

Supporting Information

Copper acetate-DMSO promoted methylthiolation of arenes and heteroarenes

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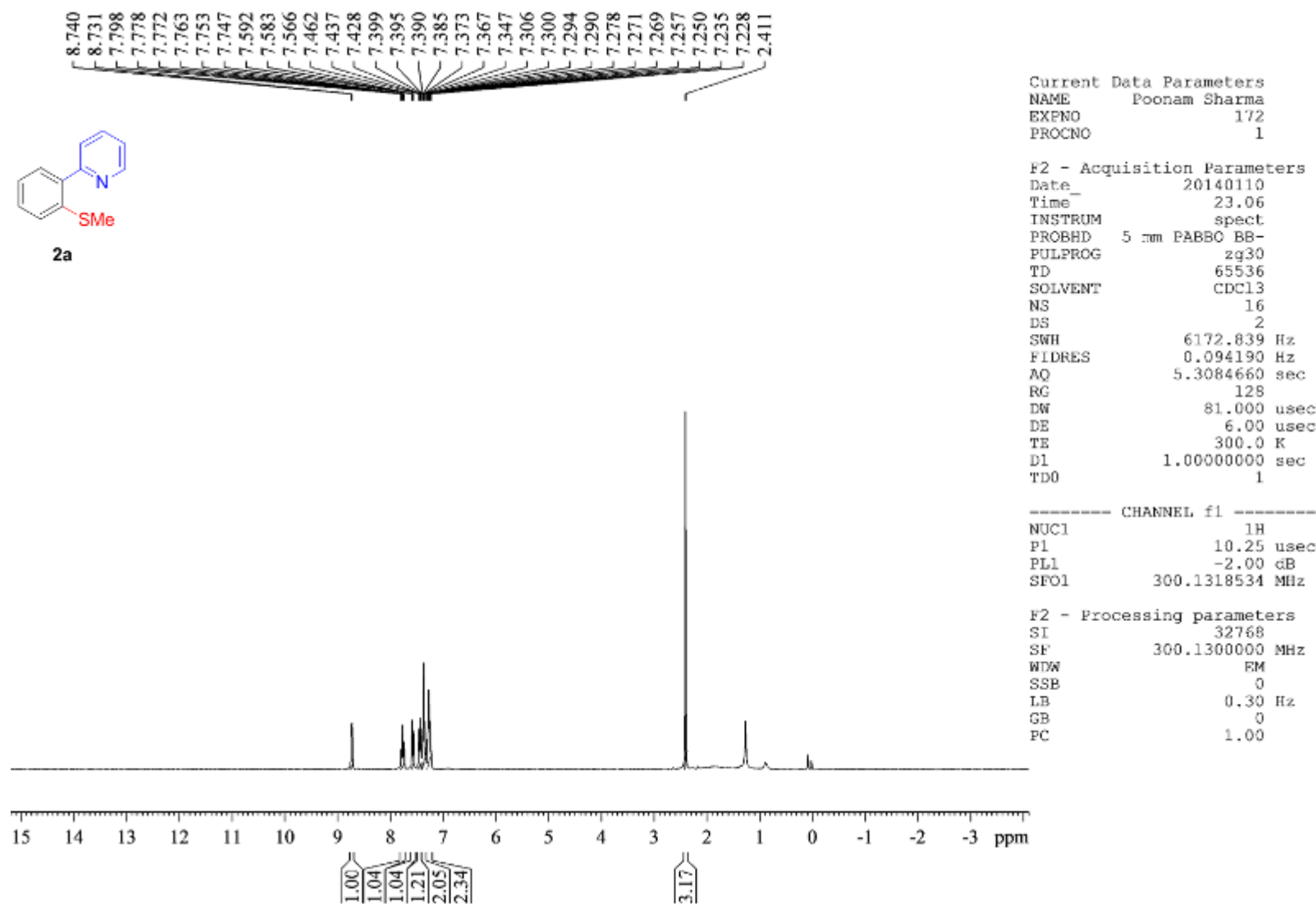
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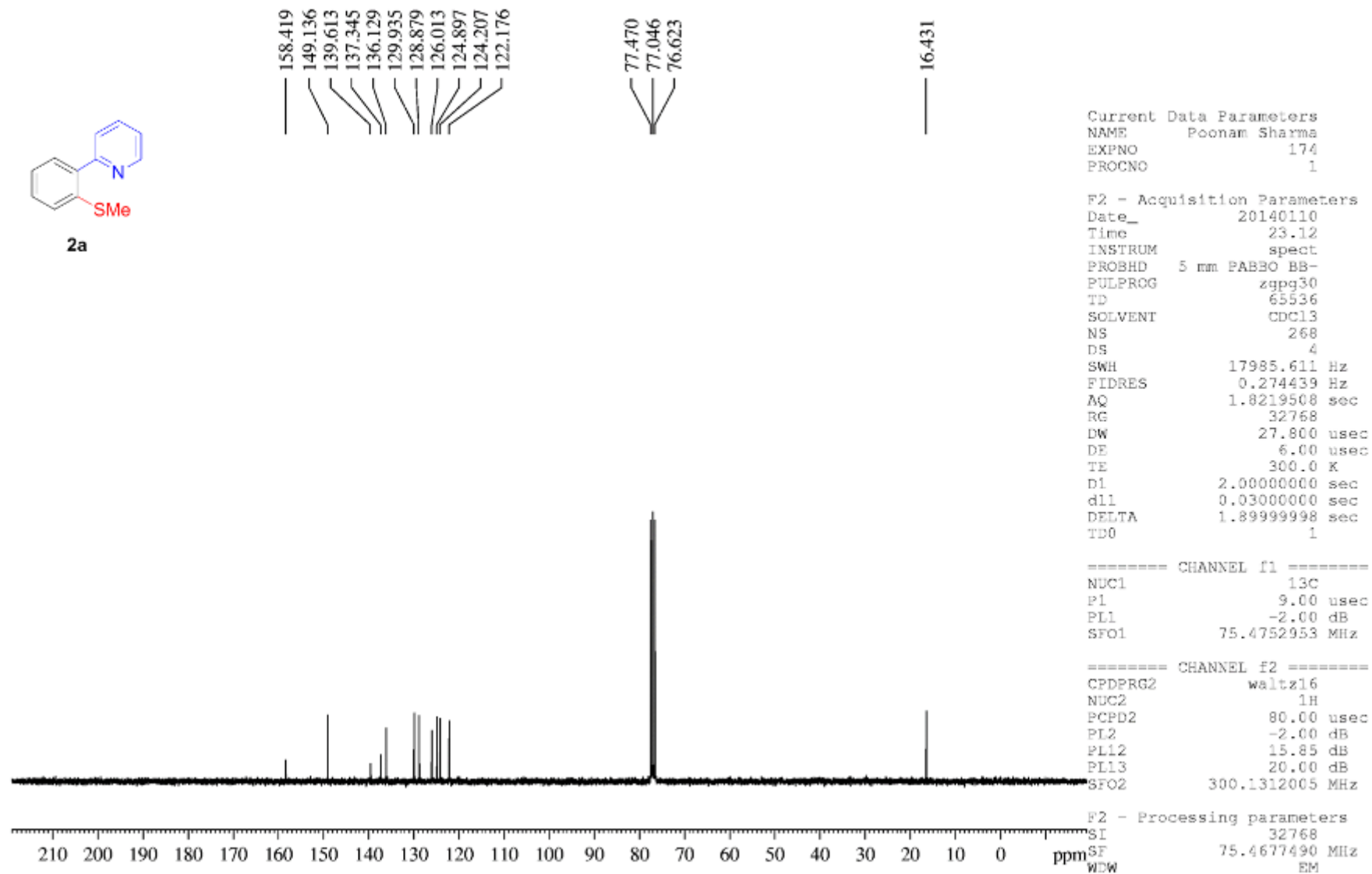
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1. Copies of ^1H NMR, ^{13}C NMR and Mass spectra (Spectrum 1-56)

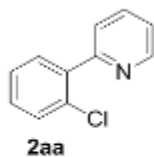


Spectrum 1. 300 MHz ^1H NMR of compound **2a**



Spectrum 2. 75 MHz ^{13}C NMR of compound 2a

8.720
7.843
7.817
7.793
7.768
7.743
7.667
7.641
7.612
7.605
7.582
7.493
7.474
7.468
7.424
7.397
7.371
7.363
7.355
7.339
7.332
7.315
7.299
7.275
7.264

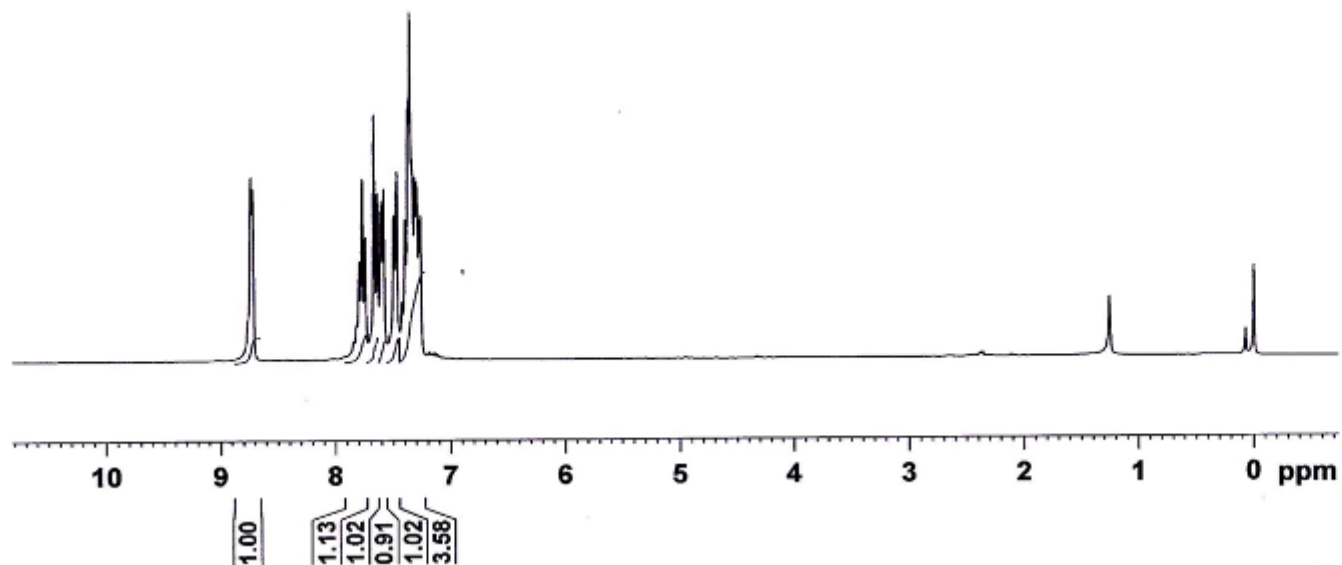


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EXPNO     1
PROCNO    1
Date_     20141119
Time      10.48
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   zg30
TD        14422
SOLVENT   CDCl3
NS        16
DS        0
SWH       6009.615 Hz
FIDRES    0.416698 Hz
AQ        1.1999604 sec
RG        203
DW        83.200 usec
DE        6.50 usec
TE        6645.2 K
D1        1.00000000 sec
TD0       1
  
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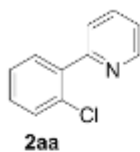
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===== CHANNEL f1 =====
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P1        12.15 usec
PL1       0.00 dB
PL1W      14.39310932 W
SFO1      300.1312005 MHz
SI        32768
SF        300.1300008 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



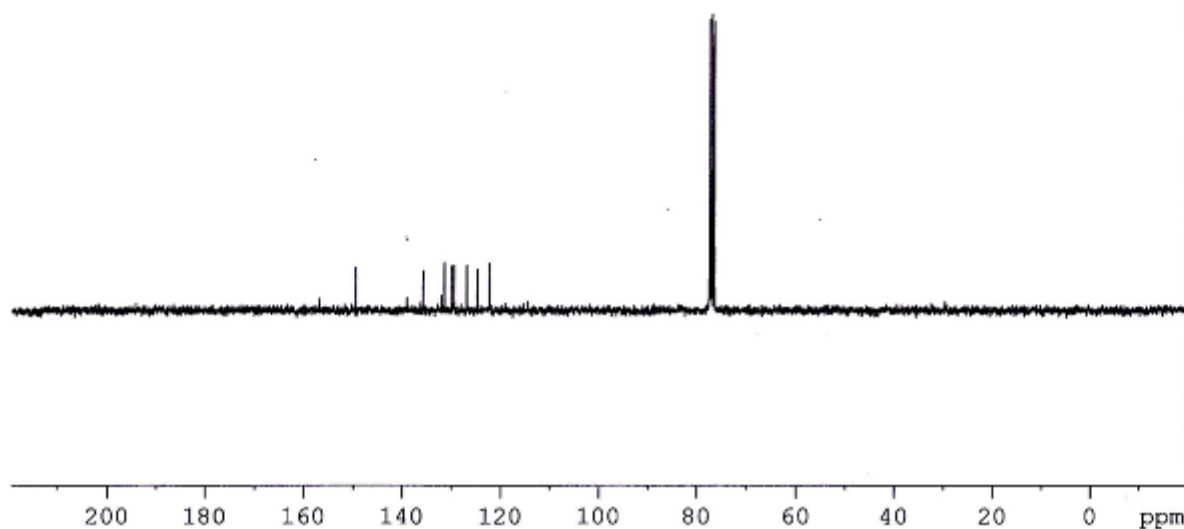
Spectrum 3. 300 MHz ^1H NMR of compound 2aa

pycuc1



156.88
149.54
139.18
135.84
132.13
131.52
130.09
129.57
127.00
124.86
122.39

77.61
77.19
76.77



```

NAME          13c-new
EXPNO          46
PROCNO         1
Date_          20141119
Time           10.54
INSTRUM        spect
PROBHD         5 mm Multinucl
PULPROG        zgpg30
TD             65536
SOLVENT        CDCl3
NS             218
DS             1
SWH            18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG             10
DW            27.733 usec
DE             6.50 usec
TE            6645.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0            1
  
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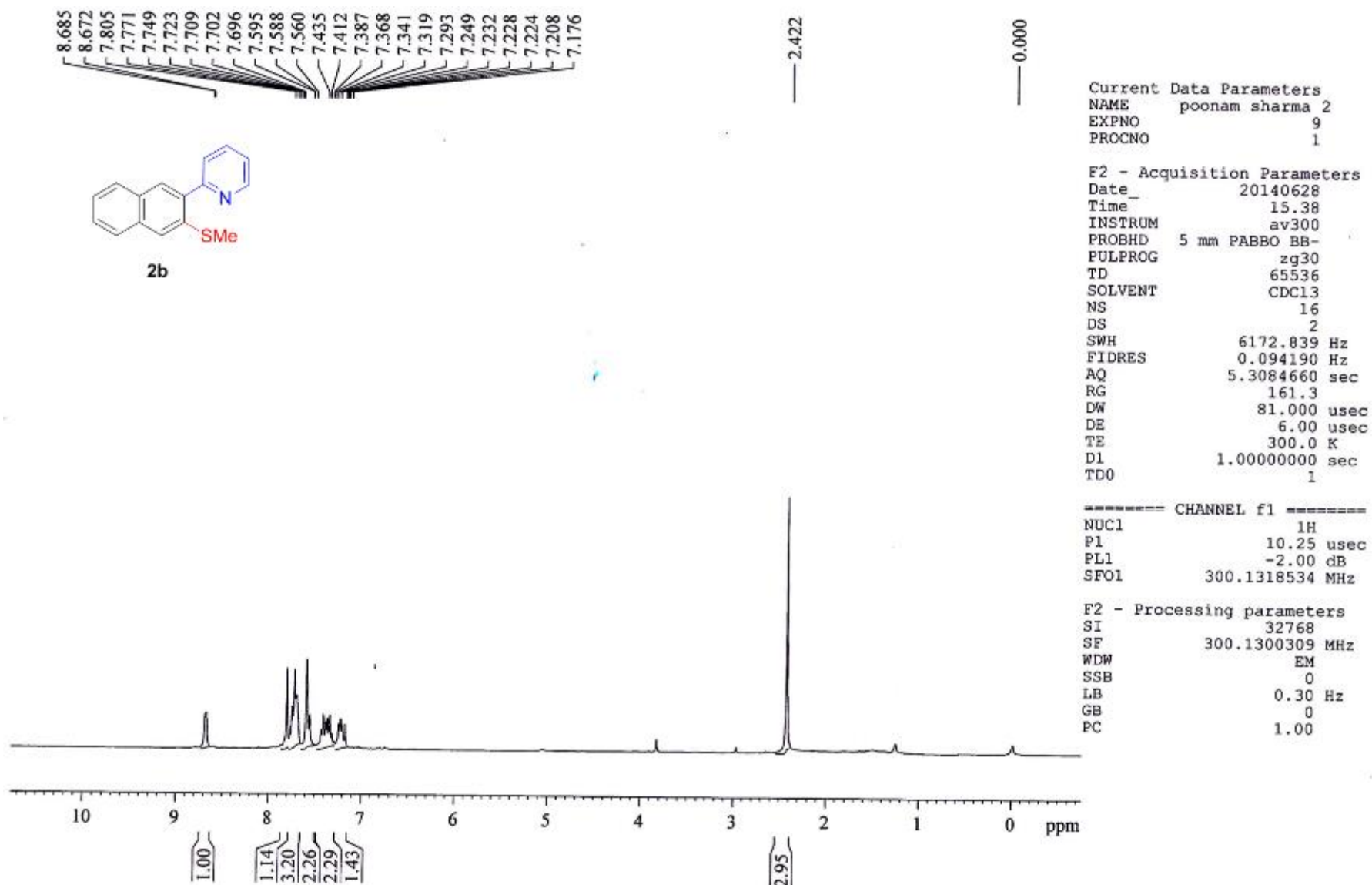
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===== CHANNEL f1 =====
NUC1           13C
P1             9.00 usec
PL1            -2.00 dB
PL1W          48.56907654 W
SFO1           75.4752953 MHz
  
```

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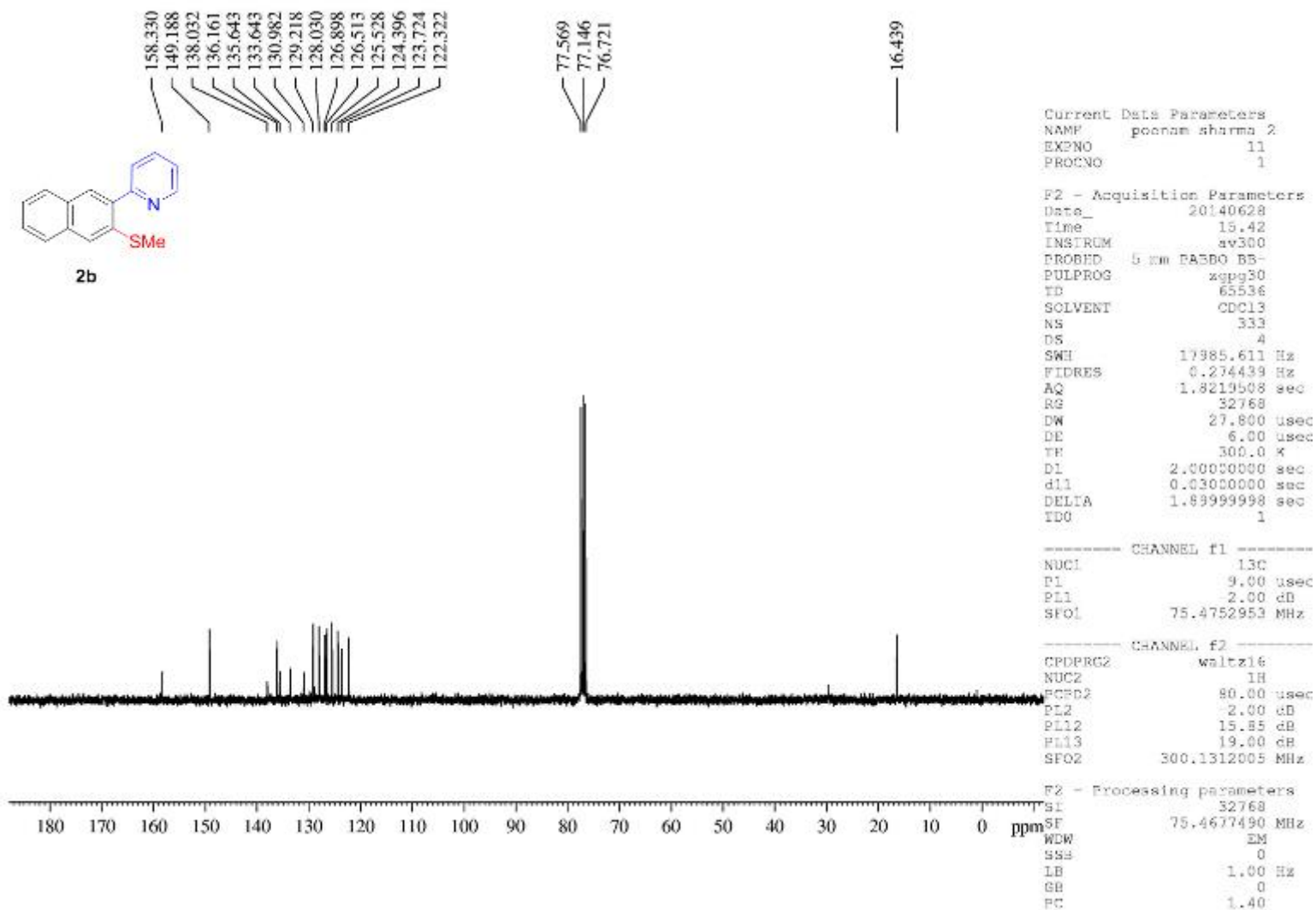
===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2            1H
PCPD2          80.00 usec
PL2             0.00 dB
PL12           16.37 dB
PL13           20.37 dB
PL2W          14.39310932 W
PL12W          0.33201259 W
PL13W          0.13217659 W
SFO2           300.1312005 MHz
SI             32768
SF            75.4677490 MHz
WDW            EM
SSB            0
LB             2.00 Hz
GB             0
PC             1.40
  
```

Spectrum 4. 75 MHz ^{13}C NMR of compound **2aa**

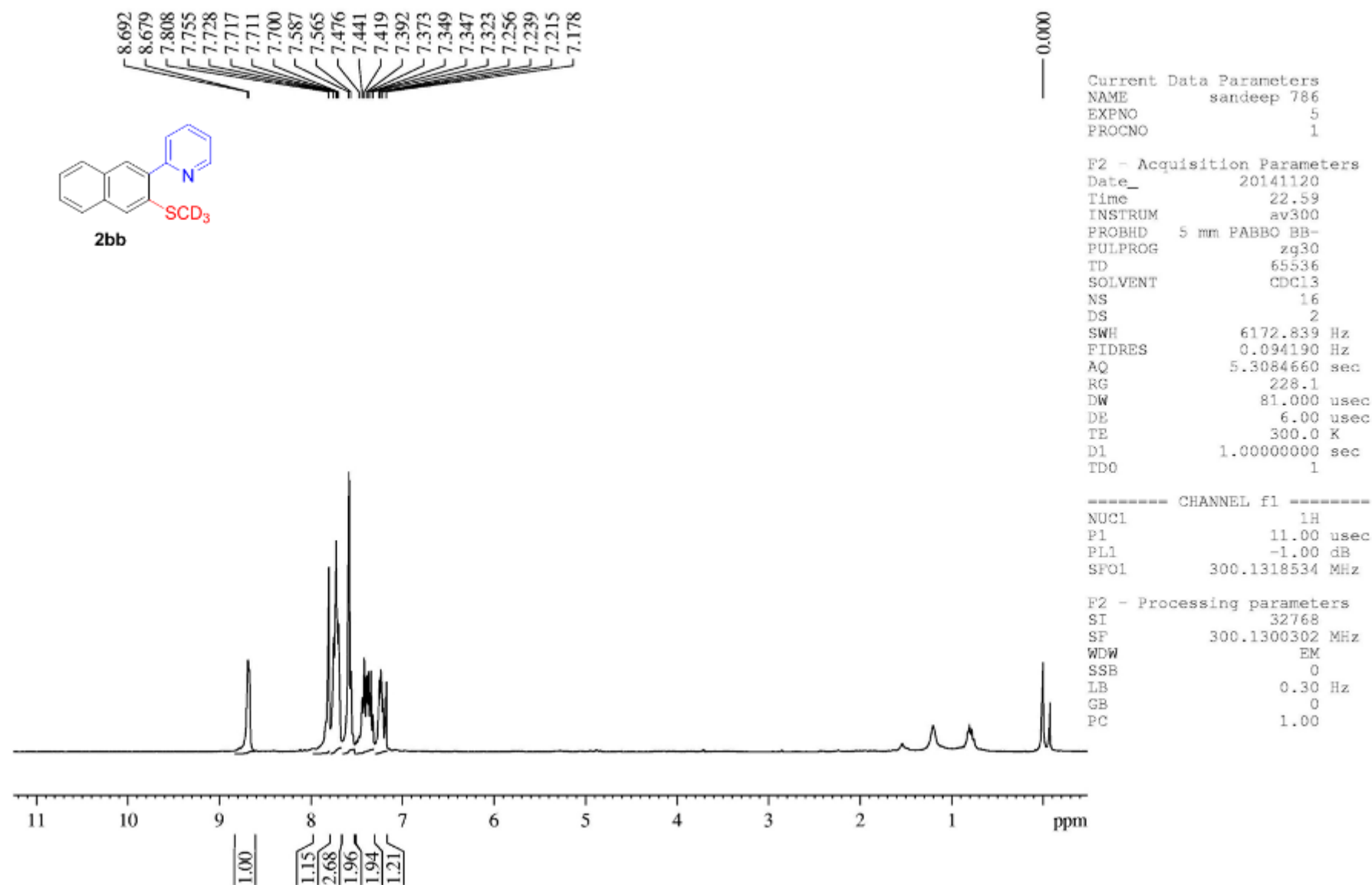


Spectrum 5. 300 MHz ¹H NMR of compound **2b**

2 nap pySMe C13

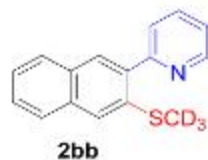


Spectrum 6. 75 MHz ^{13}C NMR of compound 2b



Spectrum 7. 300 MHz ^1H NMR of compound **2bb**

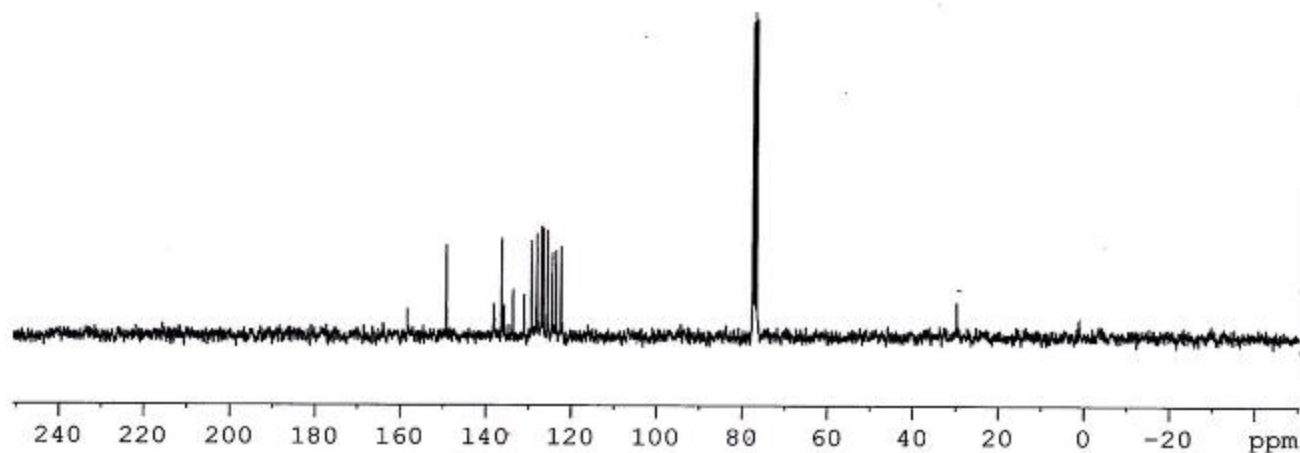
ddmsonap



158.46
149.35
138.12
136.35
135.76
133.76
131.06
129.35
128.18
127.06
126.65
125.66
124.52
123.67
122.49
77.63
77.20
76.78

—29.84

—1.17



```

NAME          13c-2
EXPNO         1289
PROCNO        1
Date_         20141112
Time          9.01
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       zgpg30
TD            65536
SOLVENT       CDC13
NS            116
DS            1
SWH           22727.273 Hz
FIDRES        0.346791 Hz
AQ            1.4418420 sec
RG            12.7
DW            22.000 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
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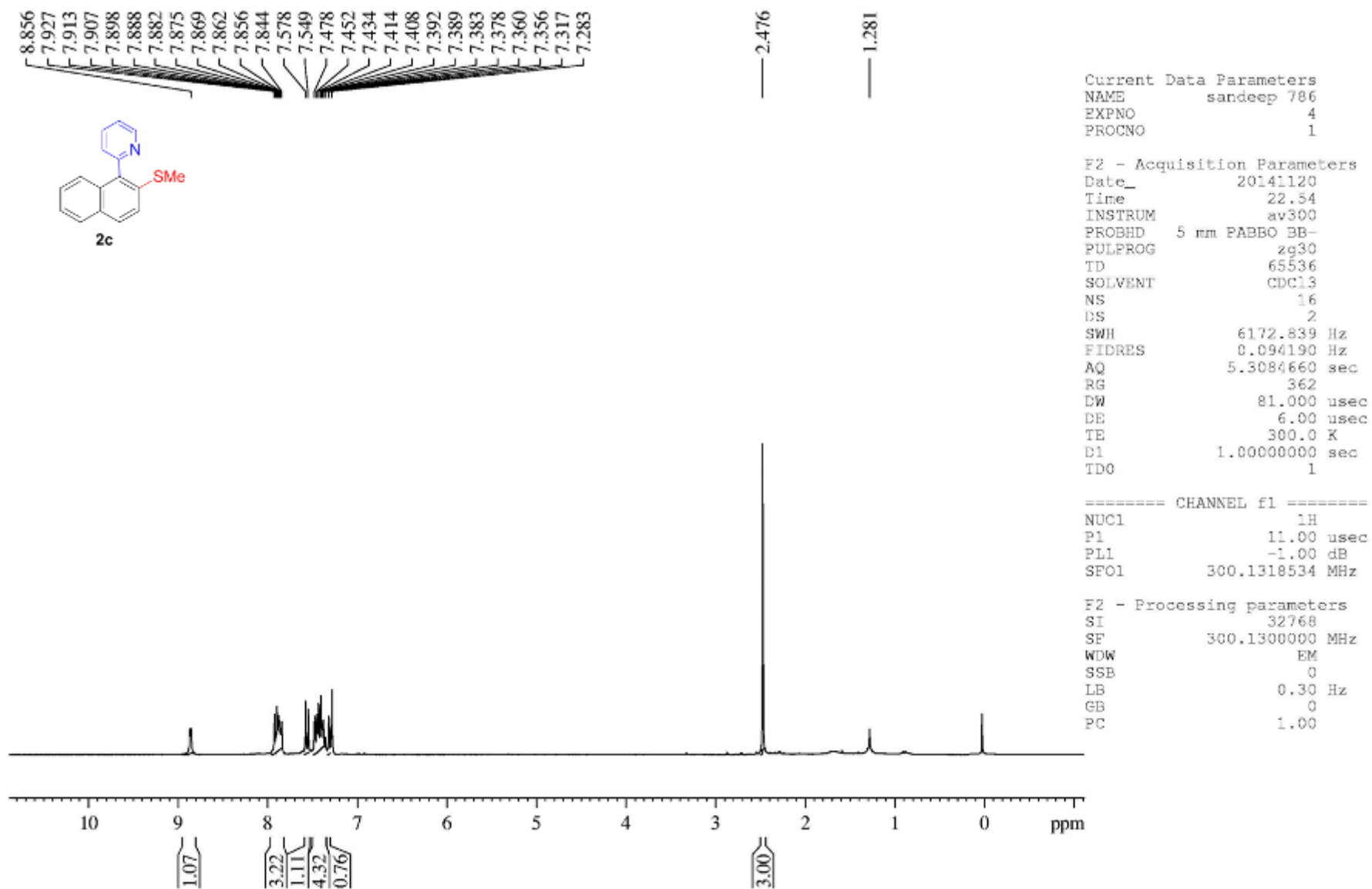
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===== CHANNEL f1 =====
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P1            9.00 usec
PL1           -2.00 dB
PL1W          48.56907654 W
SFO1          75.4752953 MHz
  
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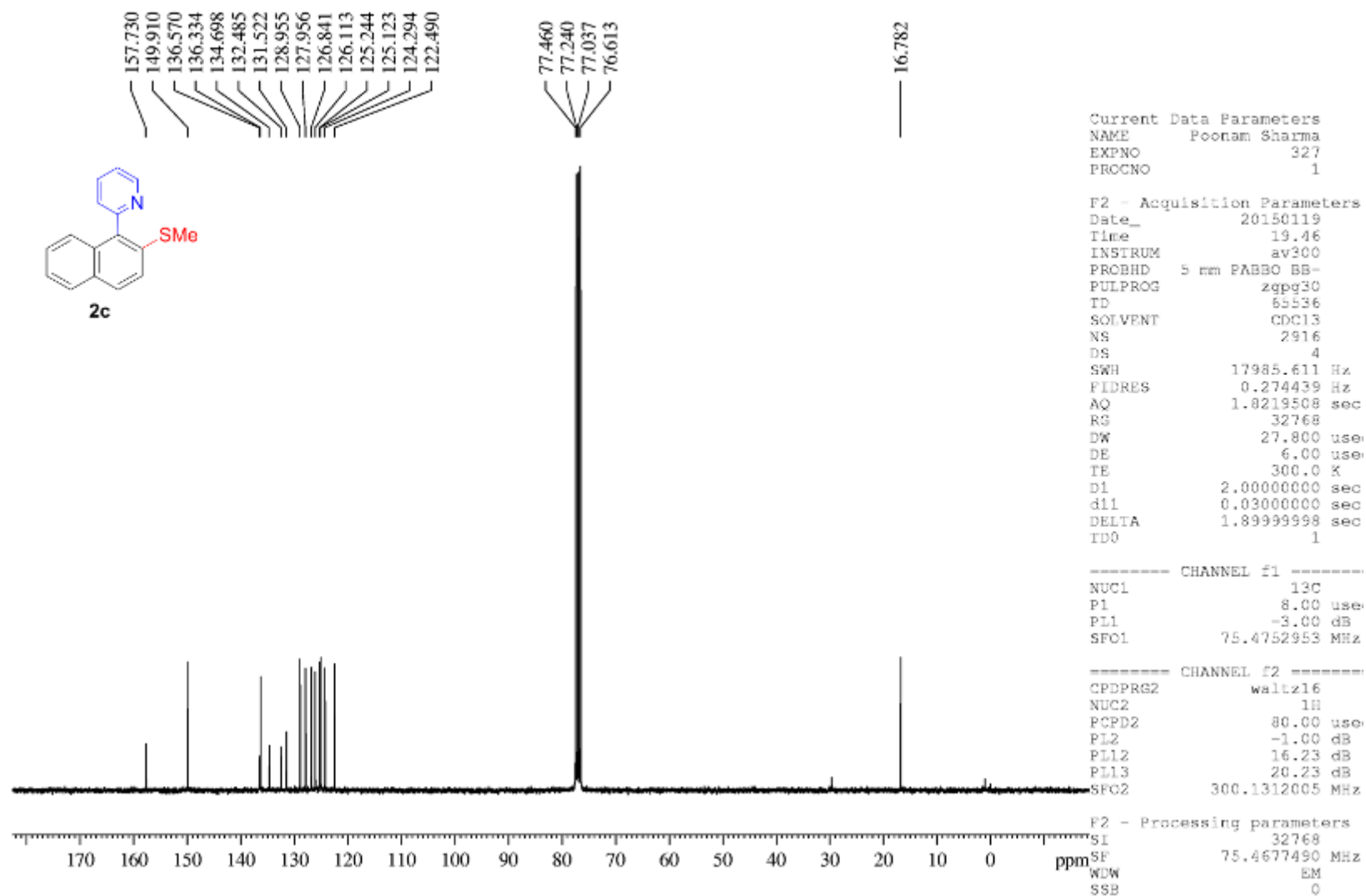
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          16.37 dB
PL13          20.37 dB
PL2W          14.39310932 W
PL12W         0.33201259 W
PL13W         0.13217659 W
SFO2          300.1312005 MHz
SI            32768
SF            75.4677376 MHz
WDW           EM
SSB           0
LB            5.00 Hz
GB            0
PC            1.40
  
```

Spectrum 8. 75 MHz ^{13}C NMR of compound **2bb**

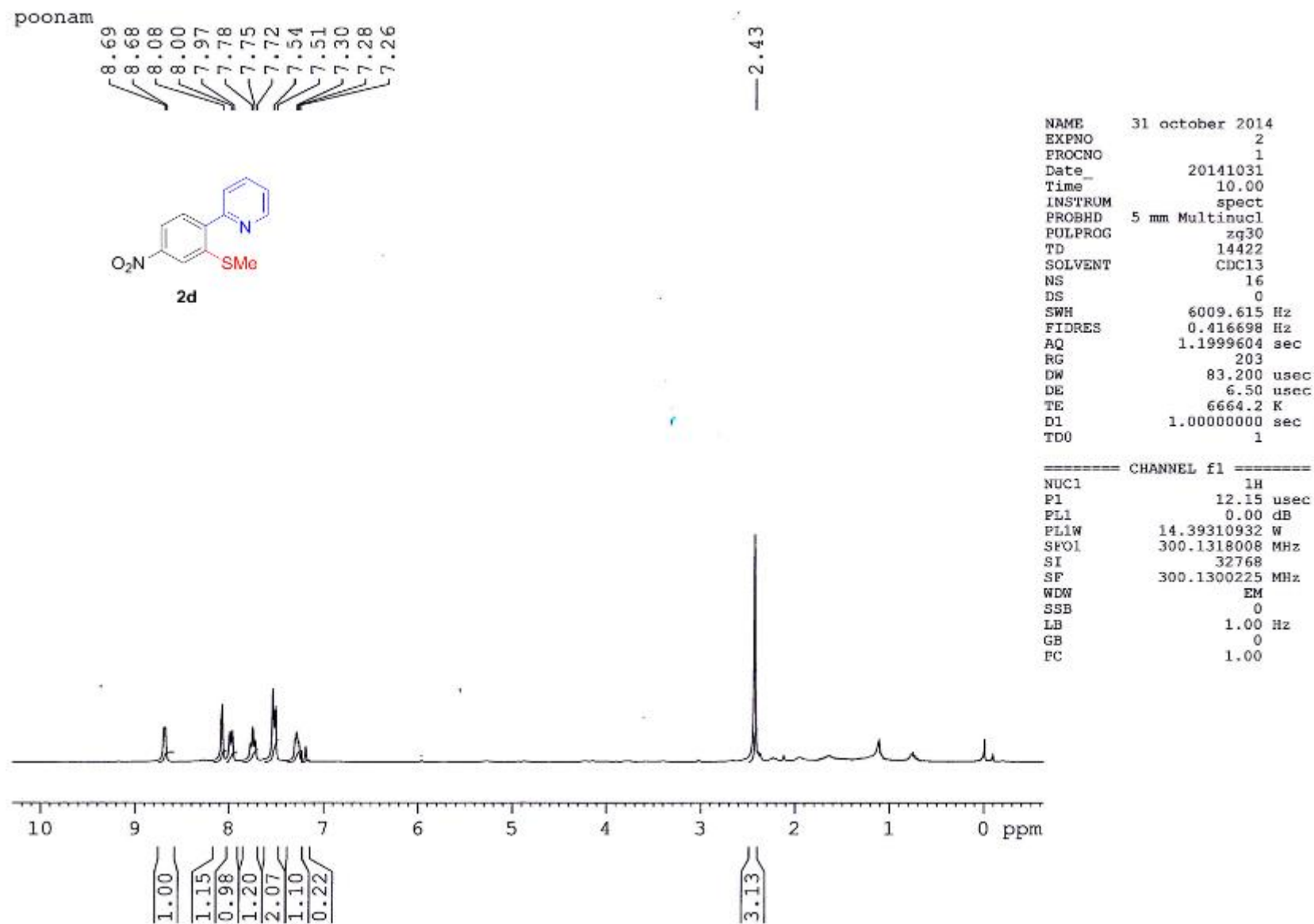


Spectrum 9. 300 MHz ^1H NMR of compound **2c**

PS-1

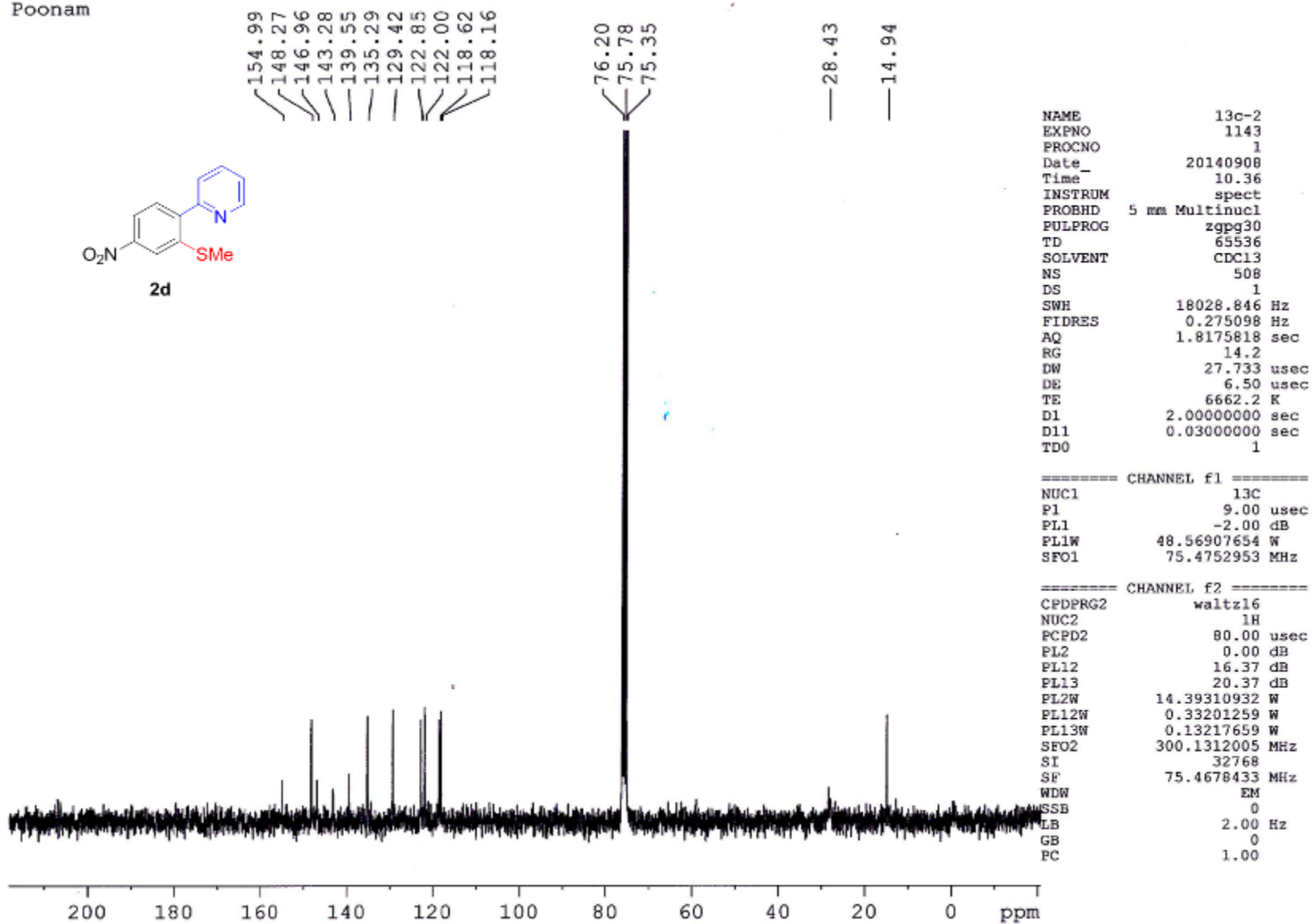


Spectrum 10. 75 MHz ^{13}C NMR of compound **2c**

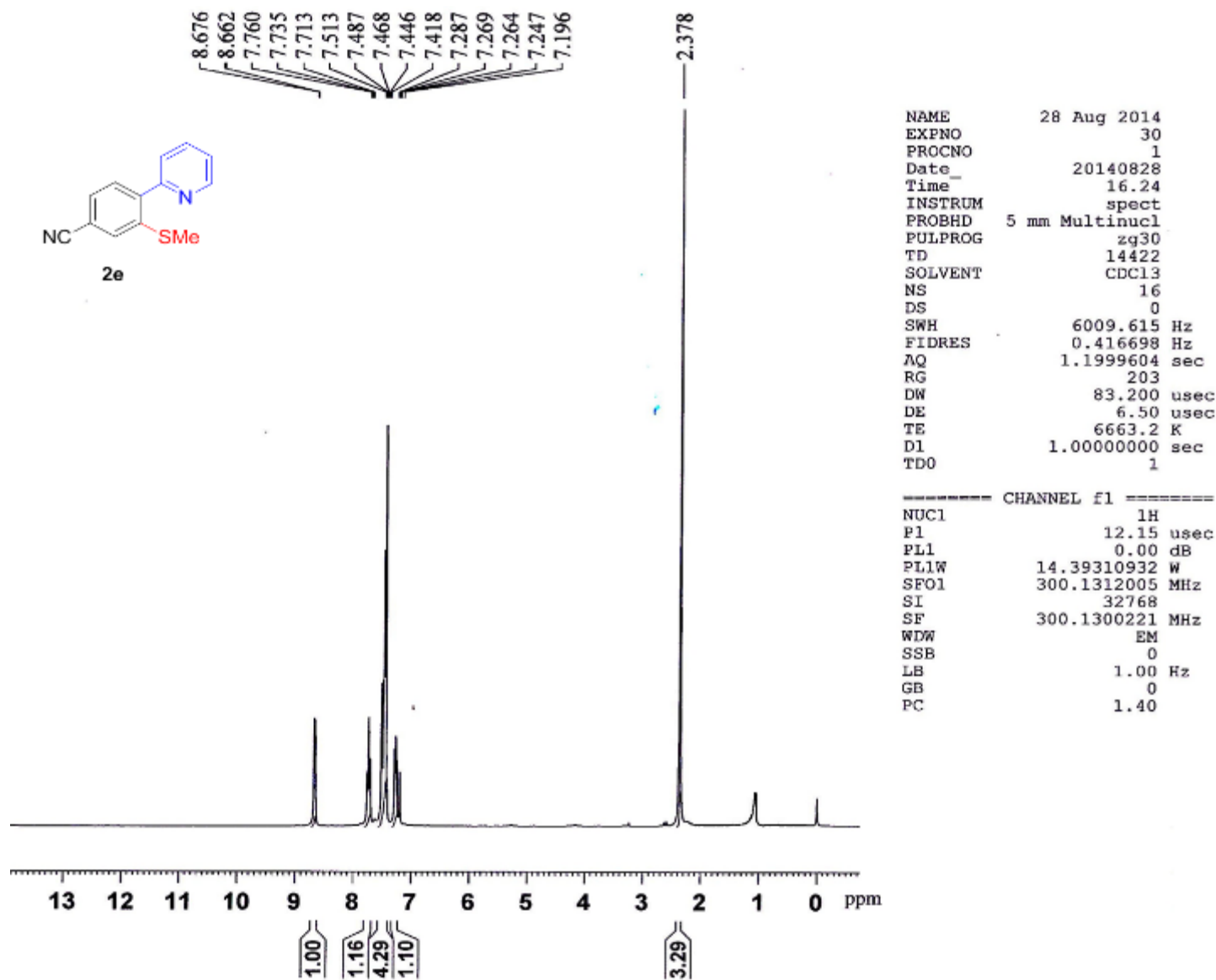


Spectrum 11. 300 MHz ^1H NMR of compound 2d

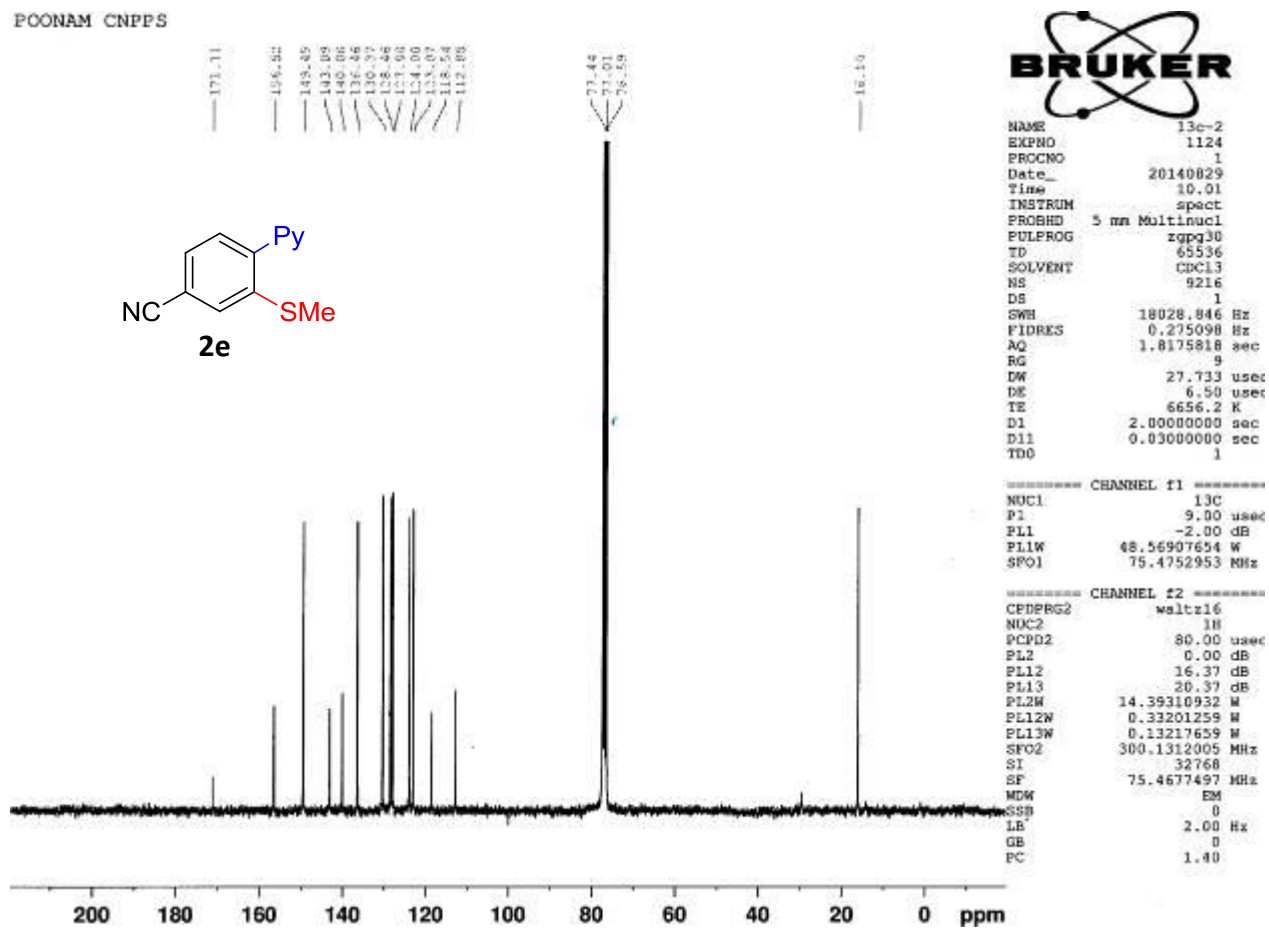
Poonam



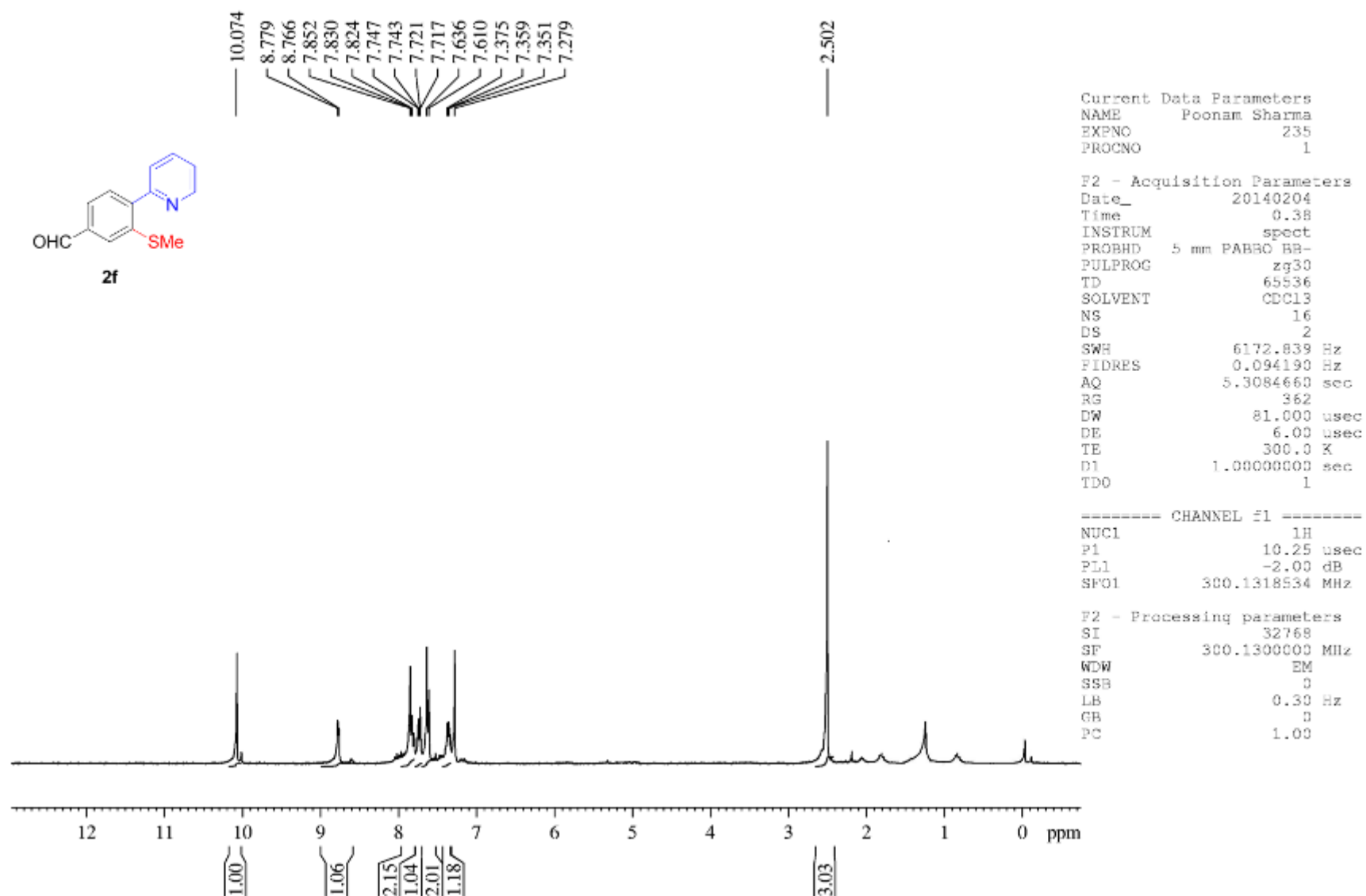
Spectrum 12. 75 MHz ¹³C NMR of compound **2d**



Spectrum 13. 300 MHz ¹H NMR of compound **2e**

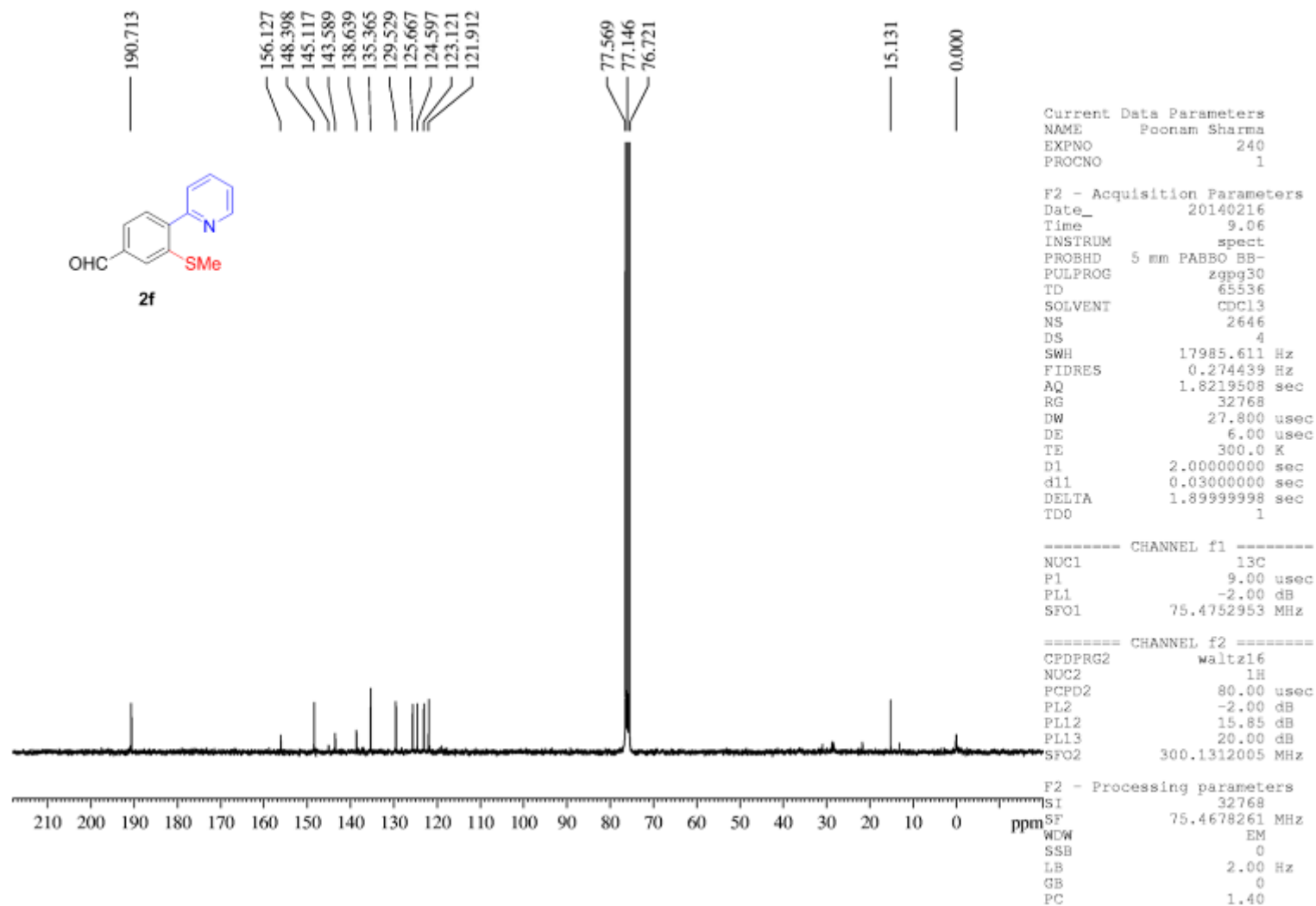


Spectrum 14. 75 MHz ^{13}C NMR of compound **2e**

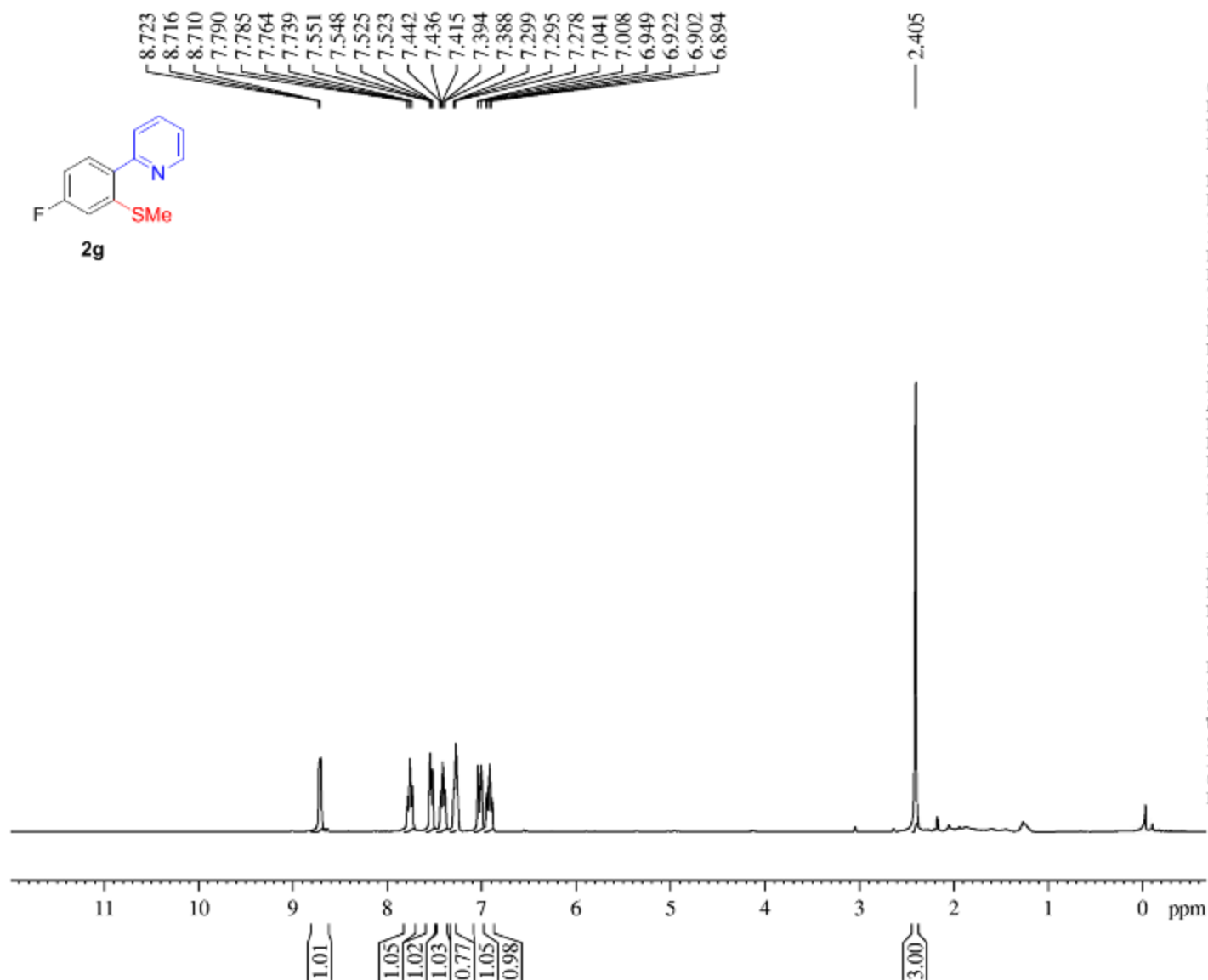


Spectrum 15. 300 MHz ¹H NMR of compound **2f**

formyl ppp c13



Spectrum 16. 75 MHz ^{13}C NMR of compound **2f**



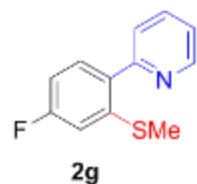
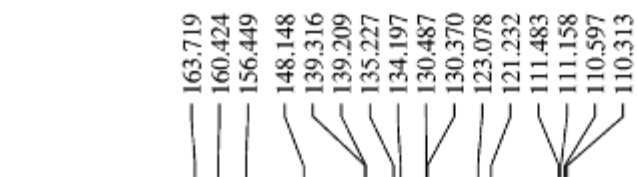
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 EXPNO 206
 PROCNO 1

F2 - Acquisition Parameters
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 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 128
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 -2.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Spectrum 17. 300 MHz ¹H NMR of compound **2g**



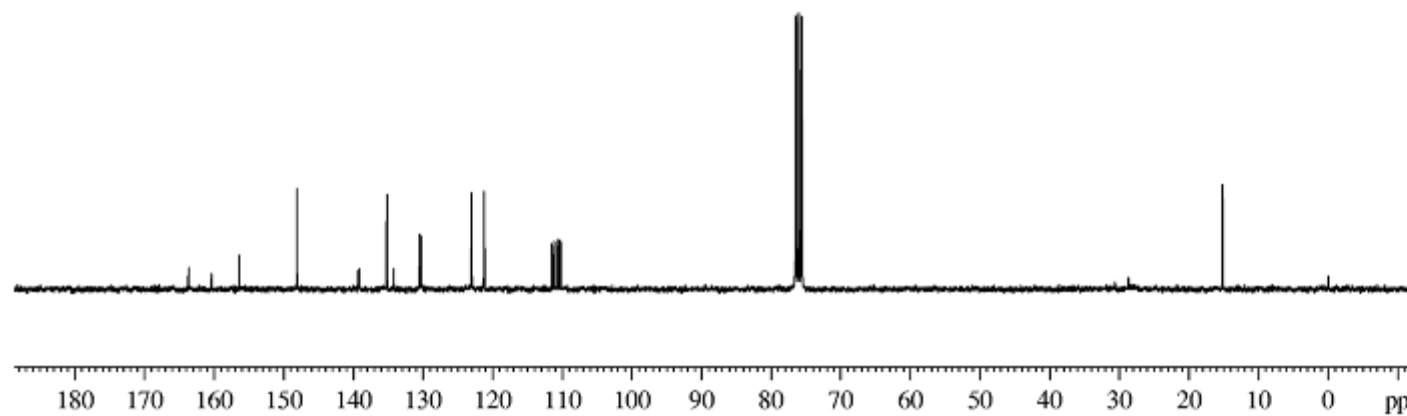
Current Data Parameters
NAME Poonam Sharma
EXPNO 208
PROCNO 1

F2 - Acquisition Parameters
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PULPROC zgpg30
TD 65536
SOLVENT CDCl3
NS 411
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

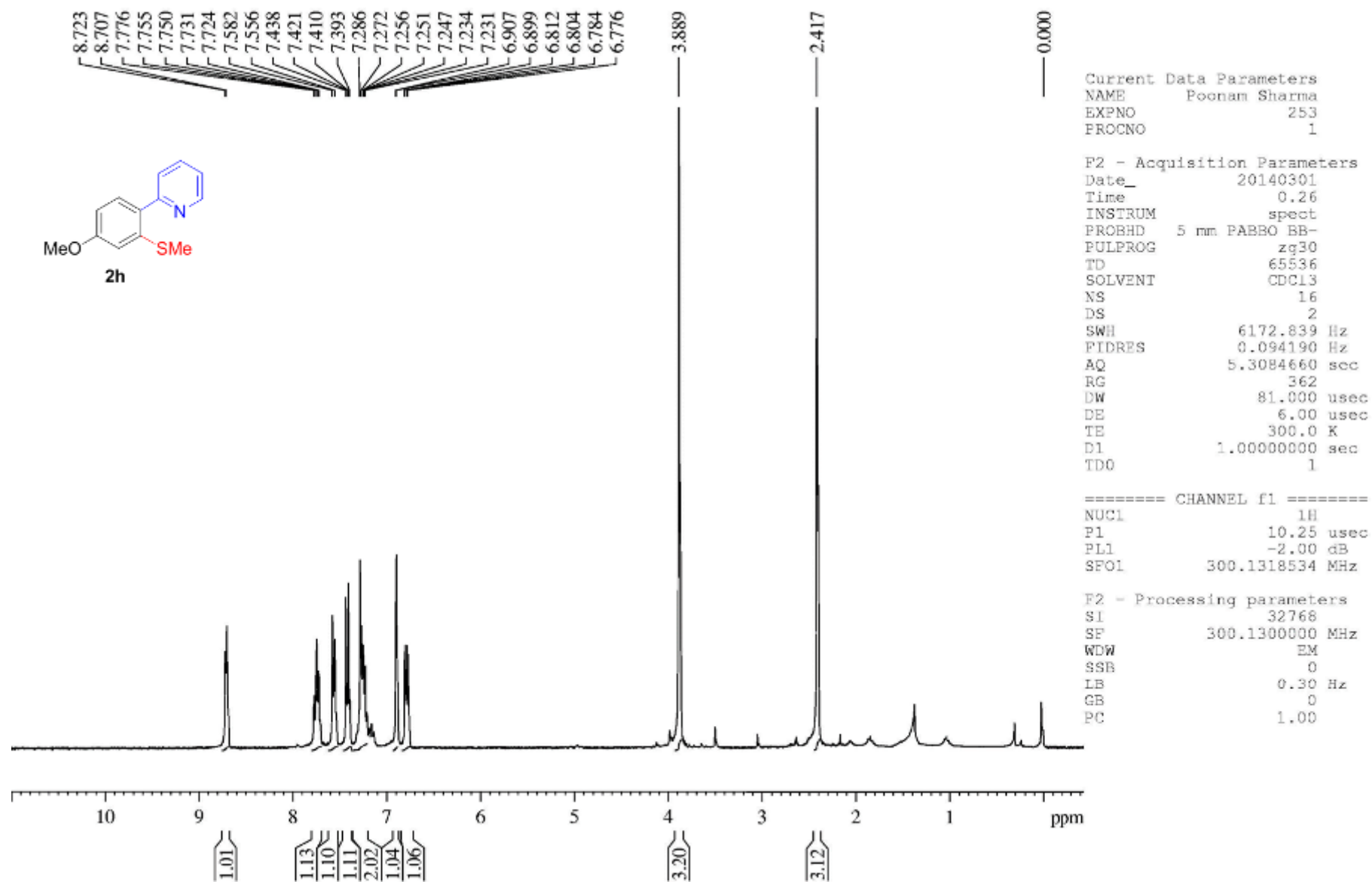
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 15.85 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

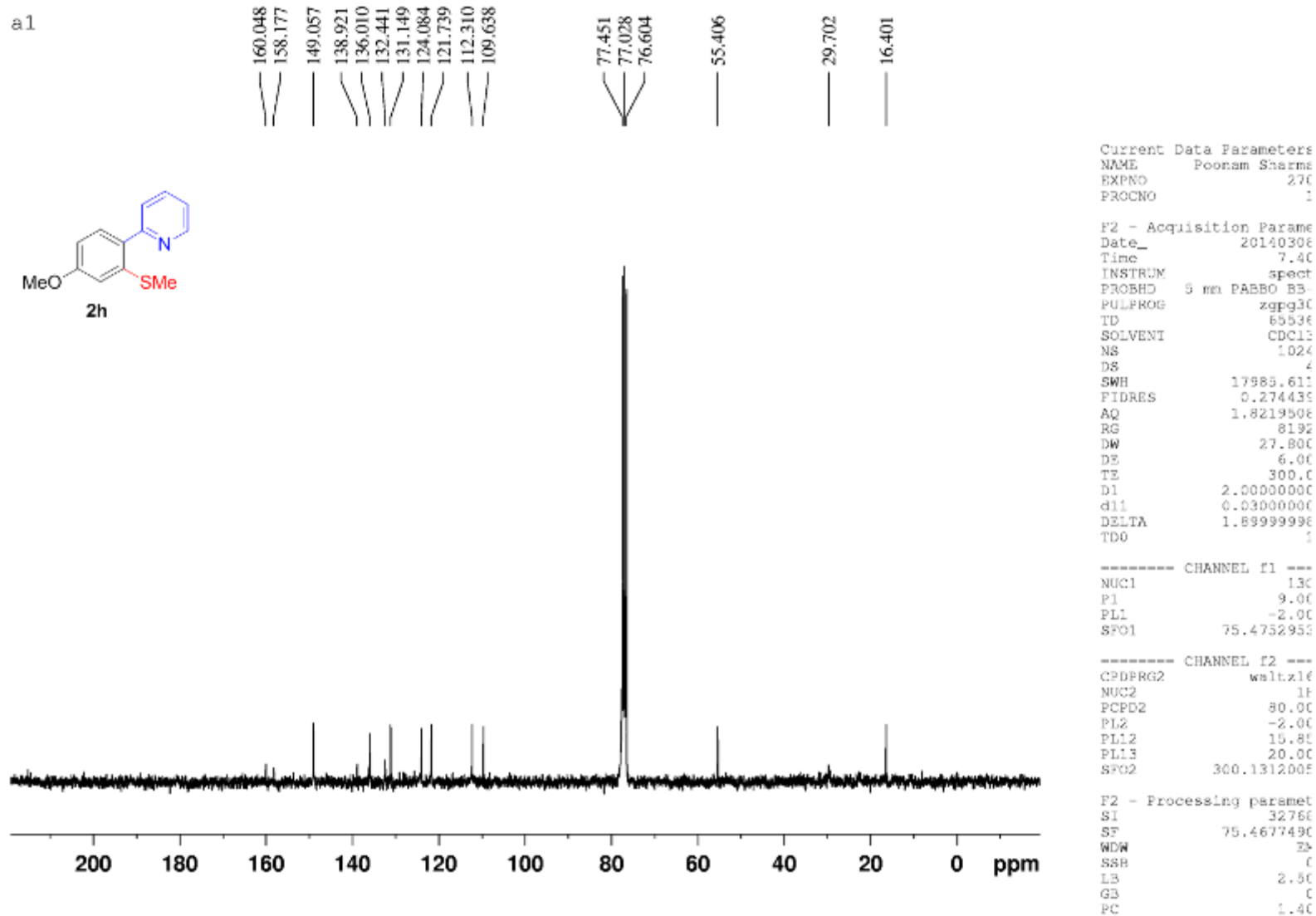
F2 - Processing parameters
SI 32768
SF 75.4678263 MHz
WDW EM



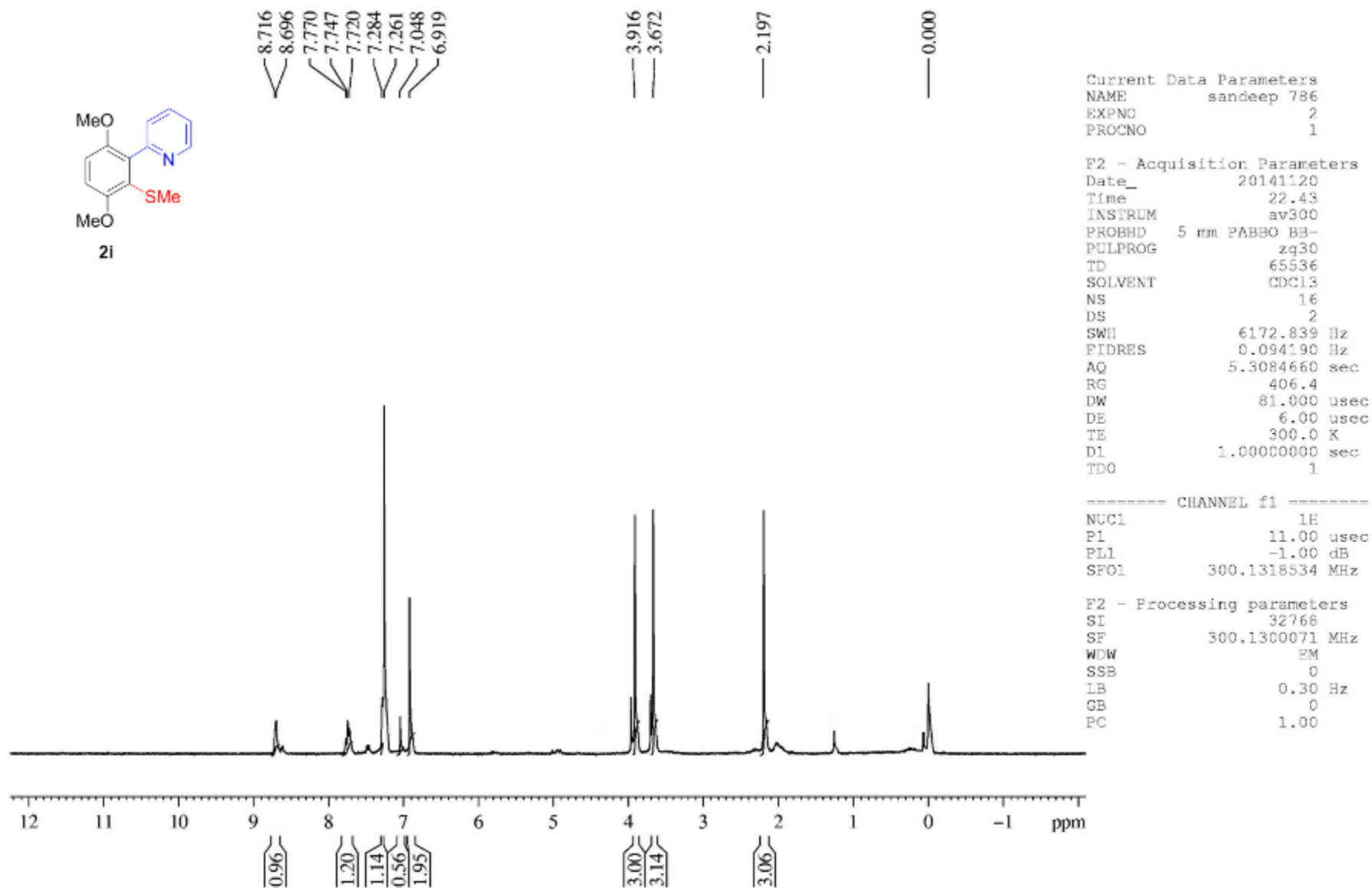
Spectrum 18. 75 MHz ^{13}C NMR of compound **2g**



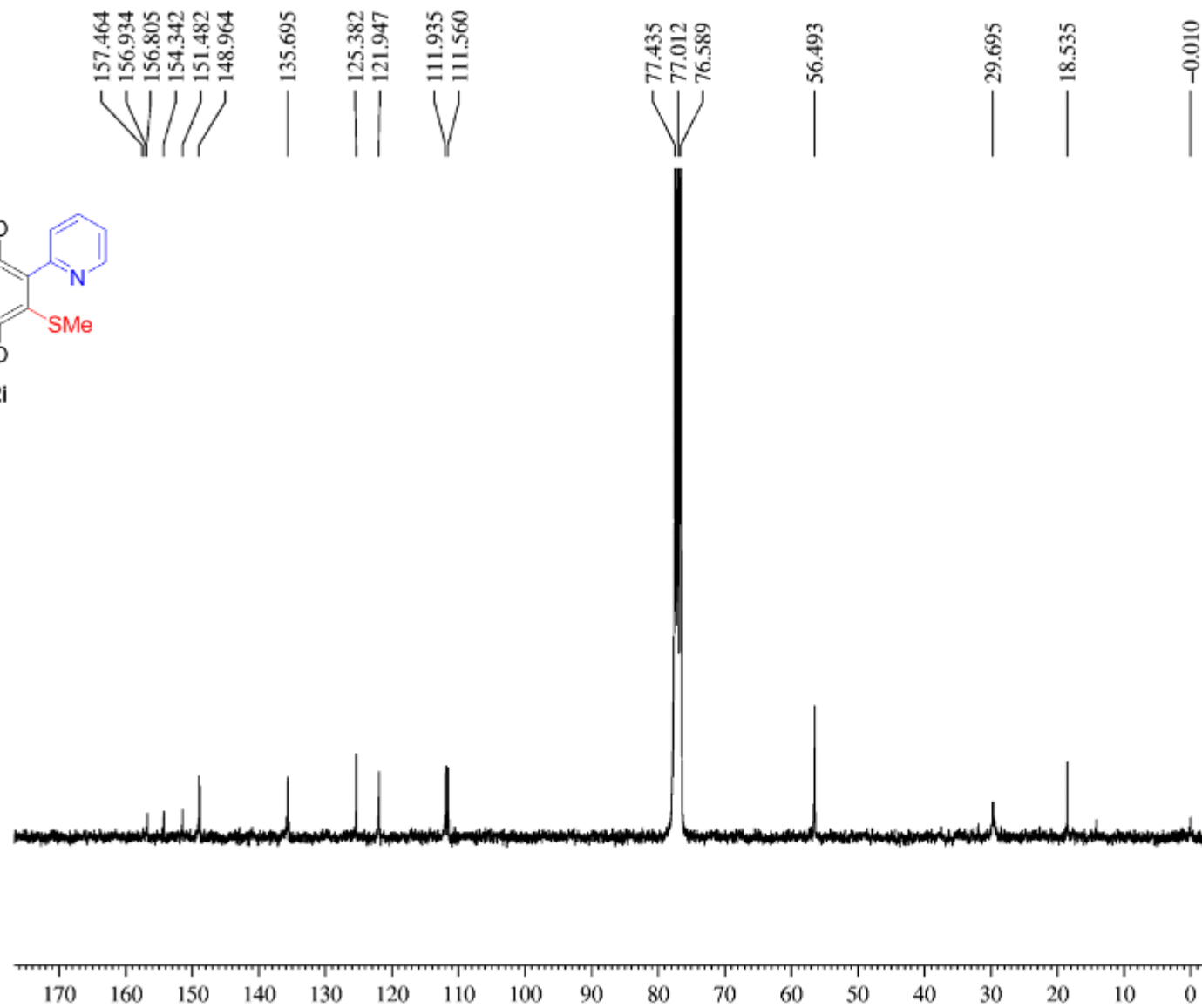
Spectrum 19. 300 MHz ¹H NMR of compound **2h**



Spectrum 20. 75 MHz ^{13}C NMR of compound **2h**



Spectrum 21. 300 MHz ¹H NMR of compound **2i**



Current Data Parameters
NAME Poonam Sharma
EXPNO 257
PROCNO 1

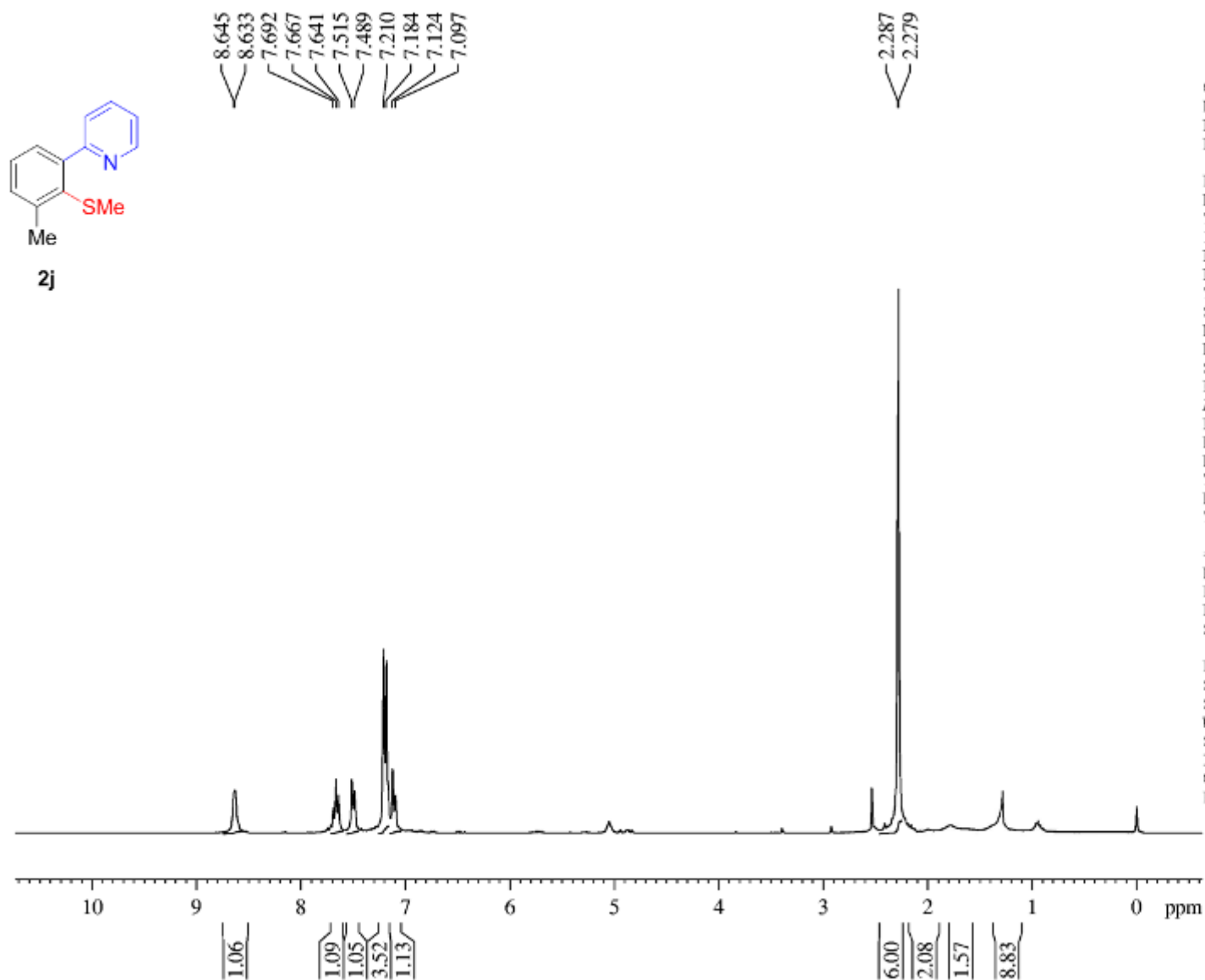
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Time 22.40
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TD 65536
SOLVENT CDCl3
NS 15836
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 15.85 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM

Spectrum 22. 75 MHz ^{13}C NMR of compound **2i**



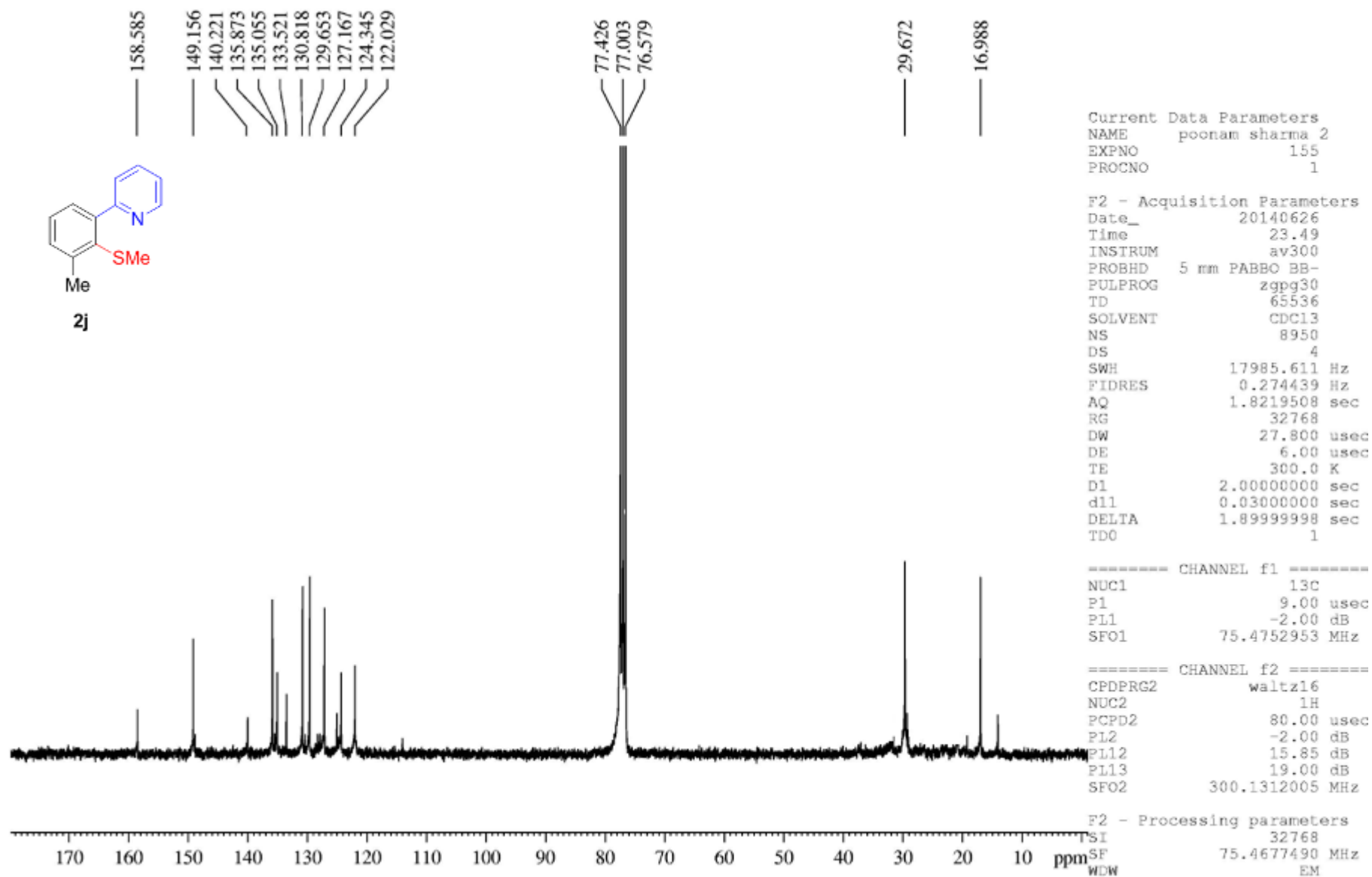
Current Data Parameters
 NAME poonam sharma 2
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
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 Time 17.07
 INSTRUM av300
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 10
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 181
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

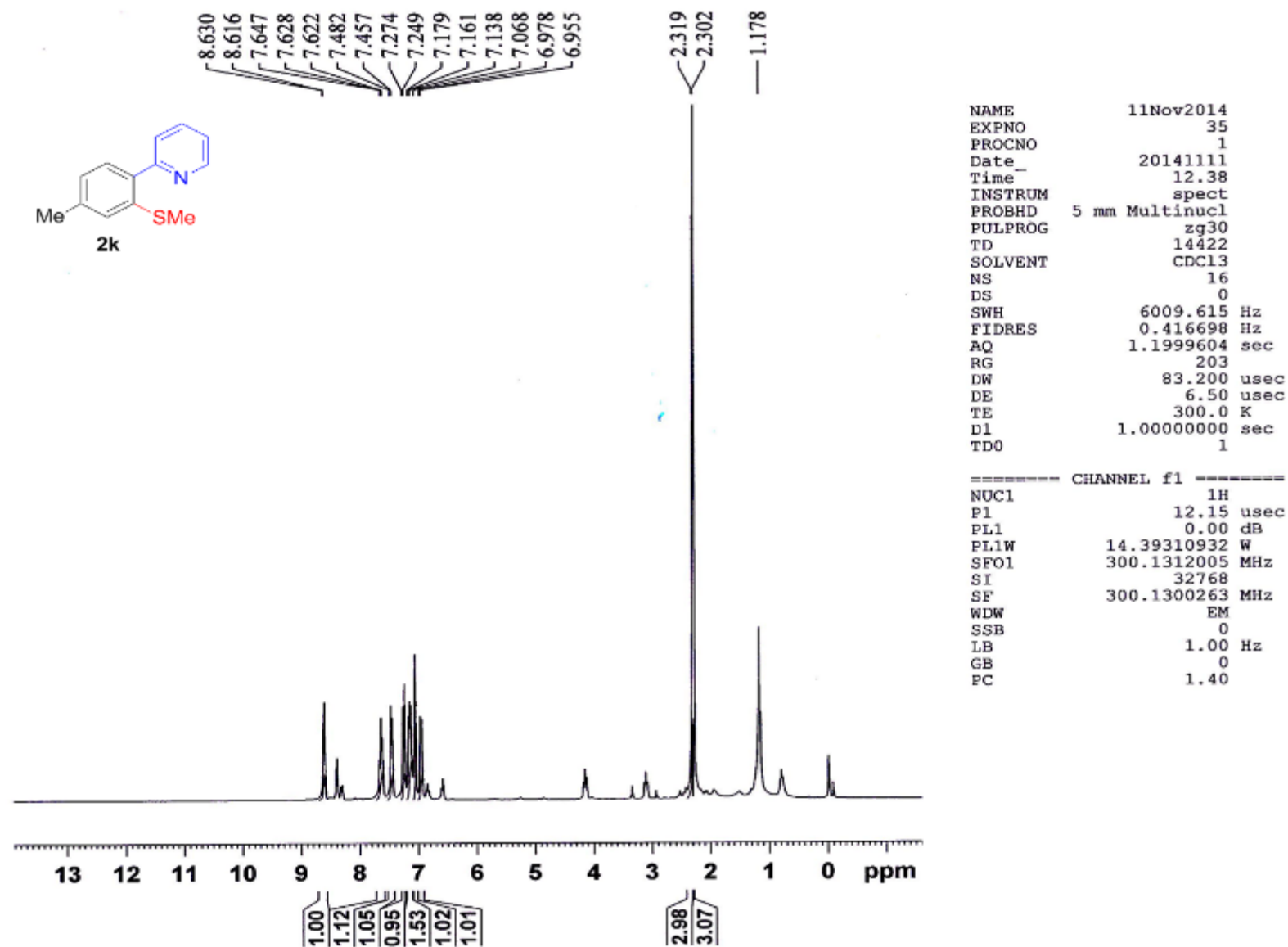
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 P1 10.25 usec
 PL1 -2.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
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 SF 300.1300286 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Spectrum 23. 300 MHz ¹H NMR of compound **2j**



Spectrum 24. 75 MHz ^{13}C NMR of compound 2j



Spectrum 25. 300 MHz ¹H NMR of compound **2k**

4mephpysme

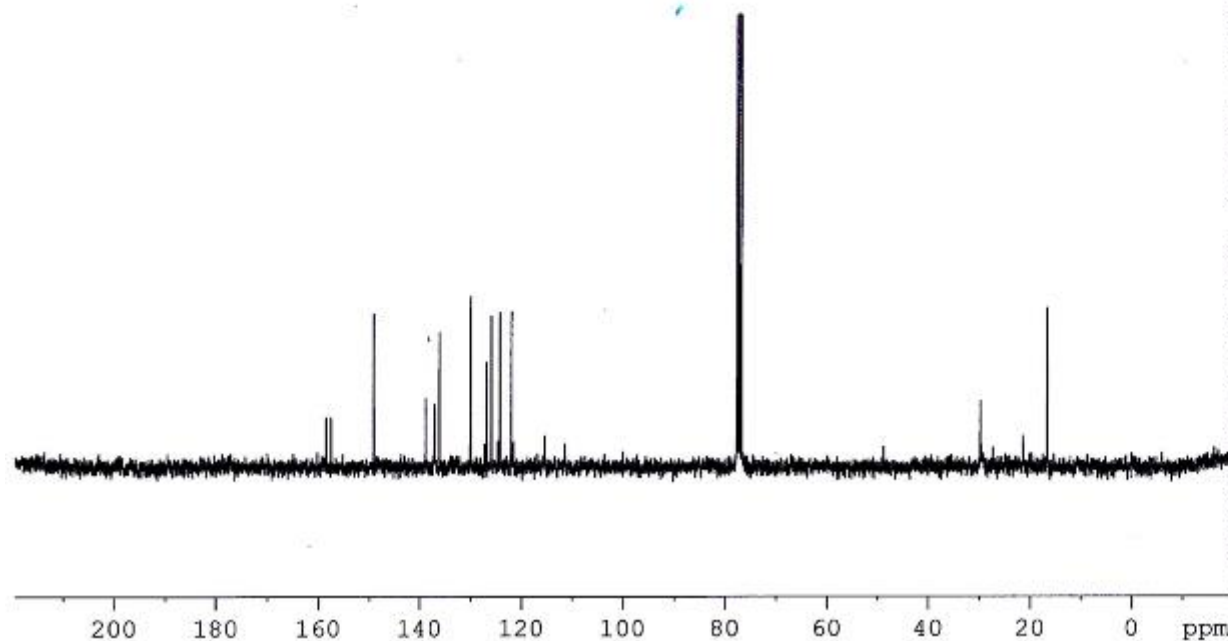


158.59
157.58
149.19
138.87
137.08
136.14
130.04
126.91
125.96
124.33
122.06

77.61
77.19
76.77

29.82

16.64

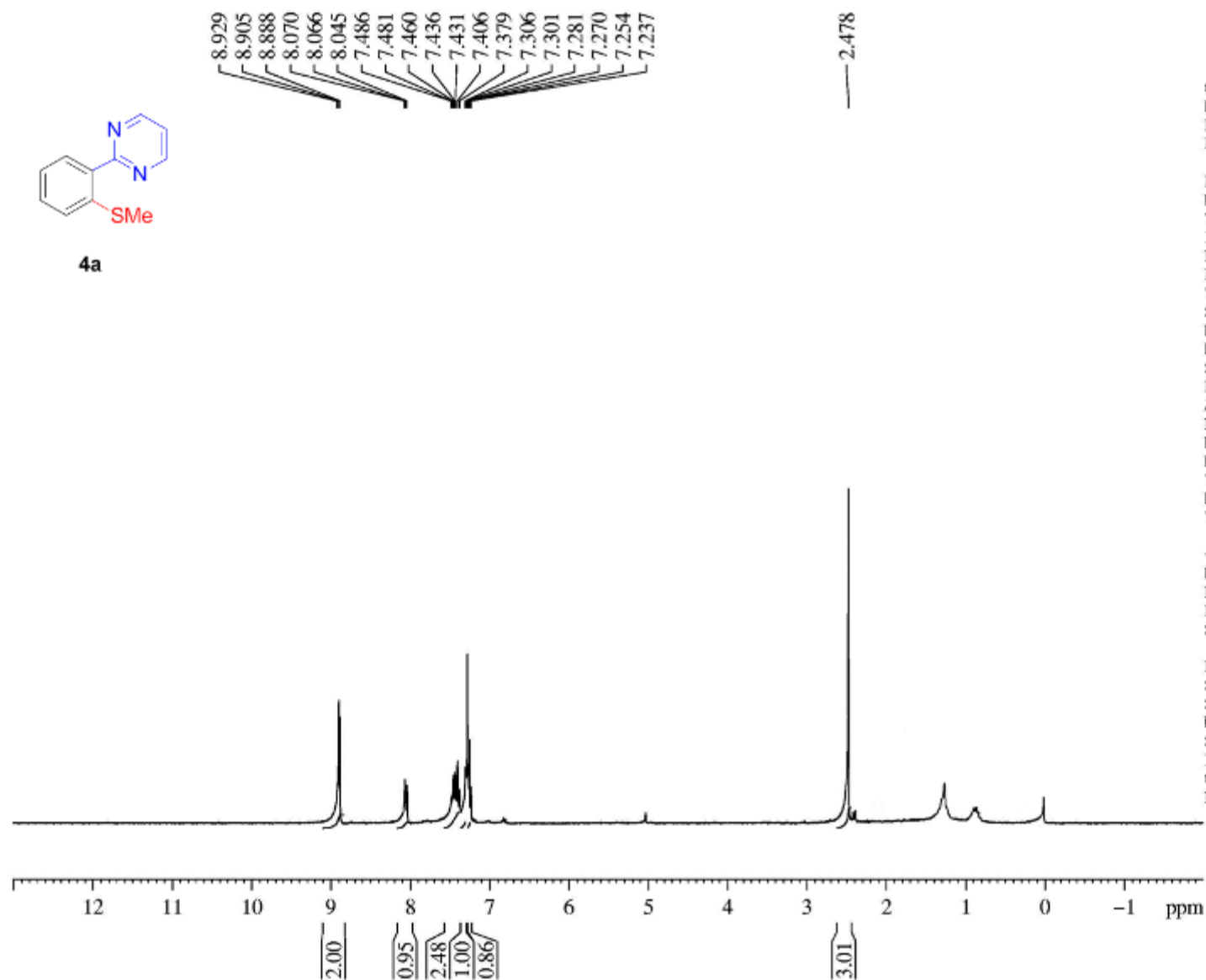


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PROCNO 1
Date 20141105
Time 17.40
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 145
DS 1
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 10
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
PL1W 48.56907654 W
SFO1 75.4752953 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 16.37 dB
PL13 20.37 dB
PL2W 14.39310932 W
PL12W 0.33201259 W
PL13W 0.13217659 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677380 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

Spectrum 26. 75 MHz ^{13}C NMR of compound 2k



Current Data Parameters
 NAME poonam sharma 2
 EXPNO 28
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141130
 Time 10.34
 INSTRUM av300
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 9
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 322.5
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

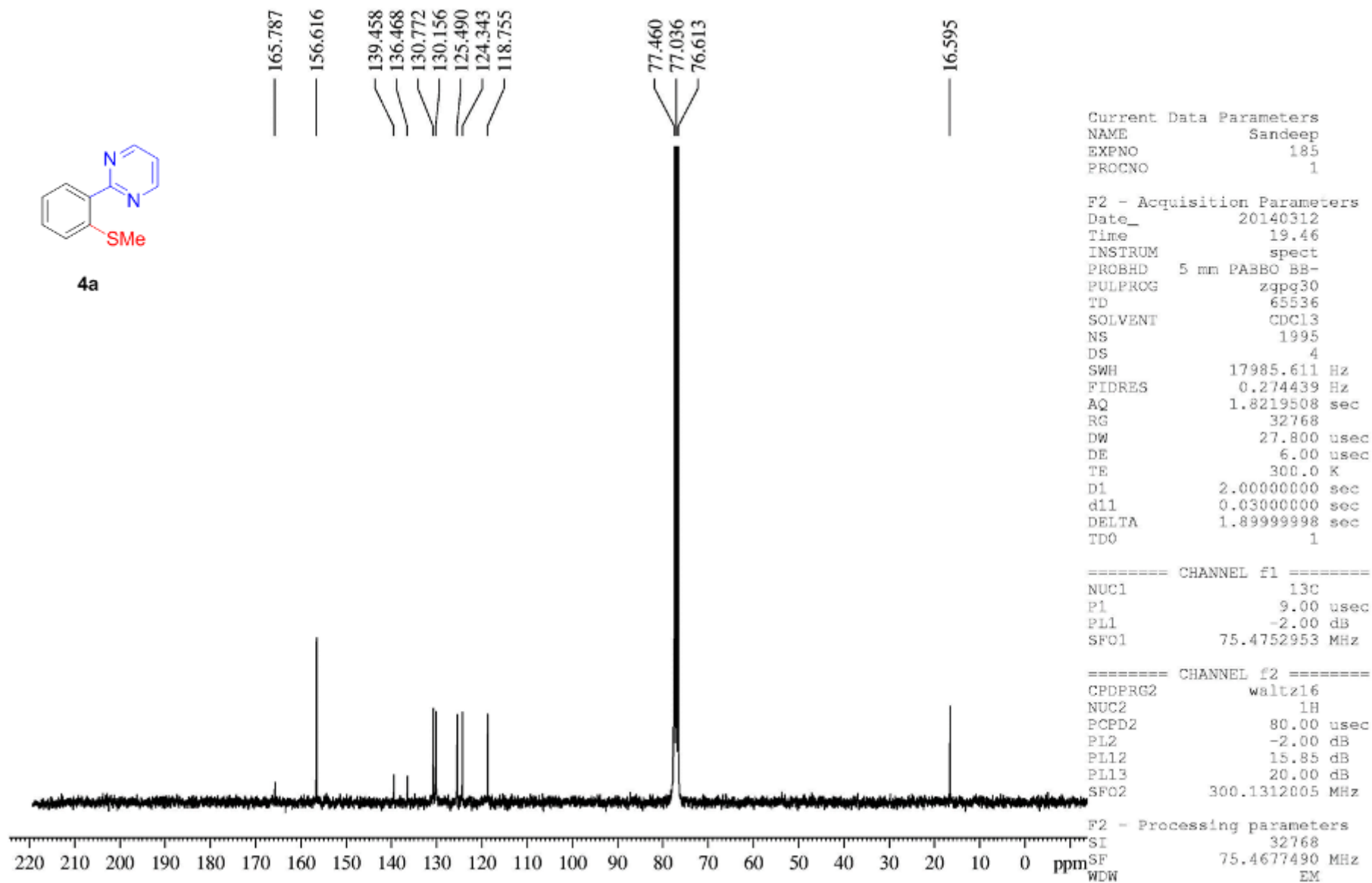
----- CHANNEL f1 -----
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 PL1 -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
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 SF 300.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

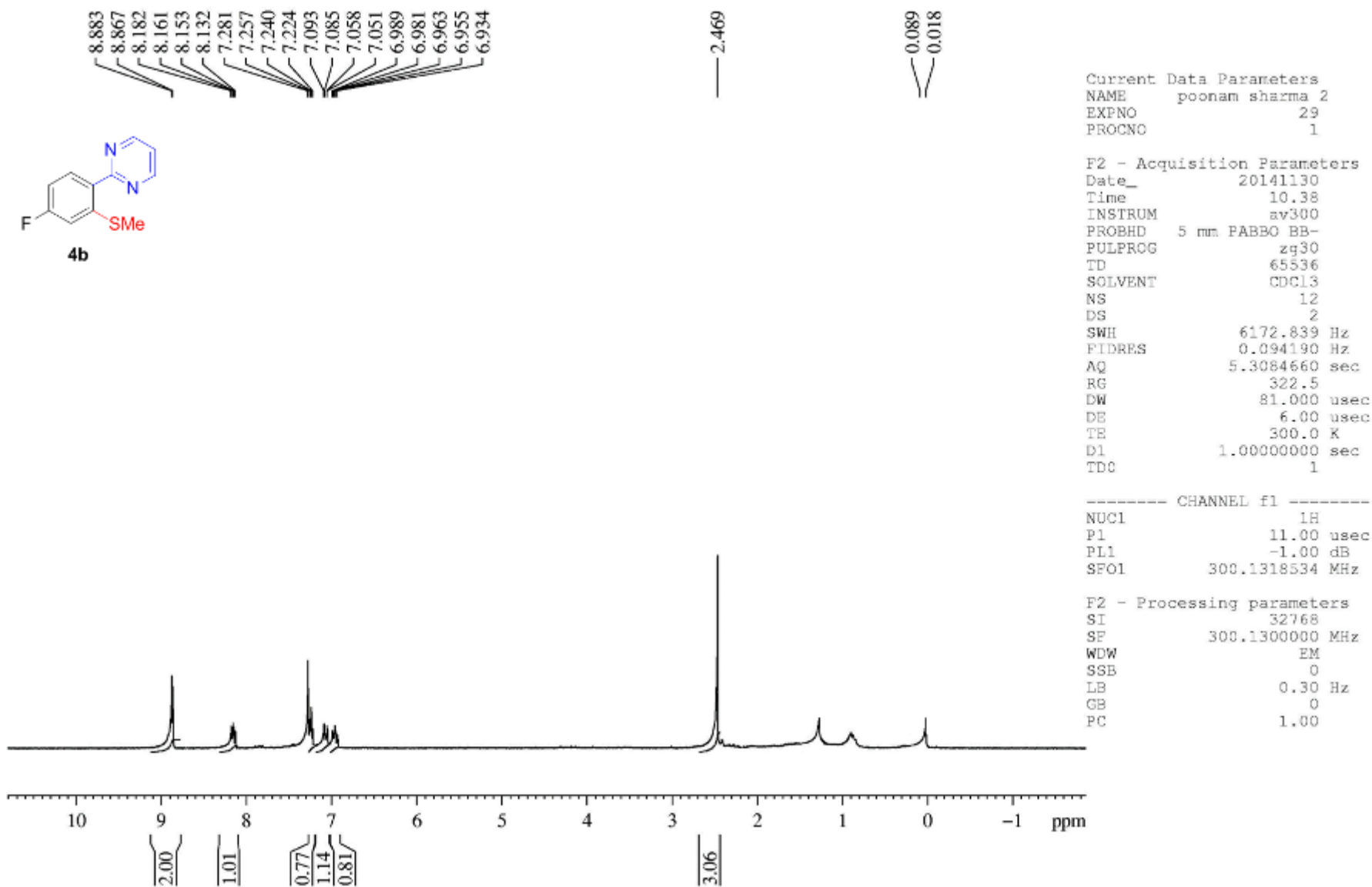
Spectrum 27. 300 MHz ^1H NMR of compound **4a**



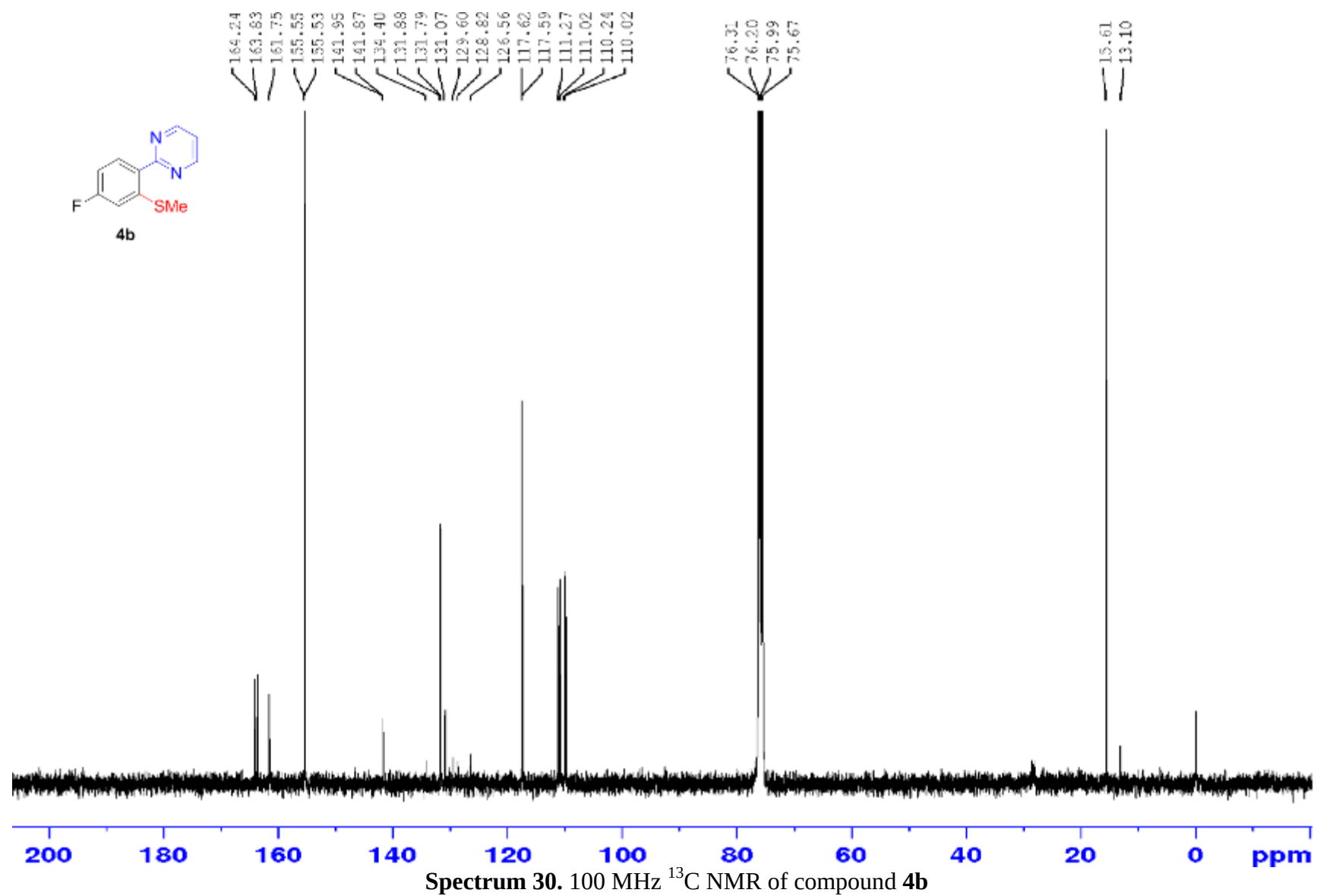
4a

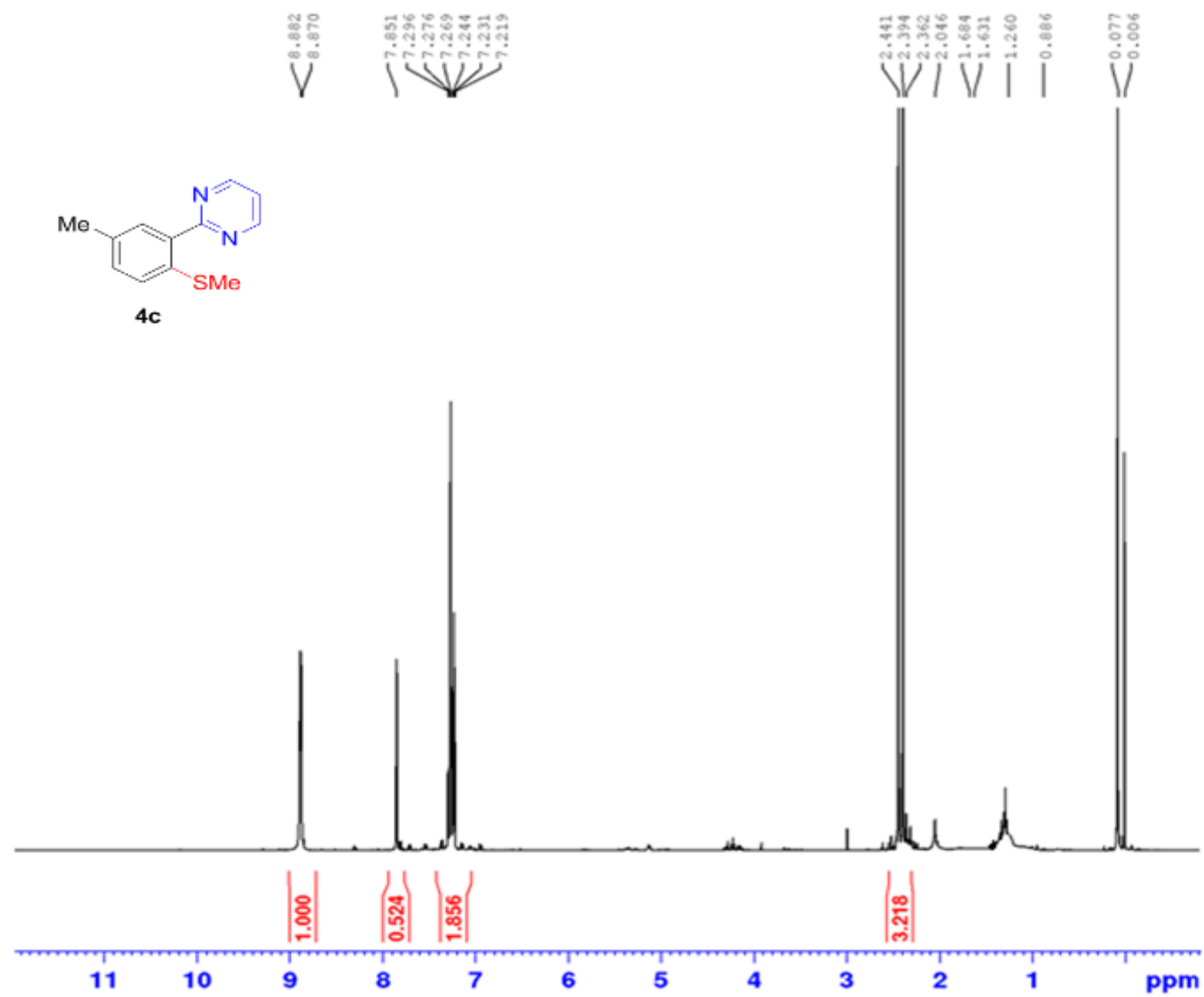


Spectrum 28. 75 MHz ^{13}C NMR of compound 4a



Spectrum 29. 300 MHz ¹H NMR of compound **4b**





Spectrum 31. 400 MHz ¹H NMR of compound