404525000	-5.665103000
7	2.583451000	-0.155517000	-3.728380000
6	3.314596000	0.715869000	-4.638979000
1	3.416786000	1.724286000	-4.225784000
1	2.817222000	0.784899000	-5.597007000
1	4.307065000	0.304507000	-4.797136000
6	3.288468000	-0.343554000	-2.477702000
1	4.325035000	-0.577805000	-2.699040000
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1	3.261595000	0.552390000	-1.847115000
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1	-2.370356000	-2.369281000	0.884475000
1	-1.492415000	-3.620084000	0.000000000

E = -1130.9596886

Optimised geometry (M05-2X/cc-pVTZ) of the lowest excited triplet state of donor

26

6	-0.699494000	-1.984696000	-1.579813000
1	-1.348674000	-2.490619000	-2.270733000
6	0.712586000	-1.988287000	-1.574356000
1	1.364529000	-2.495957000	-2.261412000
6	-1.119951000	-1.125866000	-0.588330000
6	1.129697000	-1.132324000	-0.579508000
7	0.003512000	-0.600438000	0.023273000
6	0.002562000	-0.090040000	1.389677000
1	0.929610000	0.449070000	1.543117000
1	-0.819870000	0.606714000	1.501488000
6	2.481524000	-0.734462000	-0.220742000
6	-2.471980000	-0.727823000	-0.233831000
7	3.476120000	-1.738099000	-0.168360000
7	-3.475286000	-1.724276000	-0.227161000
6	3.137973000	-3.046055000	0.373126000
1	2.220957000	-3.407673000	-0.072840000
1	3.012677000	-3.001240000	1.458233000
1	3.943136000	-3.736822000	0.140797000
6	-3.169259000	-3.050067000	0.290627000

1	-3.936582000	-3.741558000	-0.045868000
1	-3.149209000	-3.050587000	1.383537000
1	-2.208395000	-3.379624000	-0.081235000
6	-4.781178000	-1.301247000	-0.030921000
1	-5.509408000	-2.094940000	0.015407000
6	-5.135522000	-0.012405000	0.098323000
1	-6.174031000	0.226614000	0.253813000
6	-4.143354000	1.021569000	0.057934000
6	-2.833014000	0.603524000	-0.121081000
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1	-3.885716000	4.280634000	0.632822000
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1	-5.930313000	3.783256000	-0.382208000
1	-6.342914000	2.124638000	-0.808783000
1	-5.090531000	2.974286000	-1.721766000
6	2.849591000	0.596926000	-0.137060000
1	2.061852000	1.318723000	-0.279839000
6	4.159546000	1.010444000	0.055002000
6	5.141627000	-0.029997000	0.148561000
1	6.178102000	0.205602000	0.322047000
6	4.779803000	-1.319558000	0.049896000
1	5.500714000	-2.116310000	0.137305000
7	4.560767000	2.350553000	0.194763000
6	5.574454000	2.785540000	-0.755600000
1	5.157854000	2.898396000	-1.763765000
1	6.385246000	2.067806000	-0.800524000
1	5.978766000	3.742284000	-0.434011000
6	3.491240000	3.316773000	0.288309000
1	3.919052000	4.288061000	0.522002000
1	2.808060000	3.036722000	1.085621000
1	2.923498000	3.409974000	-0.647059000
6	-0.121955000	-1.220874000	2.398589000
1	0.696056000	-1.926597000	2.270912000
1	-1.062592000	-1.747572000	2.257890000
1	-0.090593000	-0.830377000	3.413158000

E = -1130.9219956

Optimised geometry (M05-2X/cc-pVTZ) of the lowest excited triplet state of donor **26**, in DMF

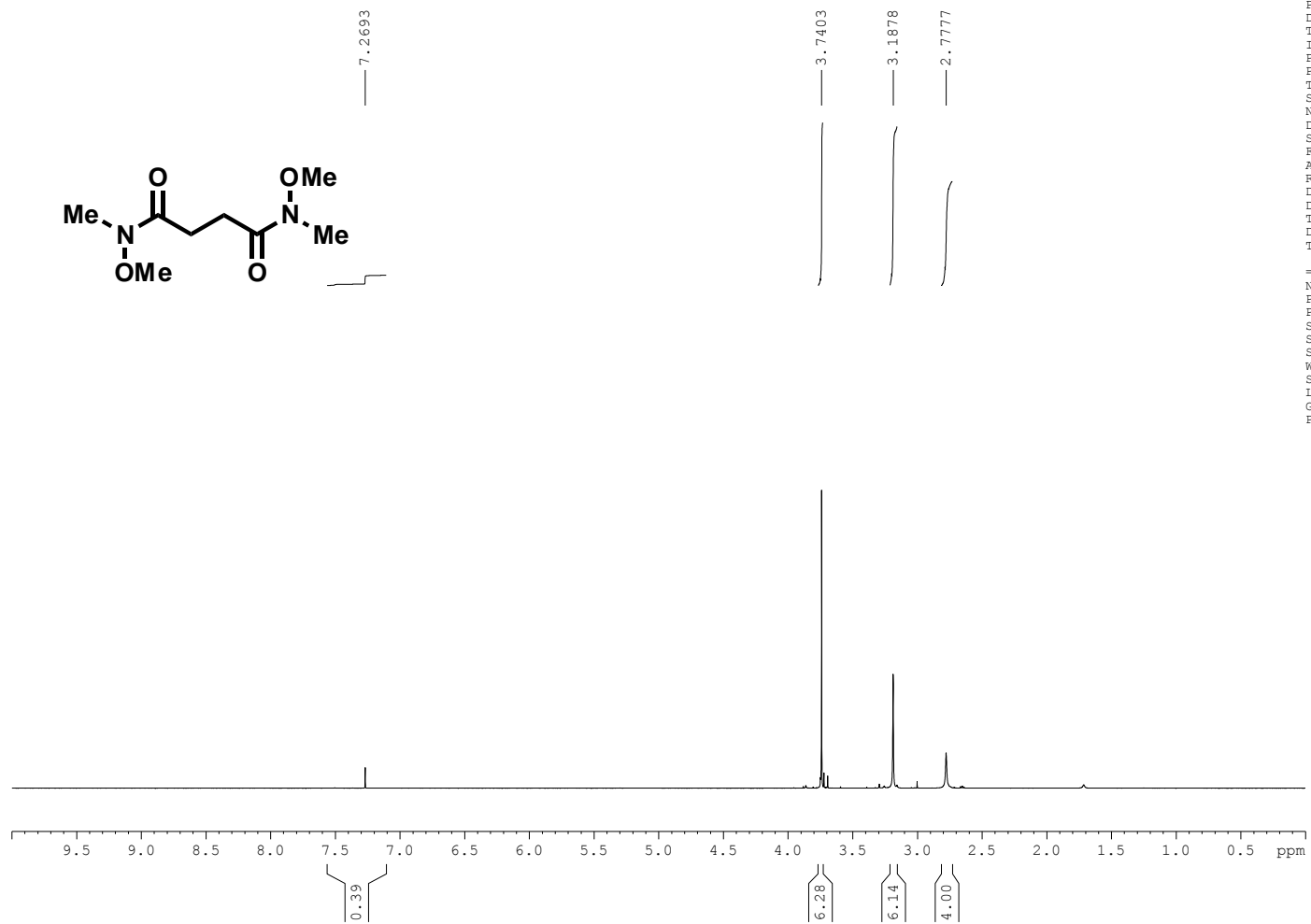
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1	2.972752000	-3.019157000	1.413486000
1	3.988111000	-3.723430000	0.143193000
6	-3.160285000	-3.059512000	0.309671000
1	-3.987679000	-3.723795000	0.082350000
1	-3.011547000	-3.035959000	1.391150000
1	-2.263329000	-3.437710000	-0.161128000
6	-4.781728000	-1.309811000	-0.002447000
1	-5.507954000	-2.103974000	0.061182000
6	-5.141943000	-0.019616000	0.105964000
1	-6.182460000	0.213309000	0.256248000
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7	4.554565000	2.352509000	0.212464000
6	5.594601000	2.797663000	-0.708780000
1	5.205981000	2.898229000	-1.728682000
1	6.420504000	2.096524000	-0.722252000
1	5.968837000	3.763740000	-0.381287000
6	3.477265000	3.317812000	0.276288000
1	3.897949000	4.291467000	0.510030000
1	2.775527000	3.043539000	1.059227000
1	2.932371000	3.399048000	-0.672484000

6	-0.071641000	-1.177841000	2.414643000
1	0.772526000	-1.854190000	2.297467000
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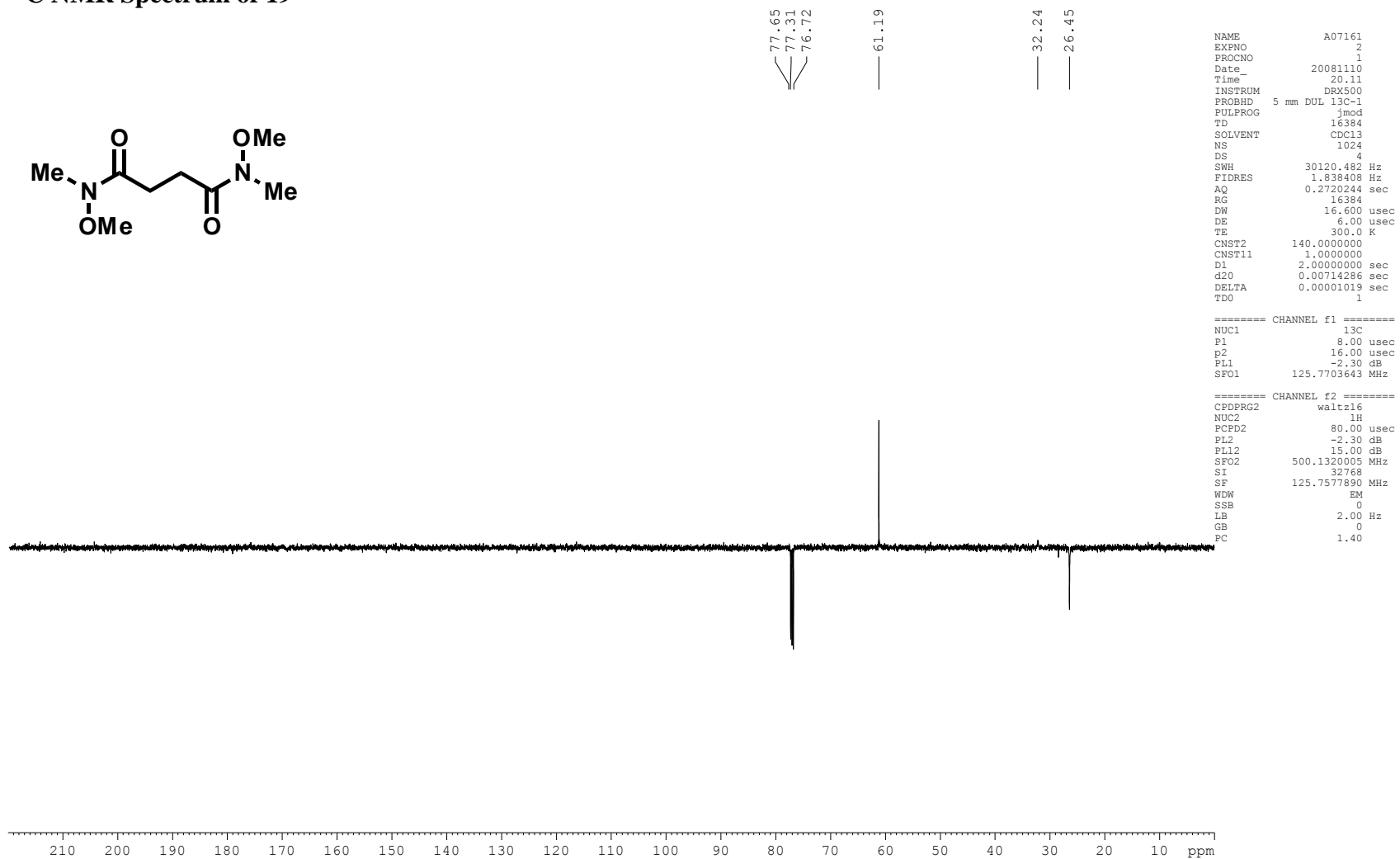
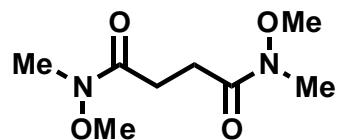
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¹H NMR Spectrum of 19

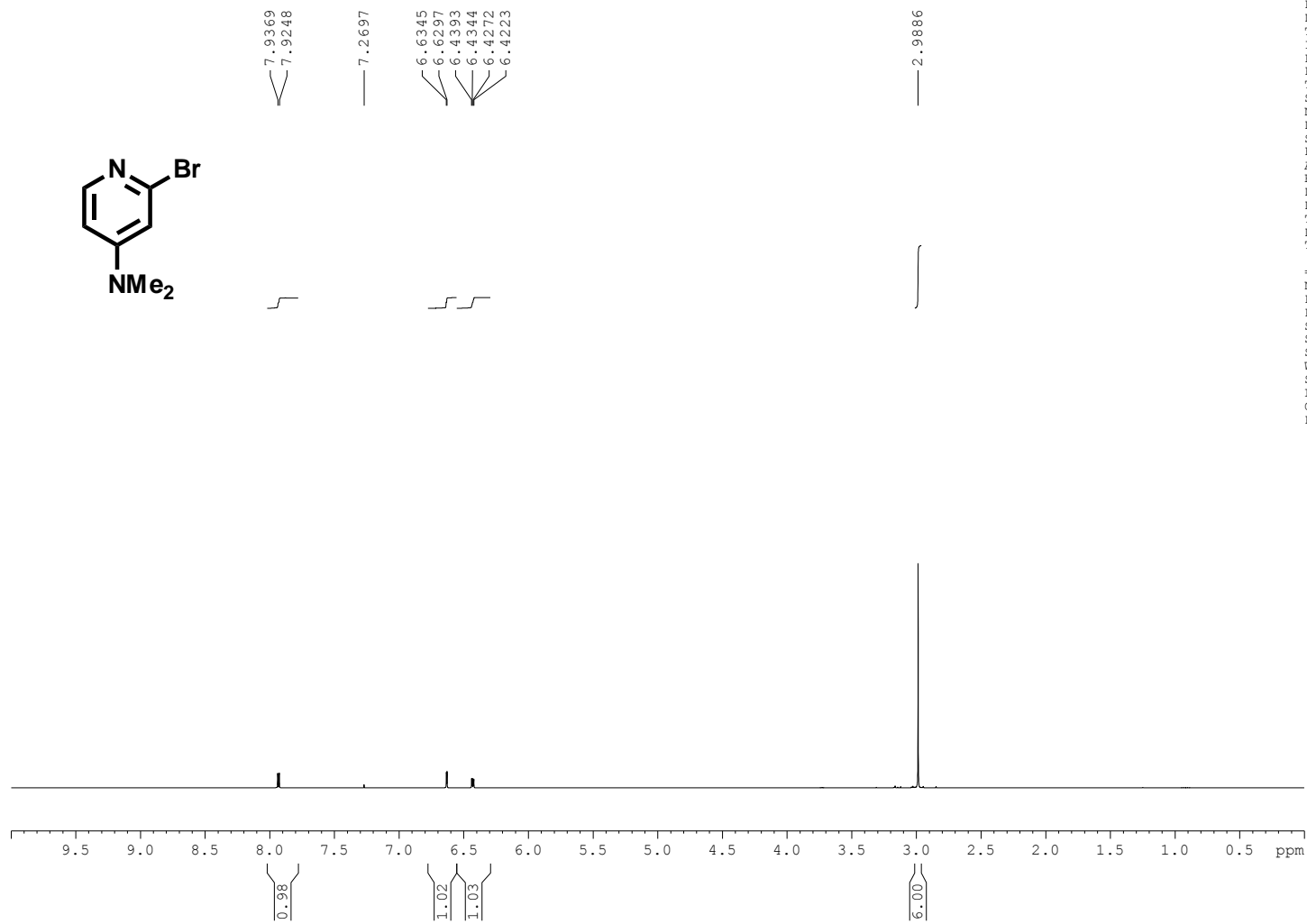


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SOLVENT      CDCl3
NS           16
DS           2
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FIDRES       0.156983 Hz
AQ           3.1850996 sec
RG           203.2
DW           48.600 usec
DE           6.00 usec
TE           300.0 K
D1           1.00000000 sec
TD0          1
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NUC1         1H
P1           12.00 usec
PL1         -2.70 dB
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WDW          EM
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¹³C NMR Spectrum of 19



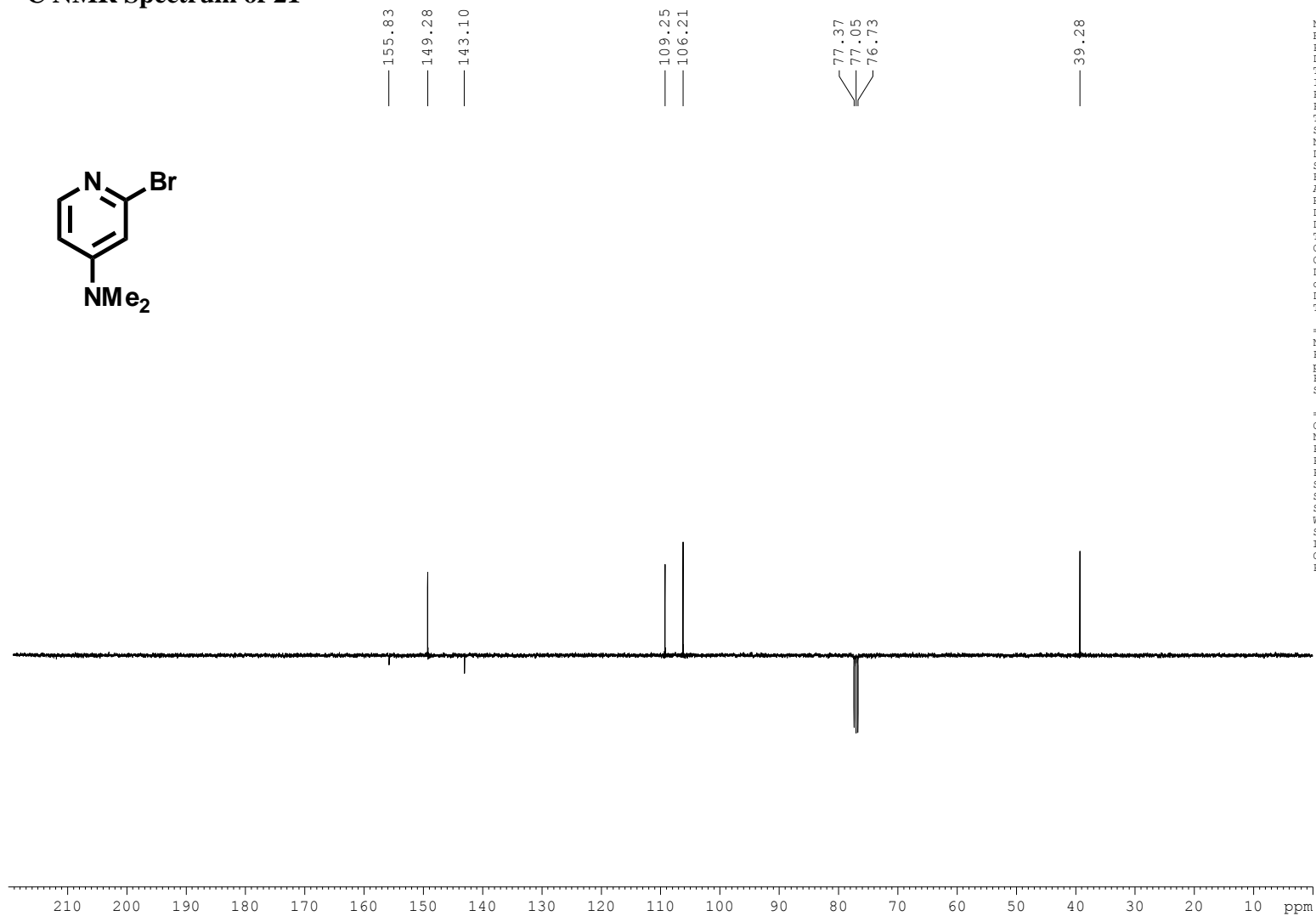
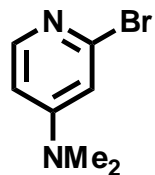
¹H NMR Spectrum of 21



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TD            65536
SOLVENT       CDCl3
NS            16
DS            2
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AQ            3.1850996 sec
RG            161.3
DW            48.600 usec
DE            6.00 usec
TE            300.0 K
D1            1.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          1H
P1            12.00 usec
PL1          -2.70 dB
SF01         500.1330885 MHz
SI           32768
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WDW           EM
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¹³C NMR Spectrum of 21

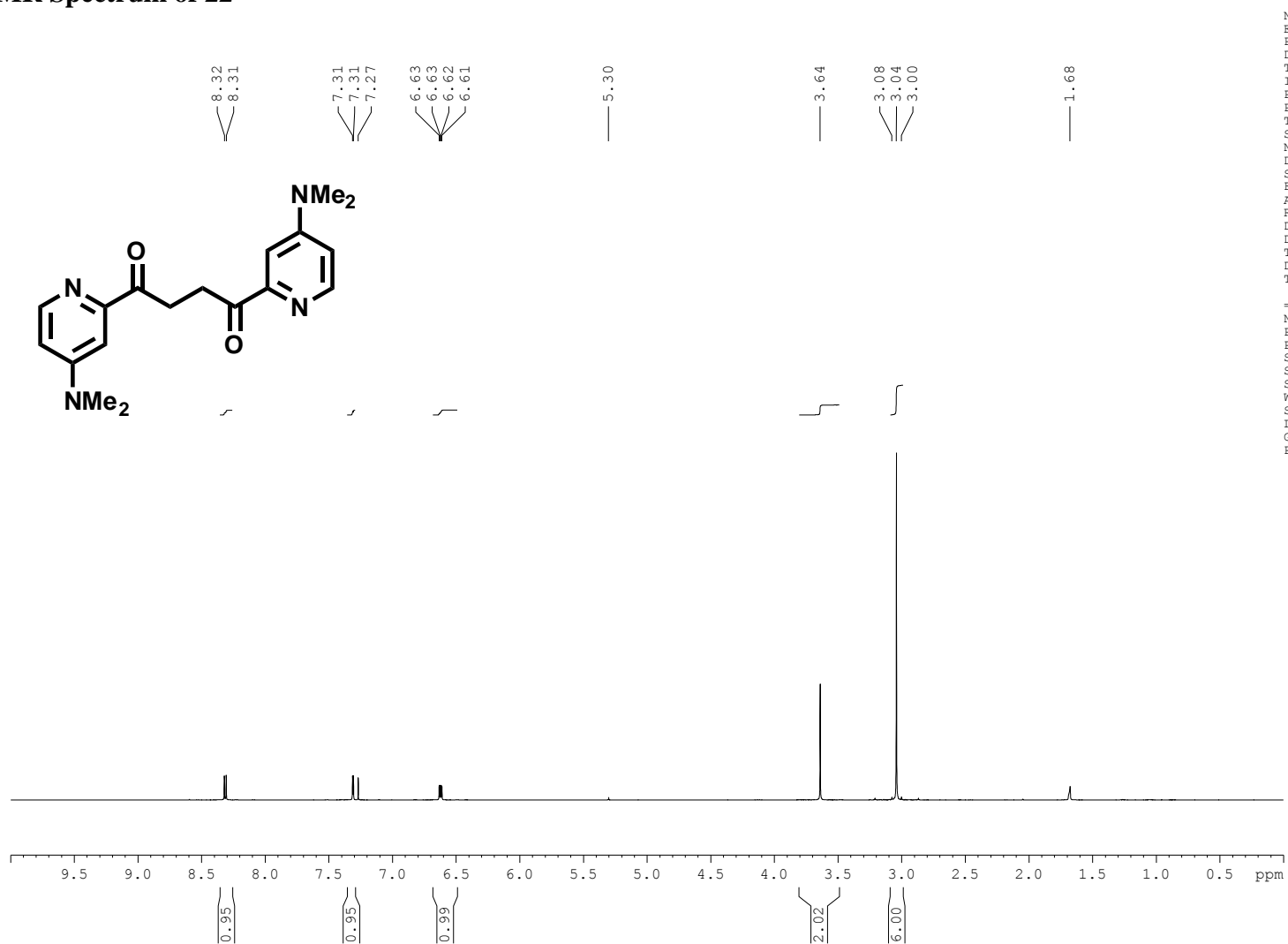


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TD            16384
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NS            512
DS            4
SWH           23980.814 Hz
FIDRES        1.463673 Hz
AQ            0.3416564 sec
RG            16384
DW            20.850 usec
DE            6.00 usec
TE            296.2 K
CNST2         145.000000
CNST11        1.0000000
D1            4.0000000 sec
d20           0.00689655 sec
DELTA         0.00001019 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.00 usec
P2            16.00 usec
PL1           -2.60 dB
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          17.00 dB
SFO2          400.1316005 MHz
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WDW           EM
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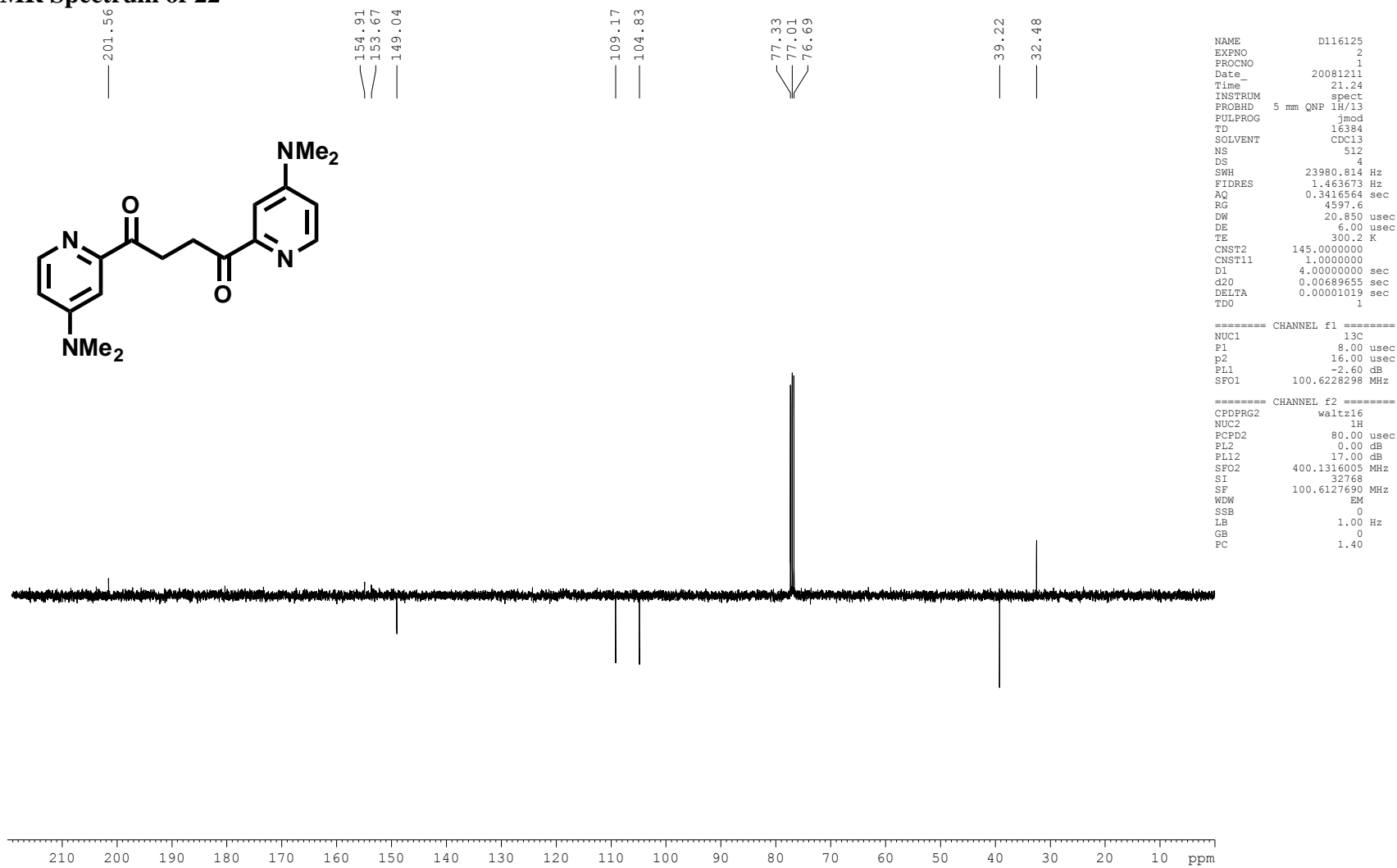
¹H NMR Spectrum of 22



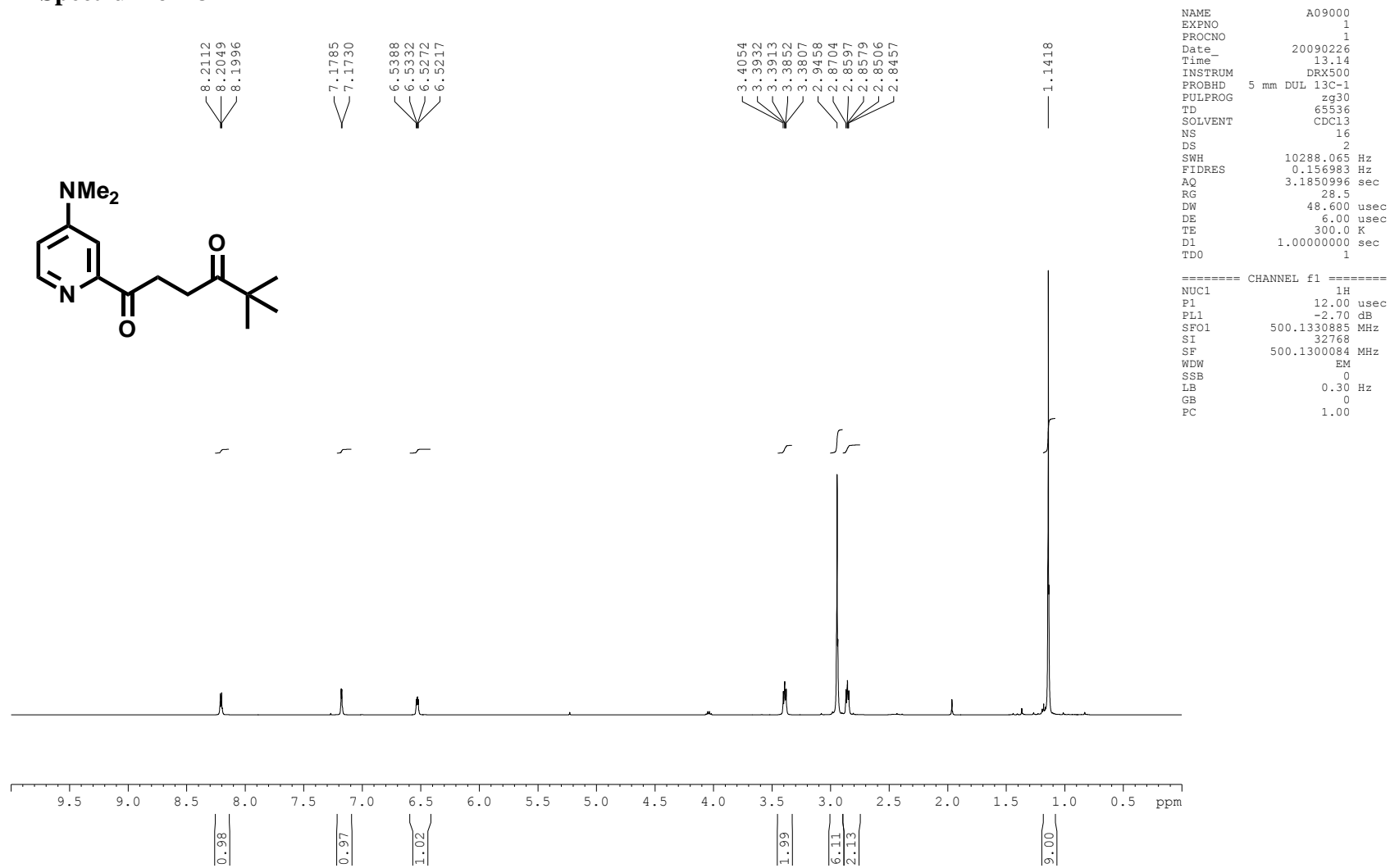
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TD            32768
SOLVENT       CDCl3
NS            16
DS            2
SWH           8278.146 Hz
FIDRES        0.252629 Hz
AQ            1.9792372 sec
RG            456.1
DW            60.400 usec
DE            6.00 usec
TE            300.2 K
D1            2.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            12.00 usec
PL1           1.10 dB
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SI            32768
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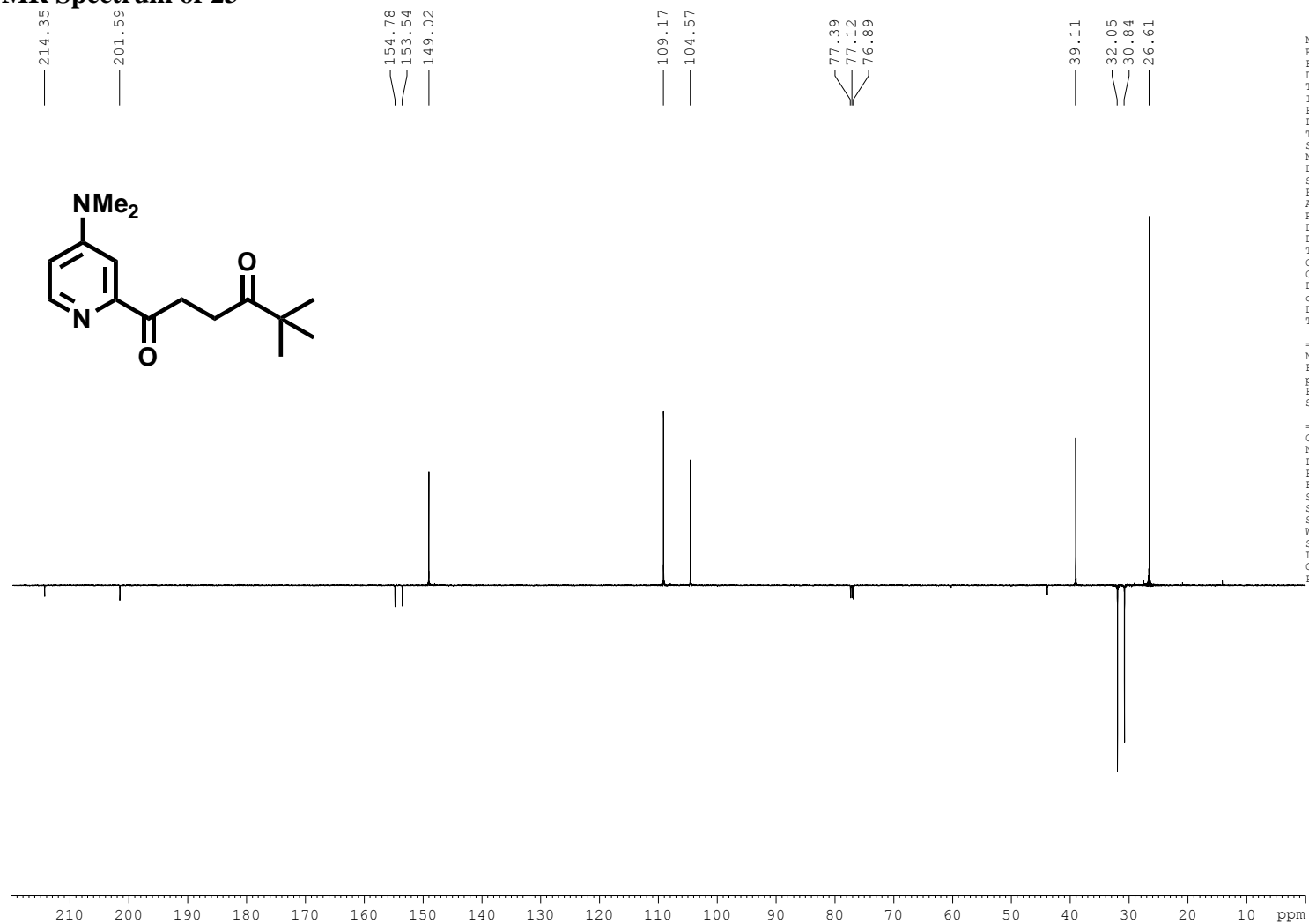
¹³C NMR Spectrum of 22



¹H NMR Spectrum of 23



¹³C NMR Spectrum of 23

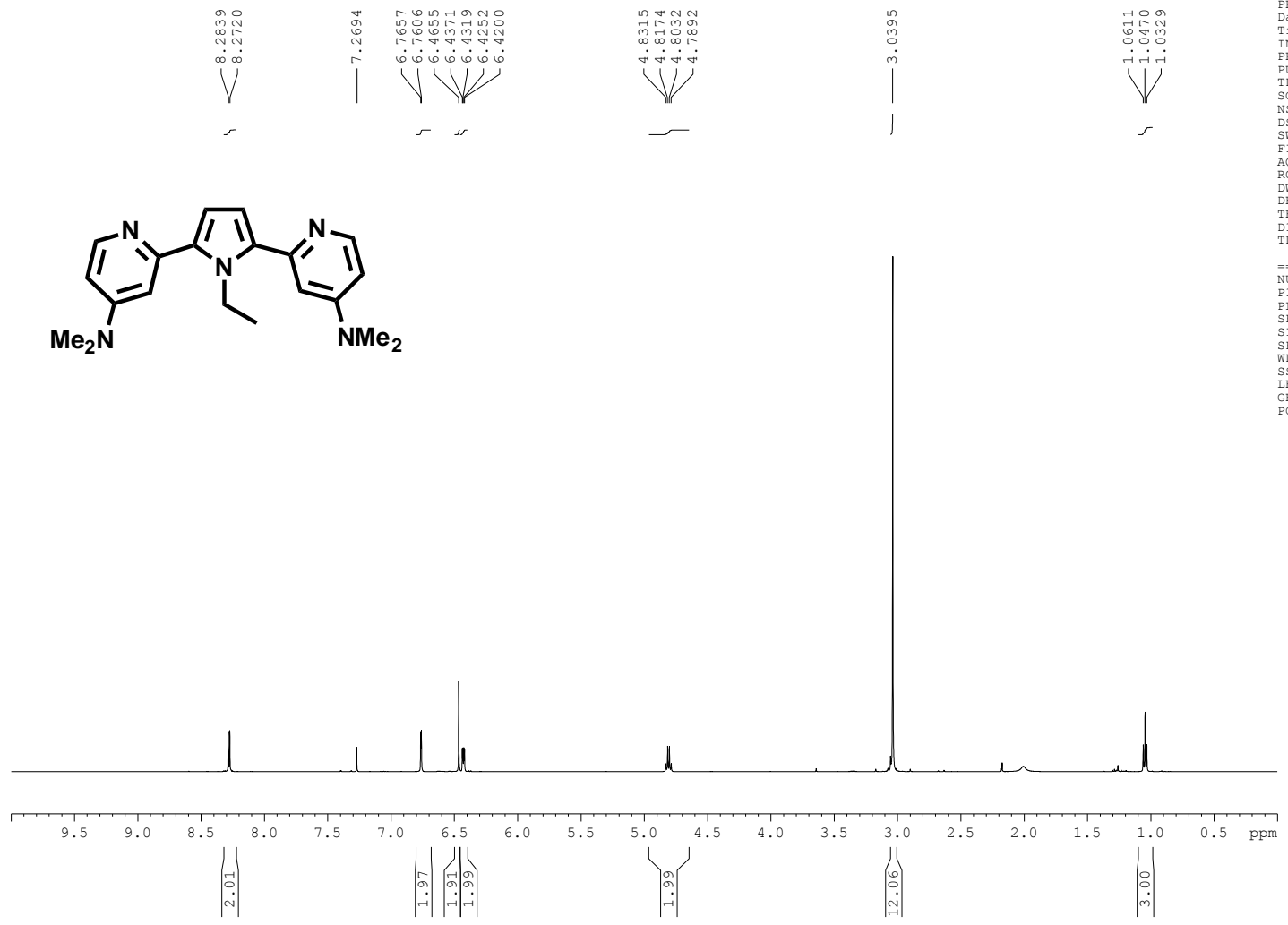


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PULPROG       jmod
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           30120.482 Hz
FIDRES        1.838408 Hz
AQ            0.2720244 sec
RG            16384
DW            16.600 usec
DE            6.00 usec
TE            300.0 K
CNST2         140.0000000
CNST11        1.0000000
DI            2.00000000 sec
d20           0.00714286 sec
DELTA         0.00001019 sec
TDO           1

===== CHANNEL f1 =====
NUC1           13C
P1             8.00 usec
p2            16.00 usec
PL1           -2.30 dB
SFO1          125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL2           -2.30 dB
PL12          15.00 dB
SFO2          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.40
```

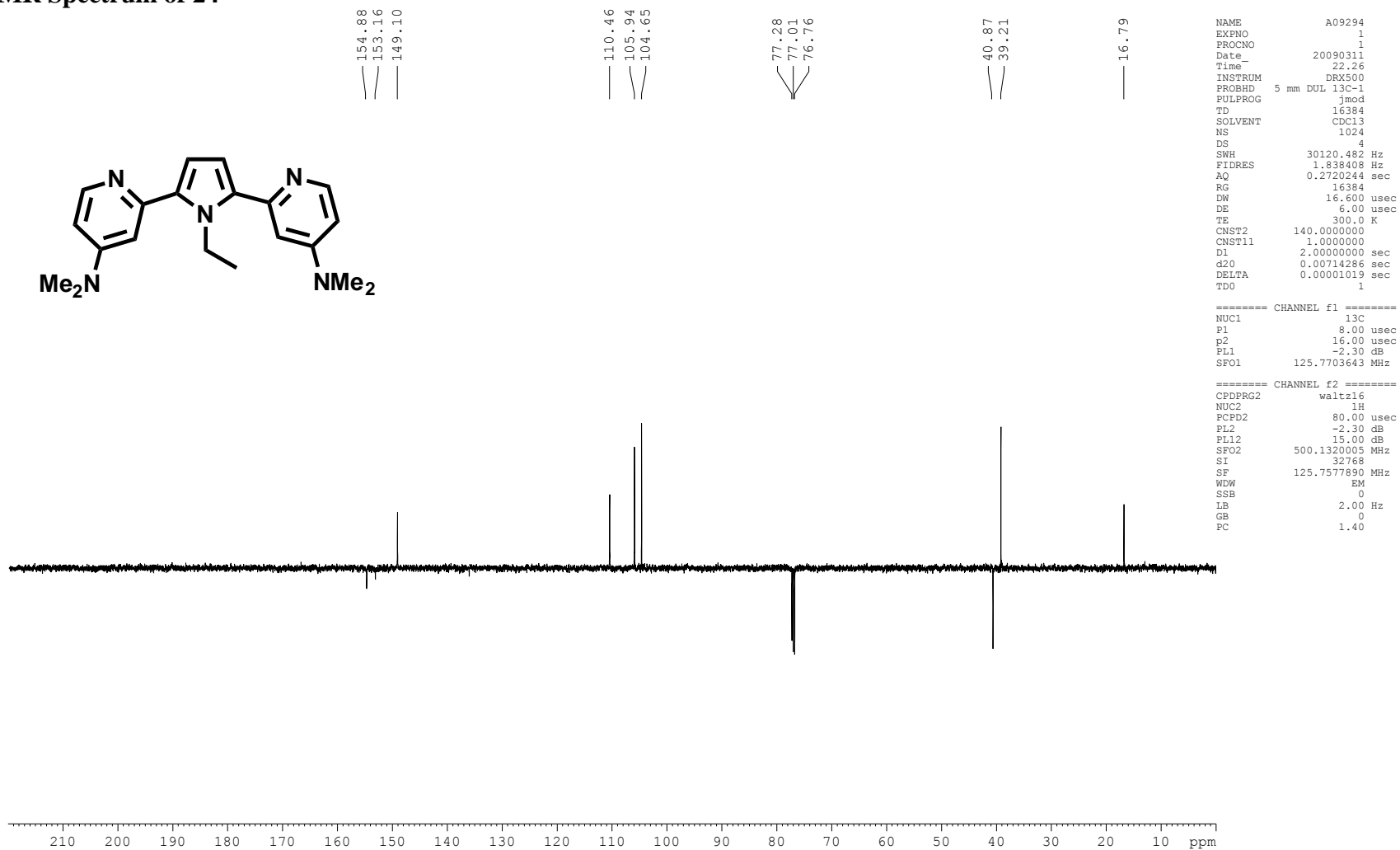
¹H NMR Spectrum of 24



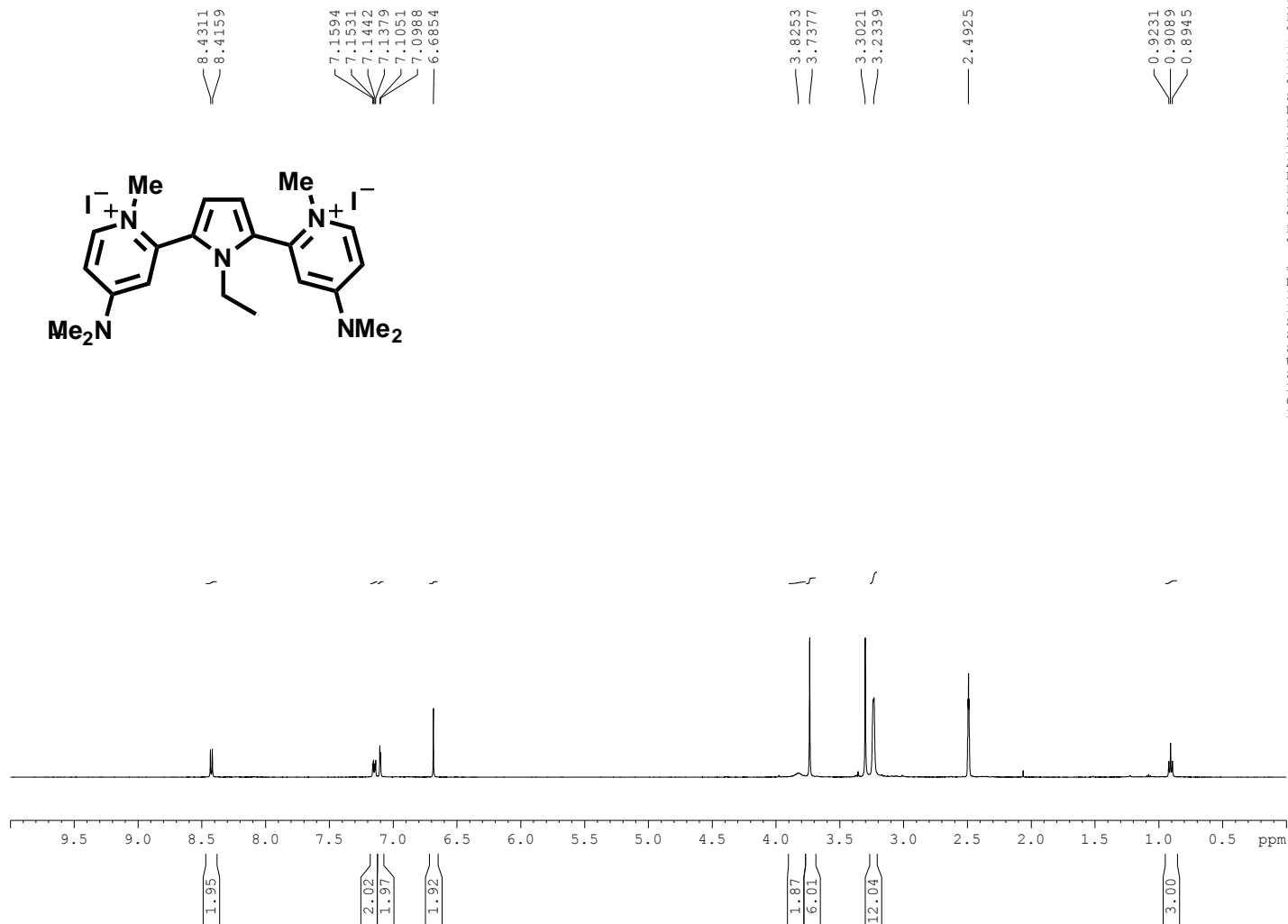
```
NAME           A11548
EXPNO          1
PROCNO         1
Date_          20090729
Time           16.52
INSTRUM        DRX500
PROBHD         5 mm DUL 13C-1
PULPROG        zg30
TD              65536
SOLVENT        CDCl3
NS              16
DS              2
SWH            10288.065 Hz
FIDRES         0.156983 Hz
AQ             3.1850996 sec
RG             322.5
DW             48.600 usec
DE             6.00 usec
TE             300.0 K
D1             1.00000000 sec
TDO            1

===== CHANNEL f1 =====
NUC1           1H
P1             12.00 usec
PL1           -2.70 dB
SFO1          500.1330885 MHz
SI            32768
SF            500.1300084 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

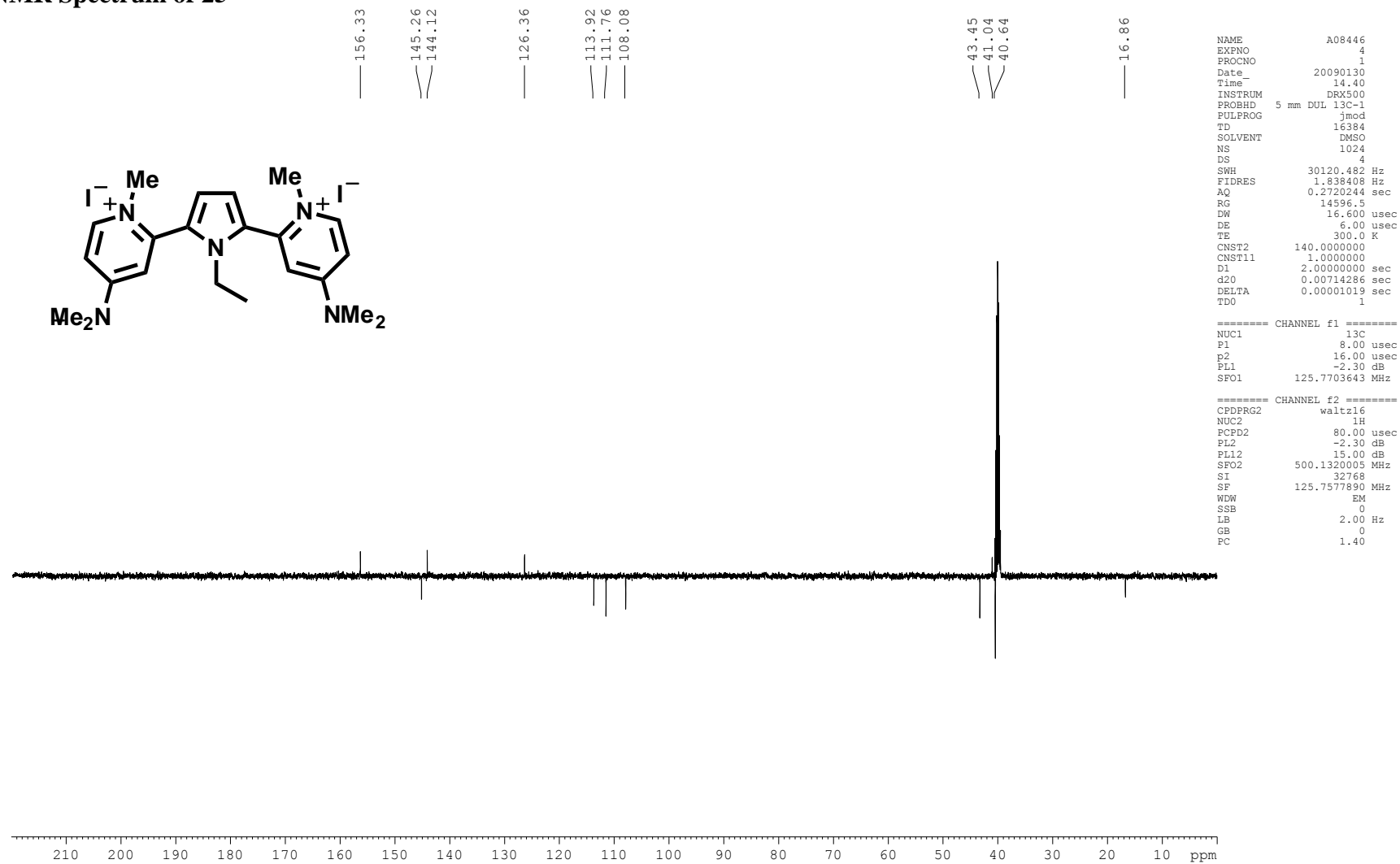

¹³C NMR Spectrum of 24



¹H NMR Spectrum of 25

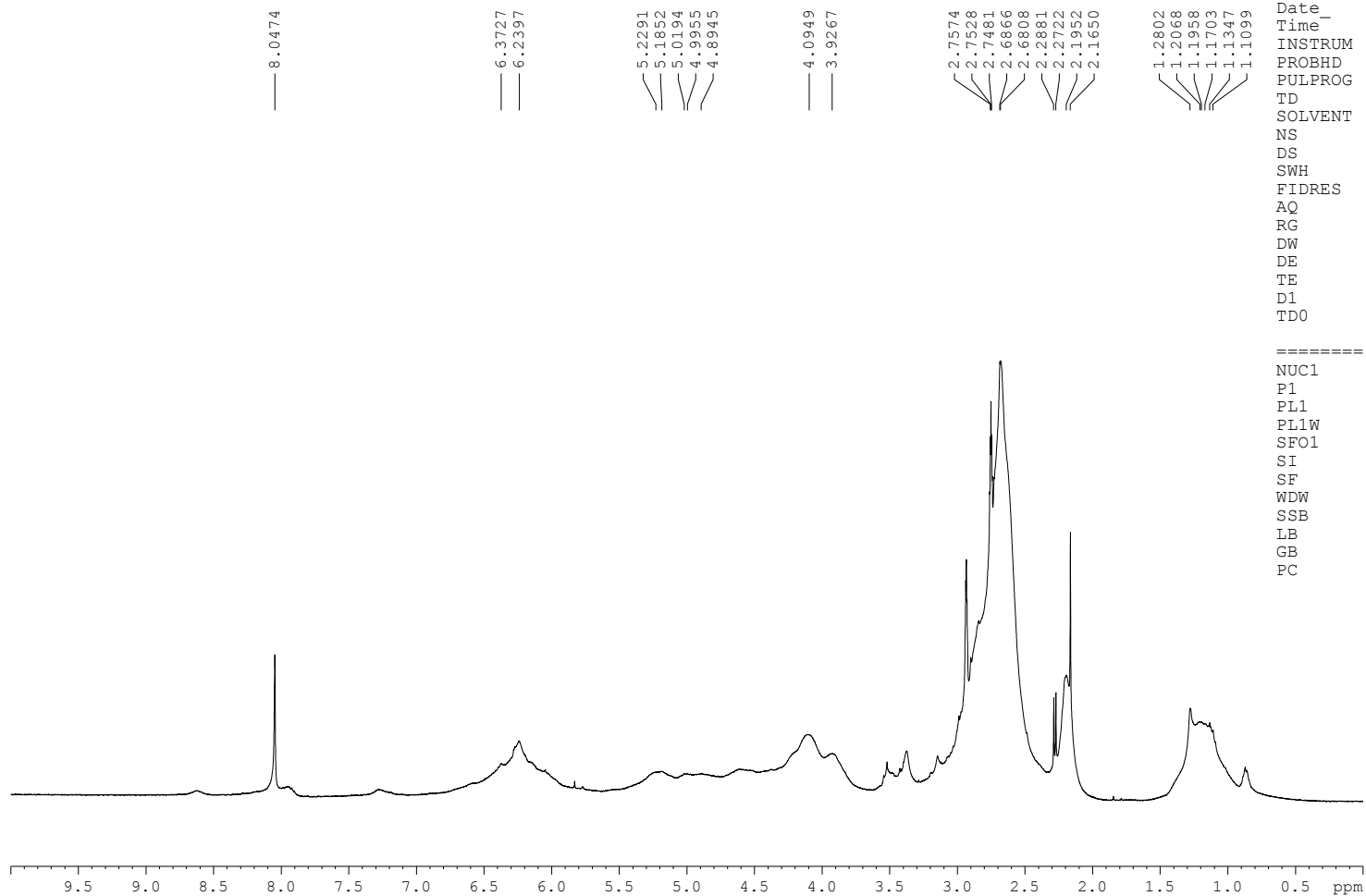


¹³C NMR Spectrum of 25



The broad NMR spectrum obtained for donor 26 in d₇-DMF.

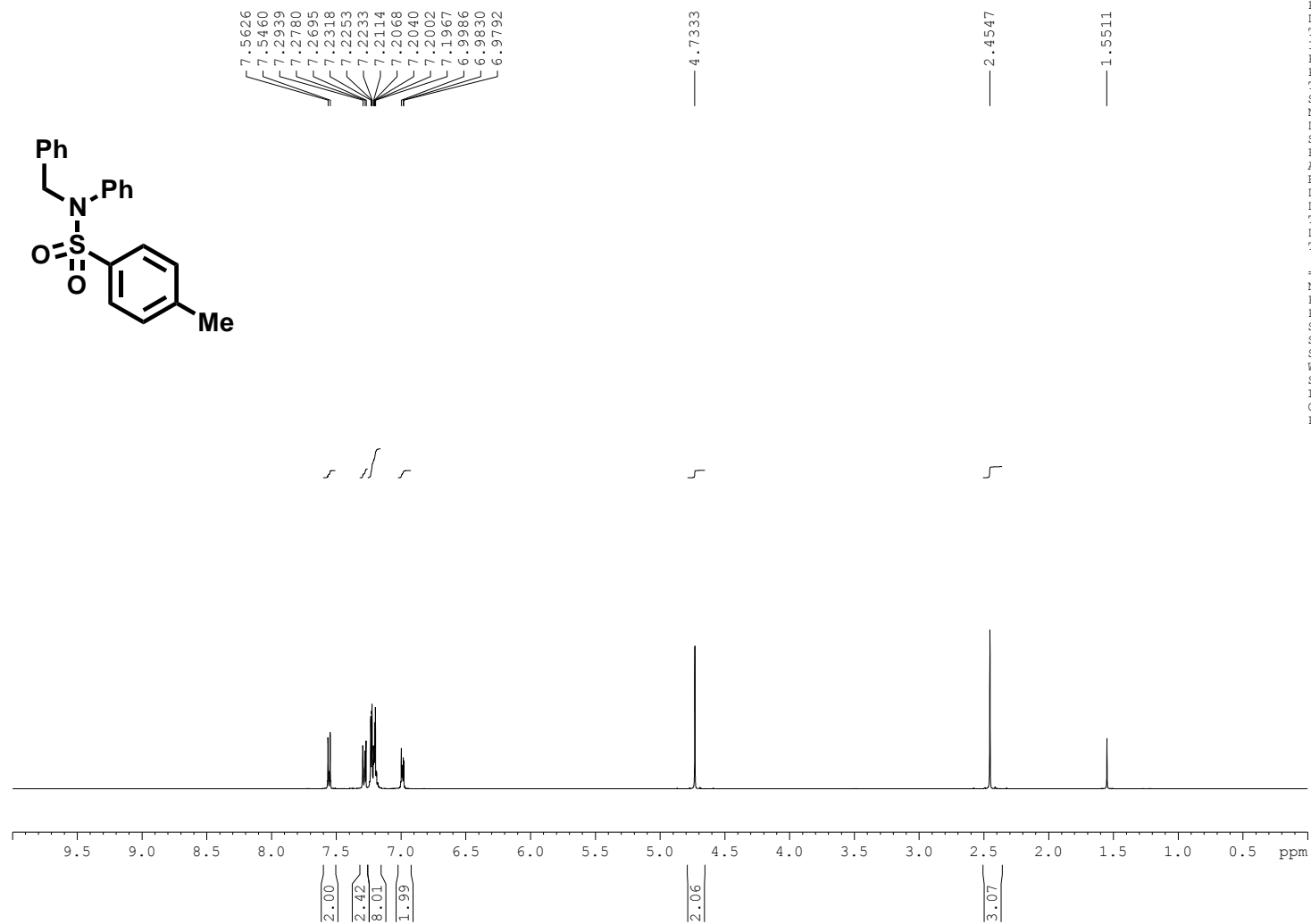
HF279 Pyrroldiylidene Donor



```
NAME          D140710
EXPNO         1
PROCNO        1
Date_         20110129
Time_         9.43
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            32564
SOLVENT       DMF
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.252539 Hz
AQ            1.9799412 sec
RG            101
DW            60.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
TD0           1
```

```
===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1           -4.00 dB
PL1W         19.93825150 W
SFO1         400.1324710 MHz
SI            32768
SF           400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

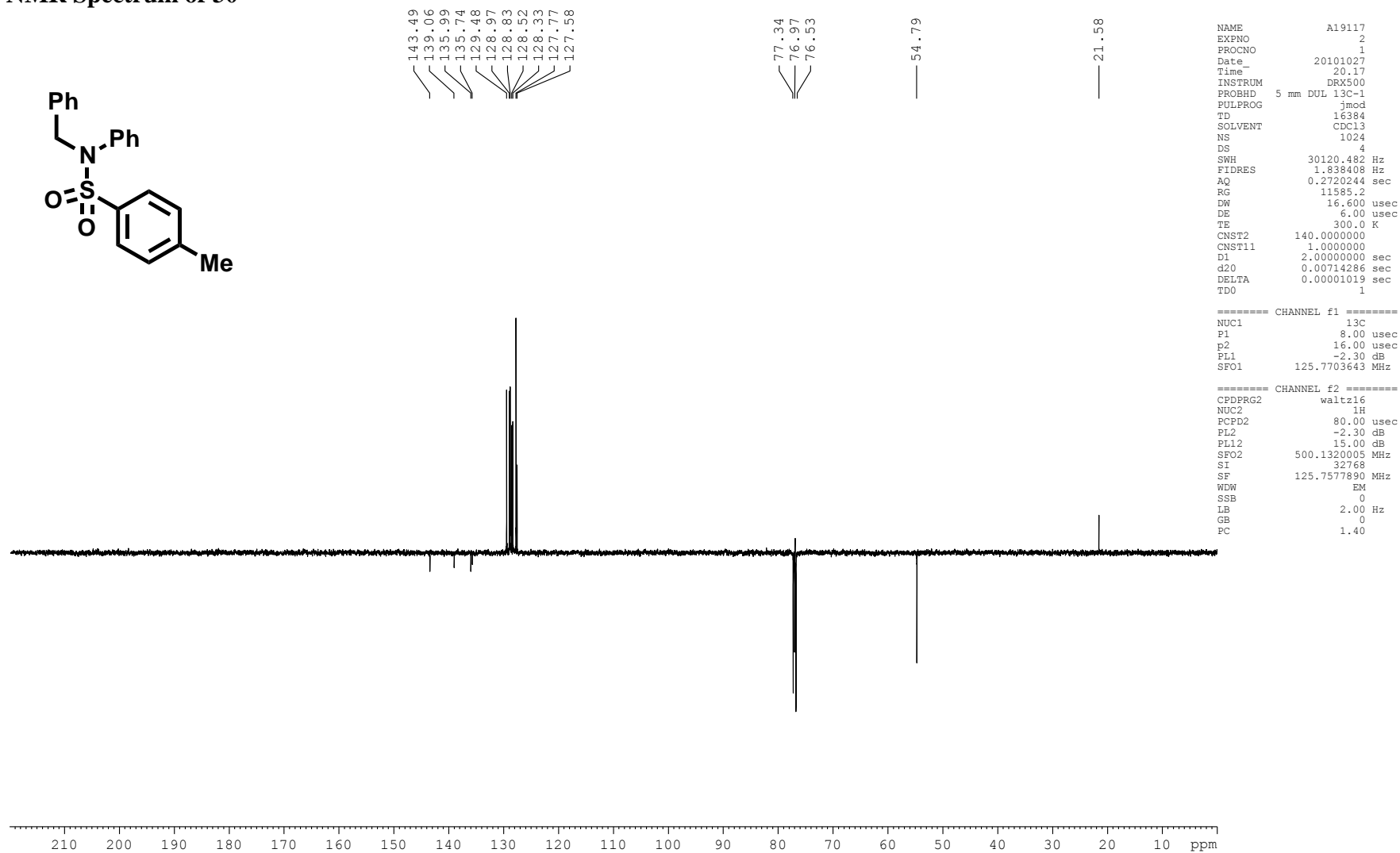
¹H NMR Spectrum of 30



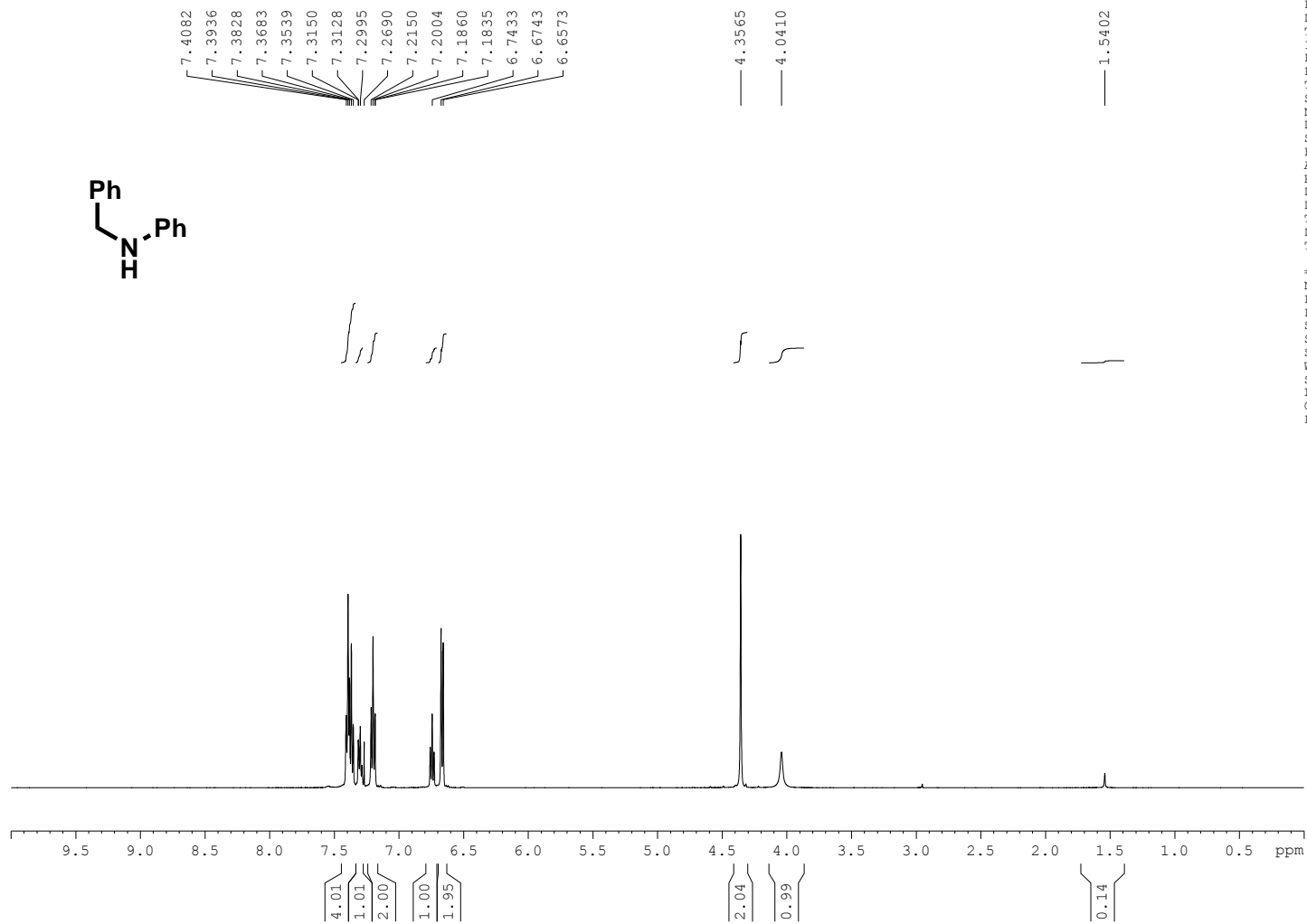
```
NAME           A19117
EXPNO          1
PROCNO         1
Date_          20101027
Time           19.36
INSTRUM       DRX500
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10288.065 Hz
FIDRES        0.156983 Hz
AQ            3.1850996 sec
RG            512
DW            48.600 usec
DE            6.00 usec
TE            300.0 K
D1            1.0000000 sec
TDO           1
```

```
===== CHANNEL f1 =====
NUC1           1H
P1             12.00 usec
PL1            -2.70 dB
SFO1          500.1330885 MHz
SI            32768
SF            500.1300084 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB            0
PC            1.00
```

¹³C NMR Spectrum of 30

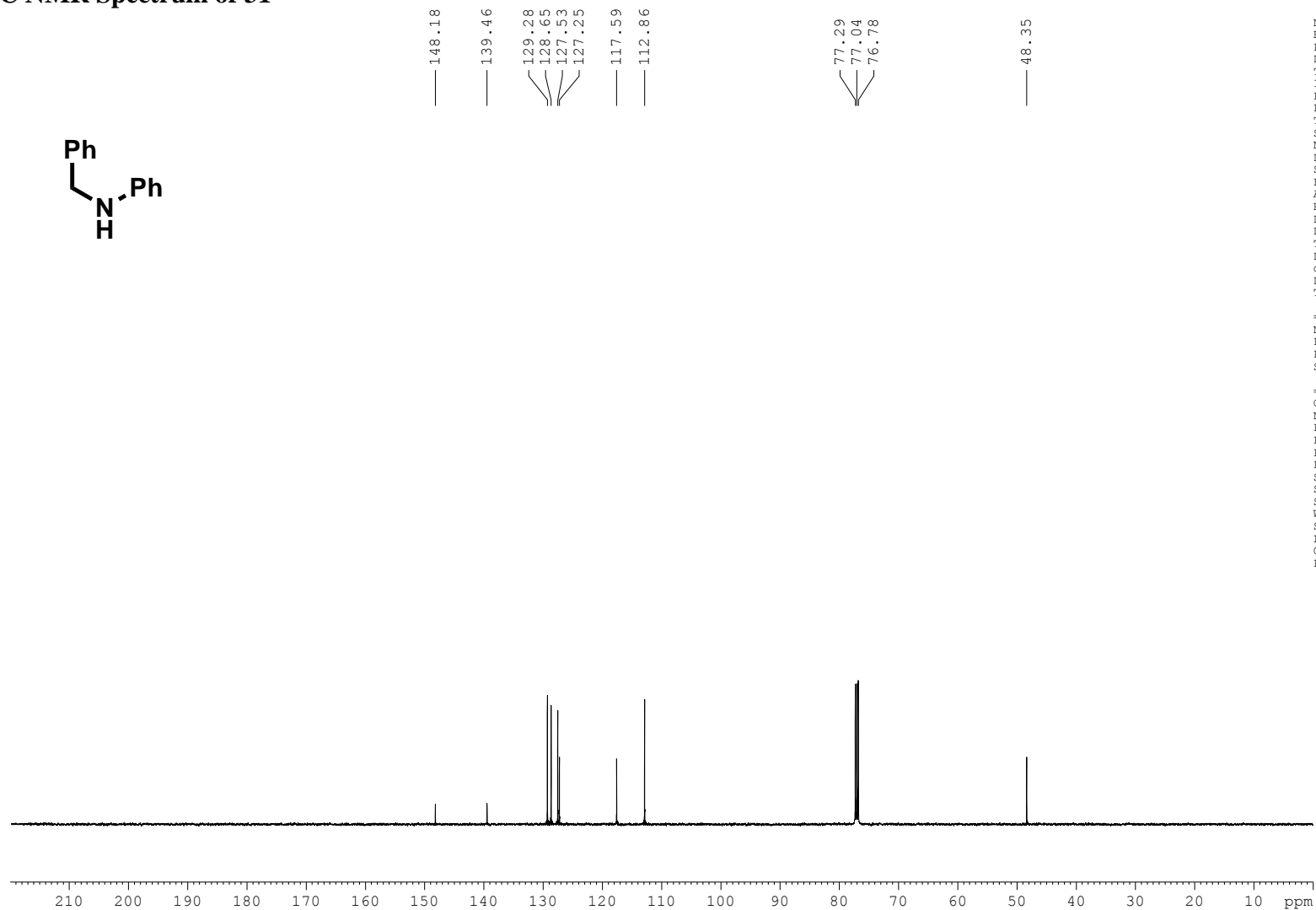
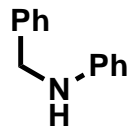


¹H NMR Spectrum of 31



```
NAME          A19116
EXPNO         1
PROCNO       1
Date_        20101027
Time_        19.08
INSTRUM      DRX500
PROBHD       5 mm DUL 13C-1
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           16
DS           2
SWH          10288.065 Hz
FIDRES       0.156983 Hz
AQ           3.1850996 sec
RG           322.5
RG           322.5
DW           48.600 usec
DE           6.00 usec
TE           300.0 K
D1           1.00000000 sec
TDO          1
===== CHANNEL f1 =====
NUC1          1H
P1           12.00 usec
PL1          -2.70 dB
SFO1         500.1330885 MHz
SI           32768
SF           500.1300084 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
```

¹³C NMR Spectrum of 31

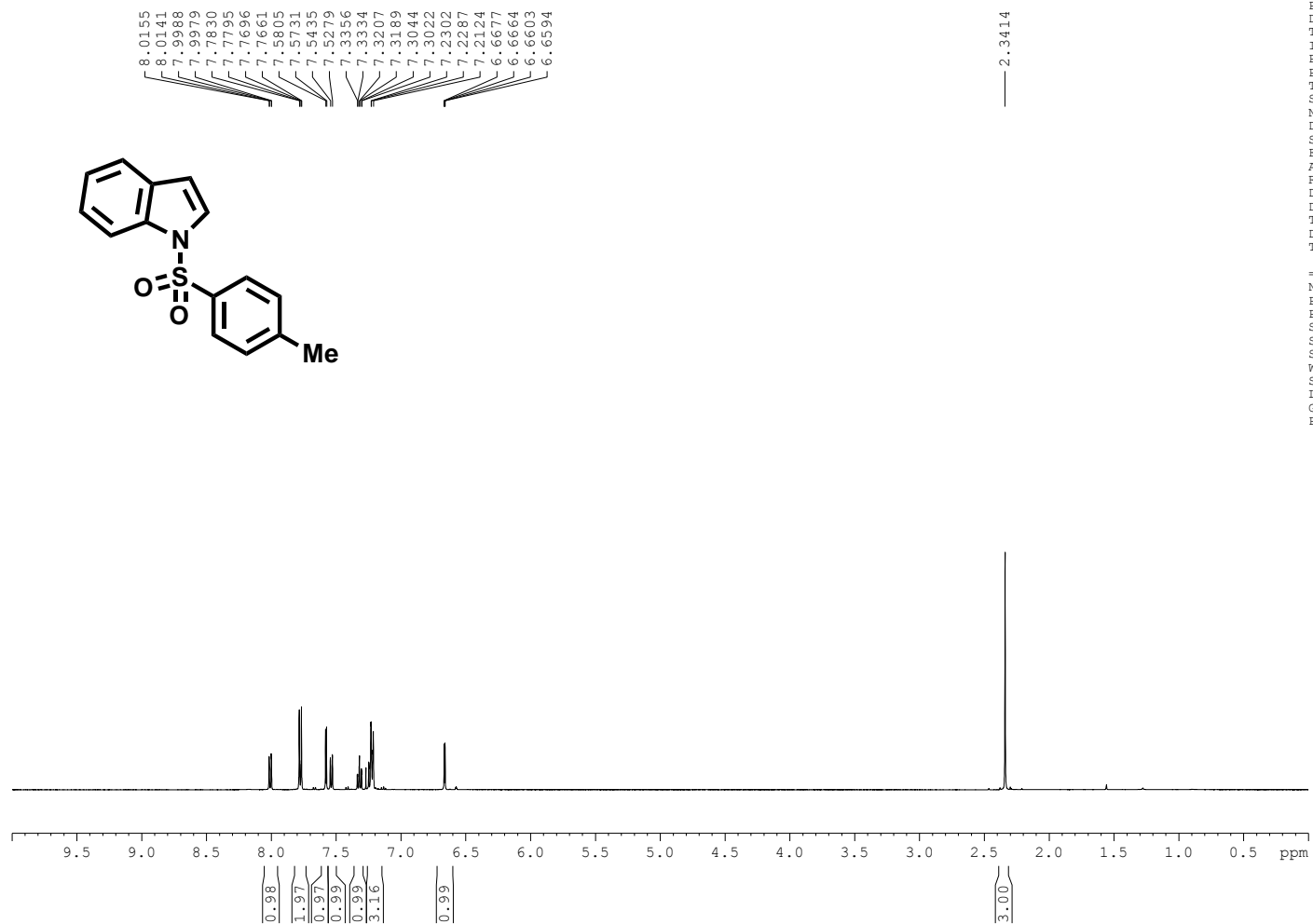


```
NAME           A19116
EXPNO           2
PROCNO          1
Date_           20101027
Time            19.27
INSTRUM         DRX500
PROBHD          5 mm DUL 13C-1
PULPROG         zgpg30
TD              16384
SOLVENT         CDCl3
NS              1024
DS              4
SWH             30120.482 Hz
FIDRES          1.838408 Hz
AQ              0.2720244 sec
RG              7298.2
DW              16.600 usec
DE              6.00 usec
TE              300.0 K
D1              0.69999999 sec
d11             0.03000000 sec
DELTA           0.59999996 sec
TD0             1
```

```
===== CHANNEL f1 =====
NUC1            13C
P1              8.00 usec
PL1             -2.30 dB
SFO1            125.7703643 MHz
```

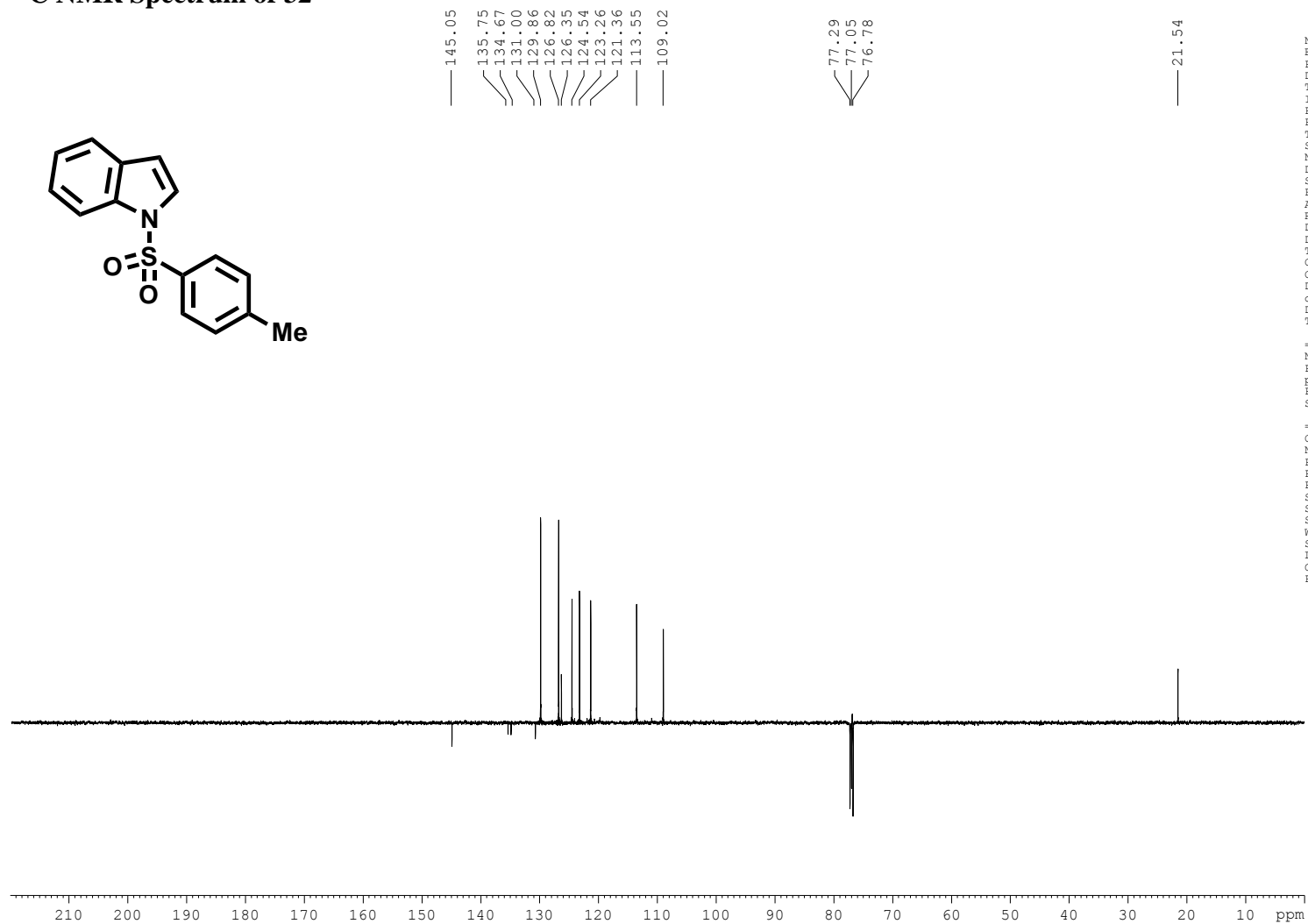
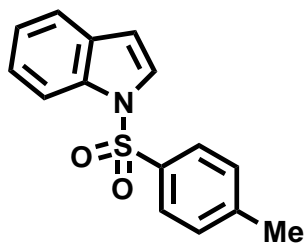
```
===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2            1H
PCPD2          80.00 usec
PL2            -2.30 dB
PL12           15.00 dB
PL13           120.00 dB
SFO2            500.1320005 MHz
SI              32768
SF              125.7577890 MHz
WDW            EM
SSB            0
LB              2.00 Hz
GB              0
PC              1.40
```


¹H NMR Spectrum of 32



```
NAME          A19119
EXPNO         1
PROCNO        1
Date_         20101027
Time_         20.53
INSTRUM       DRX500
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10288.065 Hz
FIDRES        0.156983 Hz
AQ            3.1850996 sec
RG            322.5
DW            48.600 usec
DE            6.00 usec
TE            300.0 K
D1            1.0000000 sec
TD0           1
===== CHANNEL f1 =====
NUC1          1H
P1            12.00 usec
PL1           -2.70 dB
SFO1          500.1330885 MHz
SI            32768
SF            500.1300084 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

¹³C NMR Spectrum of 32



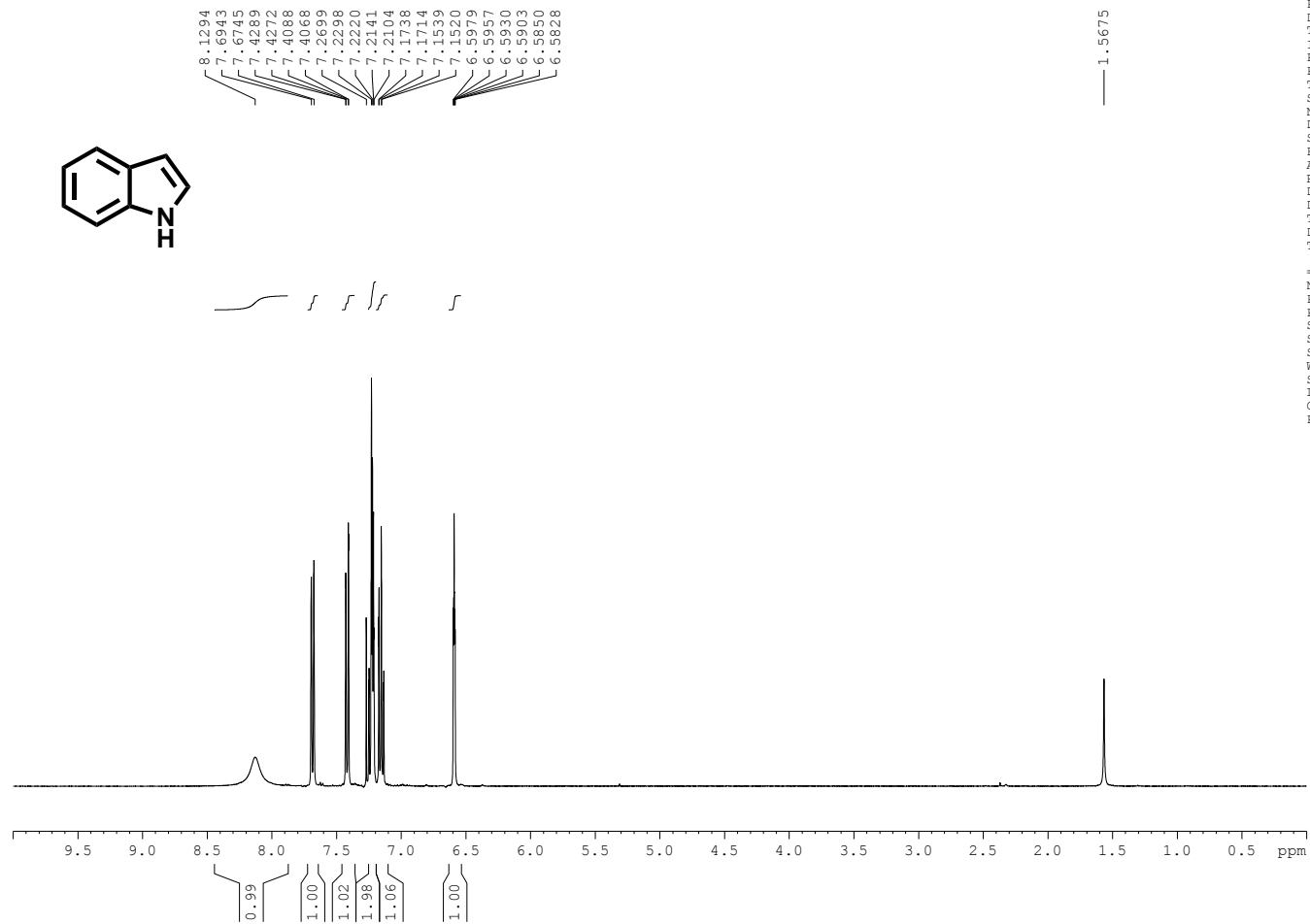
```
NAME          A19119
EXPNO         2
PROCNO        1
Date_         20101027
Time_         21.33
INSTRUM       DRX500
PROBHD        5 mm DUL 13C-1
PULPROG       jmod
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           30120.482 Hz
FIDRES        1.838408 Hz
AQ            0.2720244 sec
RG            13004
DW            16.600 usec
DE            6.00 usec
TE            300.0 K
CNST2         140.0000000
CNST11        1.0000000
D1            2.00000000 sec
d20           0.00714286 sec
DELTA         0.00001019 sec
TD0           1

===== CHANNEL f1 =====
NUC1           13C
P1             8.00 usec
p2            16.00 usec
PL1           -2.30 dB
SF01          125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL2           -2.30 dB
PL12          15.00 dB
SFO2          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.40
```

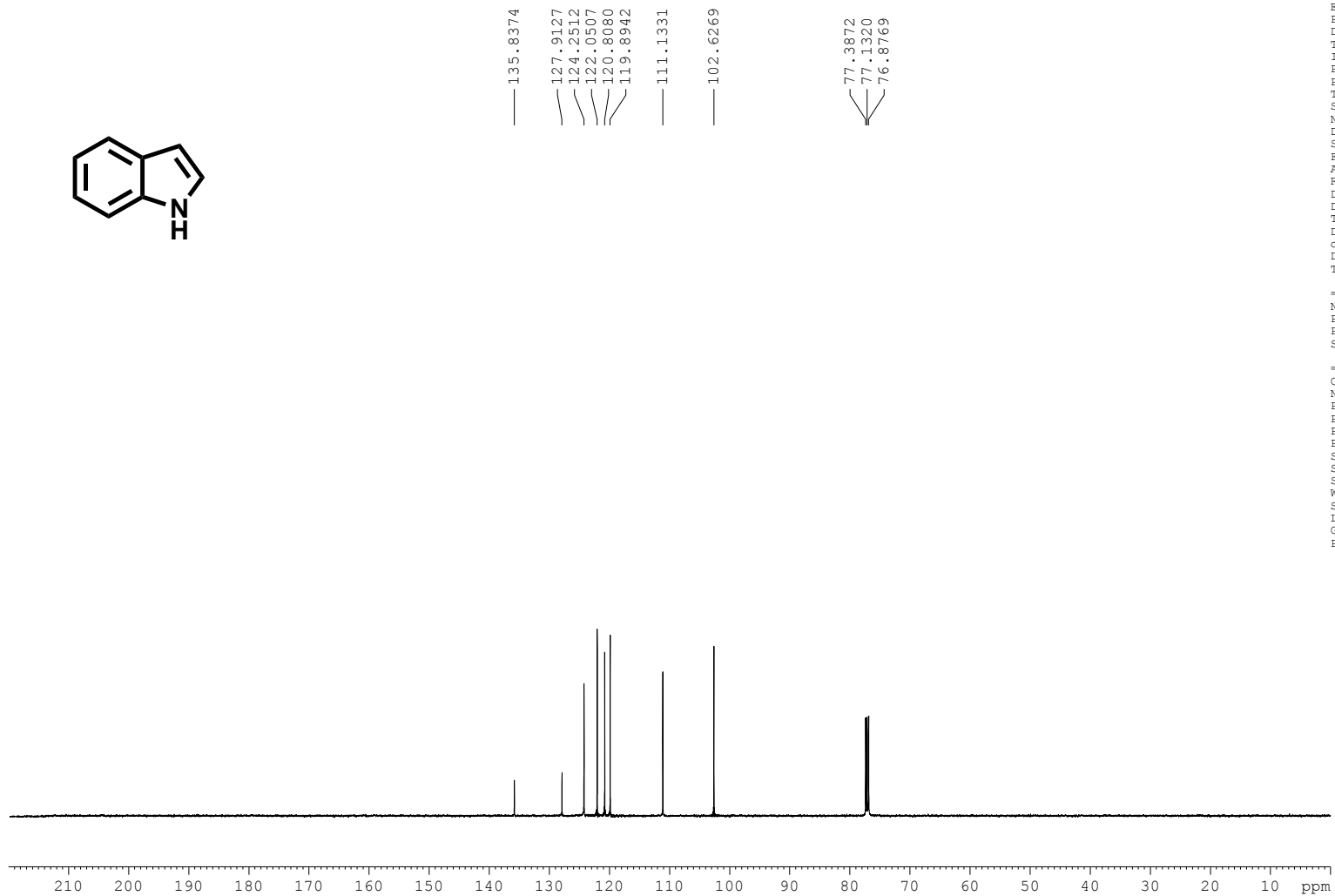
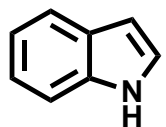
¹H NMR Spectrum of 33

HF84 PROD



```
NAME          D121803
EXPNO         1
PROCNO       1
Date_         20090623
Time         12.10
INSTRUM      spect
PROBHD       5 mm QNP 1H/13
PULPROG      zg30
TD           32768
SOLVENT      CDCl3
NS           16
DS           2
SWH          8278.146 Hz
FIDRES       0.252629 Hz
AQ           1.9792372 sec
RG           382
DW           60.400 usec
DE           6.00 usec
TE           298.2 K
D1           2.0000000 sec
TD0          1
===== CHANNEL f1 =====
NUC1         1H
P1           12.00 usec
PL1          1.10 dB
SFO1         400.1324710 MHz
SI           32768
SF           400.1300053 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           4.00
```

¹³C NMR Spectrum of 33



```
NAME          A19118
EXPNO         2
PROCNO        1
Date_         20101027
Time         20.44
INSTRUM       DRX500
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           30120.482 Hz
FIDRES        1.838408 Hz
AQ            0.2720244 sec
RG            5792.6
DW            16.600 usec
DE            6.00 usec
TE            300.0 K
D1            0.69999999 sec
d11           0.03000000 sec
DELTA         0.59999996 sec
TD0           1
```

```
===== CHANNEL f1 =====
NUC1           13C
P1             8.00 usec
PL1            -2.30 dB
SFO1          125.7703643 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL2            -2.30 dB
PL12          15.00 dB
PL13          120.00 dB
SFO2          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB            0
LB            2.00 Hz
GB            0
PC            1.40
```