

Supporting Information

Microwave Assisted $[\text{RuCl}_2(p\text{-cymene})_2]_2$ Catalyzed Regioselective *Endo*-Tandem Cyclization Involving Imine and Alkyne Activation: An Approach to benzo[4,5]imidazo[2,1-*a*]pyridine Scaffold

Sudipta Kumar Manna ^a and Gautam Panda ^{a,b*}

^aMedicinal and Process Chemistry Division, CSIR-Central Drug Research Institute,
BS 10/1, Sector 10, Jankipuram extension, Sitapur Road, Lucknow 226031, India.

^bAcademy of Scientific and Innovative Research, New Delhi 110001, India.

Fax: (+91)-522-262-3405; Phone: (+91)-522-261-2411-18 (8 line)

E-mail : gautam.panda@gmail.com; gautam_panda@cdri.res.in

1. Contents	1-6
2. Spectra	7-79

Figure 1: ^1H -NMR Spectrum of **3b**.

Figure 2: ^{13}C -NMR Spectrum of **3b**.

Figure 3: ^1H -NMR Spectrum of **4a**.

Figure 4: ^{13}C -NMR Spectrum of **4a**.

Figure 5: ^1H -NMR Spectrum of **4b**.

Figure 6: ^{13}C -NMR Spectrum of **4b**.

Figure 7: ^1H -NMR Spectrum of **4c**.

Figure 8: ^{13}C -NMR Spectrum of **4c**.

Figure 9: ^1H -NMR Spectrum of **4d**.

Figure 10: ^{13}C -NMR Spectrum of **4d**.

Figure 11: ^1H -NMR Spectrum of **4e**.

Figure 12: ^{13}C -NMR Spectrum of **4e**.

Figure 13: ^1H -NMR Spectrum of **4f**.

Figure 14: ^{13}C -NMR Spectrum of **4f**.

Figure 15: ^1H -NMR Spectrum of **4g**.

Figure 16: ^{13}C -NMR Spectrum of **4g**.

Figure 17: ^1H -NMR Spectrum of **4h**.

Figure 18: ^{13}C -NMR Spectrum of **4h**.

Figure 19: ^1H -NMR Spectrum of **4i**.

Figure 20: ^{13}C -NMR Spectrum of **4i**.

Figure 21: ^1H -NMR Spectrum of **4j**.

Figure 22: ^{13}C -NMR Spectrum of **4j**.

Figure 23: ^1H -NMR Spectrum of **4k**.

Figure 24: ^{13}C -NMR Spectrum of **4k**.

Figure 25: ^1H -NMR Spectrum of **5a**.

Figure 26: ^{13}C -NMR Spectrum of **5a**.

Figure 27: ^1H -NMR Spectrum of **5b**.

Figure 28: ^{13}C -NMR Spectrum of **5b**.

Figure 29: ^1H -NMR Spectrum of **5c**.

Figure 30: ^{13}C -NMR Spectrum of **5c**.

Figure 31: ^1H -NMR Spectrum of **5d**.

Figure 32: ^{13}C -NMR Spectrum of **5d**.

Figure 33: DEPT-I -Spectrum of **5d**.

Figure 34: DEPT-II -Spectrum of **5d**.

Figure 35: HSQC -Spectrum of **5d**.

Figure 36: HMBC -Spectrum of **6d**.

Figure 37: COSY -Spectrum of **5d**.

Figure 38: ^1H -NMR Spectrum of **5e**.

Figure 39: ^{13}C -NMR Spectrum of **5e**.

Figure 40: ^1H -NMR Spectrum of **5f**.

Figure 41: ^{13}C -NMR Spectrum of **5f**.

Figure 42: ^1H -NMR Spectrum of **5g**.

Figure 43: ^{13}C -NMR Spectrum of **5g**.

Figure 44: DEPT-I -Spectrum of **5g**.

Figure 45: DEPT-II -Spectrum of **5g**.

Figure 46: HSQC -Spectrum of **5g**.

Figure 47: HMBC -Spectrum of **5g**.

Figure 48: COSY -Spectrum of **5g**.

Figure 49: ^1H -NMR Spectrum of **5h**.

Figure 50: ^{13}C -NMR Spectrum of **5h**.

Figure 51: ^1H -NMR Spectrum of **5i**.

Figure 52: ^{13}C -NMR Spectrum of **5i**.

Figure 63: ^1H -NMR Spectrum of **5j**.

Figure 54: ^{13}C -NMR Spectrum of **5j**.

Figure 55: ^1H -NMR Spectrum of **5k**.

Figure 56: ^{13}C -NMR Spectrum of **5k**.

Figure 57: ^1H -NMR Spectrum of **5l**.

Figure 58: ^{13}C -NMR Spectrum of **5l**.

Figure 59: ^1H -NMR Spectrum of **5m**.

Figure 60: ^{13}C -NMR Spectrum of **5m**.

Figure 61: ^1H -NMR Spectrum of **5n**.

Figure 62: ^{13}C -NMR Spectrum of **5n**.

Figure 63: ^1H -NMR Spectrum of **5o**.

Figure 64: ^1H -NMR Spectrum of **5p**.

Figure 65: ^1H -NMR Spectrum of **5q**.

Figure 66: ^{13}C -NMR Spectrum of **5q**.

Figure 67: ^1H -NMR Spectrum of **5r**.

Figure 68: ^{13}C -NMR Spectrum of **5r**.

Figure 69: ^1H -NMR Spectrum of **5s**.

Figure 70: ^1H -NMR Spectrum of **U**.

Figure 71: ^{13}C -NMR Spectrum of **U**.

Figure 72: DEPT-I -Spectrum of **U**.

Figure 73: DEPT-II -Spectrum of **U**.

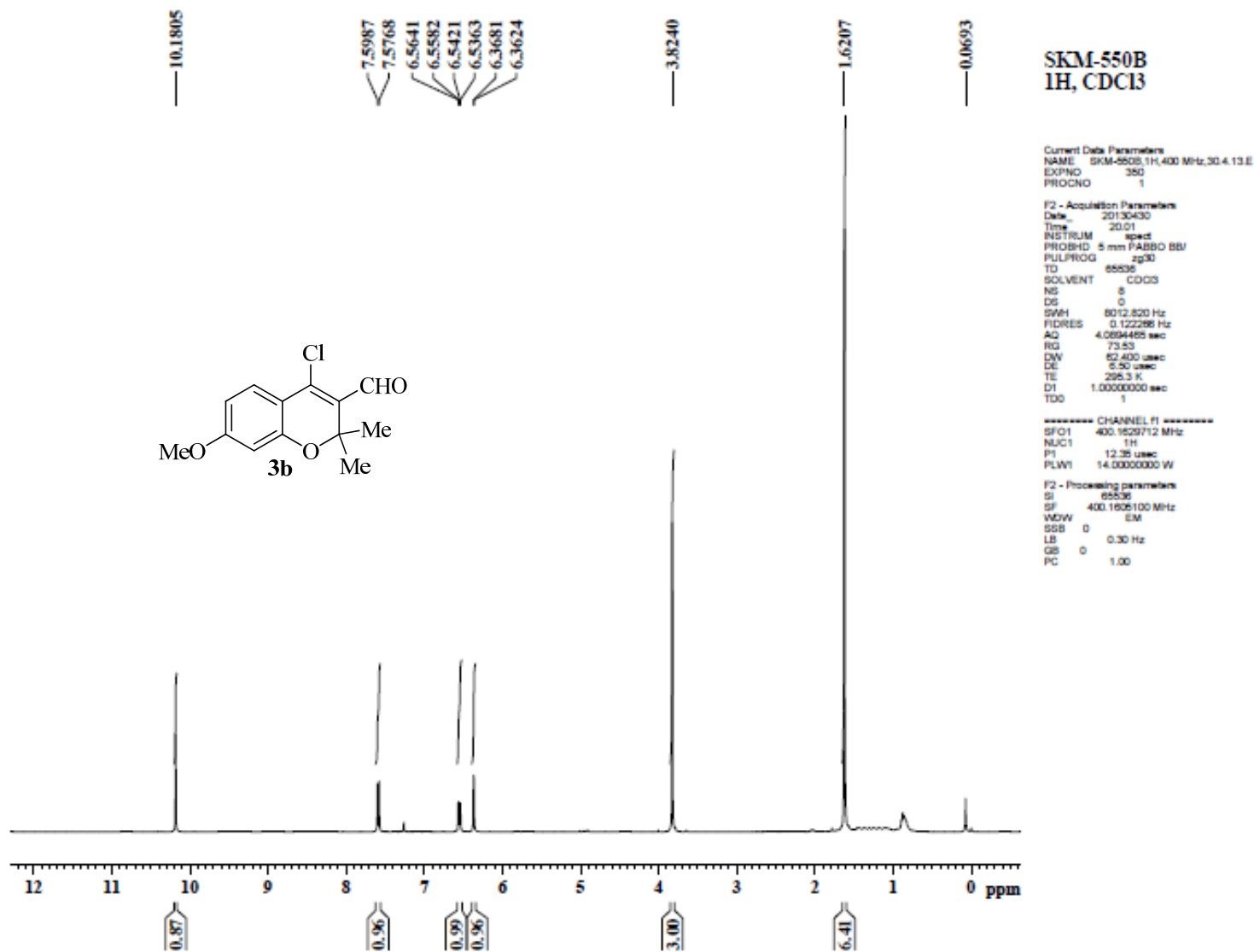


Figure 1: ¹H -NMR Spectrum of **3b**.

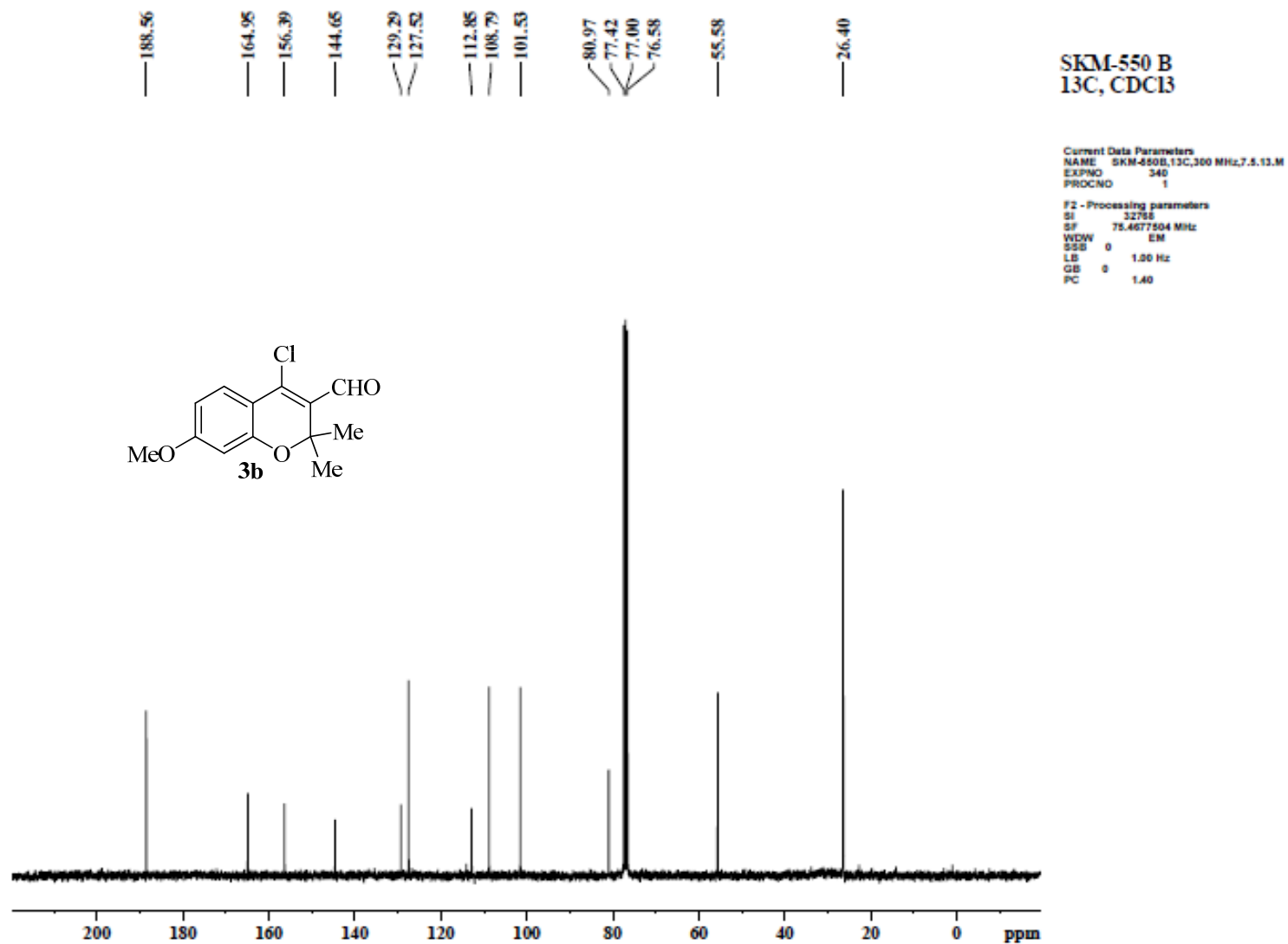


Figure 2: ¹³C -NMR Spectrum of **3b**.

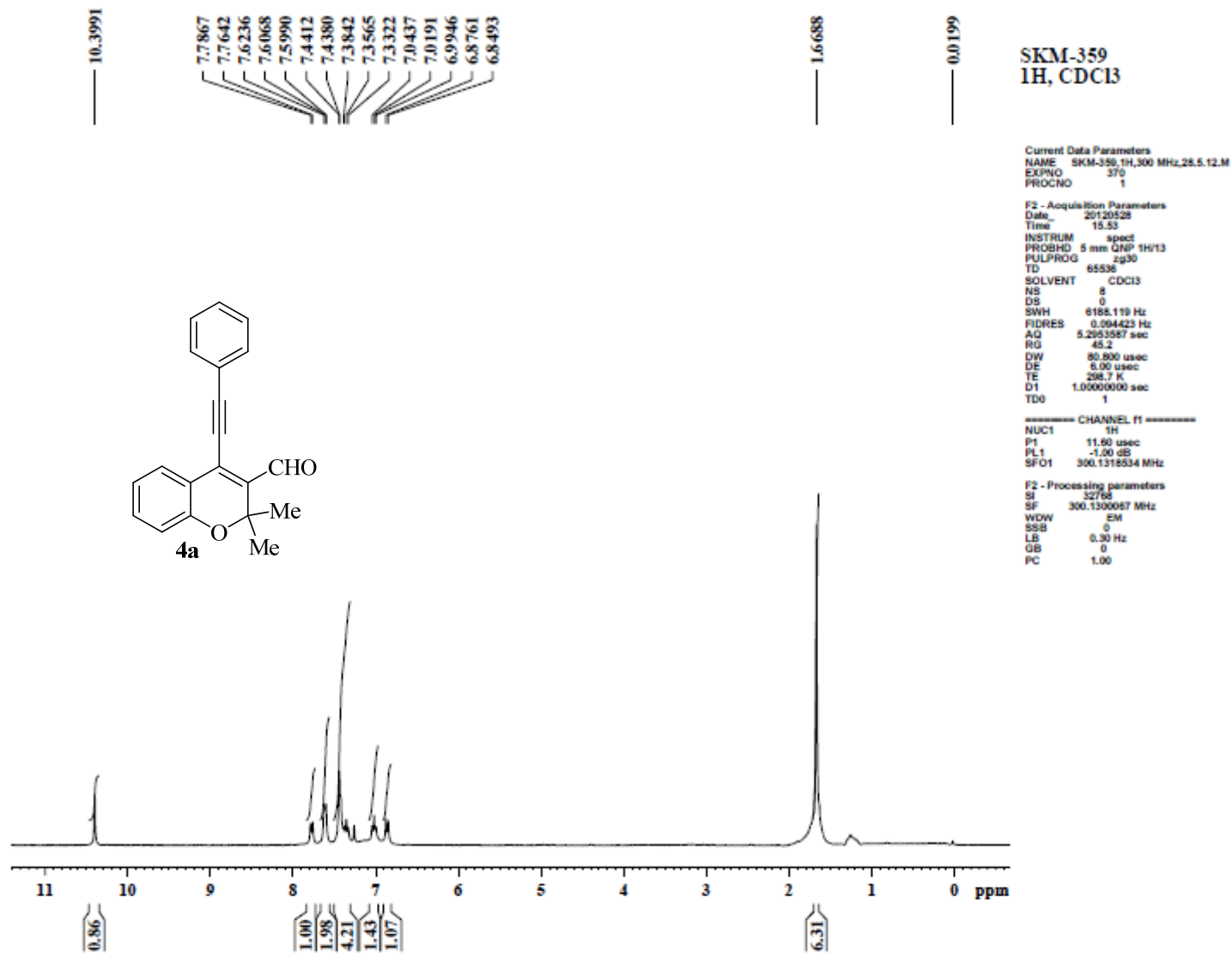


Figure 3: ¹H -NMR Spectrum of 4a.

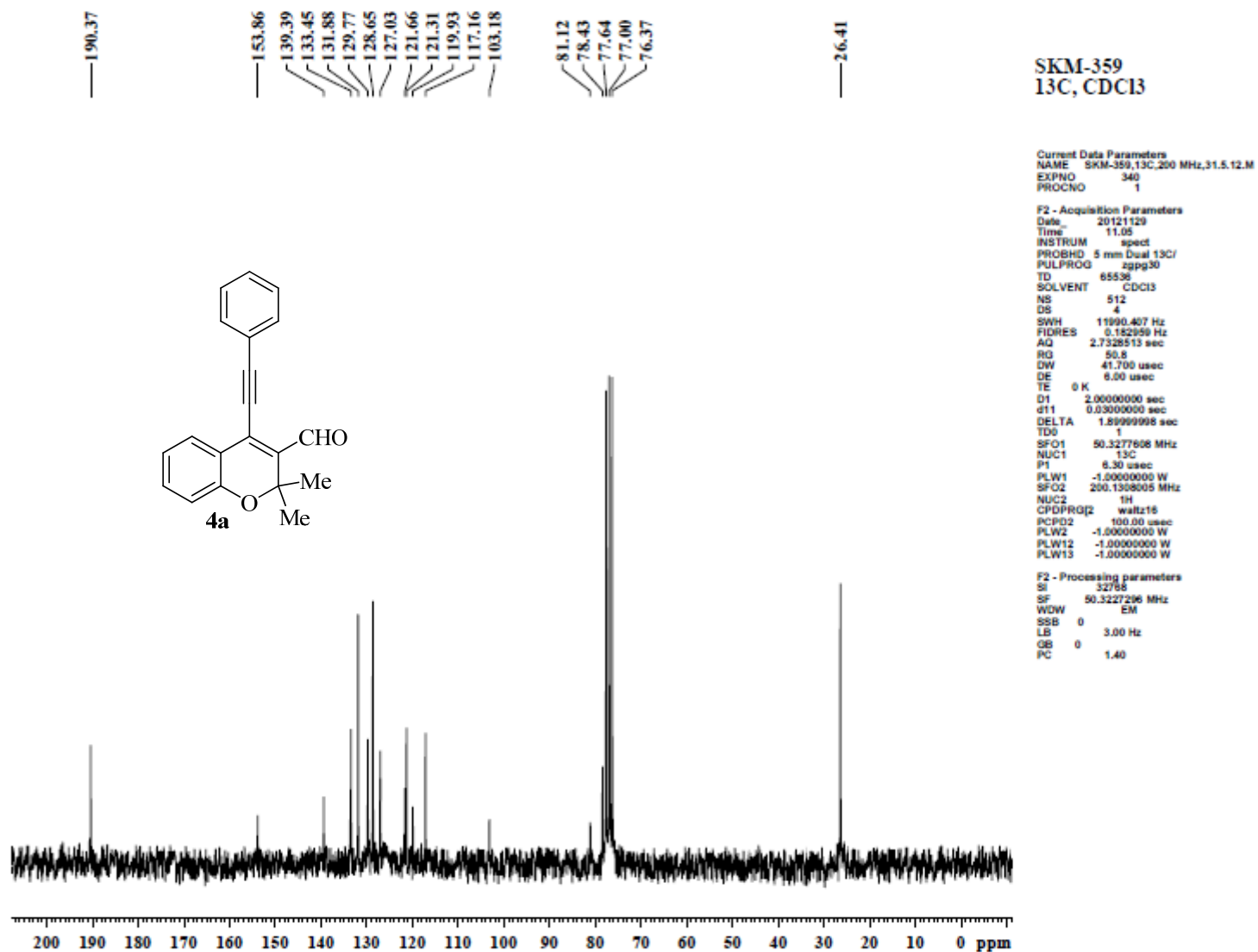


Figure 4: ¹³C -NMR Spectrum of **4a**.

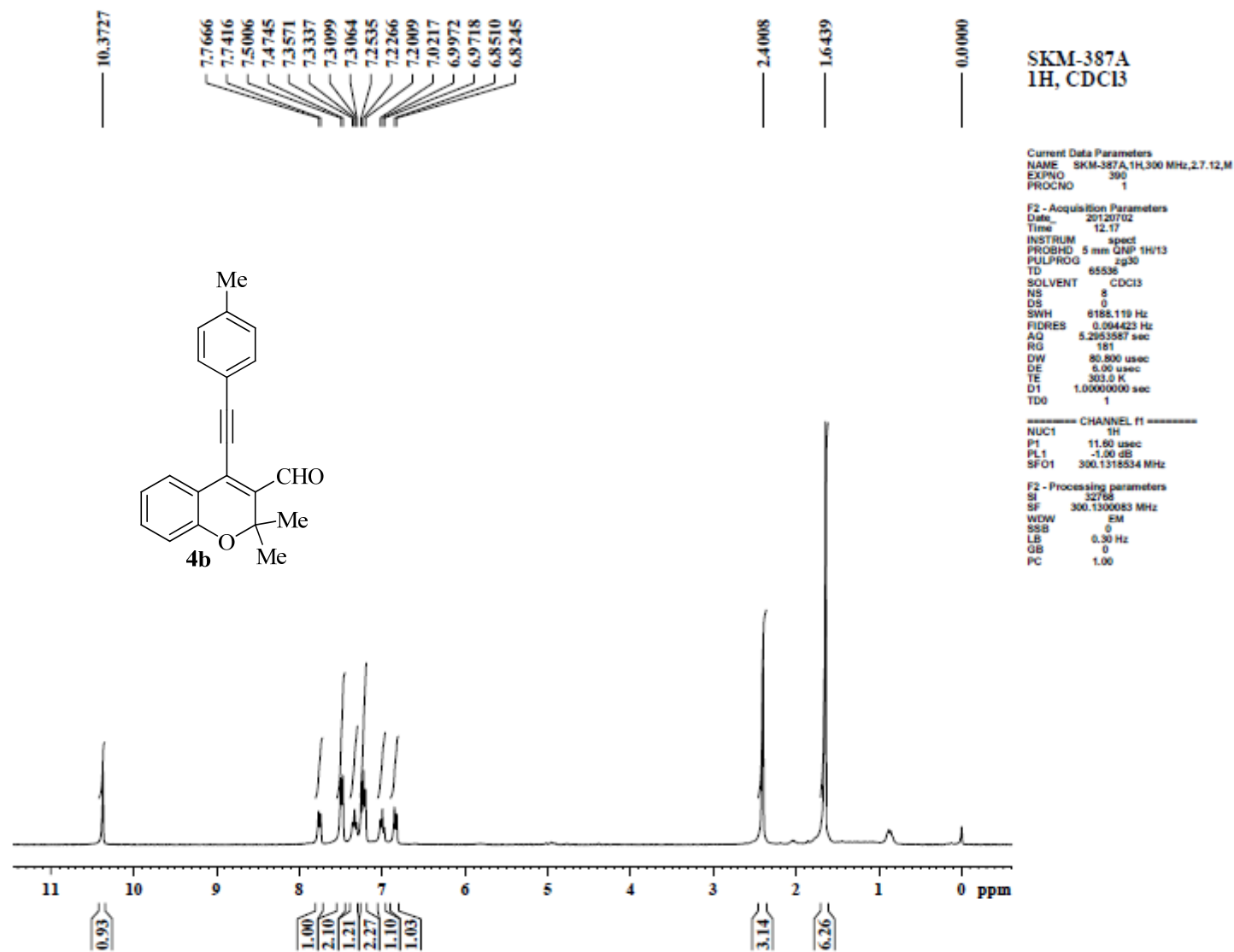
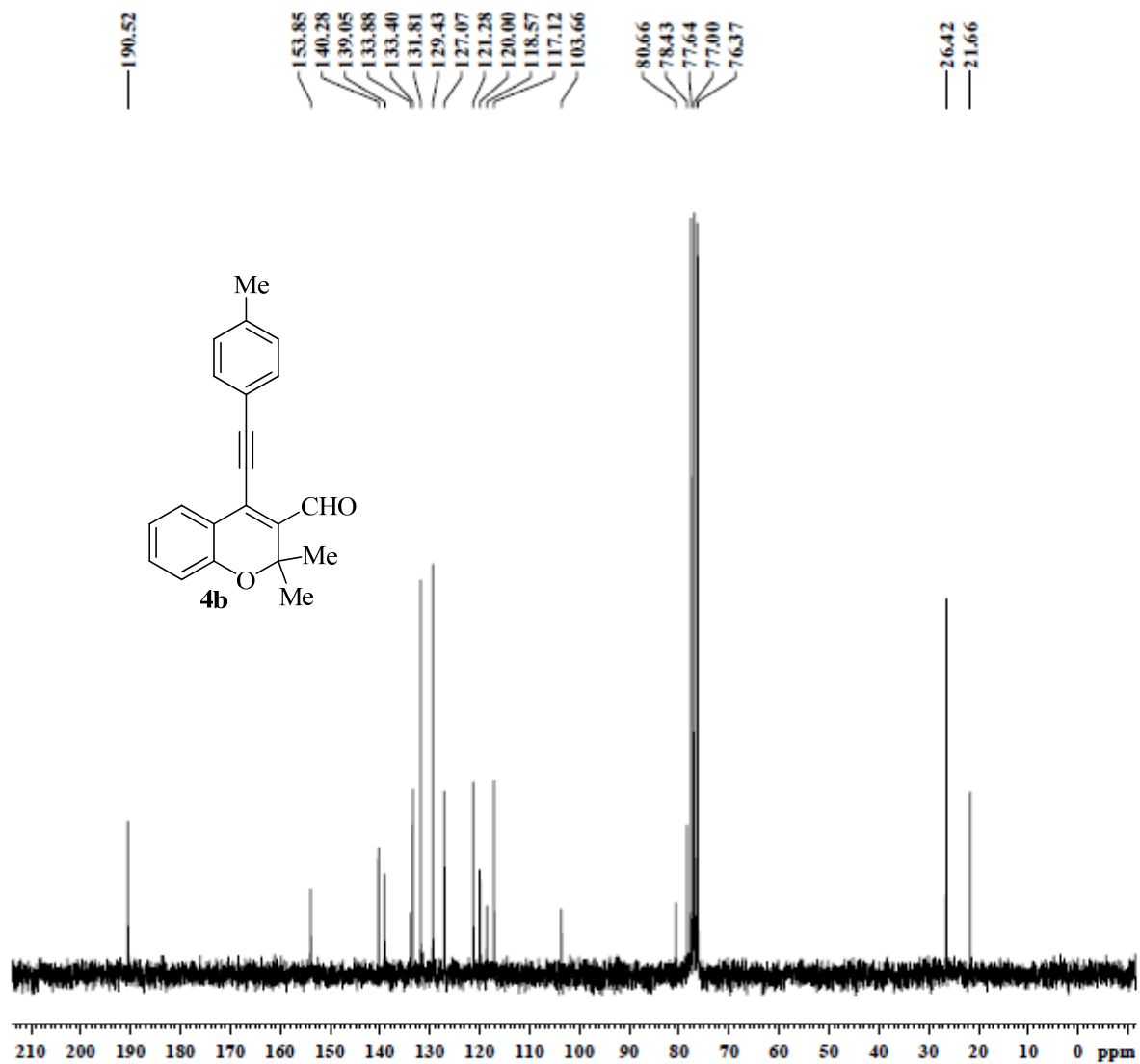


Figure 5: ¹H -NMR Spectrum of **4b**.



SKM-387A
13C, CDCl3

Current Data Parameters
NAME SKM-387A,13C,200 MHz,4.7.12.M
EXPNO 320
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120704
Time 14.25
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 11900.407 Hz
FIDRES 0.18280 Hz
AQ 2.7328513 sec
RG 57
DW 41.700 usec
DE 8.00 usec
TE 0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TDO 1
SFO1 50.3277608 MHz
NUC1 13C
P1 8.20 usec
PLW1 -1.0000000 W
SFO2 200.1308005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 100.00 usec
PLW2 -1.0000000 W
PLW12 -1.0000000 W
PLW13 -1.0000000 W

F2 - Processing parameters
SI 32768
SF 50.327296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 6: ¹³C -NMR Spectrum of **4b**.

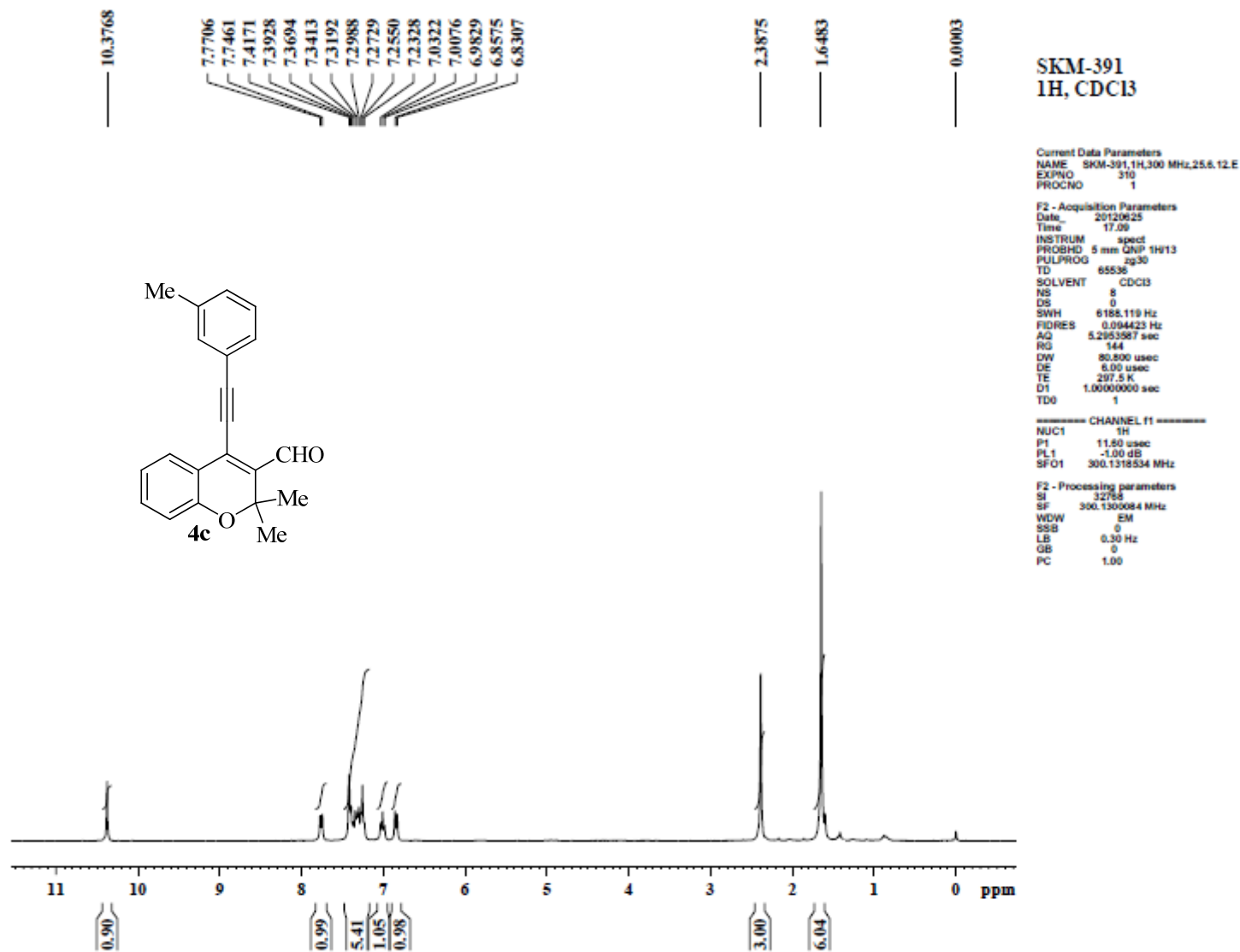
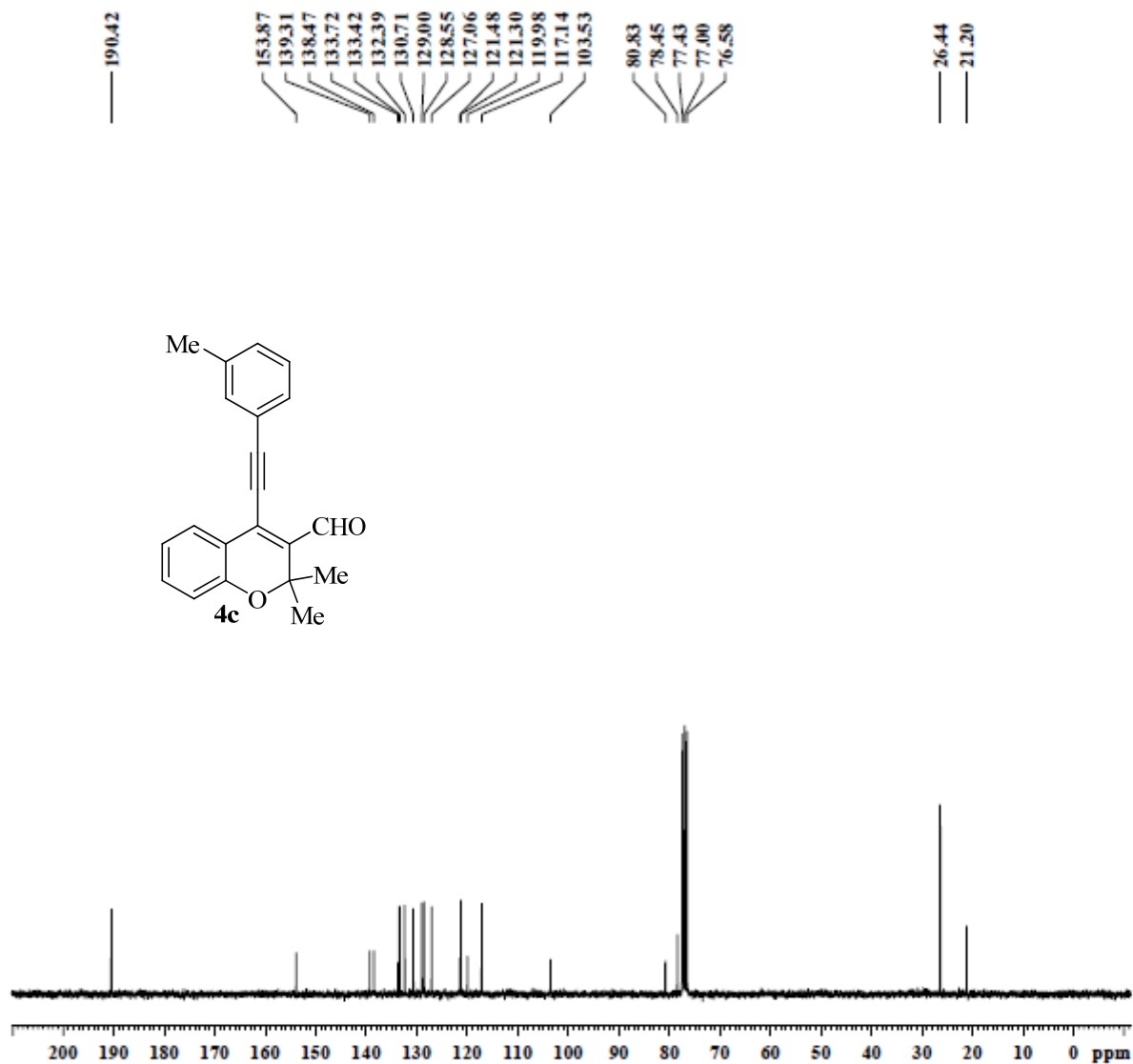


Figure 7: ^1H -NMR Spectrum of **4c**.



SKM-391
13C, CDCl3

Current Data Parameters
 NAME SKM-391,13C,200 MHz,28.6,12.M
 EXPNO 360
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120629
 Time 8.48
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275095 Hz
 AQ 1.8175818 sec
 RG 14.2
 DW 27.733 usec
 DE 6.00 usec
 TE 303.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.70 usec
 PL1 -3.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 17.00 dB
 PL13 21.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677498 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 8: ¹³C -NMR Spectrum of **4c**.

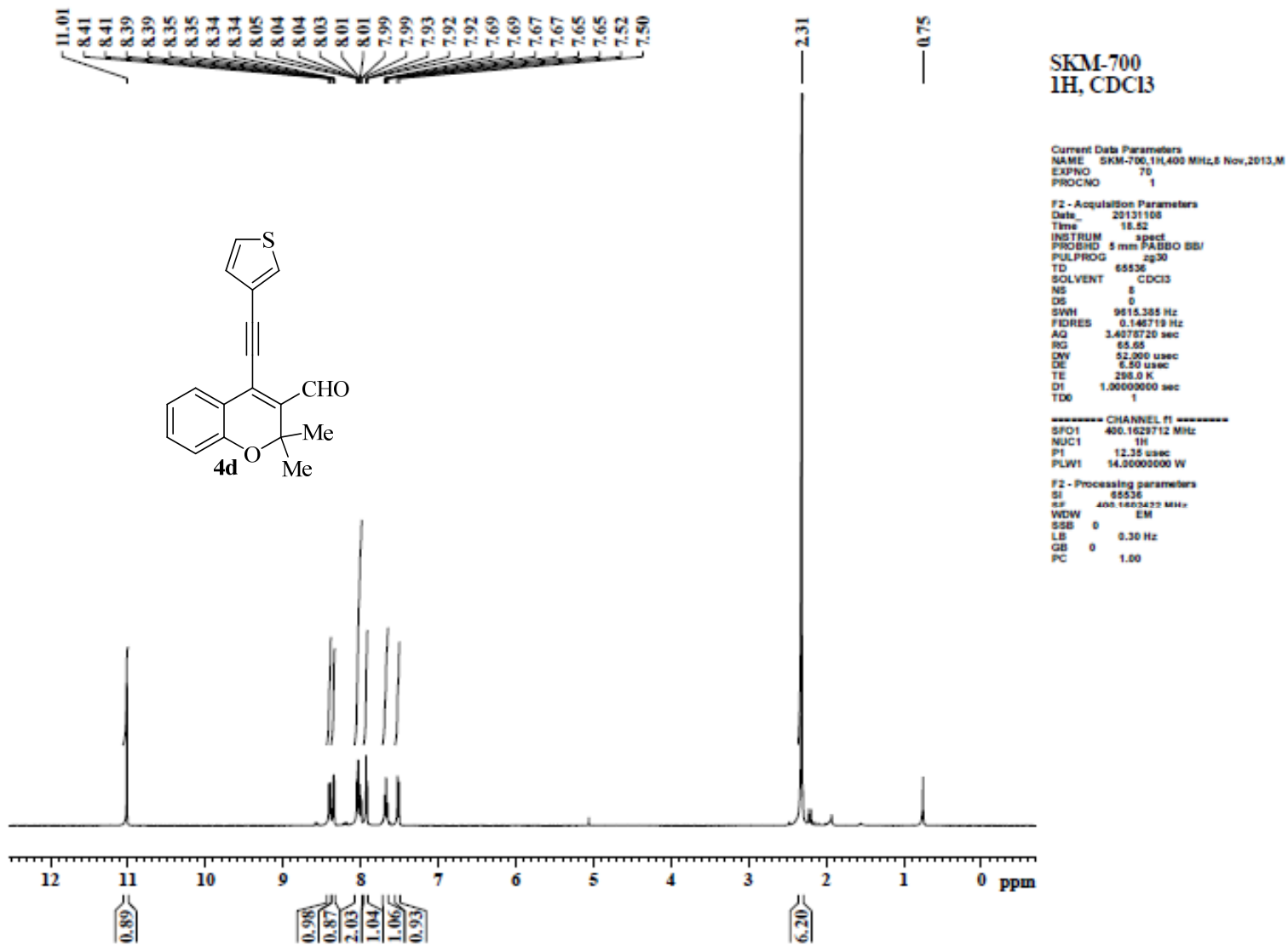
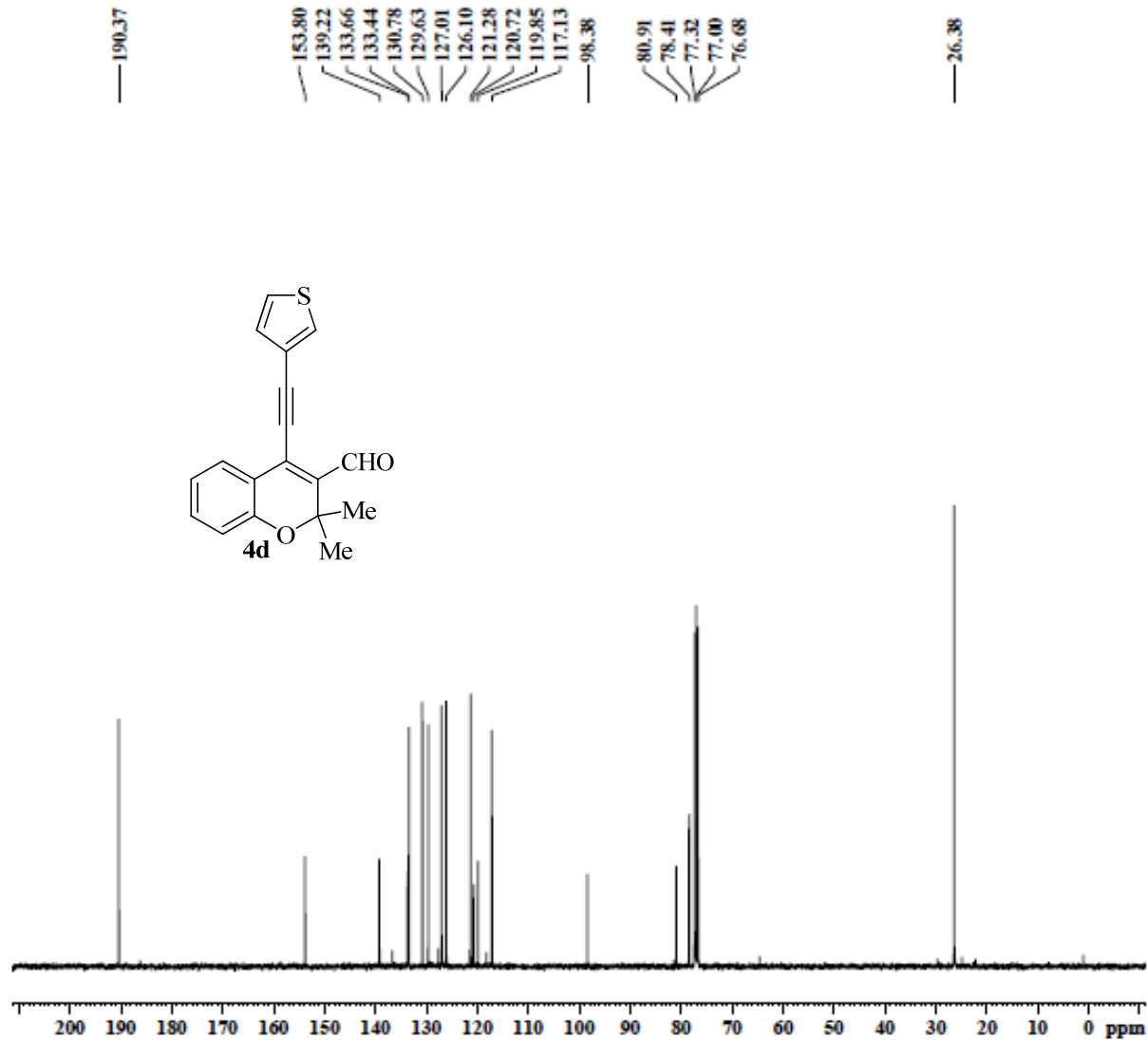


Figure 9: ¹H -NMR Spectrum of **4d**.



SKM-700
13C, CDC13

Current Data Parameters
NAME SKM-700_13C_400 MHz_11 Nov_2013_E
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131112
Time 4.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.386798 Hz
AQ 1.3631488 sec
RG 201.48
DW 20.500 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 100.6304993 MHz
NUC1 13C
P1 8.20 usec
PLW1 70.59999847 W

----- CHANNEL f2 -----
SFO2 400.1621006 MHz
NUC2 1H
CPOPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.26381999 W
PLW13 0.21353000 W

F2 - Processing parameters
SI 32768
SF 100.6304433 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 10: ¹³C -NMR Spectrum of **4d**.

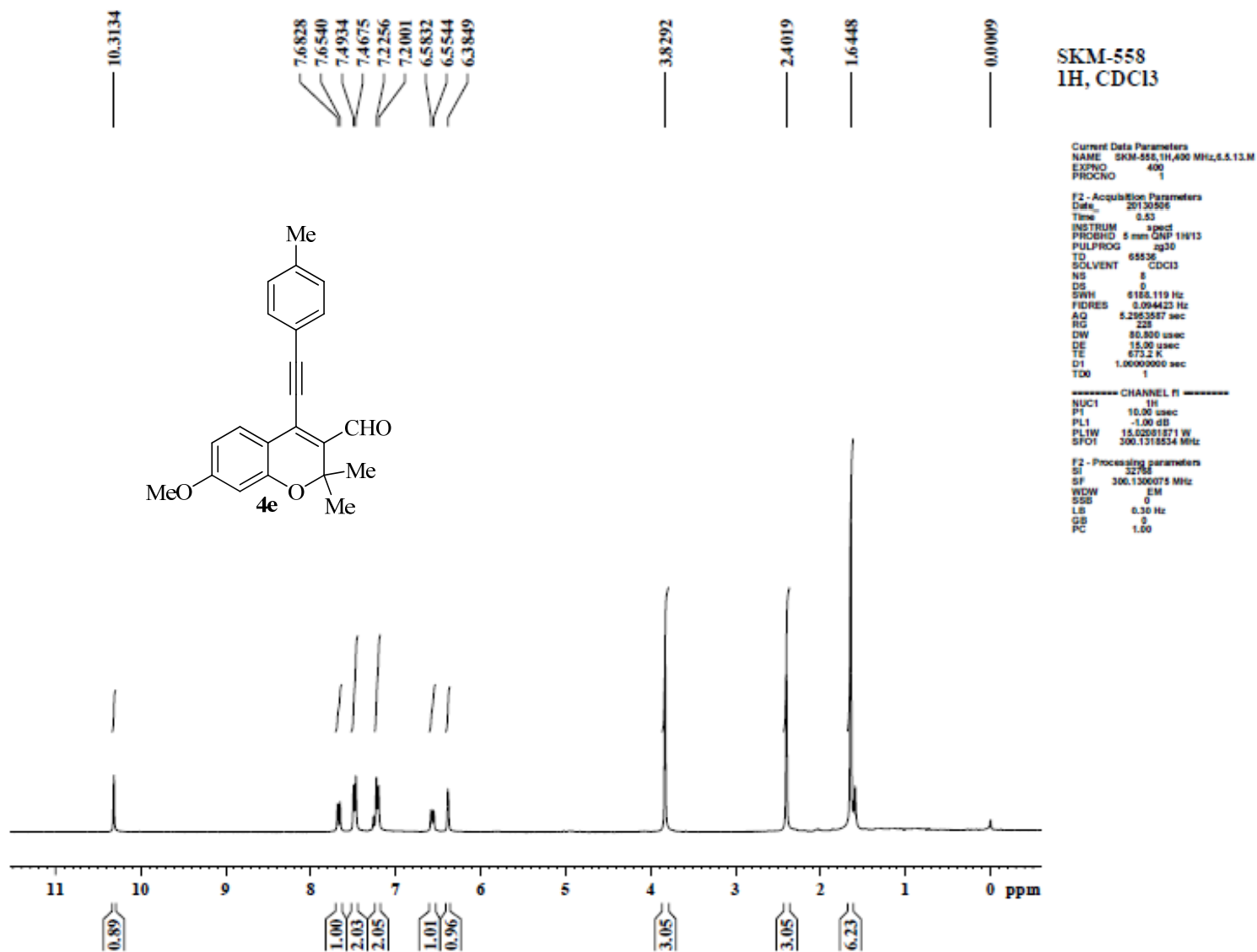


Figure 11: ¹H -NMR Spectrum of **4e**.

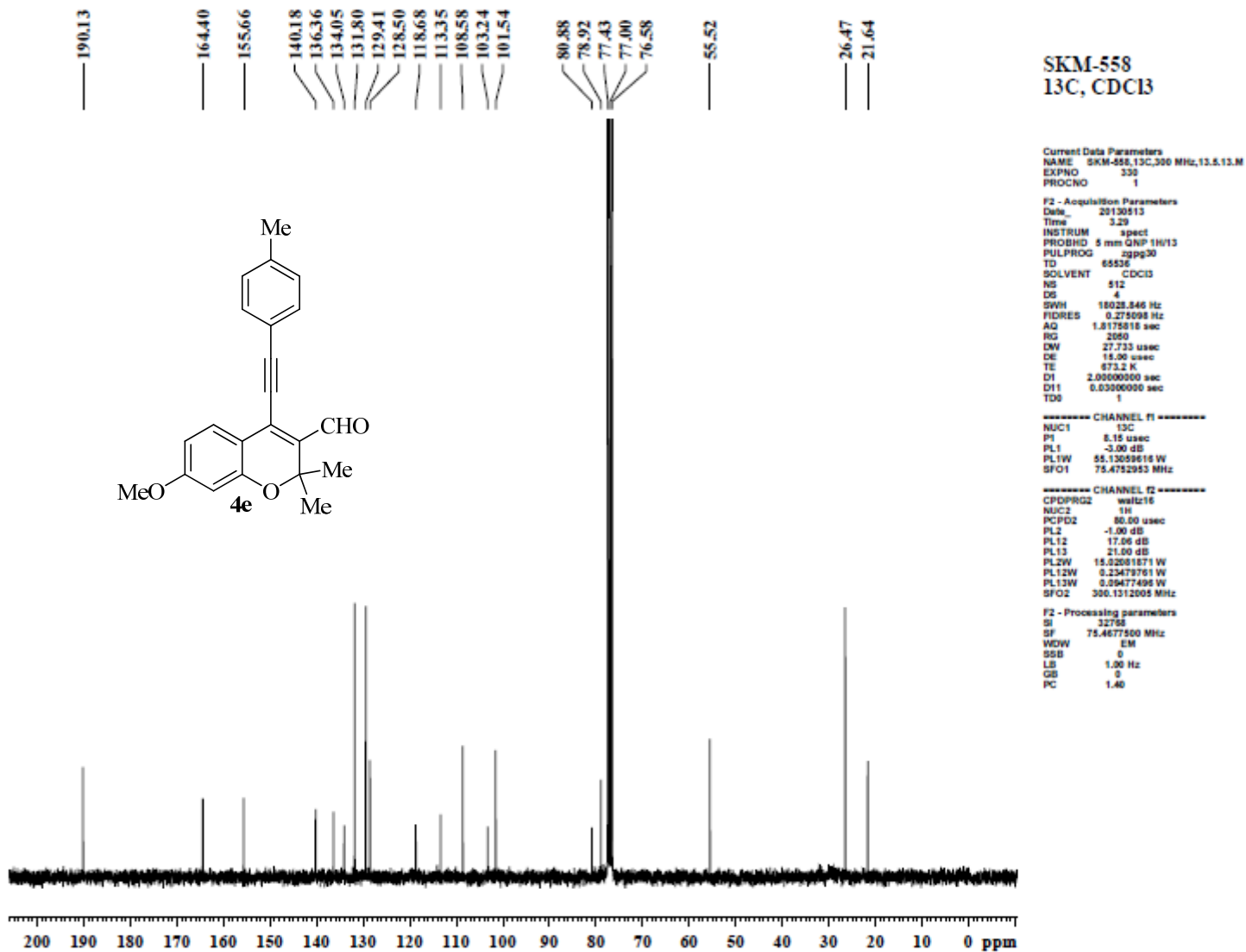


Figure 12: ^{13}C -NMR Spectrum of **4e**.

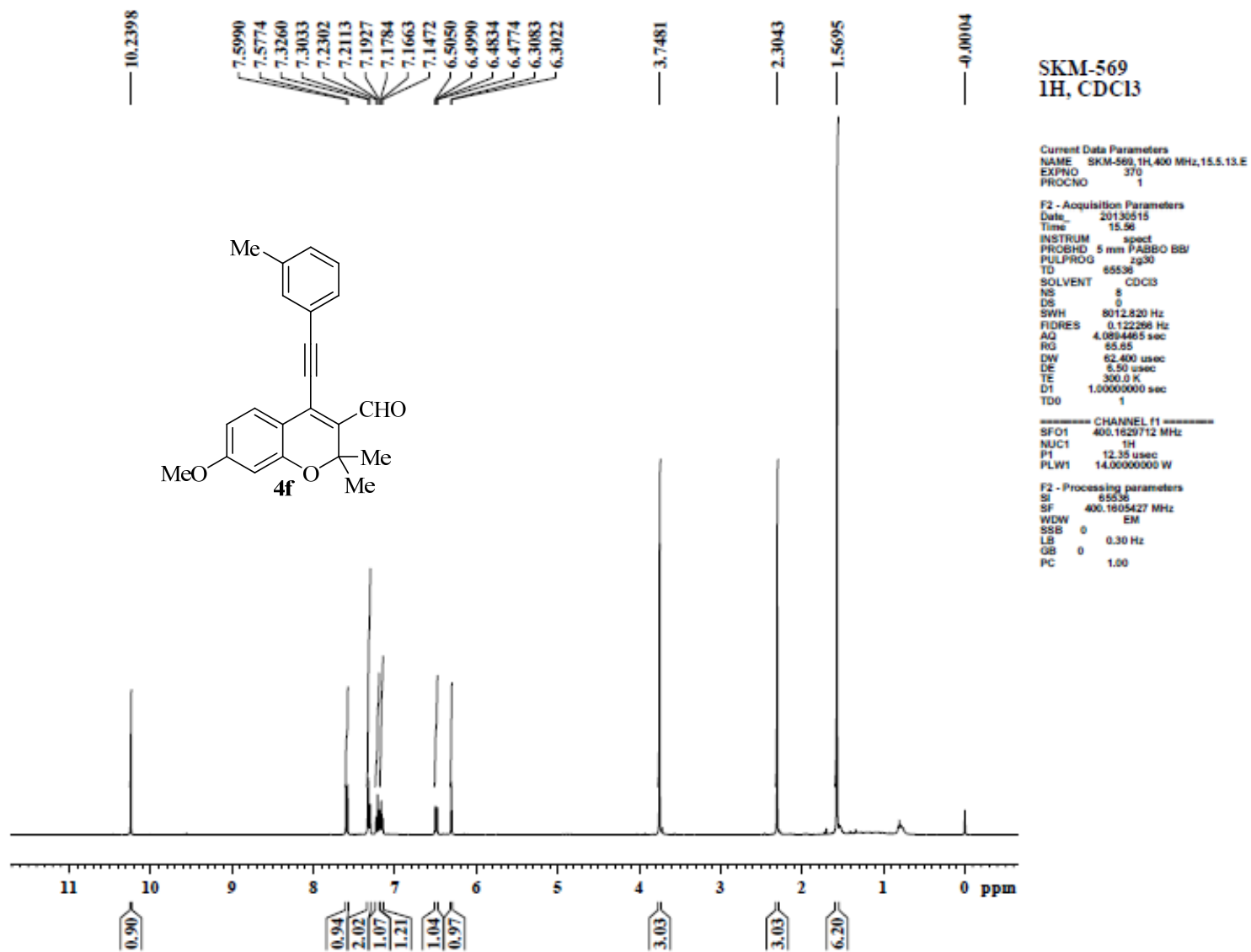


Figure 13: ¹H -NMR Spectrum of **4f**.

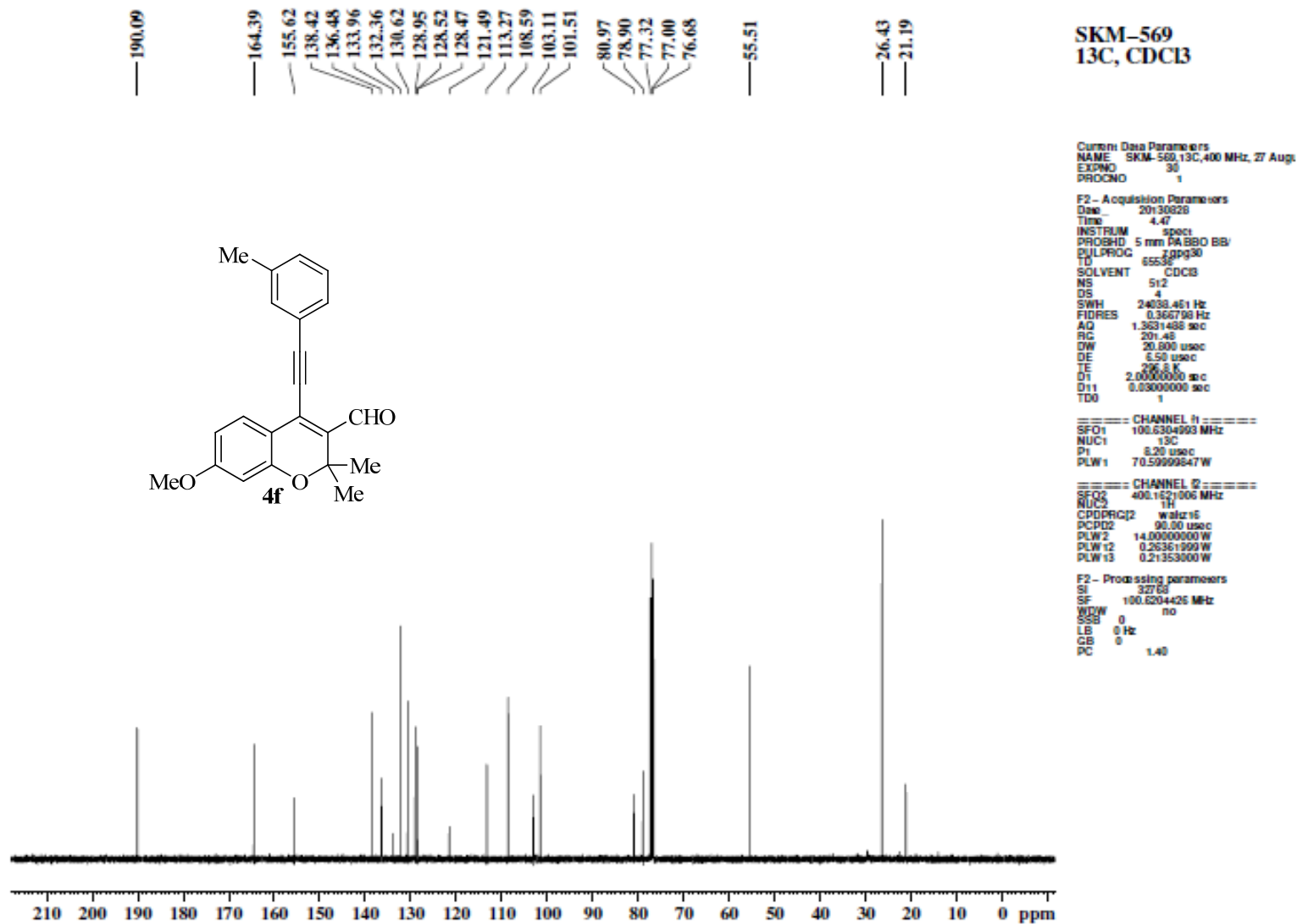


Figure 14: ¹³C -NMR Spectrum of **4f**.

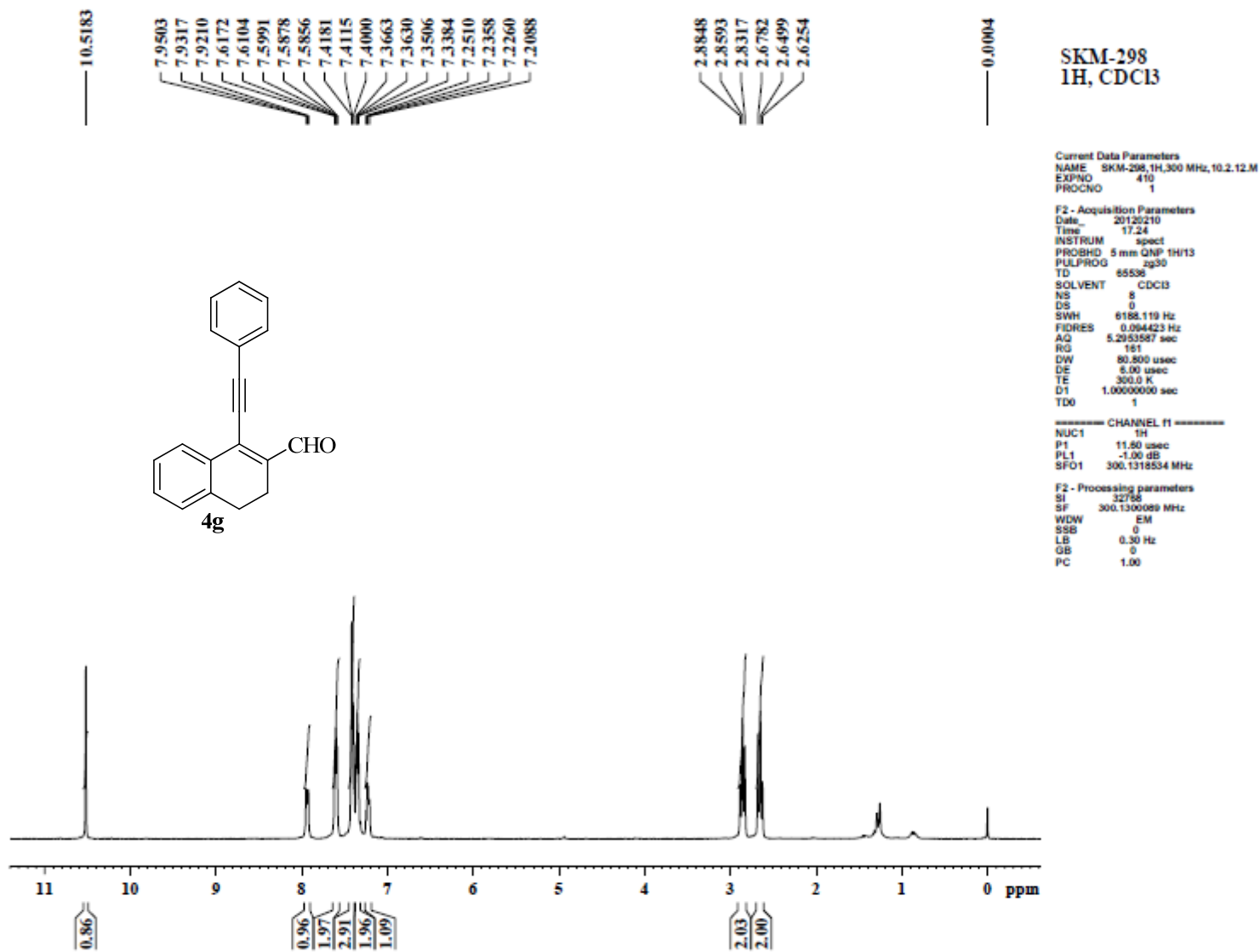


Figure 15: ¹H -NMR Spectrum of **4g**.

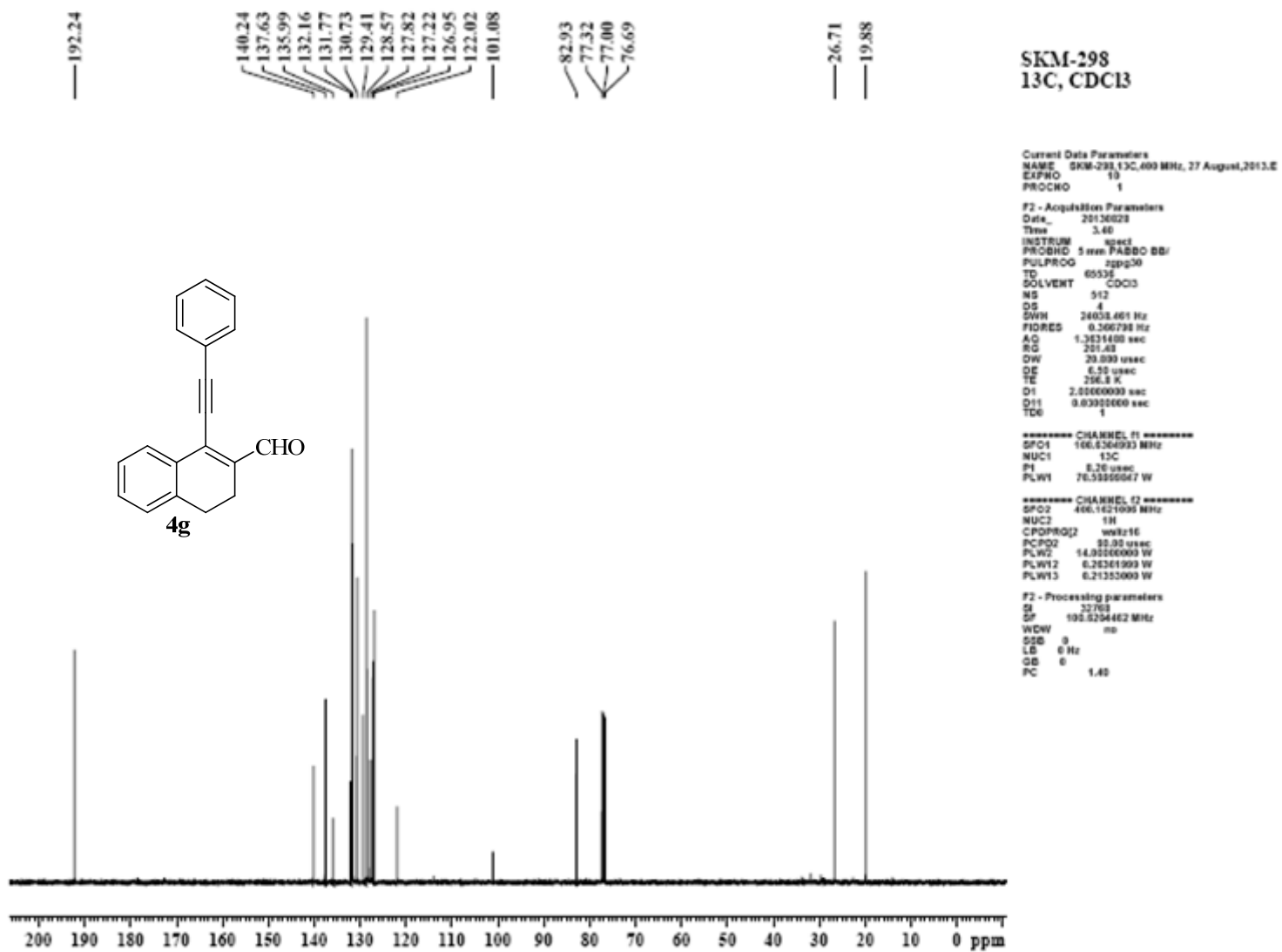


Figure 16: ^{13}C -NMR Spectrum of **4g**.

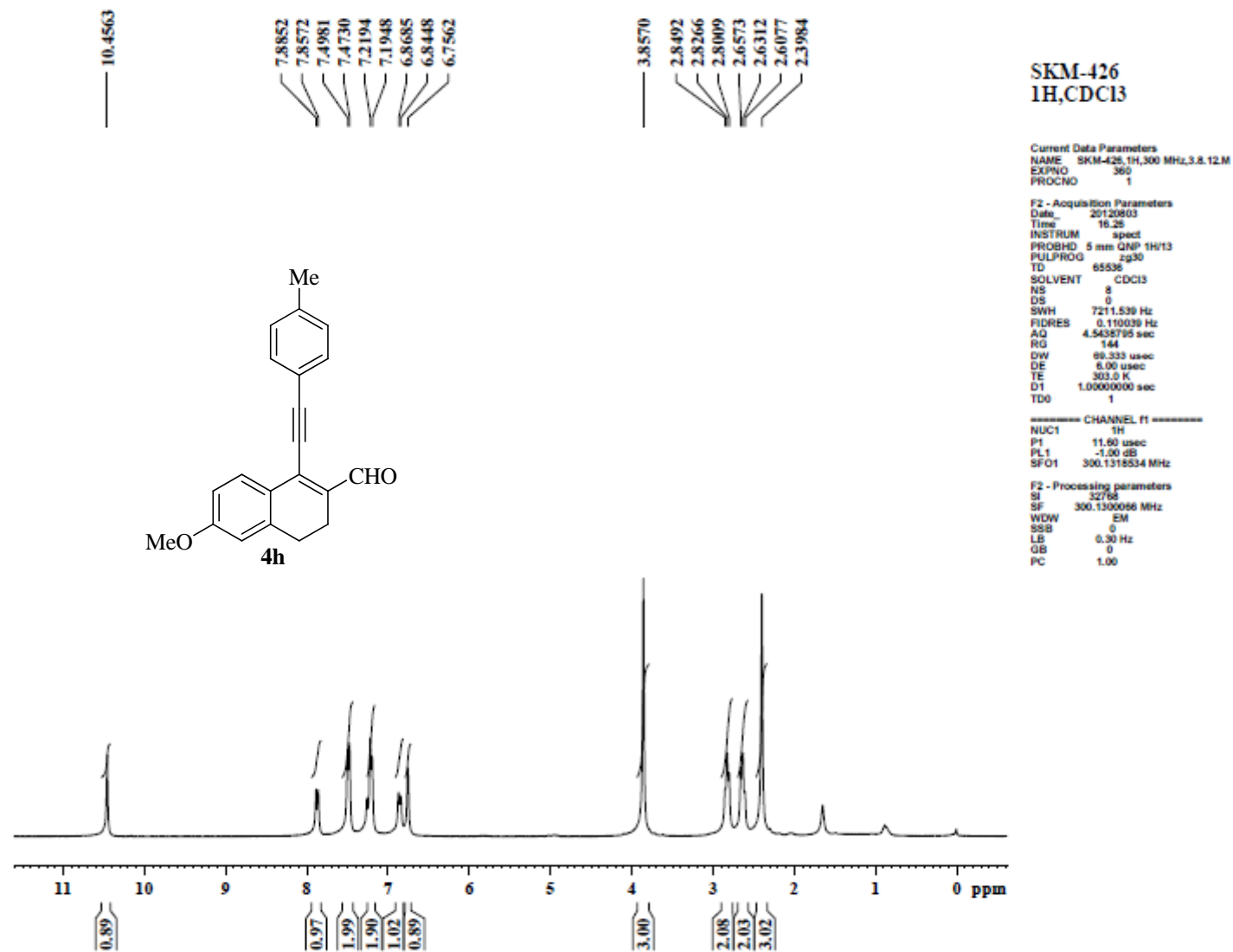
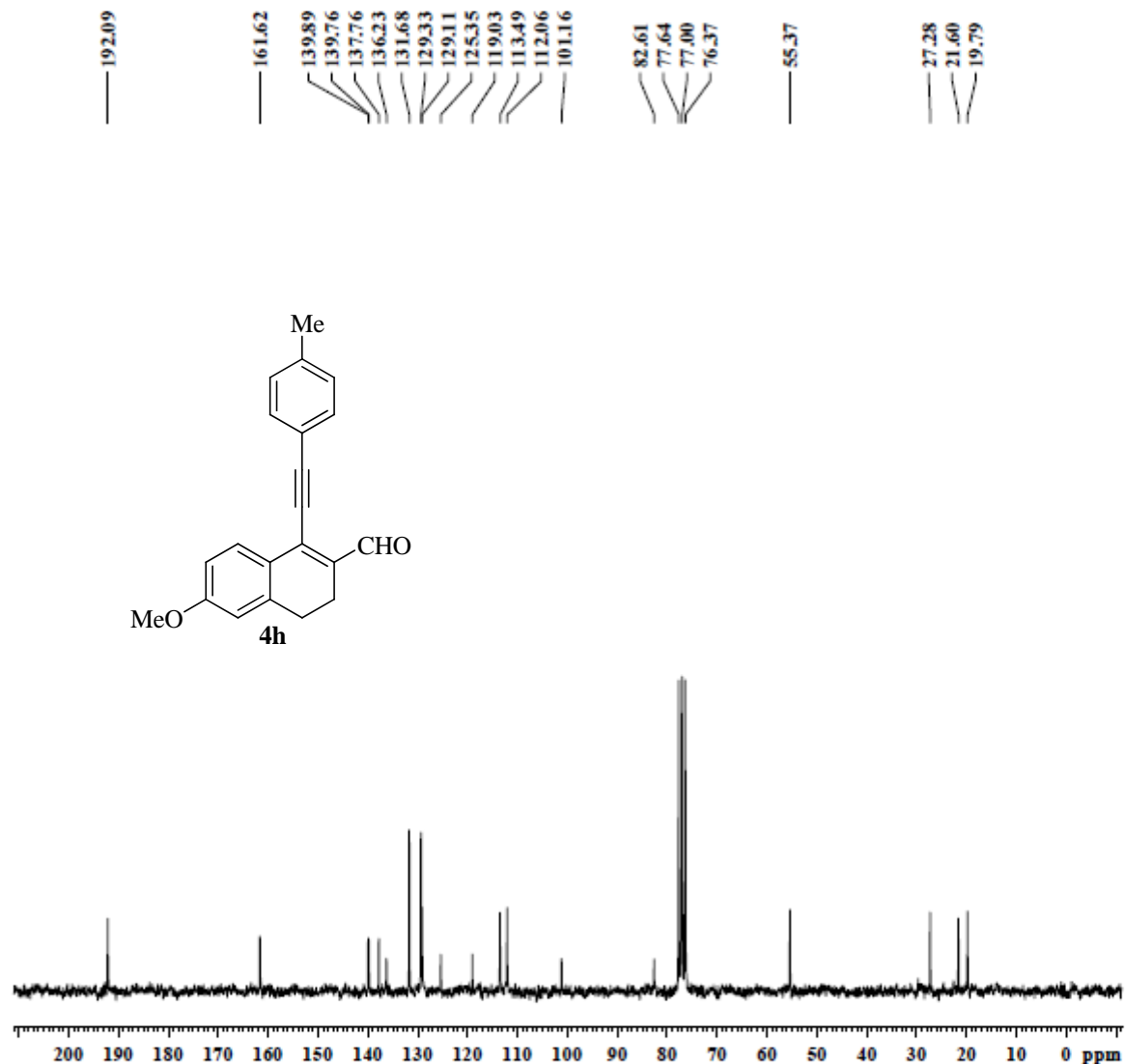


Figure 17: ¹H -NMR Spectrum of 4h.



SKM-426
13C, CDCl₃

Current Data Parameters
NAME SKM-426,13C,200 MHz,9.8.12.M
EXPNO 400
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120809
Time 10.36
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 256
DS 4
SWH 11990.407 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 50.8
DWF 41.700 usec
DE 0.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.80000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SFO1 50.3277868 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 18.00 dB
PL13 22.00 dB
SFO2 200.1308005 MHz

F2 - Processing parameters
SI 32768
SF 50.3227315 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Figure 18: ¹³C -NMR Spectrum of **4h**.

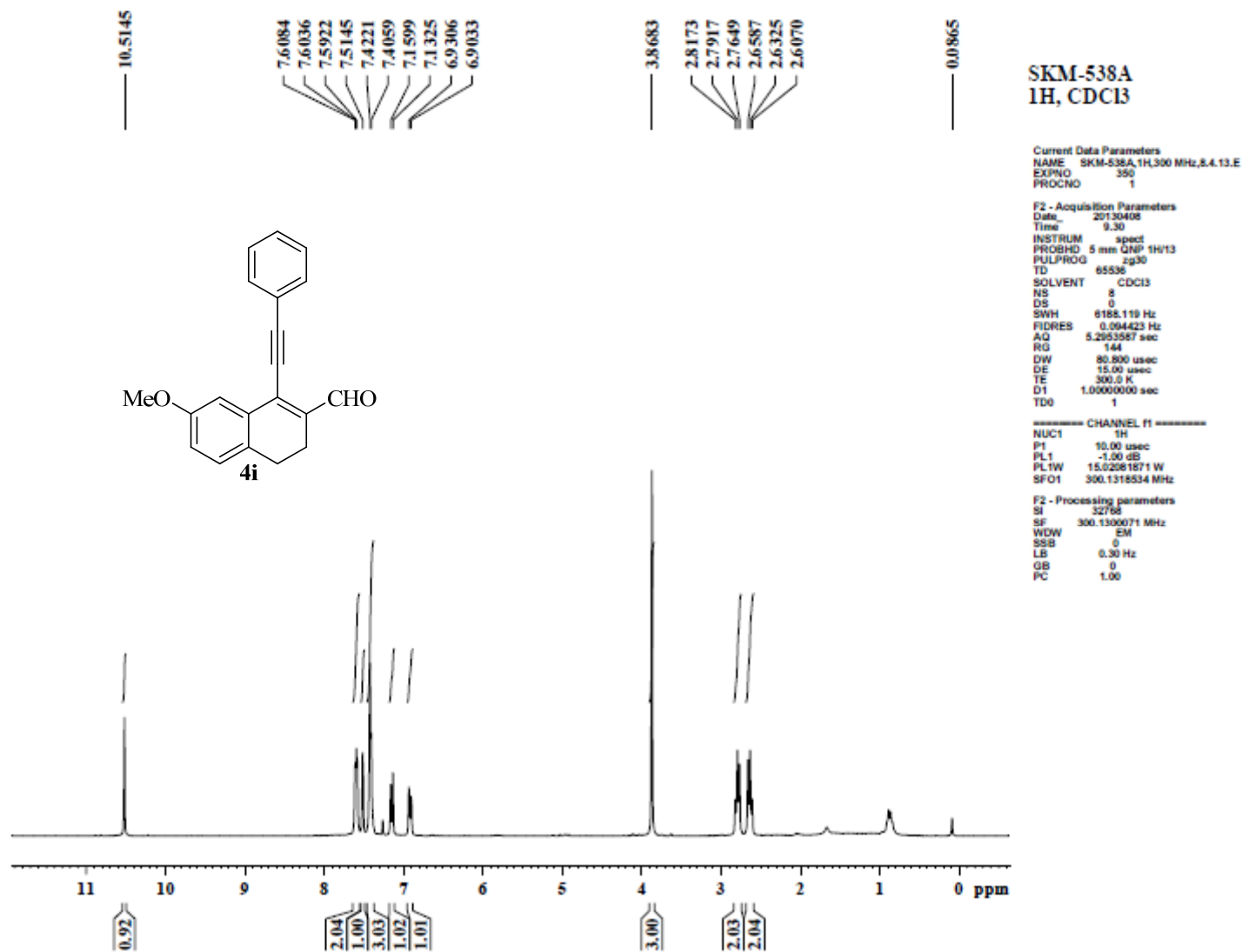


Figure 19: ^1H -NMR Spectrum of **4i**.

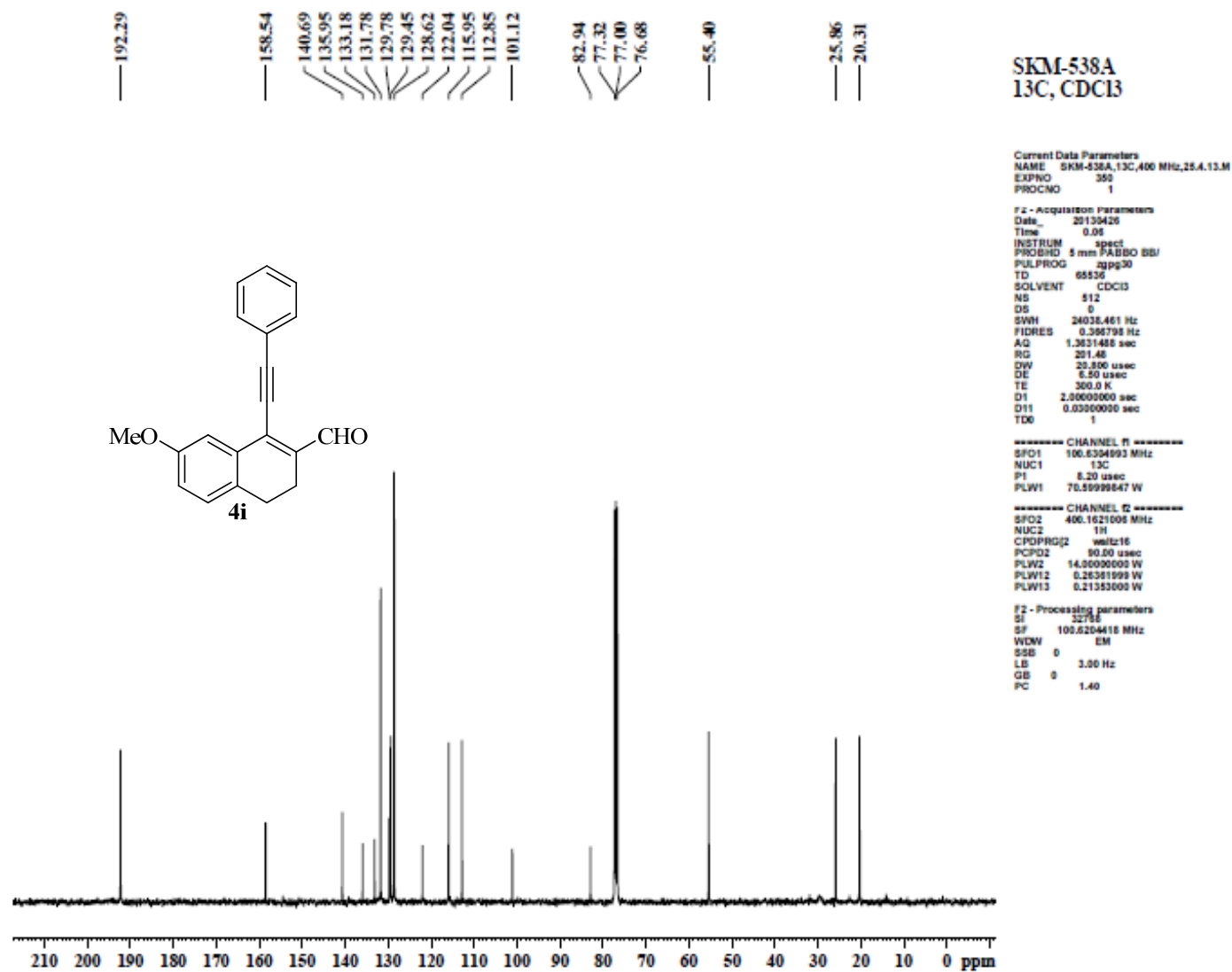


Figure 20: ^{13}C -NMR Spectrum of **4i**.

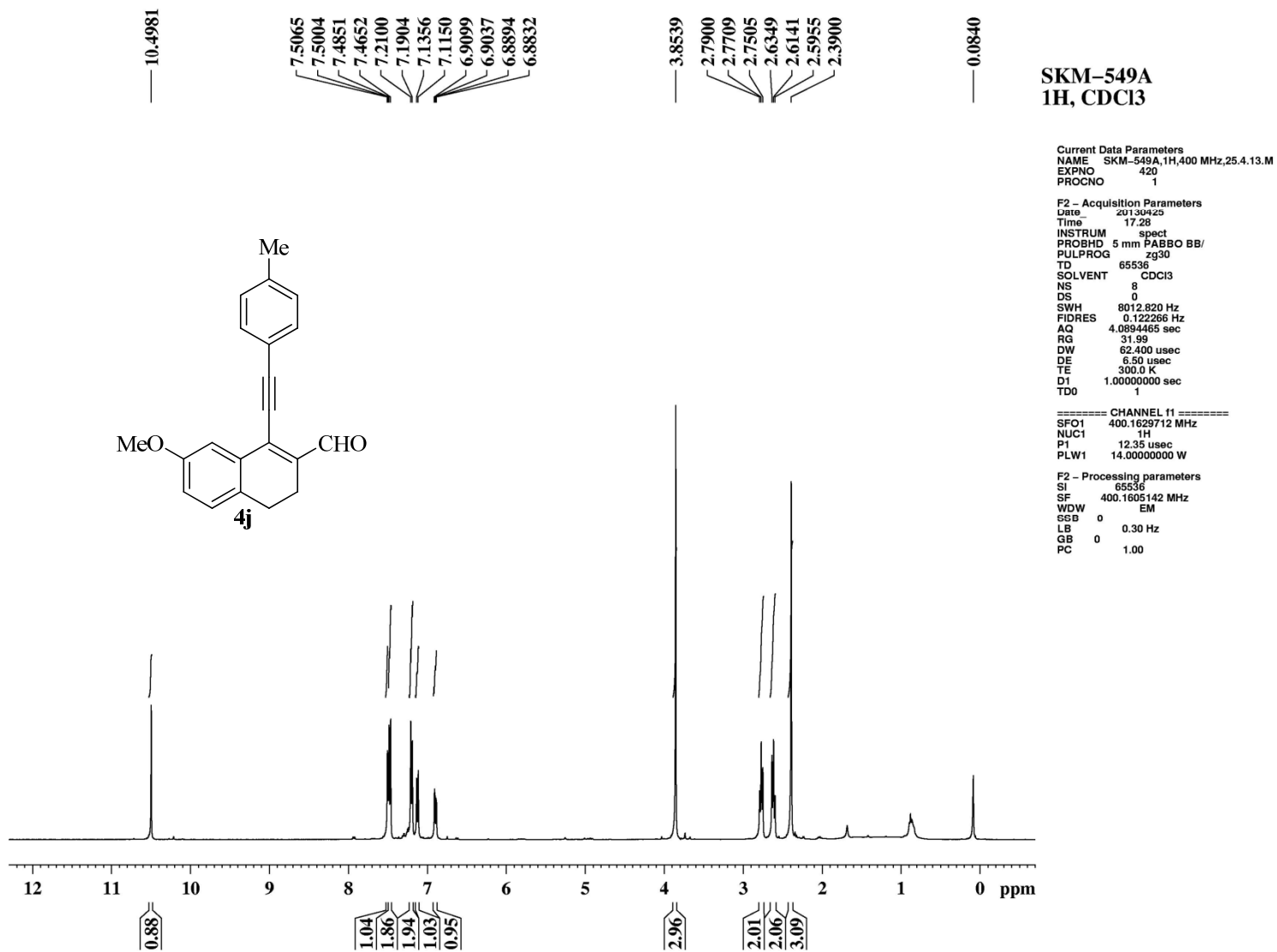
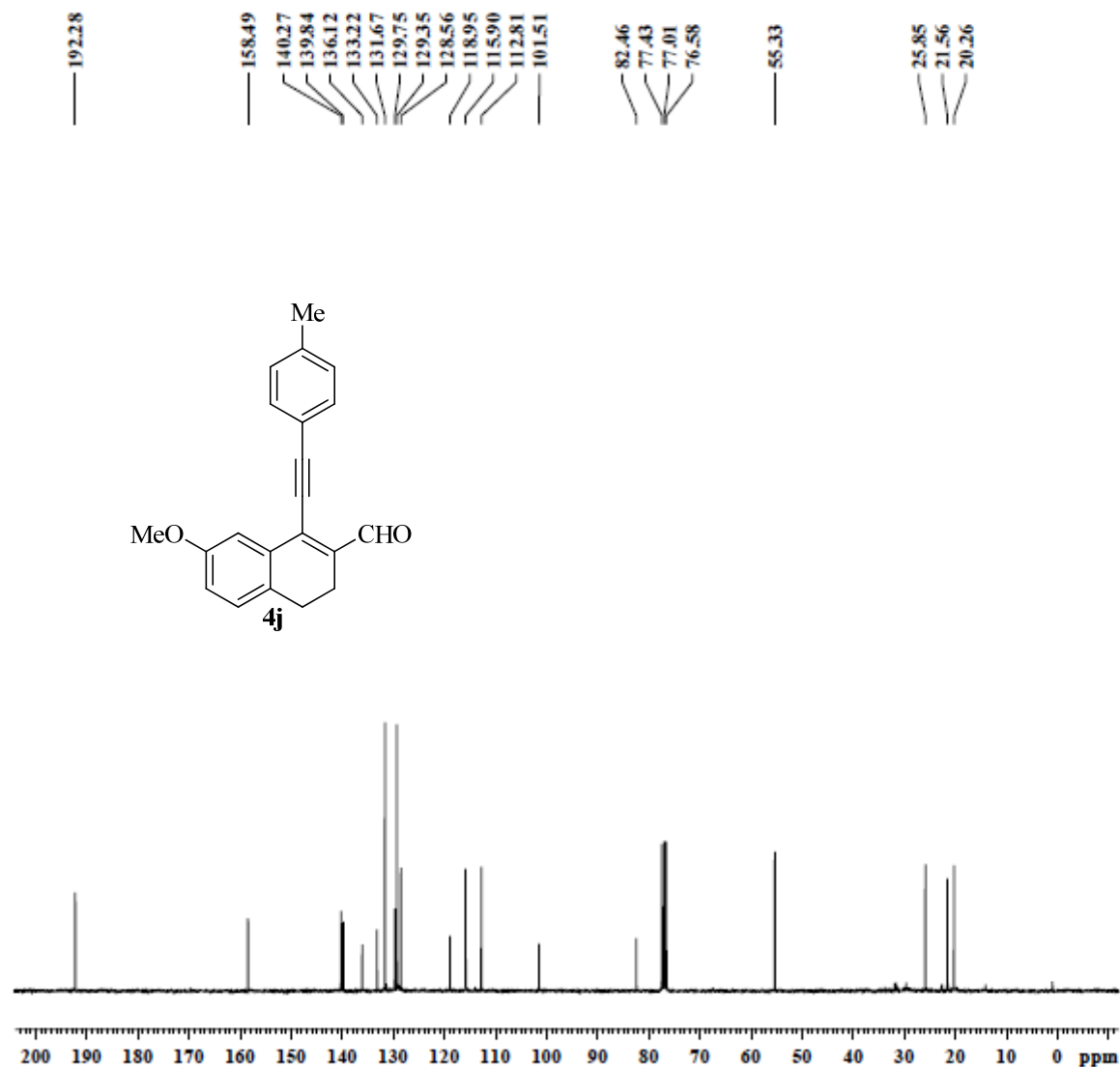


Figure 21: ¹H -NMR Spectrum of **4j**.



SKM-549A
13C, CDCl3

Current Data Parameters
NAME SKM-549A,13C,300 MHz,6.5,13.M
EXPNO 360
PROCNO 1

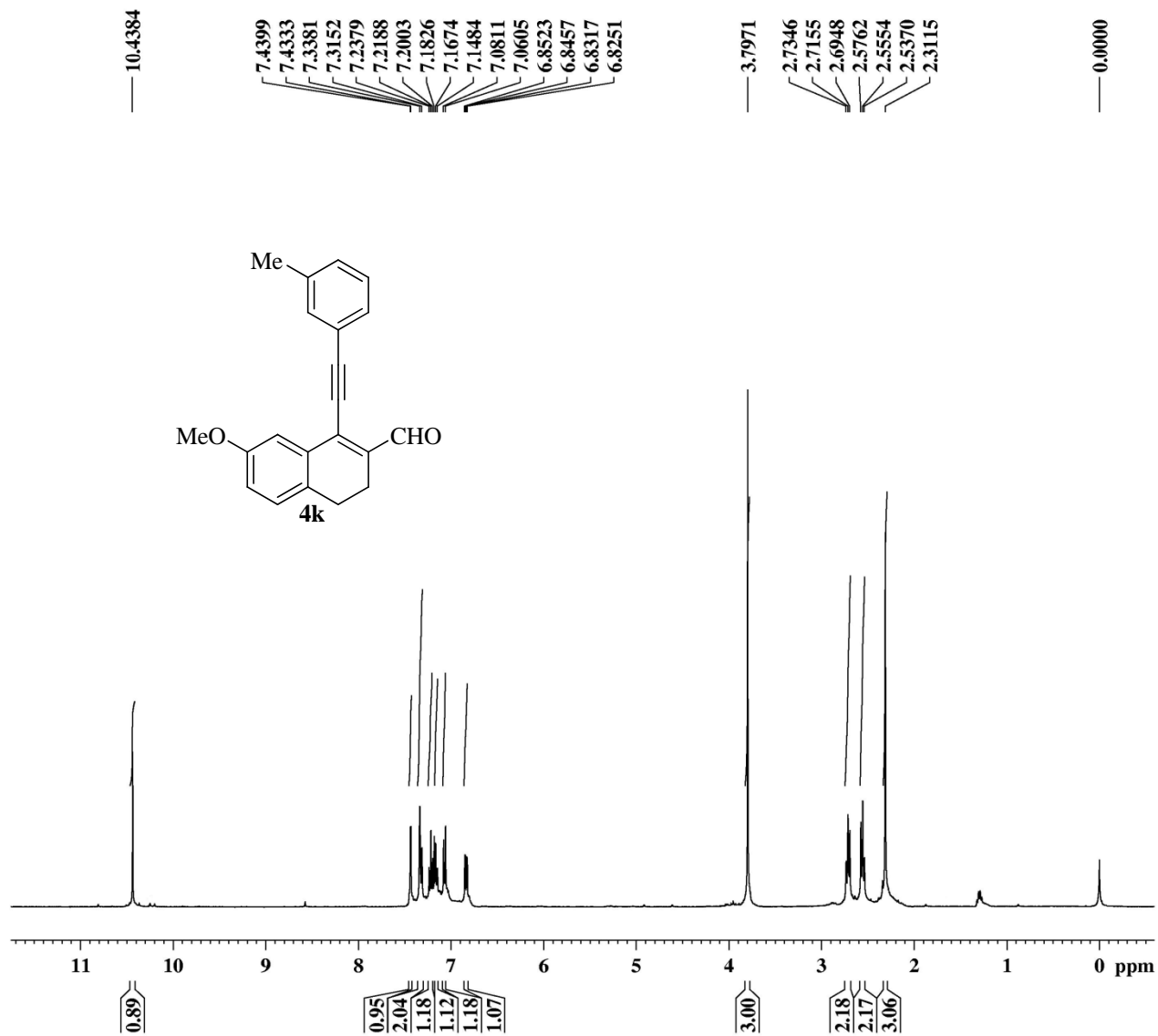
F2 - Acquisition Parameters
Date_ 20130506
Time 8.51
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2030
DW 27.733 usec
DE 15.00 usec
TE 673.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.15 usec
PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -1.00 dB
PL12 17.06 dB
PL13 21.00 dB
PL2W 15.02081871 W
PL12W 0.23437971 W
PL13W 0.0947406 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677548 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 22: ¹³C -NMR Spectrum of **4j**.



**SKM-556A
1H, CDCl3**

Current Data Parameters
 NAME SKM-556A,1H,400 MHz,29.4.1:
 EXPNO 390
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130430
 Time 13.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 58.68
 DW 62.400 usec
 DE 6.50 usec
 TE 295.7 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 12.35 usec
 PLW1 14.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605410 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 23: ¹H -NMR Spectrum of 4k.

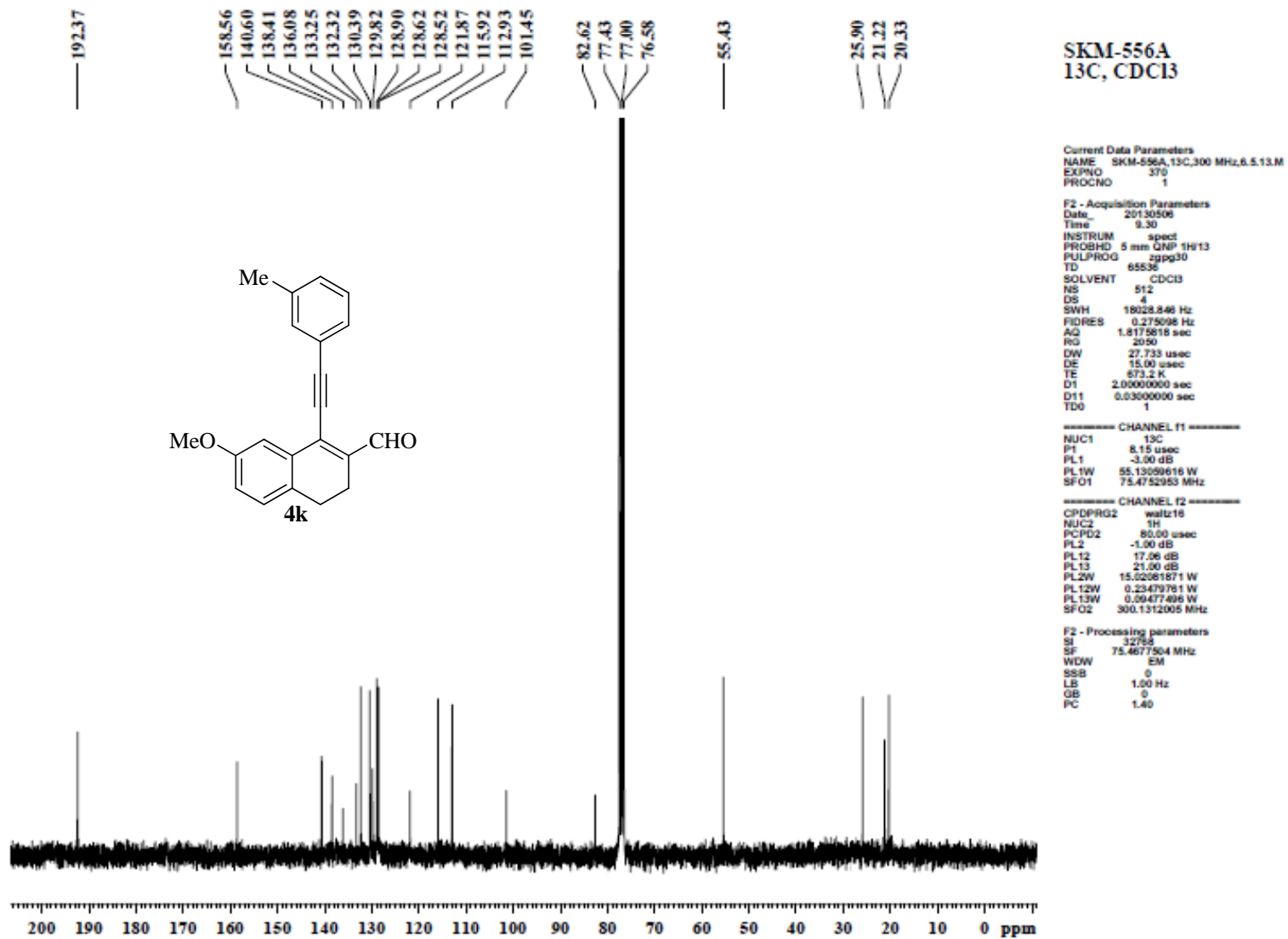


Figure 24: ^{13}C -NMR Spectrum of **4k**.

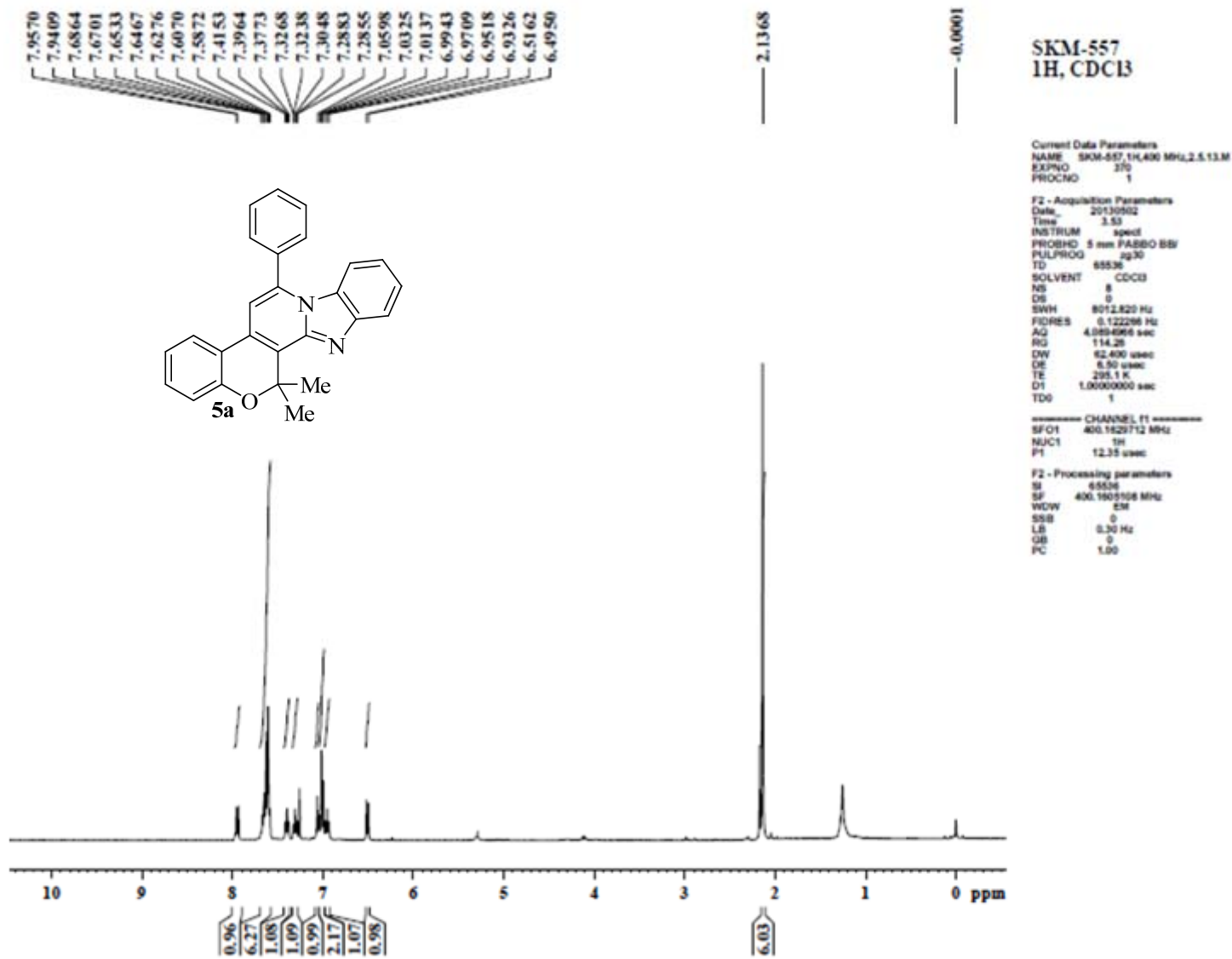


Figure 25: ^1H -NMR Spectrum of **5a**.

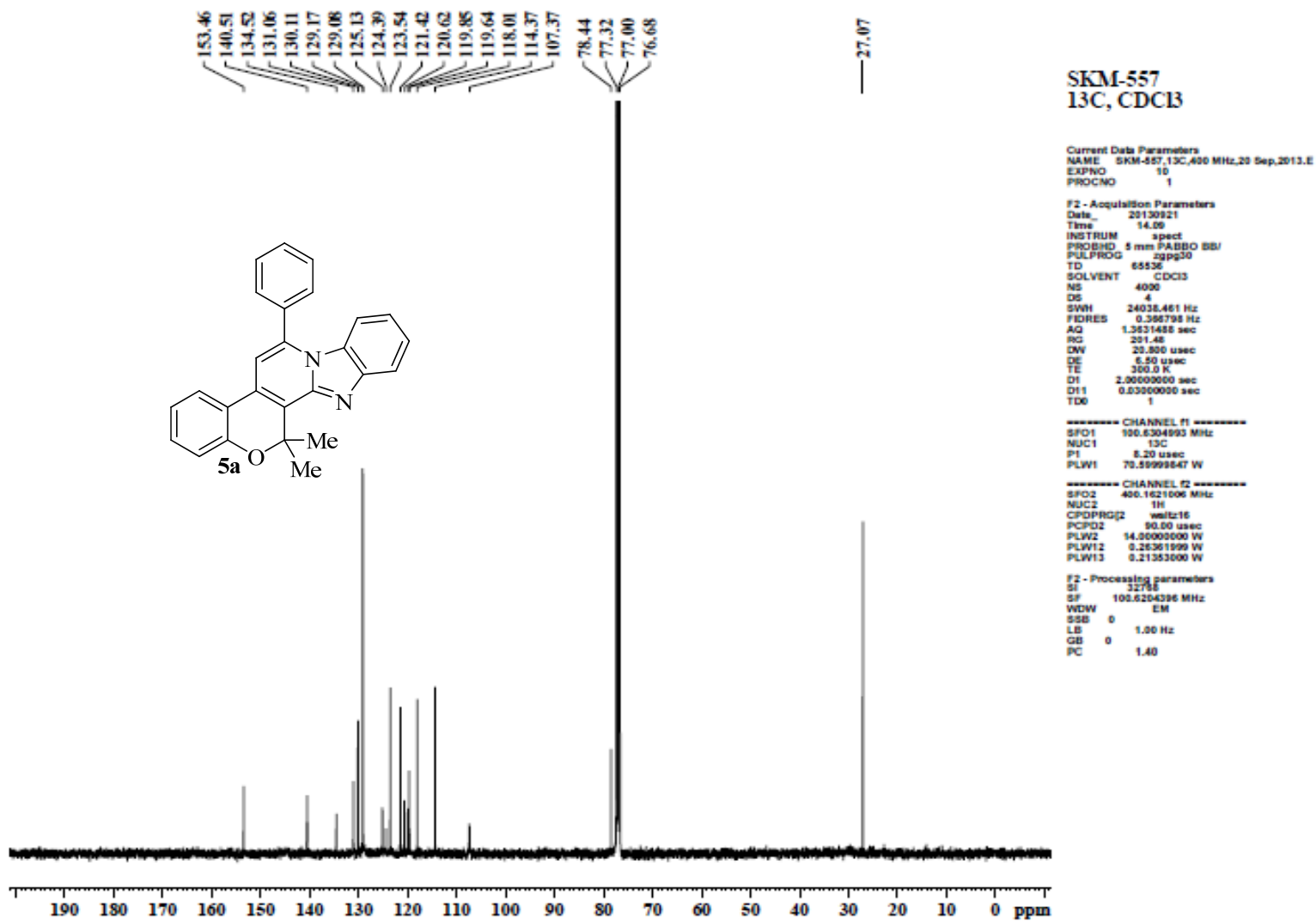


Figure 26: ^{13}C -NMR Spectrum of **5a**.

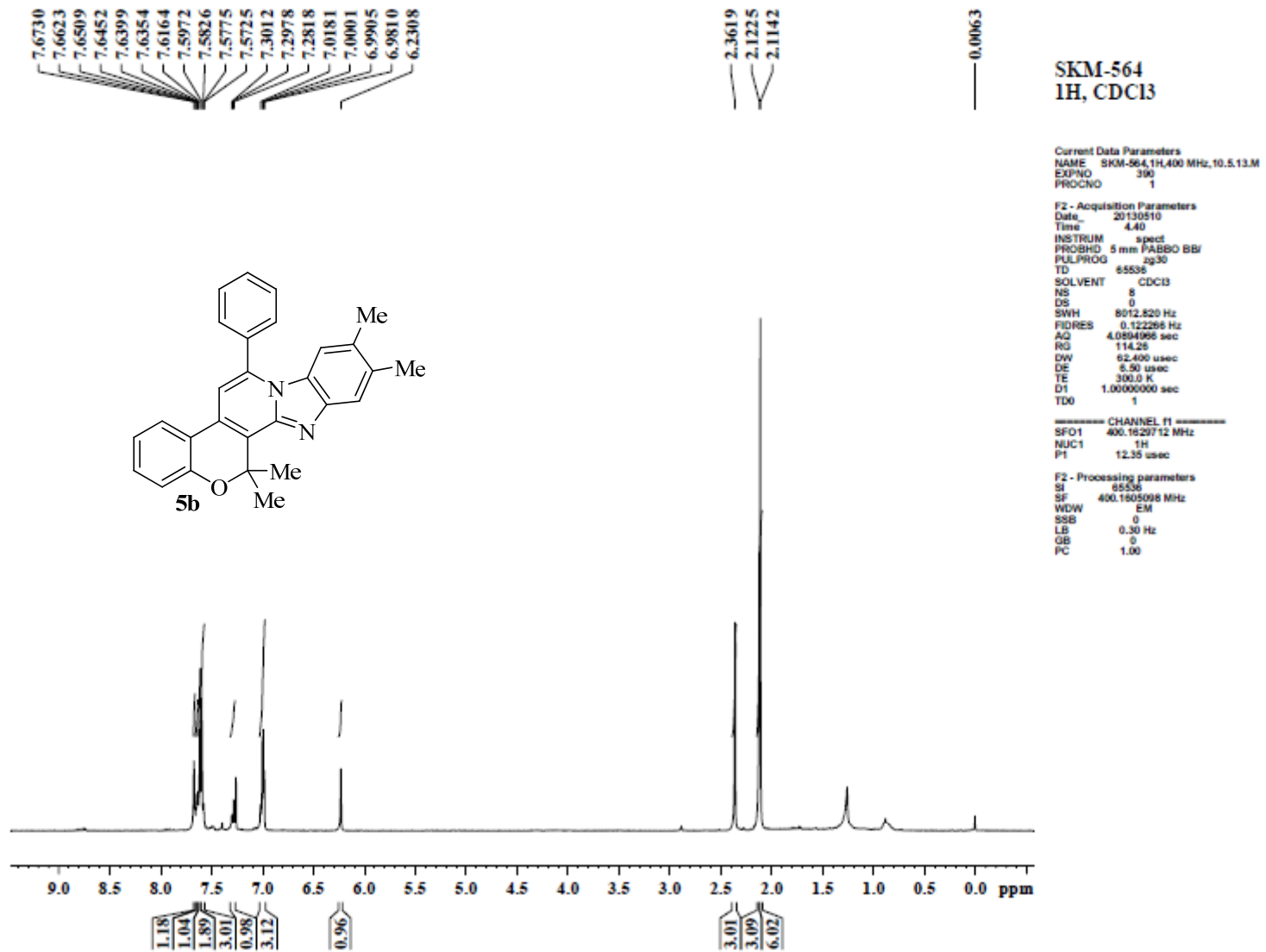


Figure 27: ¹H -NMR Spectrum of **5b**.

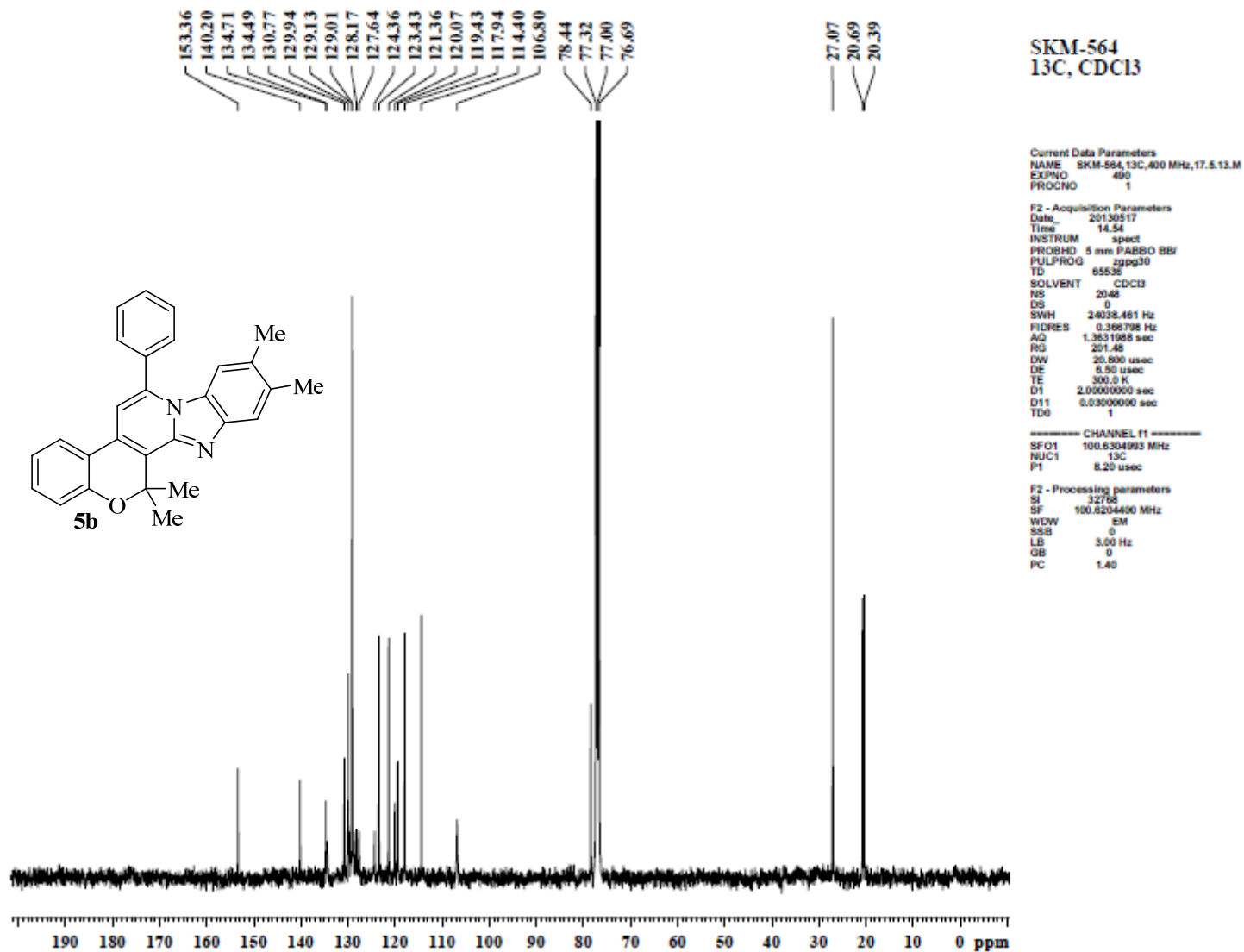


Figure 28: ¹³C -NMR Spectrum of **5b**.

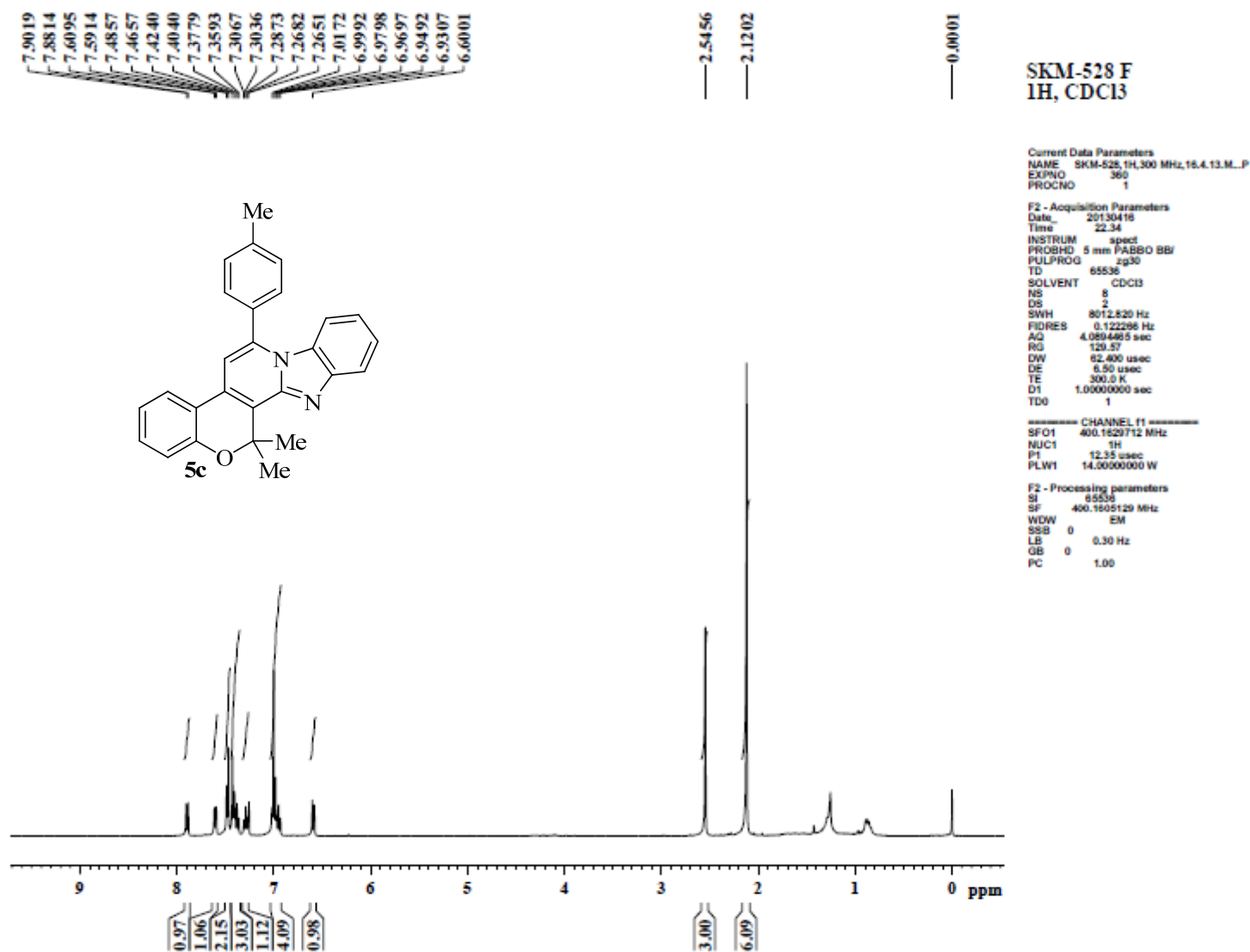


Figure 29: ^1H -NMR Spectrum of **5c**.

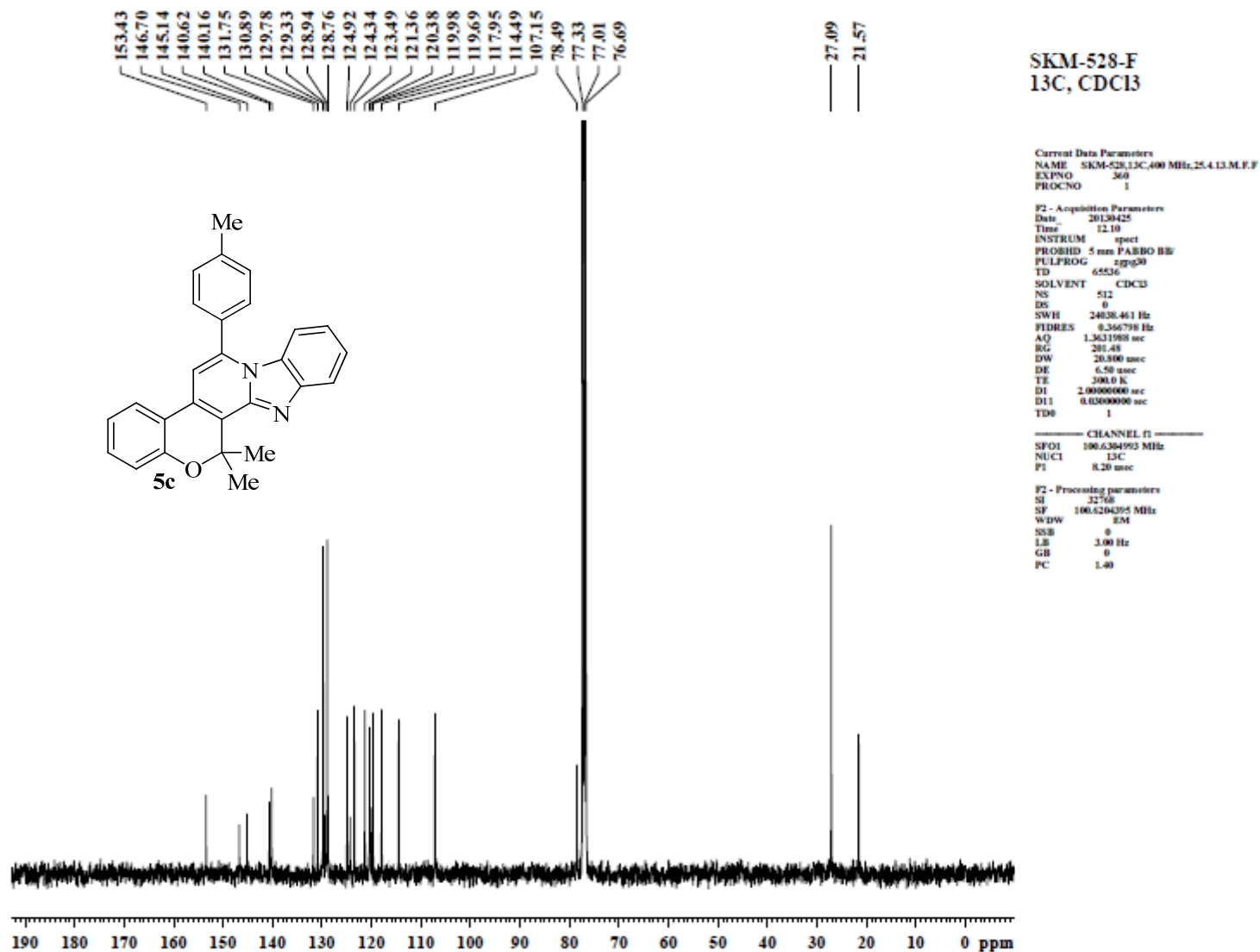


Figure 30: ¹³C -NMR Spectrum of **5c**.

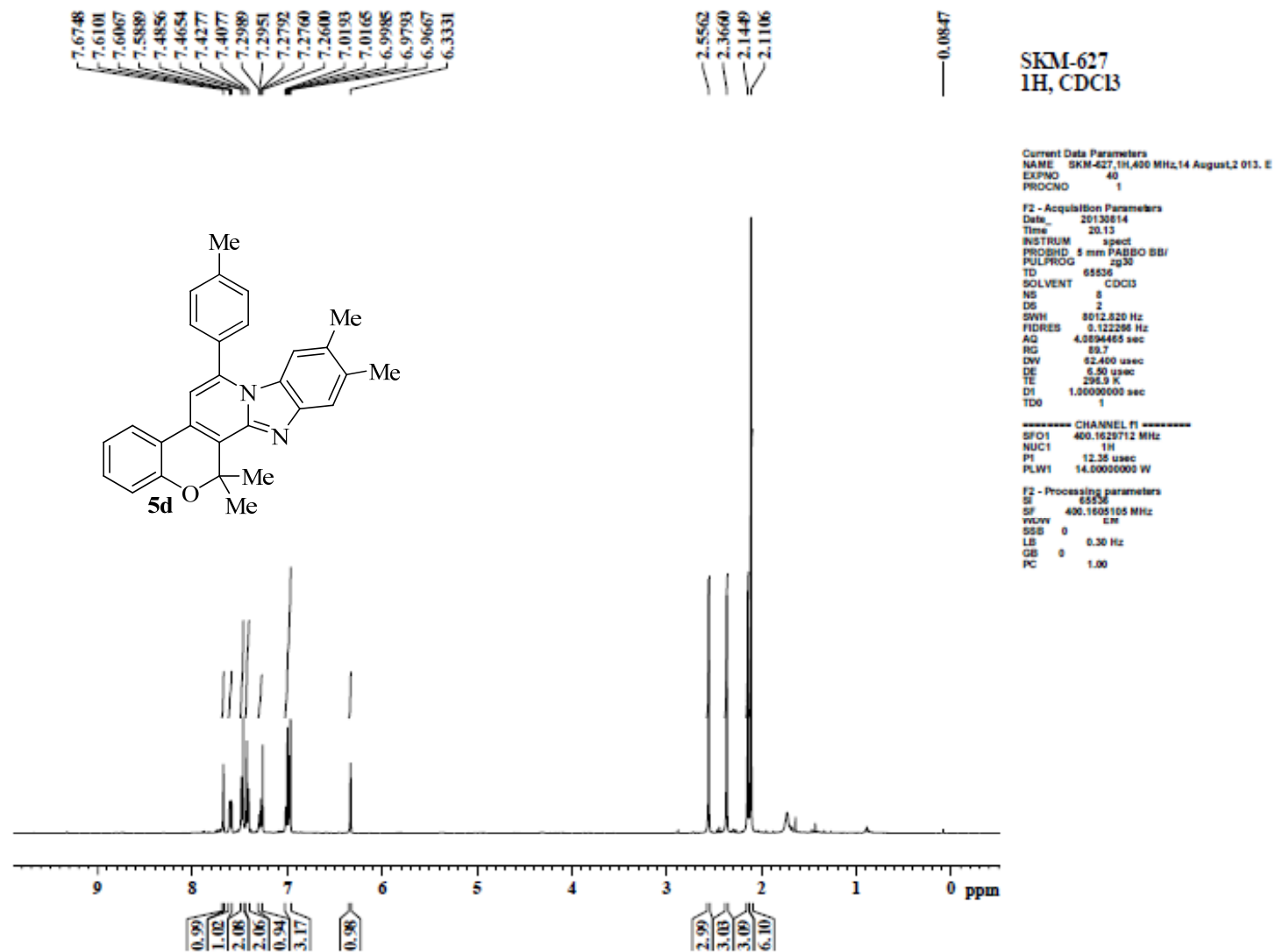


Figure 31: ¹H -NMR Spectrum of **5d**.

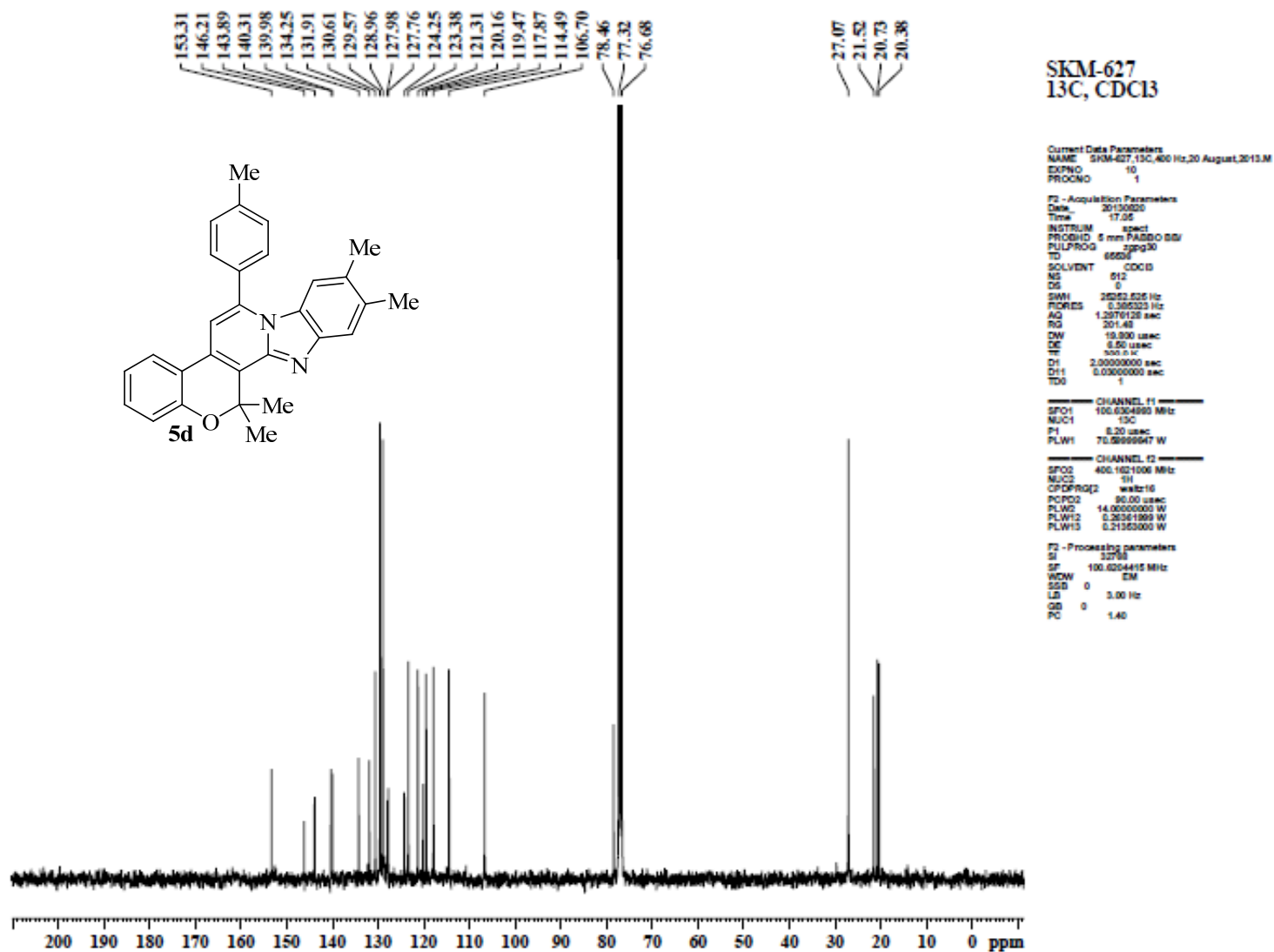


Figure 32: ^{13}C -NMR Spectrum of **5d**.

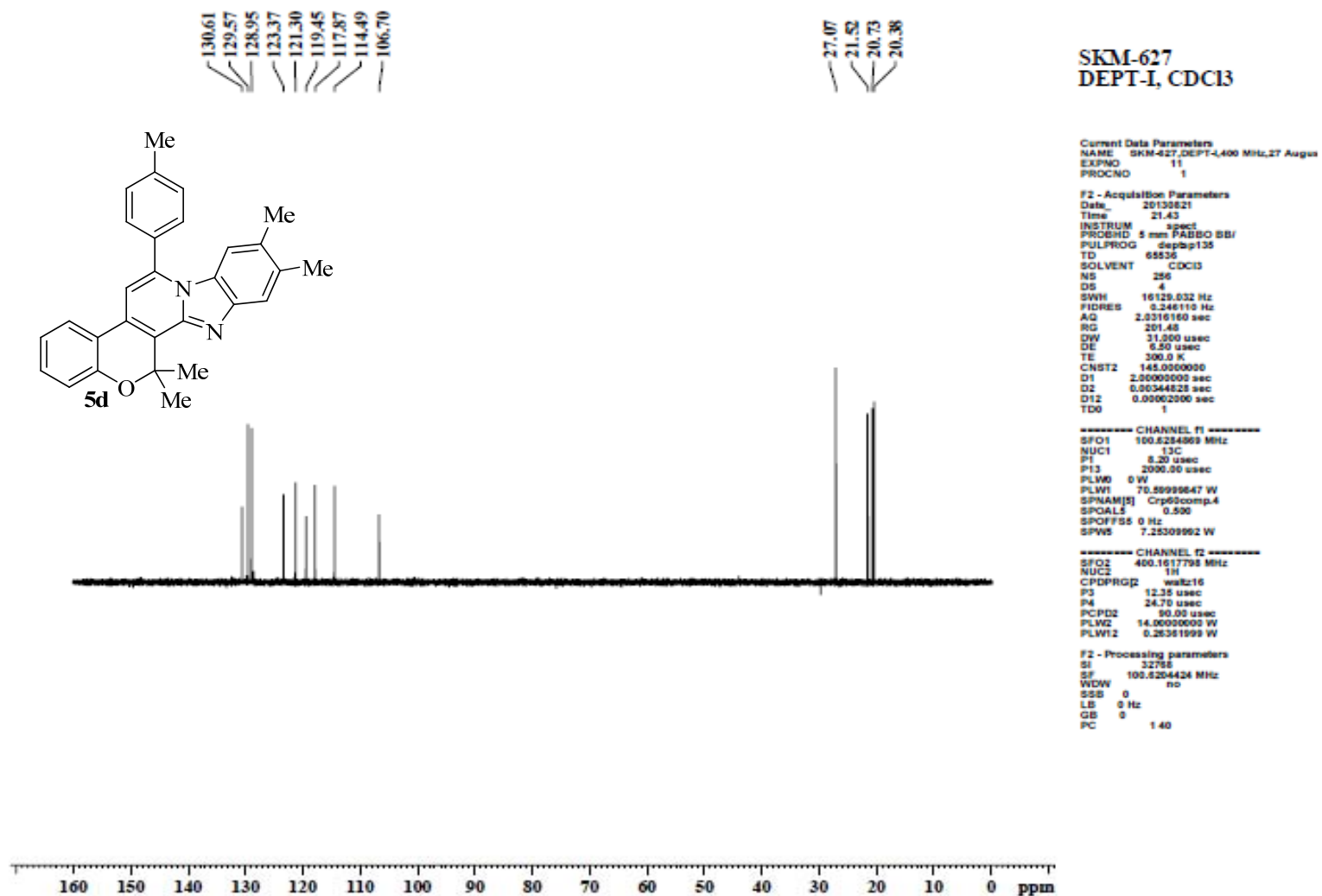


Figure 33: DEPT-I -Spectrum of **5d**.

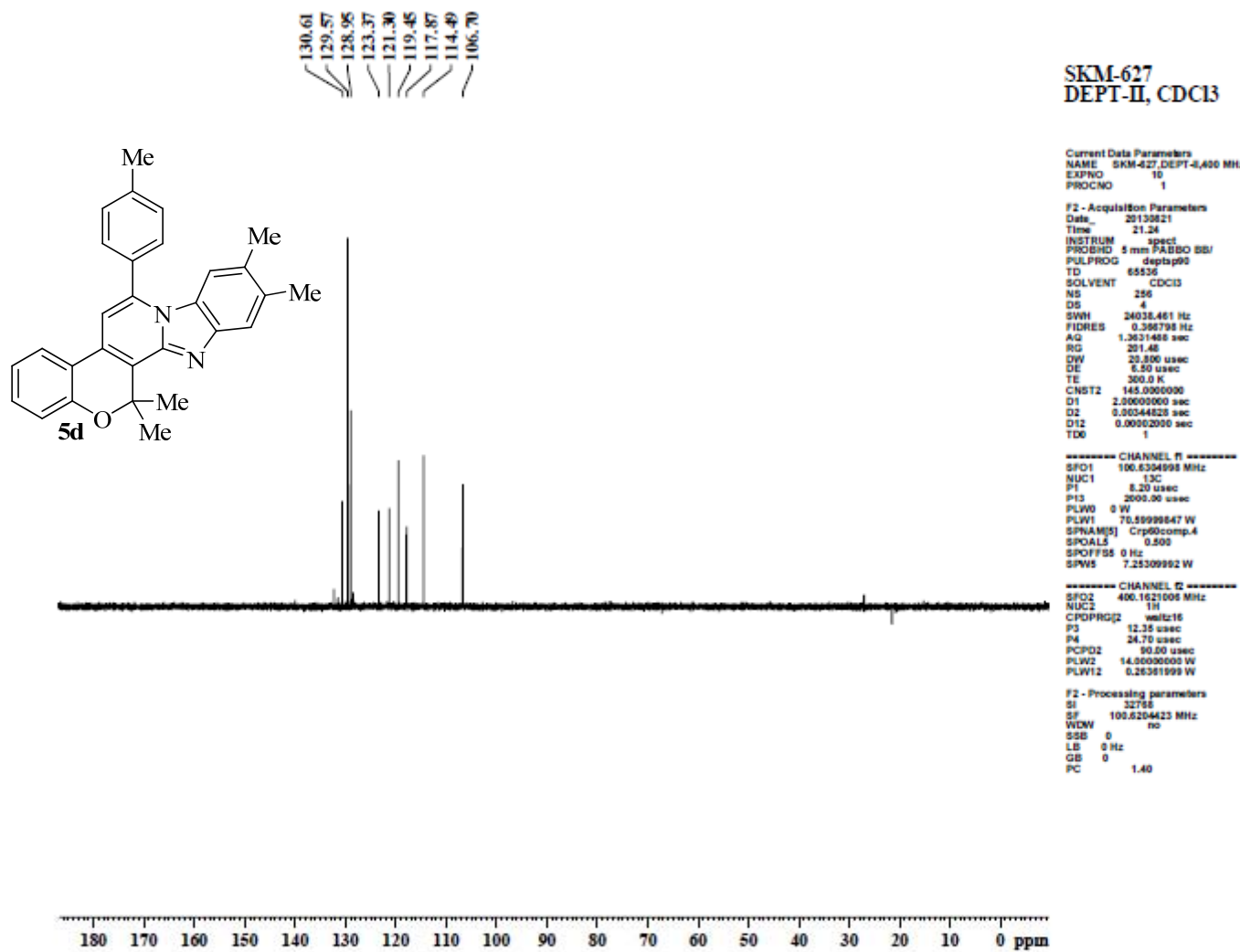
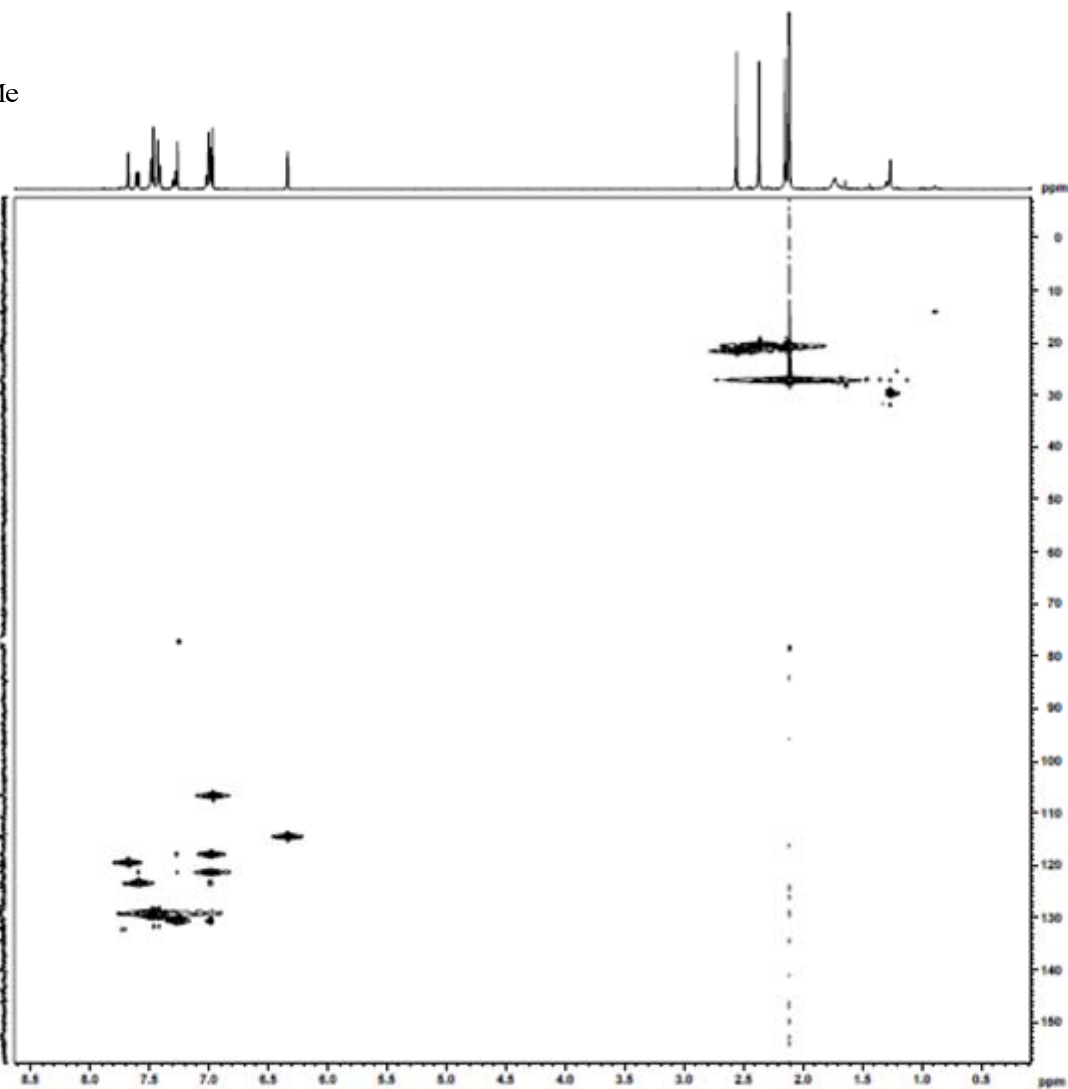
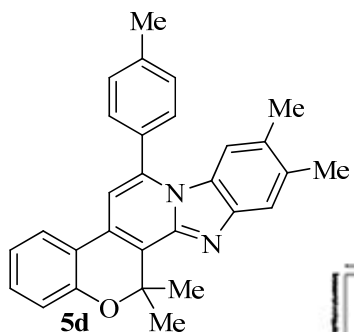


Figure 34: DEPT-II -Spectrum of 5d.



SKM-627
HSQC, CDCl3

Current Data Parameters
 NAME SKM-627.HSQC, 400 MHz, 23 A
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130824
 Time 5.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG hsqcetps2
 TD 1024
 SOLVENT CDCl3
 NS 16
 DS 16
 SWH 3424.657 Hz
 FIDRES 3.344382 Hz
 AQ 0.1495040 sec
 RG 201.68
 DW 146.000 usec
 DE 6.50 usec
 TE 300.0 K
 CNST2 145.000000
 D0 0.00000000 sec
 D1 1.44864703 sec
 D4 0.00172614 sec
 D11 0.03000000 sec
 D16 0.00020000 sec
 D24 0.0006207 sec
 RNO 0.00000000 sec
 ZGOPTNS

==== CHANNEL F1 =====
 SFO1 400.1622543 MHz
 NUC1 131
 P1 12.35 usec
 P2 24.70 usec
 P28 1000.00 usec
 PLW1 14.00000000 W

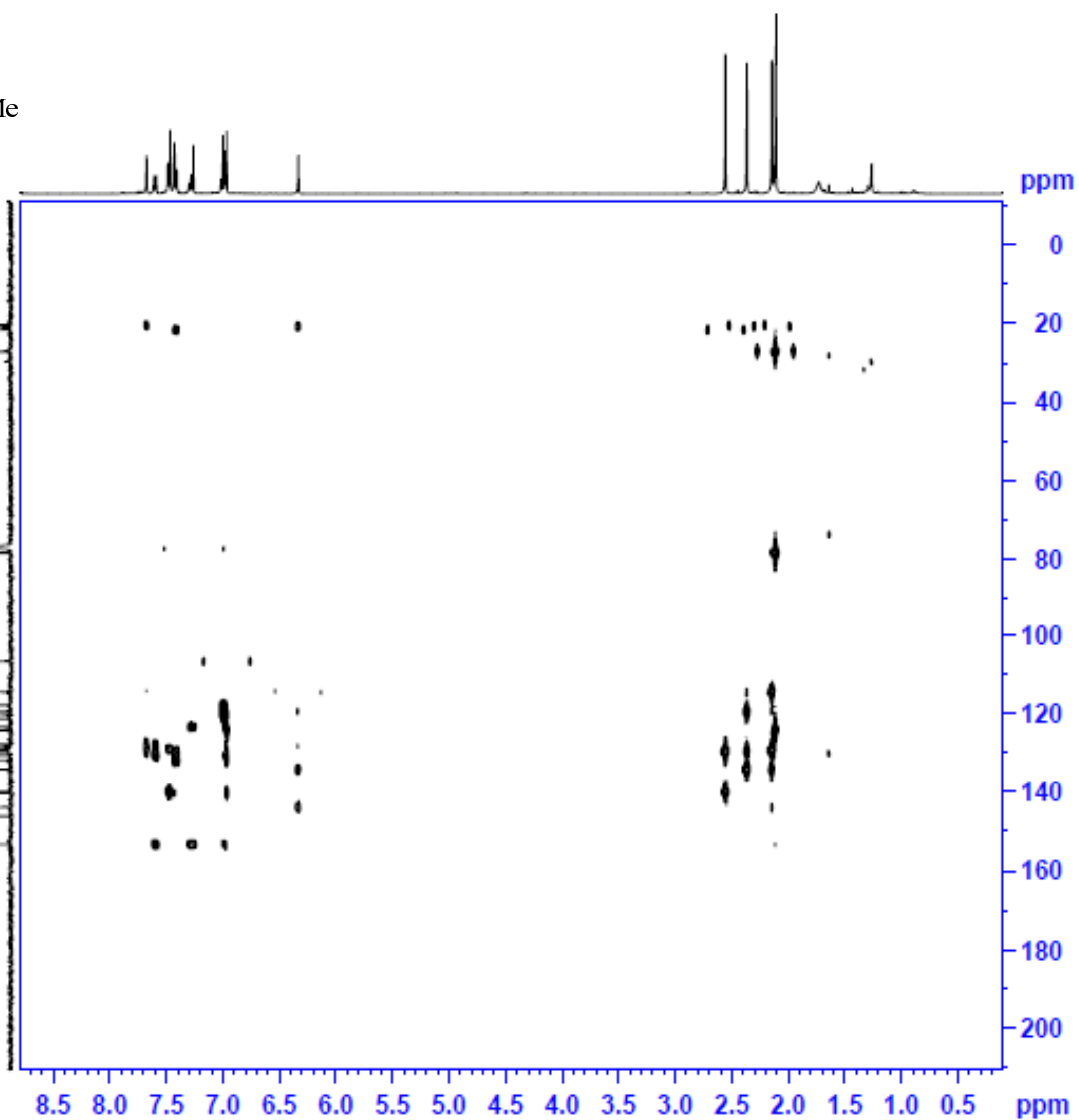
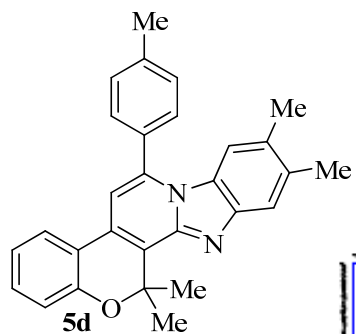
==== CHANNEL F2 =====
 SFO2 100.6279622 MHz
 NUC2 13C
 CPDPRG2 garp
 P3 8.20 usec
 P4 16.40 usec
 PCPD2 80.00 usec
 PLW2 70.59999847 W
 PLW12 0.74172999 W

==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPNAM[4] SMSQ10.100
 GPZ1 90.00 %
 GPZ2 20.10 %
 GPZ3 11.00 %
 GPZ4 -6.00 %
 P16 1000.00 usec
 P19 600.00 usec

F1 - Acquisition parameters
 TD 256
 SFO1 100.628 MHz
 FIDRES 66.104164 Hz
 SW 165.627 ppm
 FWHOOE Echo-AtBecho

F2 - Processing parameters

Figure 35: HSQC -Spectrum of 5d.



SKM-627
HMBC, CDCl₃

Current Data Parameters
 NAME SKM-627, HMBC, 400 MHz, 22 Aug
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130823
 Time 1.15
 INSTRUM spect
 PROBNM 5 mm PABBO BB/
 PULPROG hmcsgplpndqf
 TD 2048
 SOLVENT CDCl₃
 NS 4
 DS 16
 SWH 5472.222 Hz
 FIDRES 1.695421 Hz
 AQ 0.2949120 sec
 RG 201.48
 DW 144.000 usec
 DE 8.50 usec
 TE 300.2 K
 CNST2 145.000000
 CNST3 10.000000
 D0 0.00000300 sec
 D1 1.40210605 sec
 D2 0.00344825 sec
 D3 0.05000000 sec
 D15 0.00020000 sec
 INO 0.00002240 sec

==== CHANNEL F1 =====
 SFO1 400.1622905 MHz
 NUC1 13C
 P1 12.35 usec
 P2 24.70 usec
 PLW1 14.00000000 W

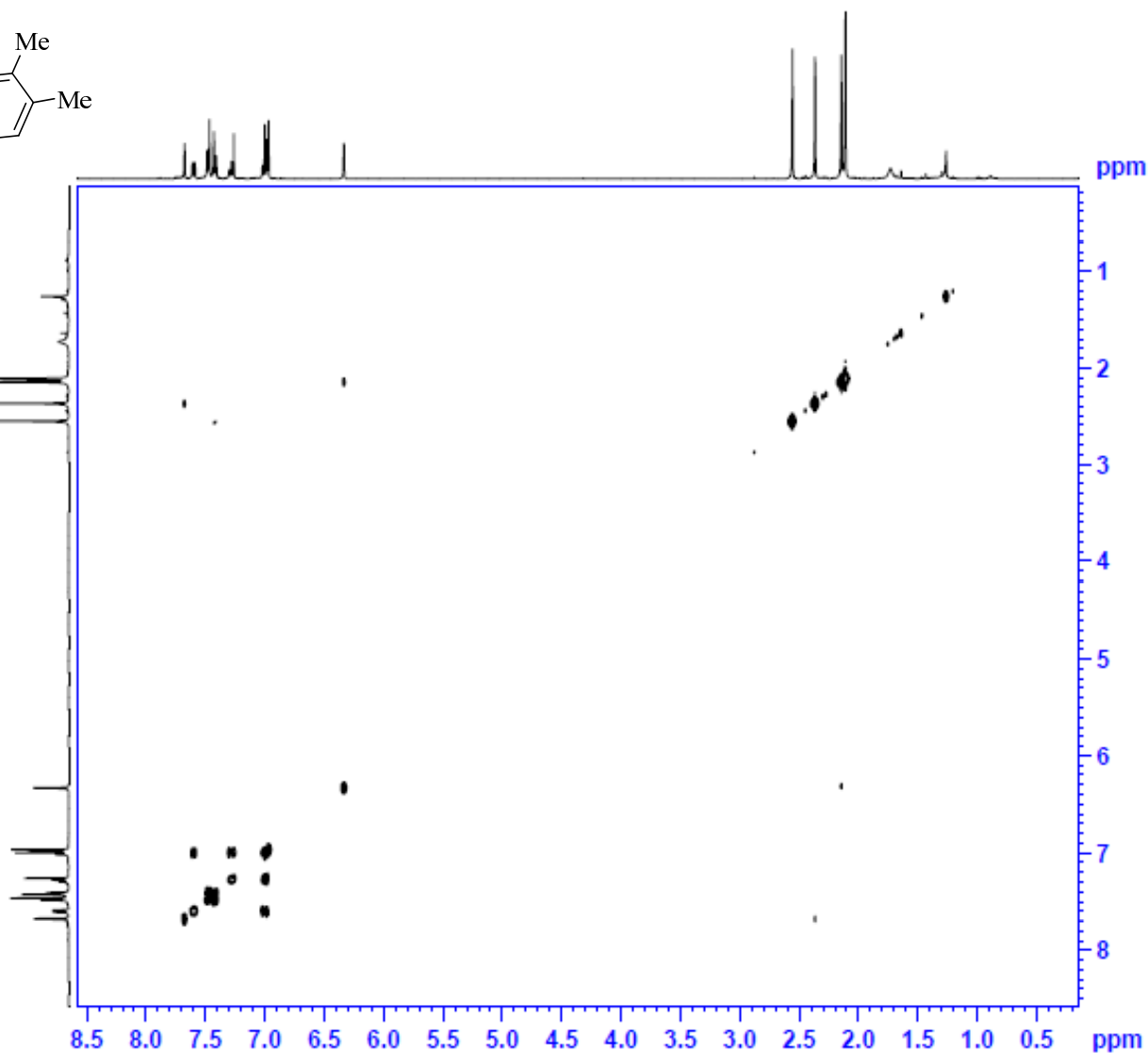
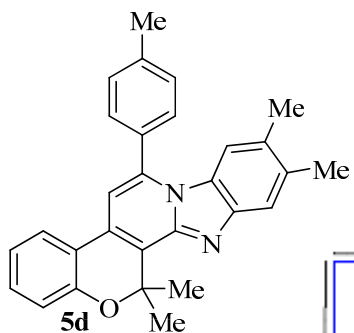
==== CHANNEL F2 =====
 SFO2 100.6304833 MHz
 NUC2 13C
 P3 8.20 usec
 PLW2 70.59998647 W

==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P15 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 100.6305 MHz
 FIDRES 174.386154 Hz
 SW 221.516 ppm
 FwMODE QF

F2 - Processing parameters
 SI 2048
 SF 400.1605118 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0

Figure 36: HMBC -Spectrum of **5d**.



SKM-627
COSY, CDC13

Current Data Parameters
NAME SKM-627_COSY_400 MHz, 271
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130208
Time 4.53
INSTRUM spect
PROBHD 5 mm PABBO BB1
PULPROG cosypppof
TD 2948
SOLVENT CDC13
NS 1
DS 8
SWH 3378.378 Hz
FIDRES 1.648590 Hz
AQ 0.3021940 sec
RG 65.85
DW 140.000 usec
DE 8.90 usec
TE 298.1 K
D0 0.0000000 sec
D1 1.0000000 sec
D11 0.0000000 sec
D12 0.0000000 sec
D13 0.0000000 sec
D18 0.0000000 sec
IND 0.0000000 sec

***** CHANNEL f1 *****
SFO1 400.1623600 MHz
NUC1 13H
P0 12.35 usec
P1 12.35 usec
P17 2500.00 usec
PLW1 14.00000000 W
PLW18 3.10079600 W

***** GRADIENT CHANNEL *****
GPRAMP1 500000.000
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 400.1623 MHz
FIDRES 26.300501 Hz
SW 0.443 ppm
FRMODE GF

F2 - Processing parameters
SI 1024
SF 400.1600000 MHz
WOW 0.50000000
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 GF
SF 400.1600000 MHz

Figure 37: COSY -Spectrum of **5d**.

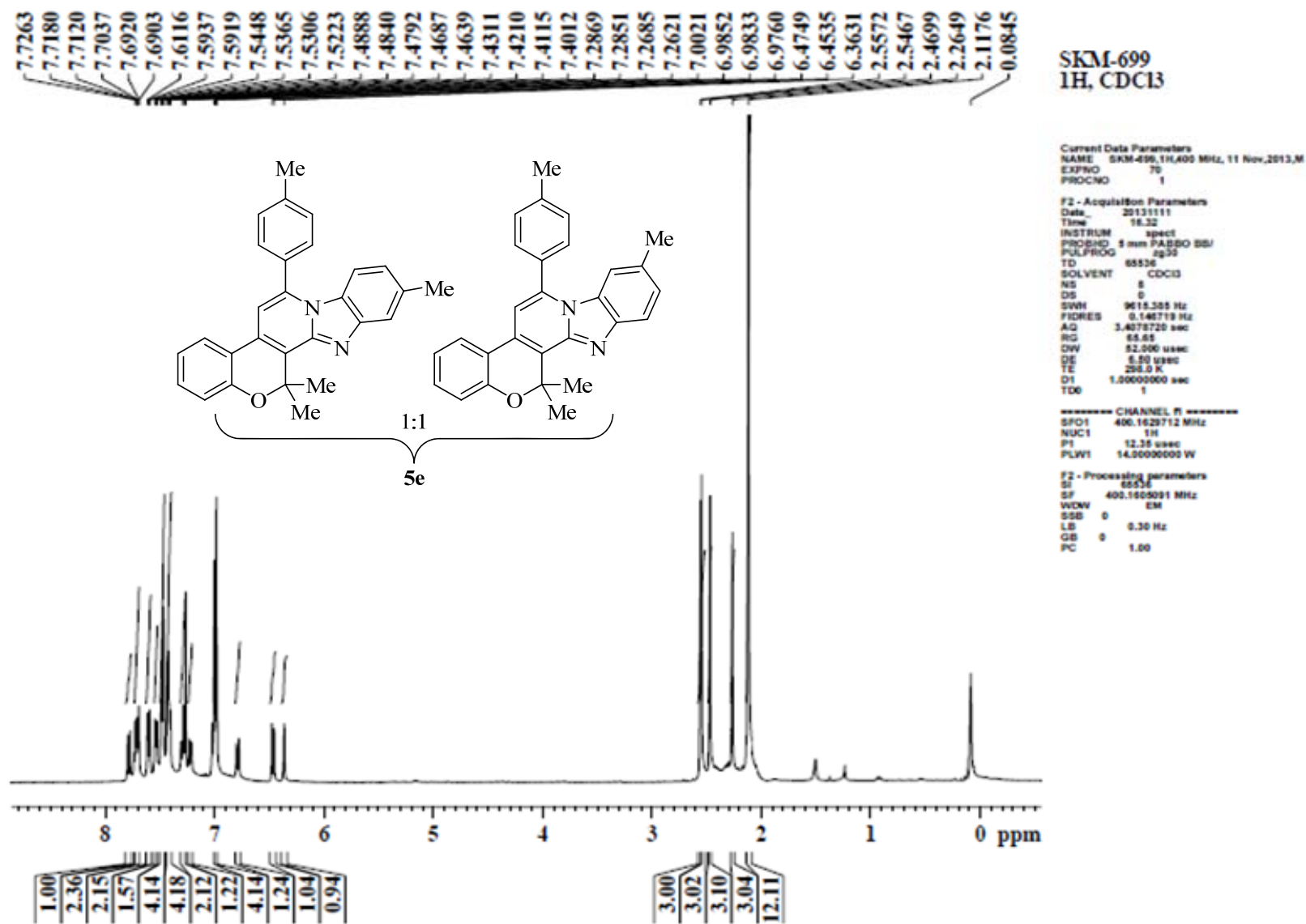


Figure 38: ¹H -NMR Spectrum of **5e**.

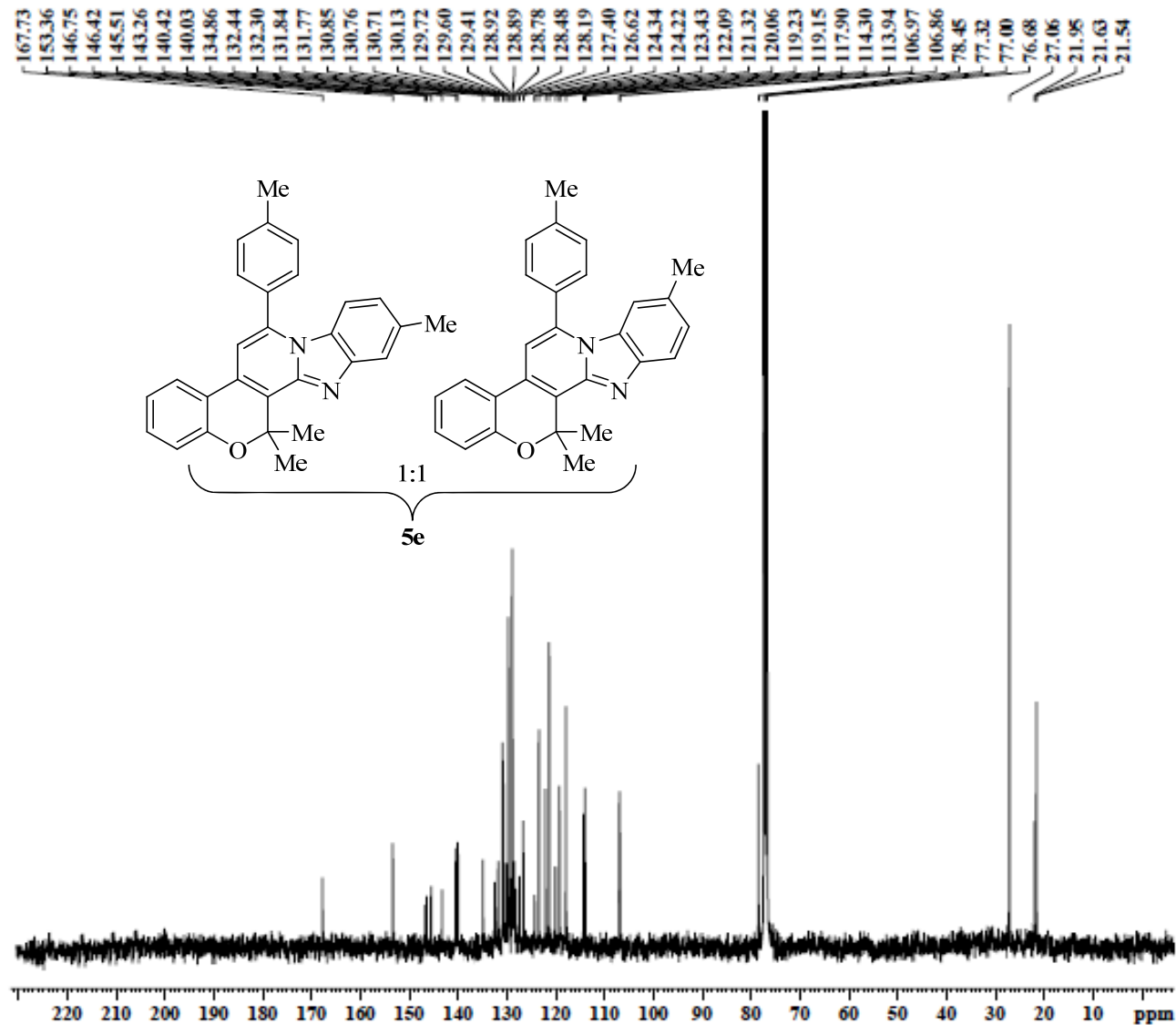


Figure 39: ¹³C -NMR Spectrum of 5e.

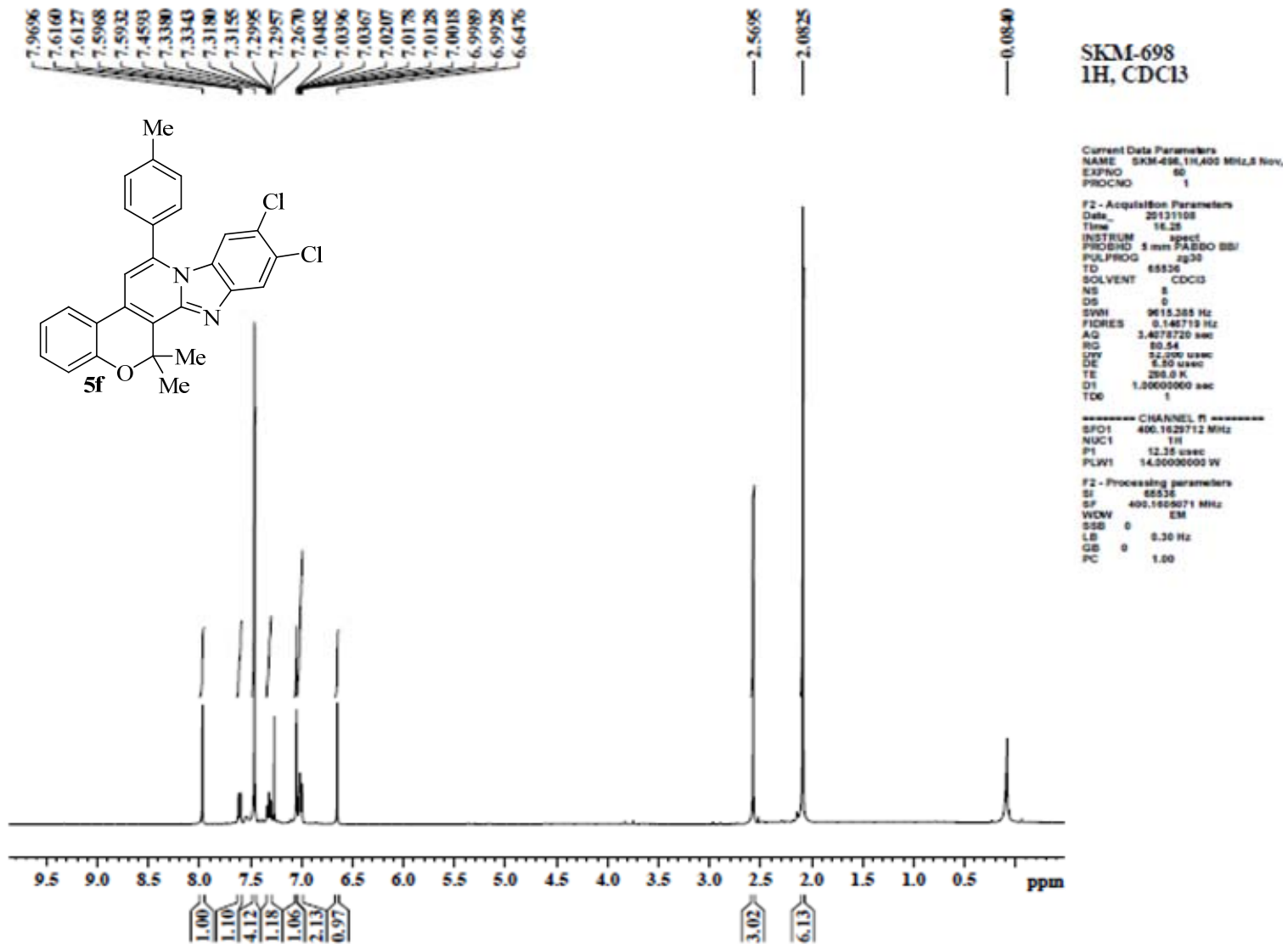


Figure 40: ¹H -NMR Spectrum of **5f**.

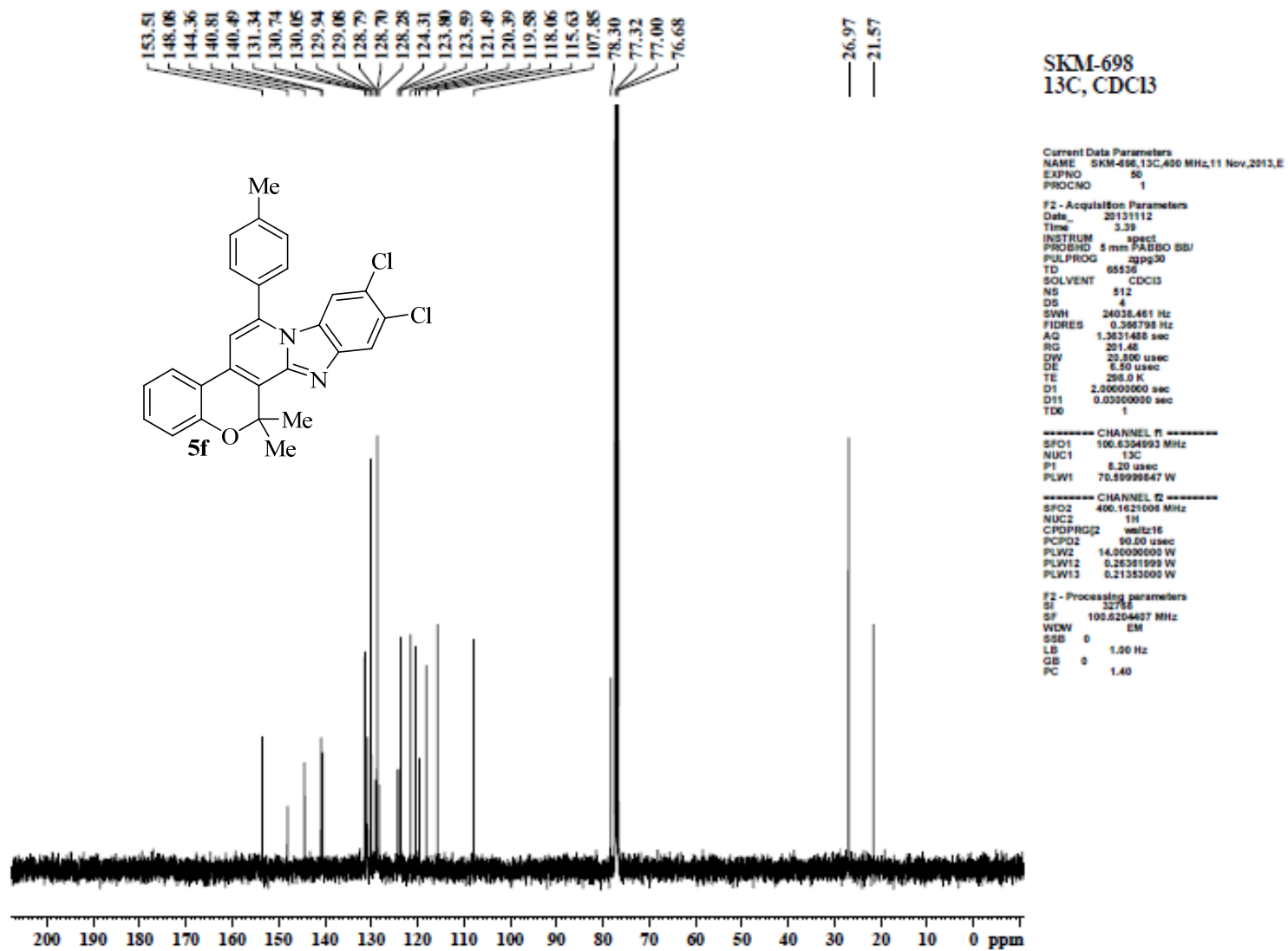


Figure 41: ^{13}C -NMR Spectrum of **5f**.

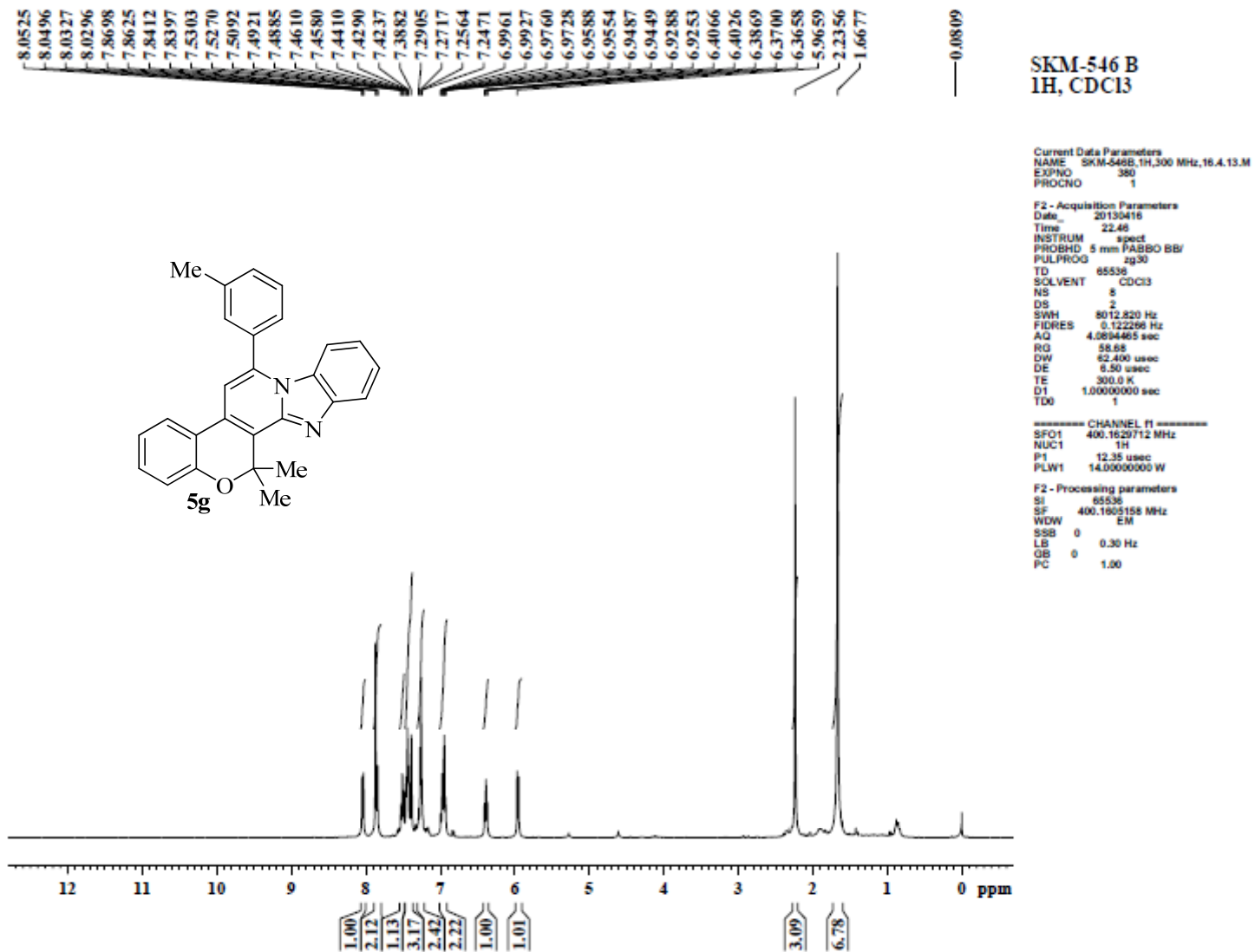


Figure 42: ^1H -NMR Spectrum of **5g**.

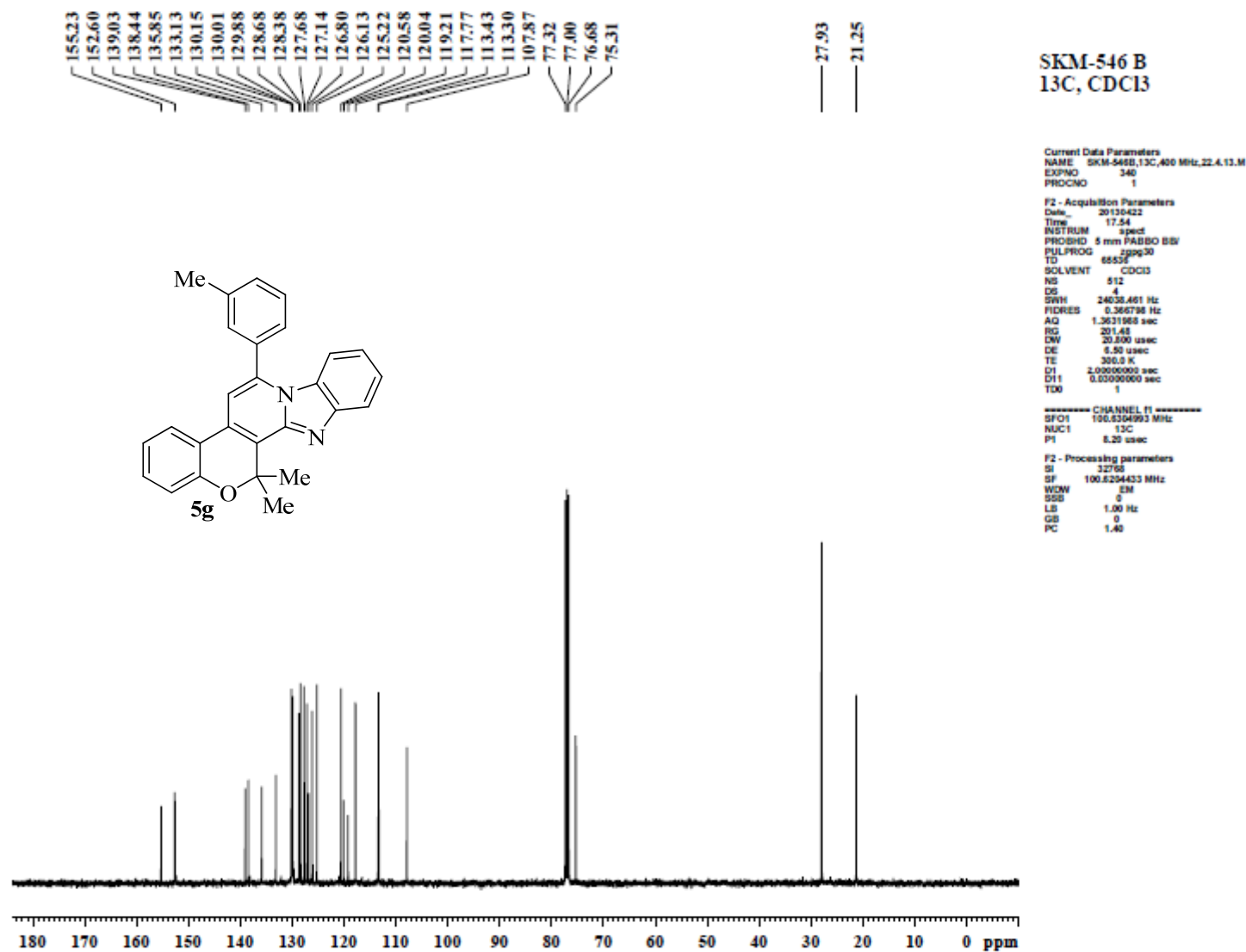


Figure 43: ^{13}C -NMR Spectrum of **5g**.

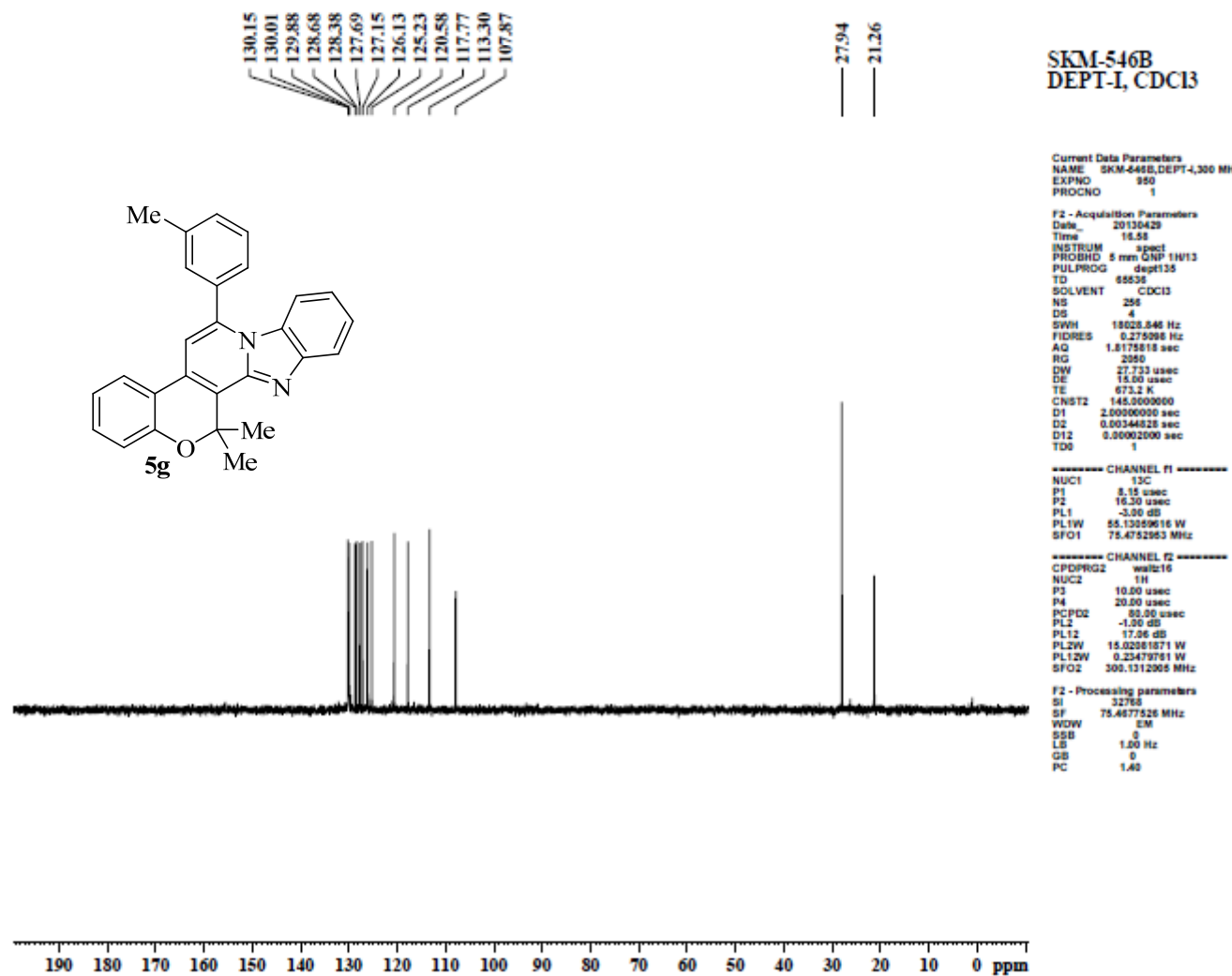
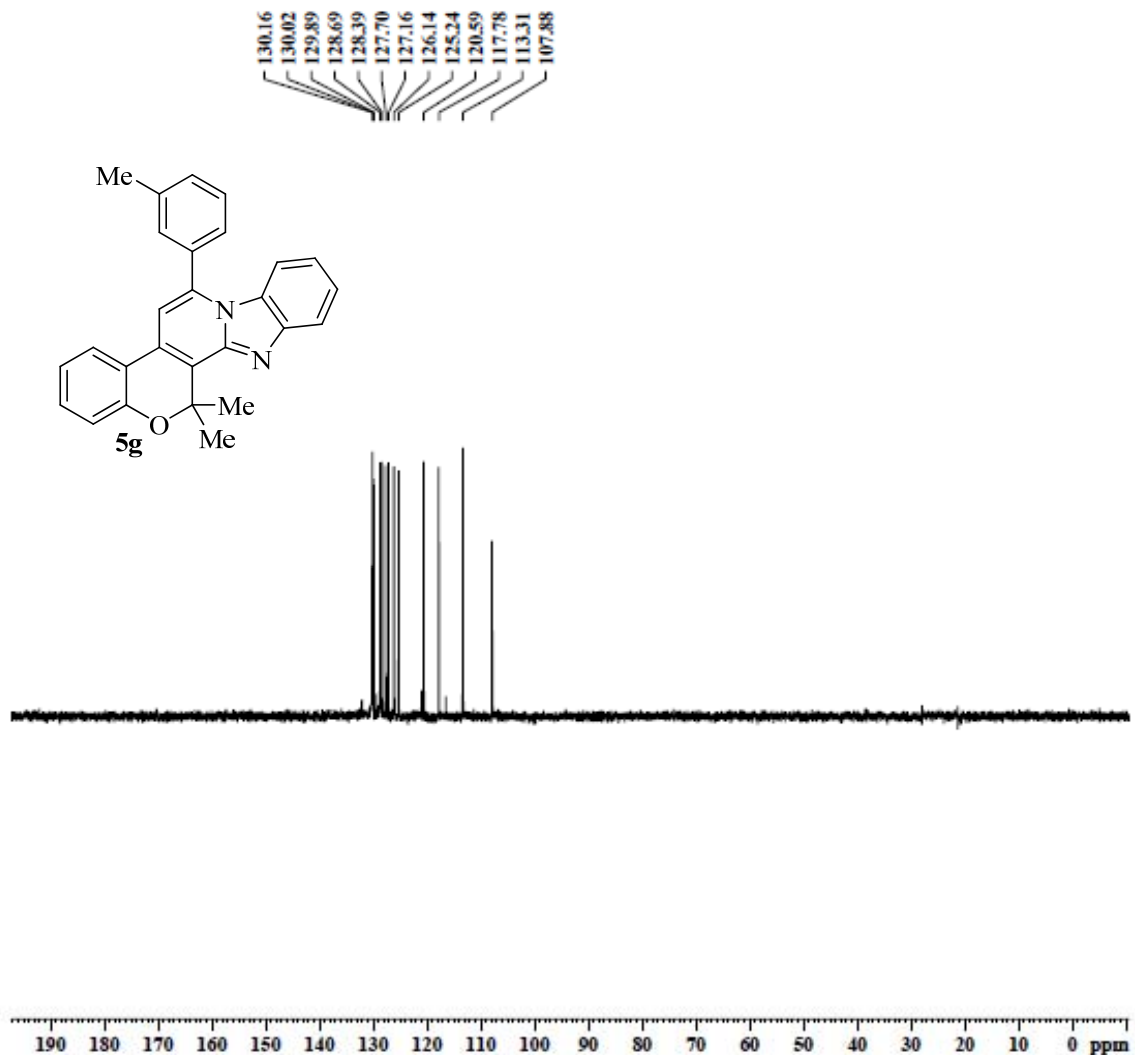


Figure 44: DEPT -I -Spectrum of 5g.



SKM-546B
DEPT-II, CDC13

Current Data Parameters
NAME SKM-546B,DEPT-II, 300 MHz,20.4.13.E
EXPNO 951
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130429
Time 17.15
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 15023.346 Hz
FIDRES 0.275958 Hz
AQ 1.8175813 sec
RG 2080
DW 27.733 usec
DE 15.50 usec
TE 673.2 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.0034622 sec
D12 0.0002000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 8.15 usec
P2 16.30 usec
PL1 -3.00 dB
PL1W 55.13259616 W
SFO1 75.4752953 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
P4 20.00 usec
PCPD2 80.00 usec
PL2 -1.30 dB
PL12 17.06 dB
PL2W 15.02081871 W
PL12W 0.25479761 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677519 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 45: DEPT -II -Spectrum of 5g.

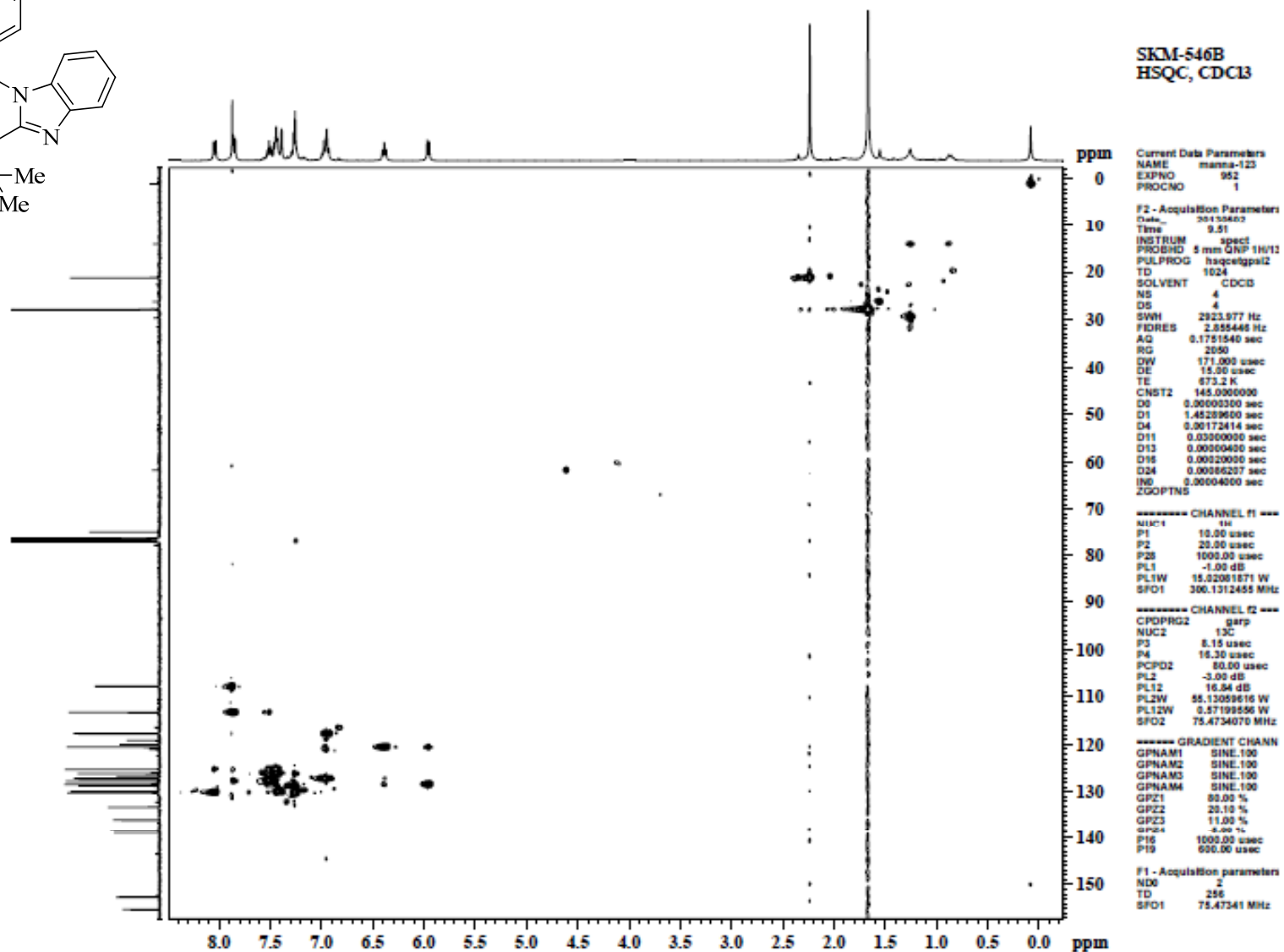
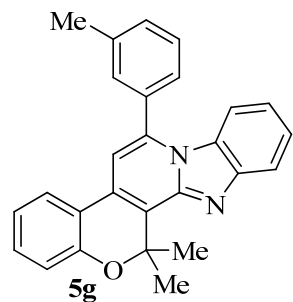


Figure 46: HSQC -Spectrum of **5g**.

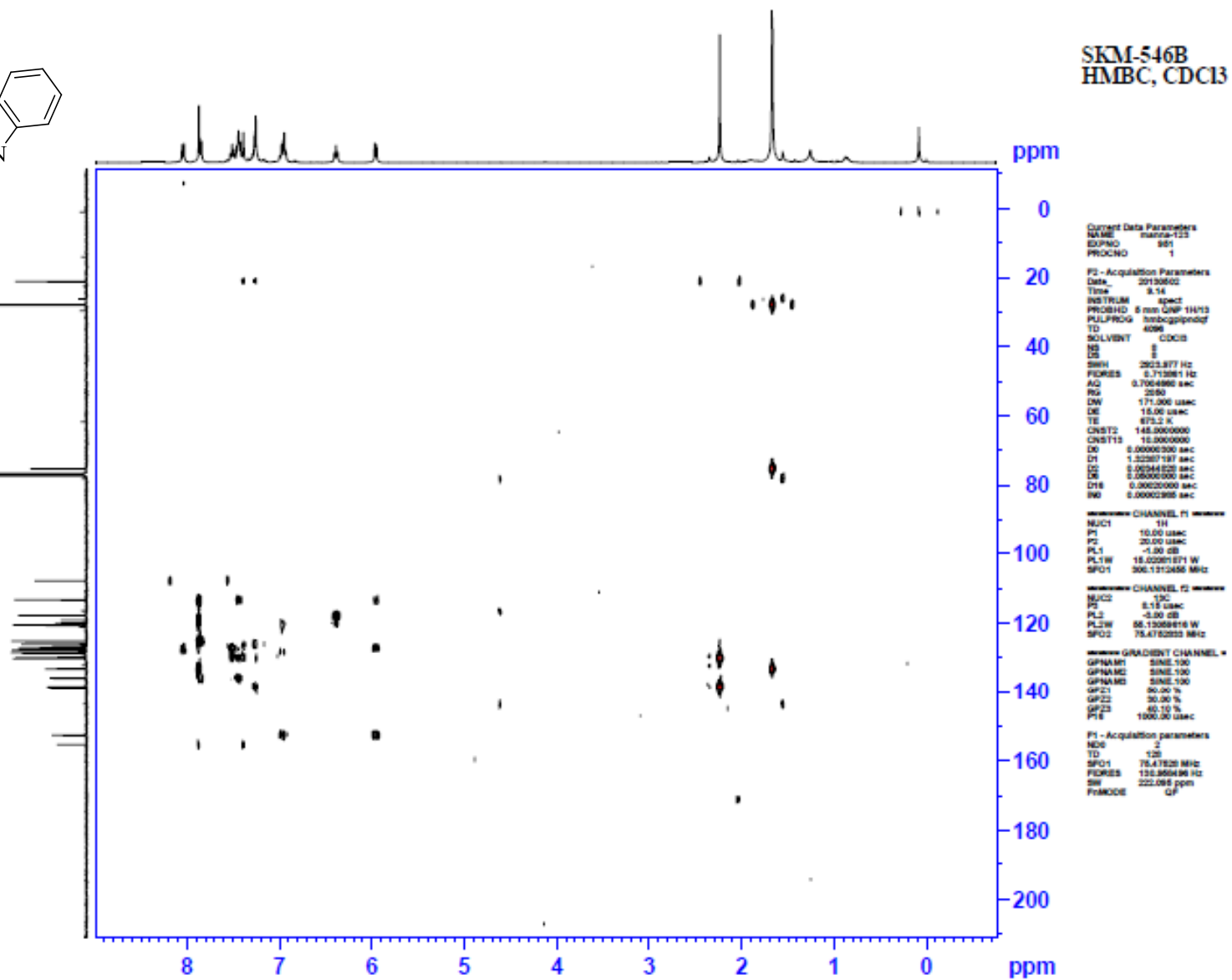
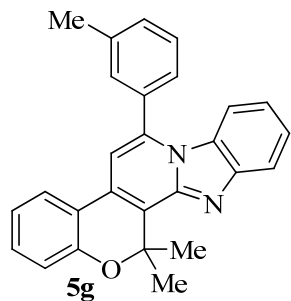
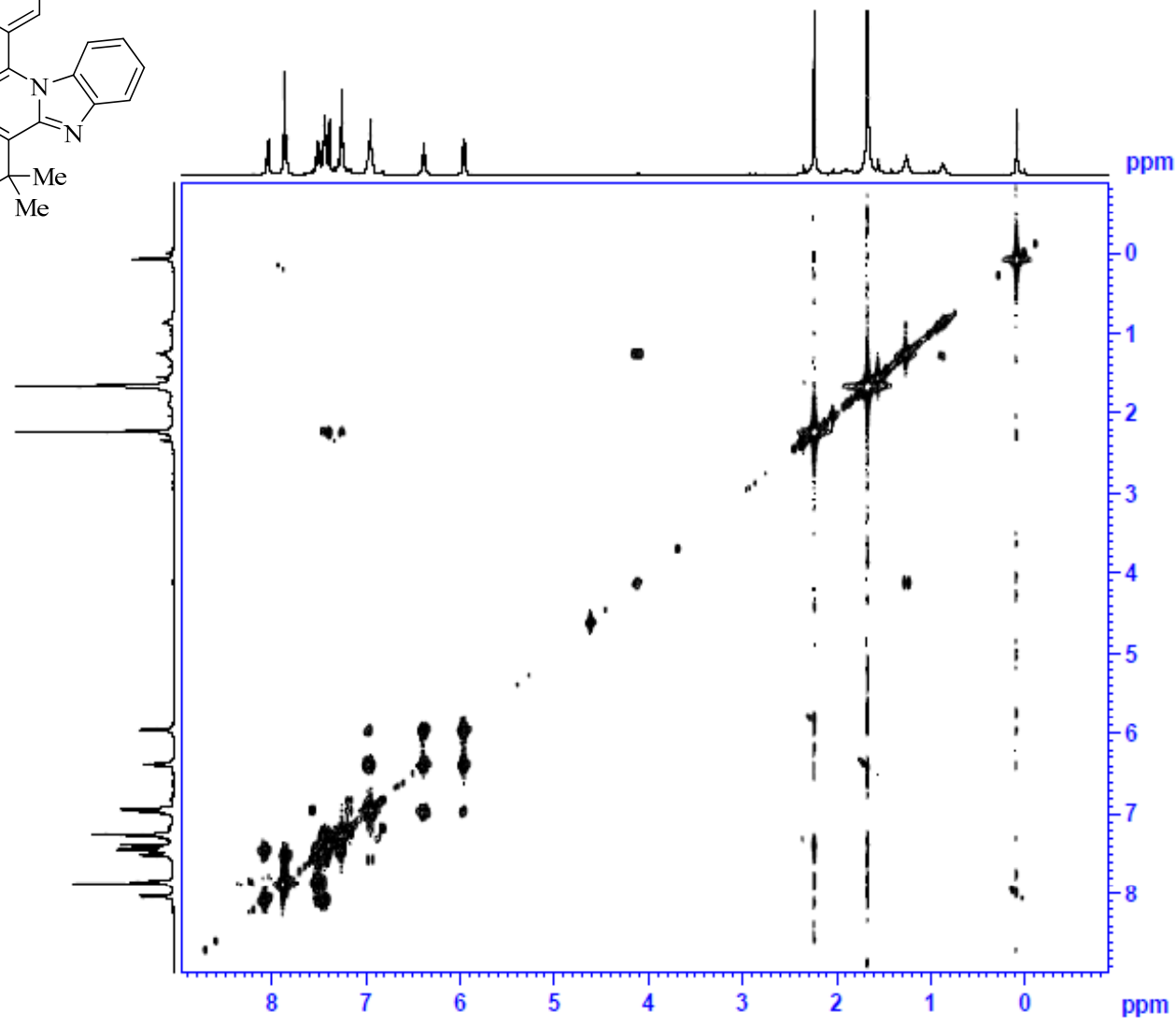
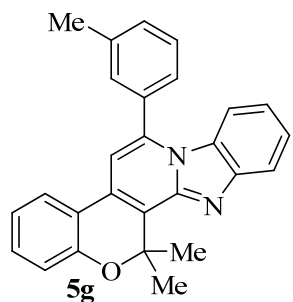


Figure 47: HMBC -Spectrum of 5g.



SKM-546B
CDCl₃, COSY

Current Data Parameters
 NAME SKM-546B,COSY,300 MHz,21.5.13.M
 EXPNO 931
 PROCNO 1

F1 - Acquisition parameters
 TD 128
 SFO1 300.1312 MHz
 FIDRES 23.113965 Hz
 SIV 9.888 ppm
 FxMODE QF

F2 - Processing parameters
 SI 1024
 SF 300.1300111 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 300.1300050 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0

Figure 48: COSY -Spectrum of 5g.

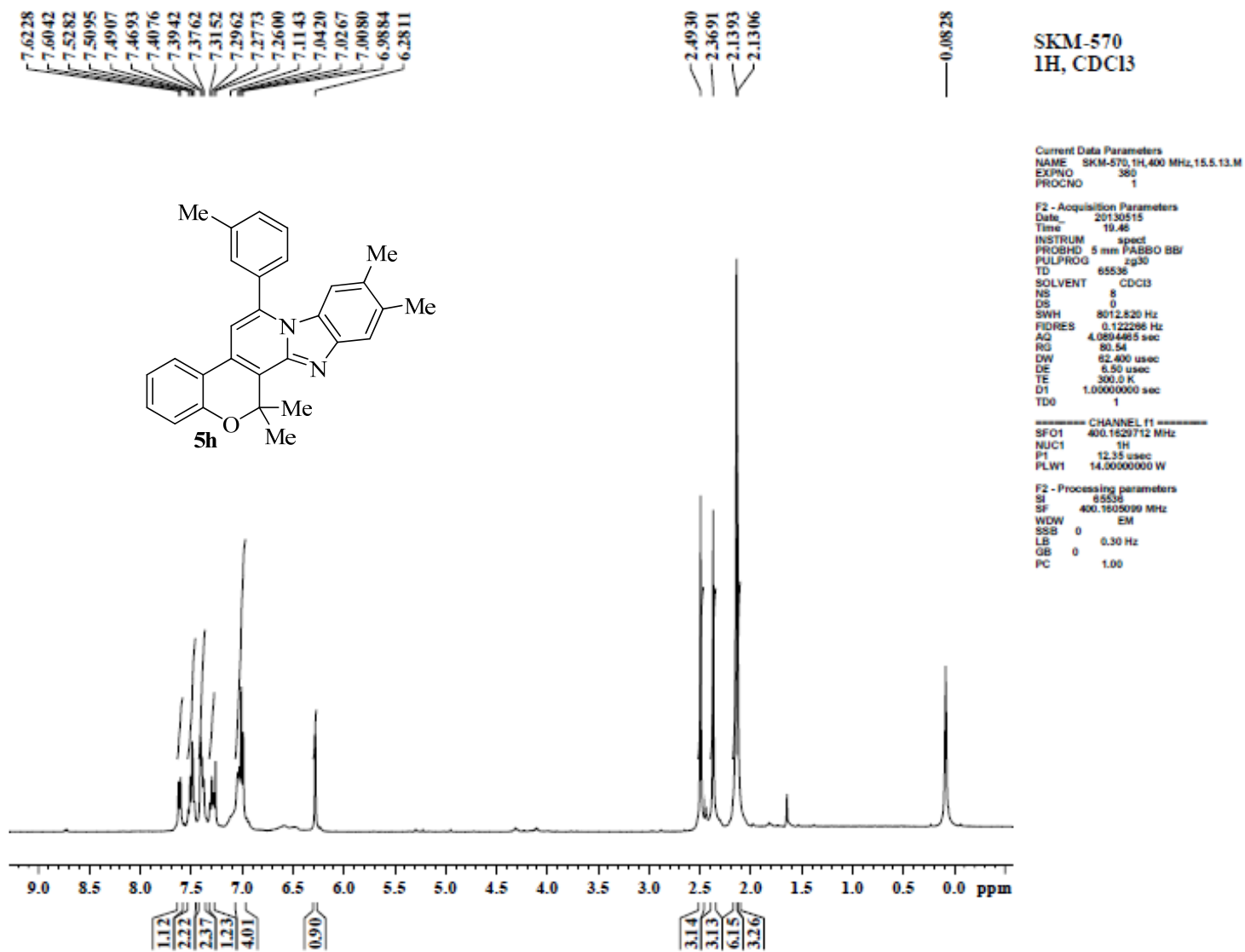


Figure 49: ¹H -NMR Spectrum of **5h**.

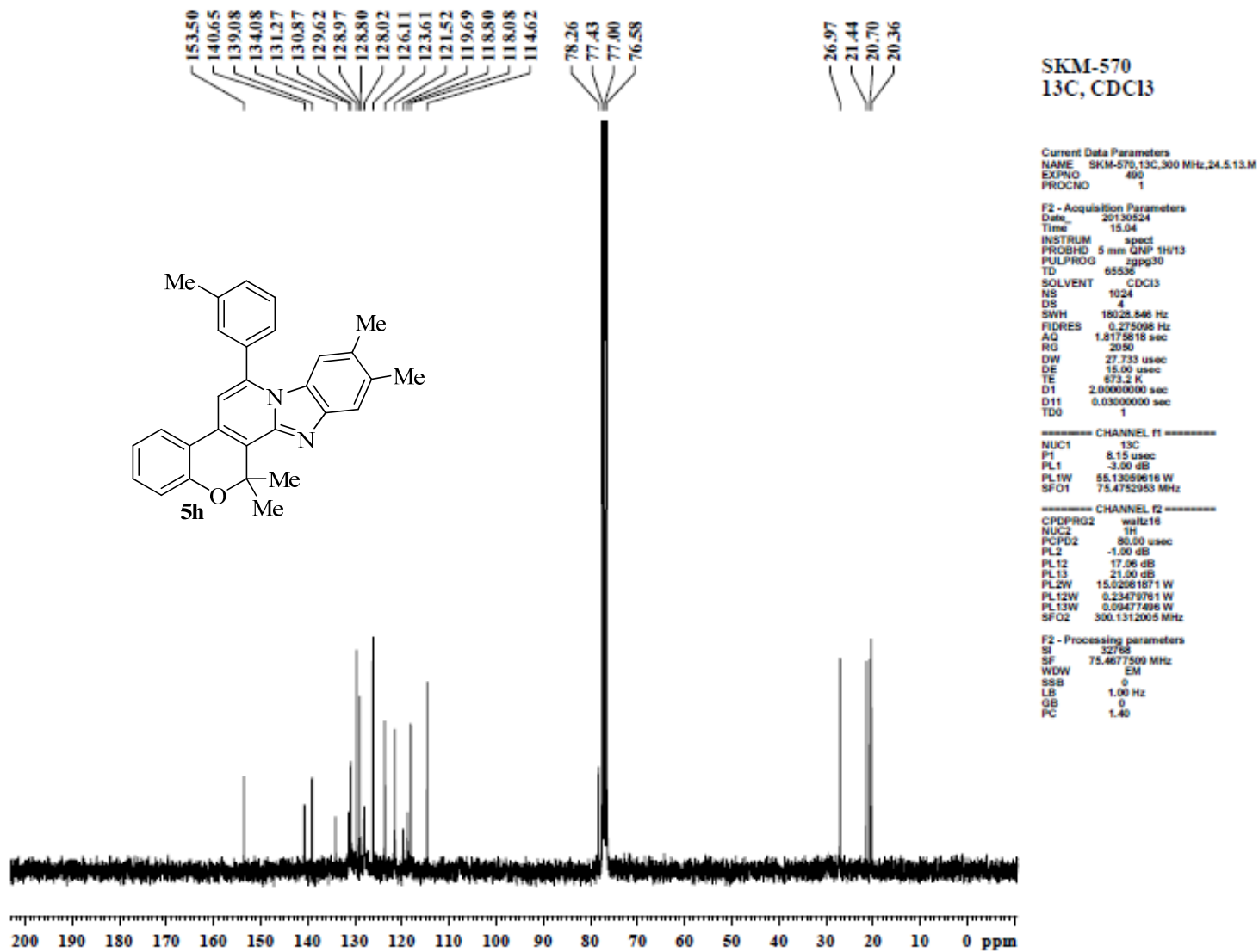


Figure 50: ^{13}C -NMR Spectrum of **5h**.

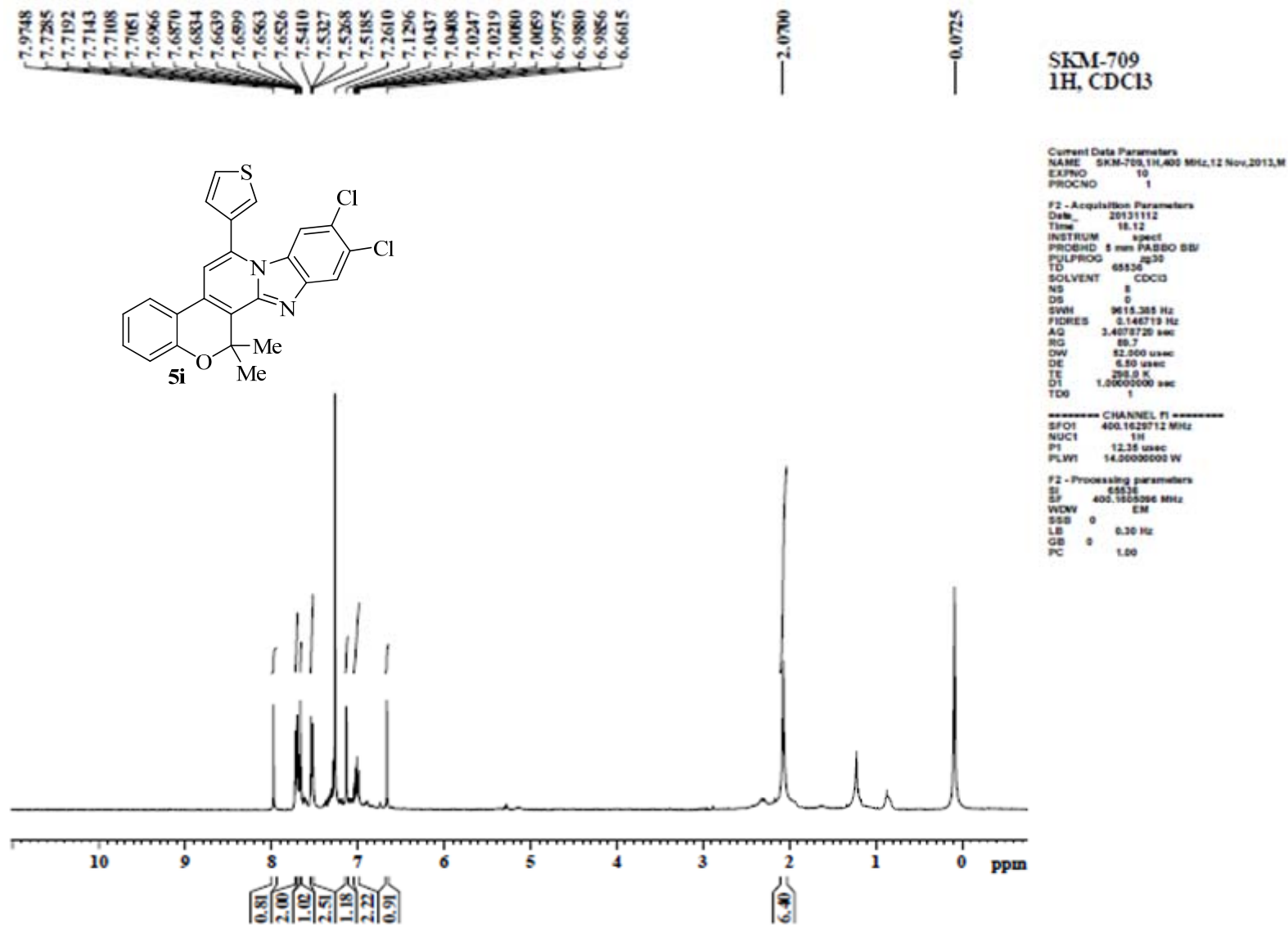


Figure 51: ¹H -NMR Spectrum of **5i**.

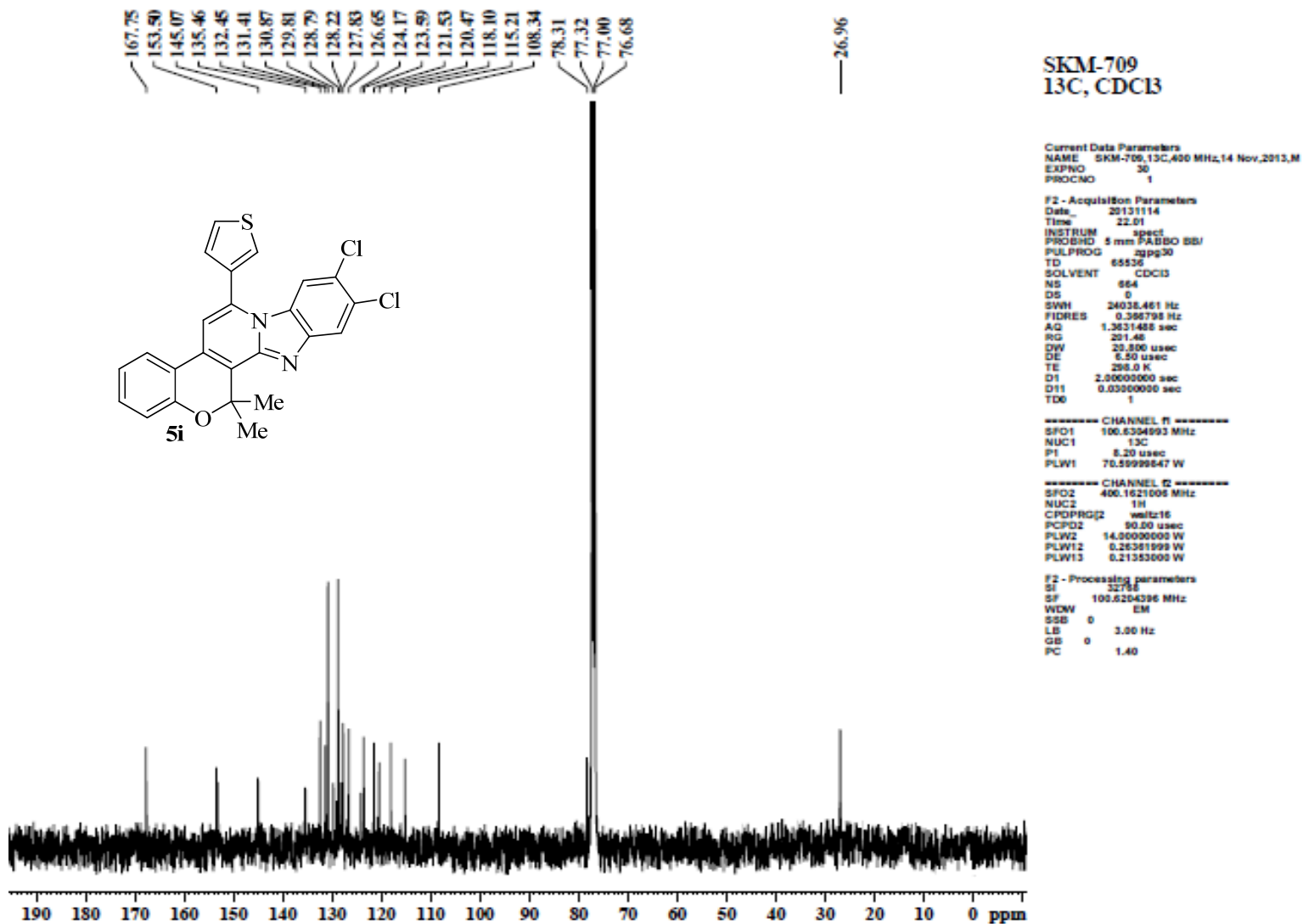


Figure 52: ^{13}C -NMR Spectrum of **5i**.

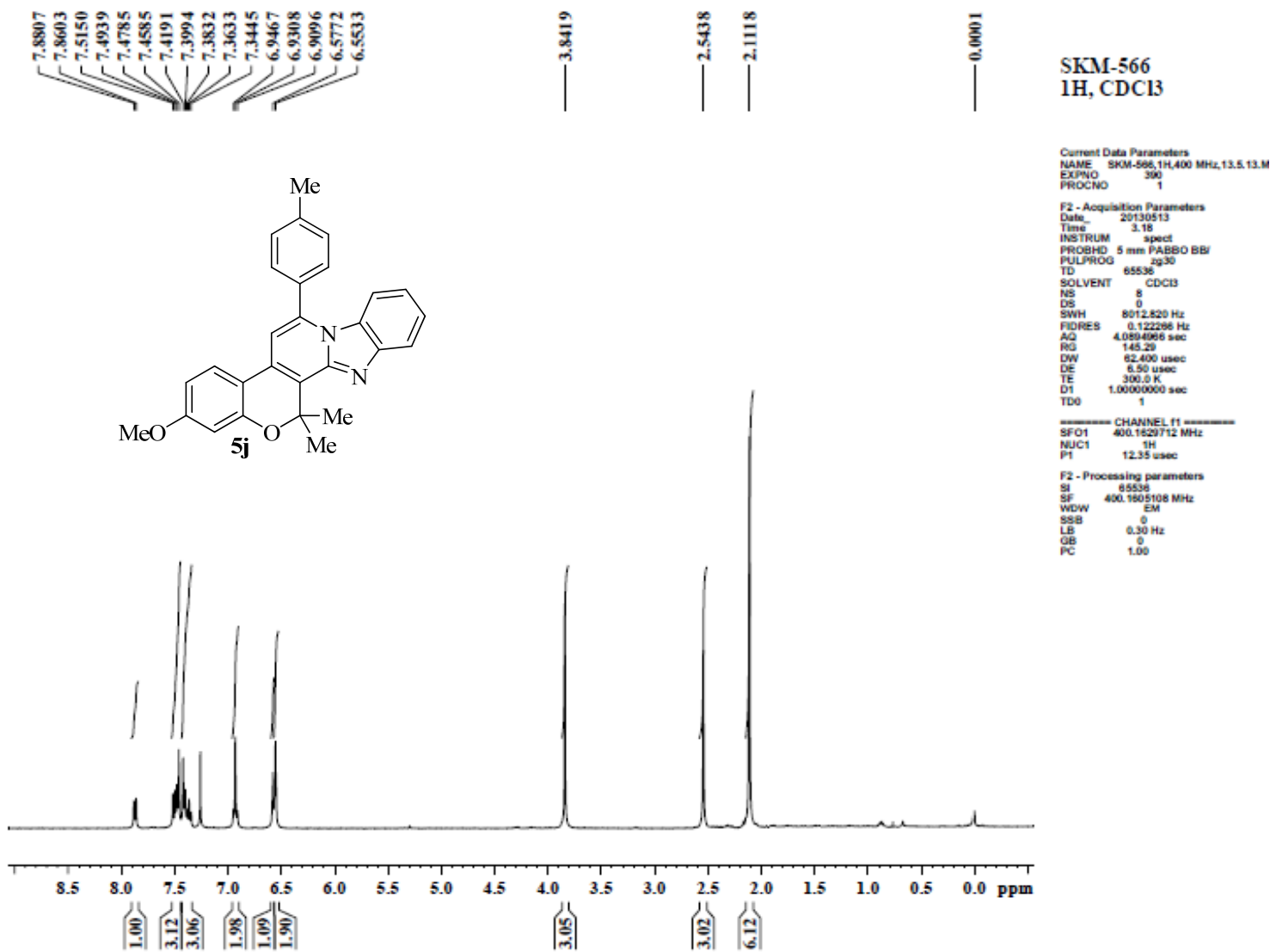


Figure 53: ¹H -NMR Spectrum of **5j**.

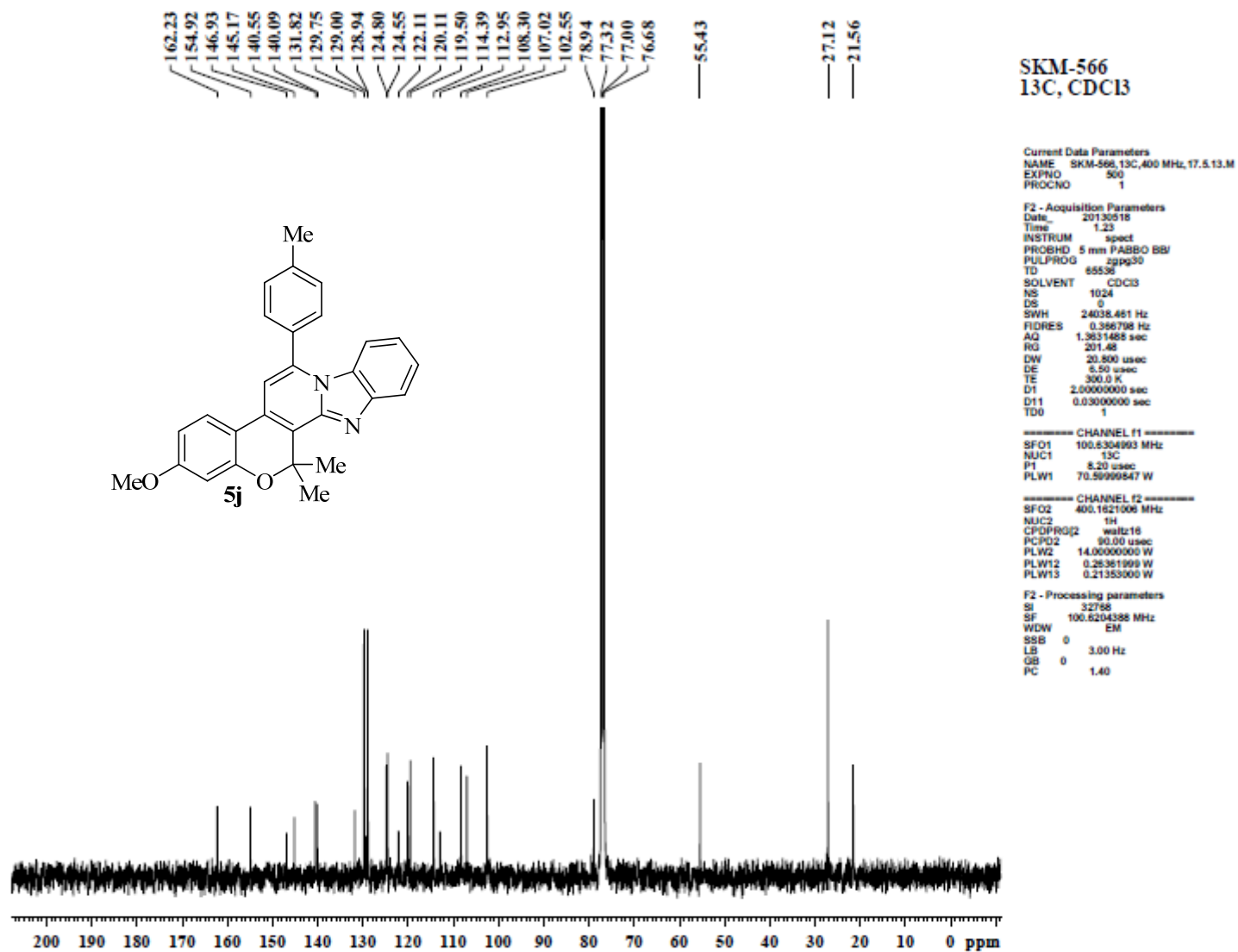


Figure 54: ^{13}C -NMR Spectrum of **5j**.

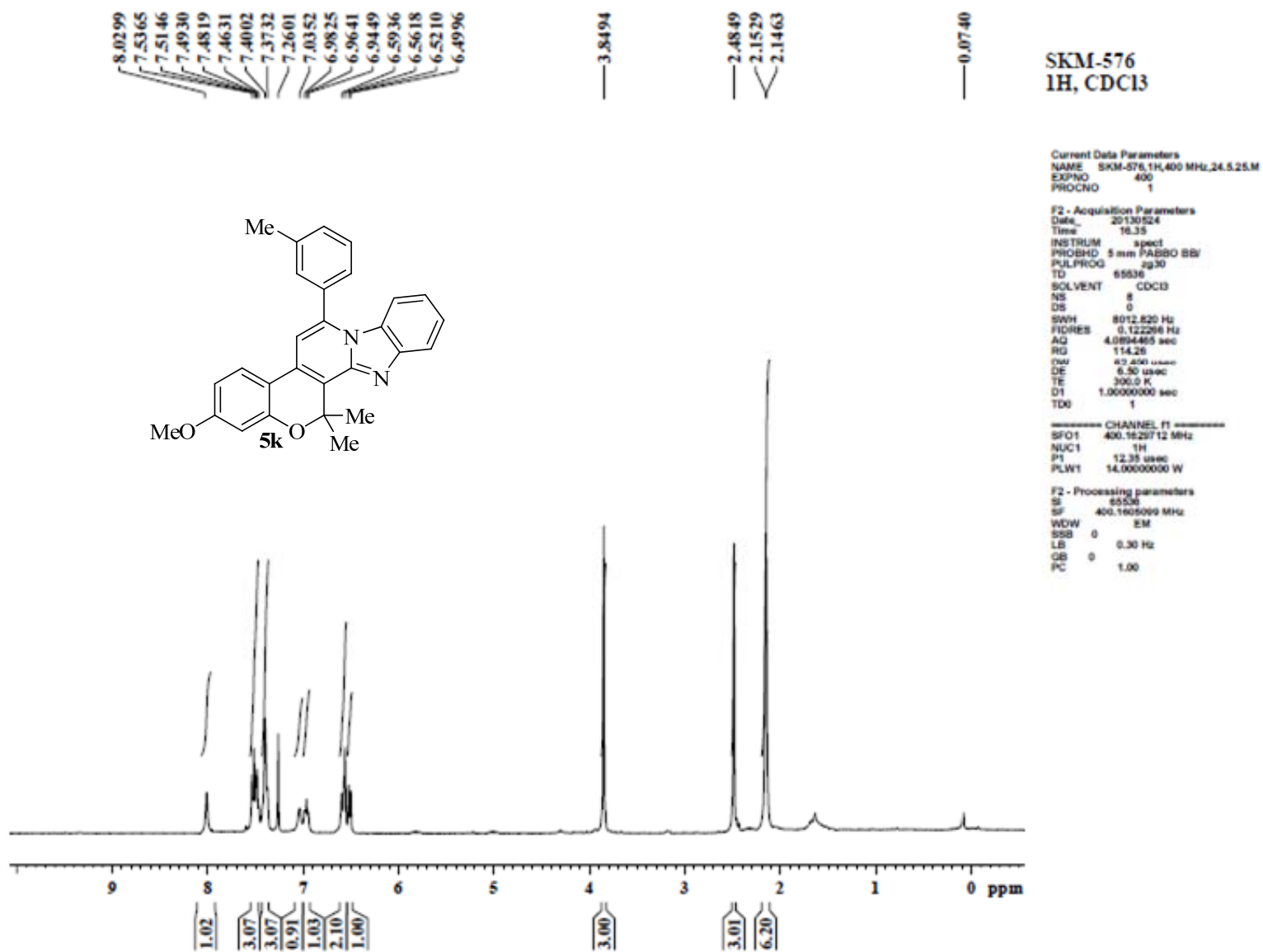


Figure 55: ¹H -NMR Spectrum of **5k**.

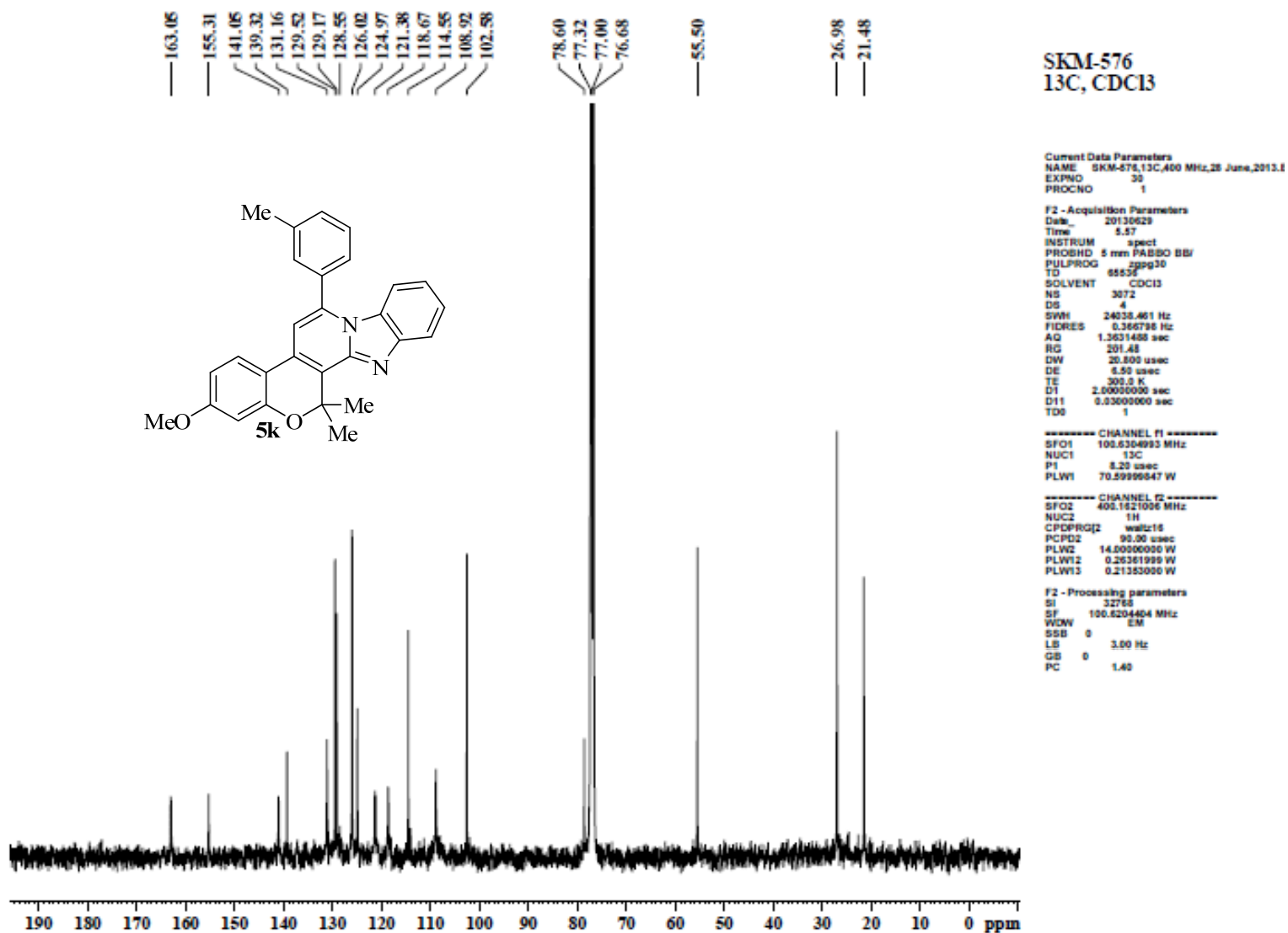
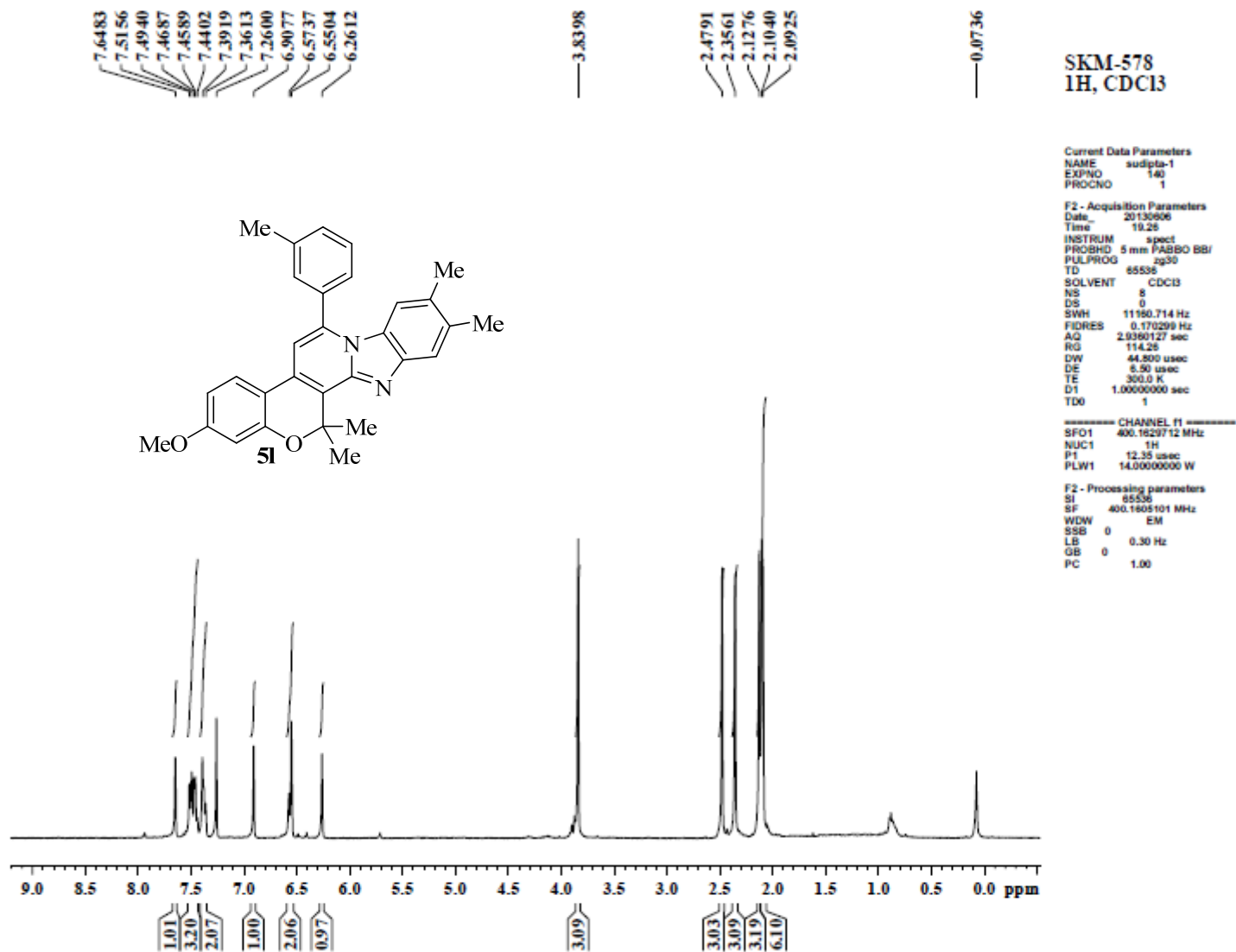


Figure 56: ^{13}C -NMR Spectrum of **5k**.



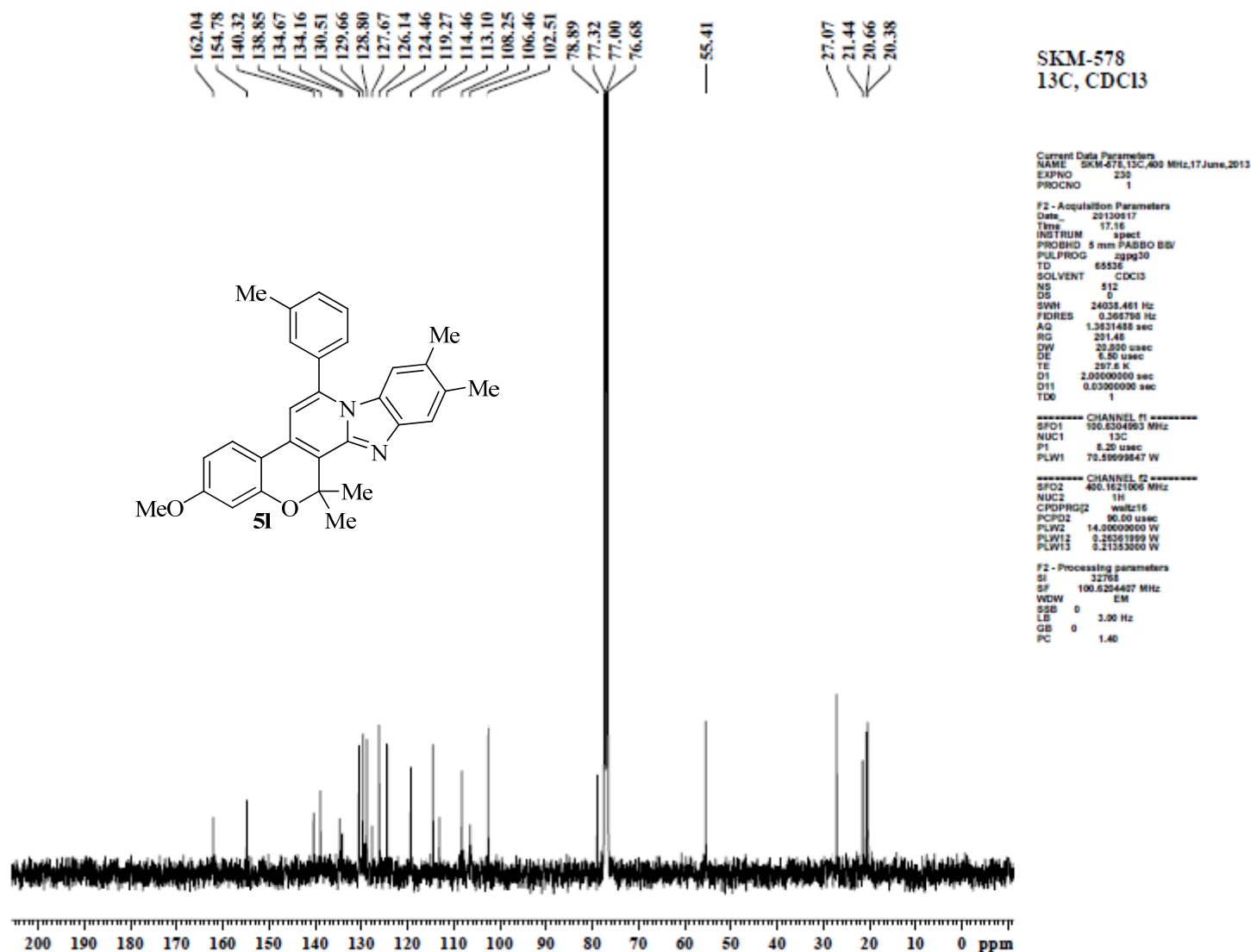


Figure 58: ^{13}C -NMR Spectrum of 5l.

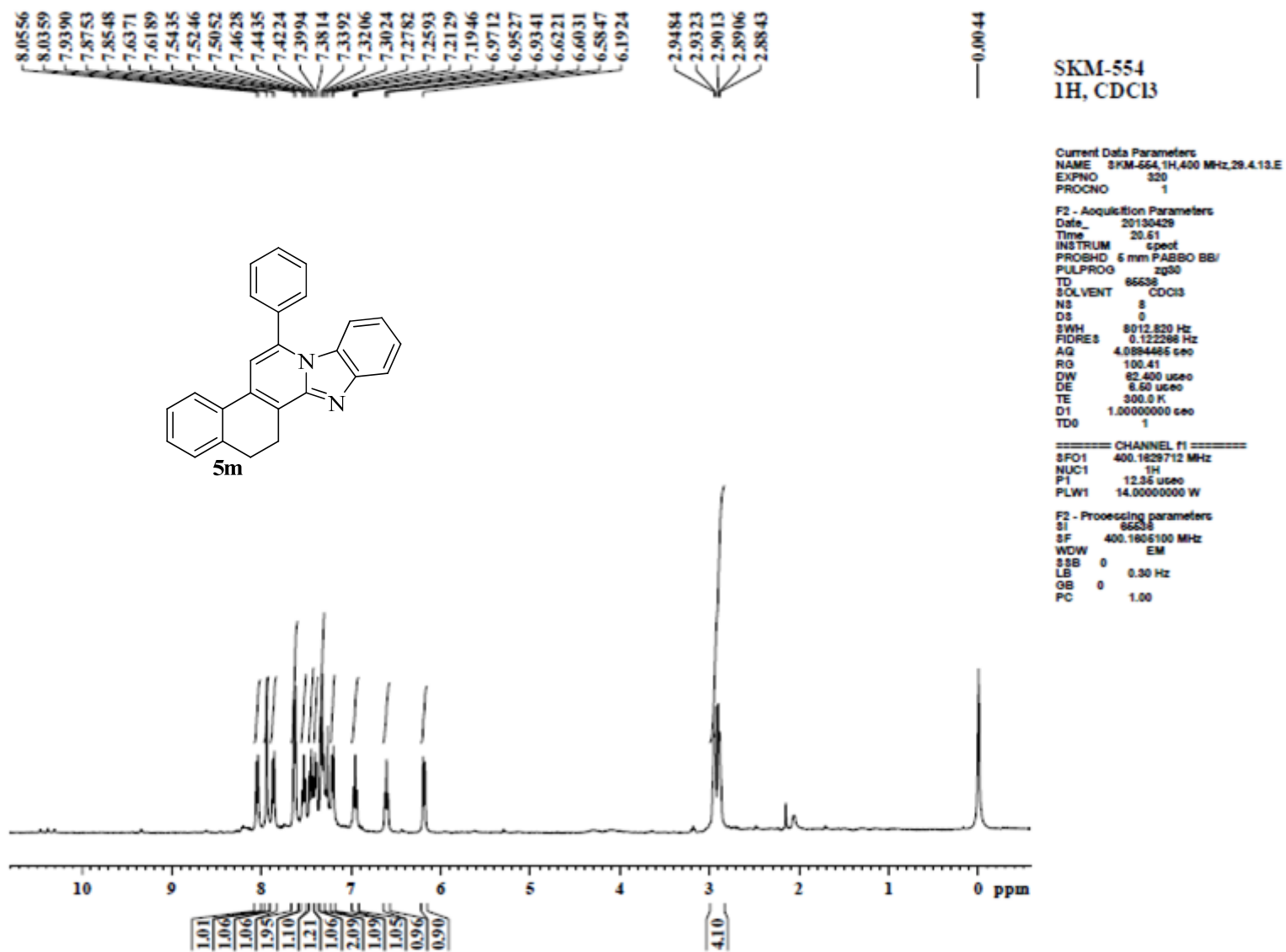


Figure 59: ^1H -NMR Spectrum of **5m**.

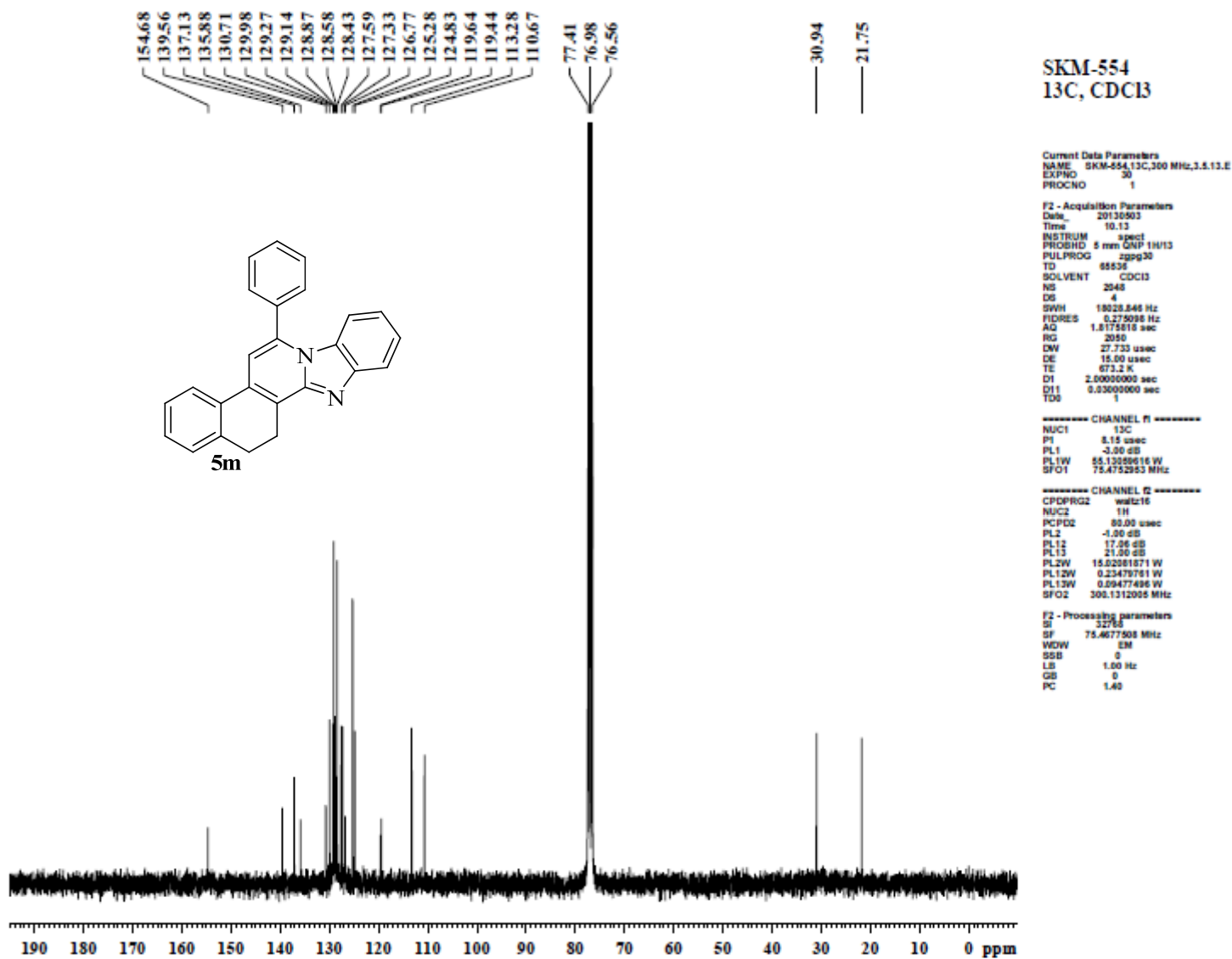


Figure 60: ¹³C -NMR Spectrum of **5m**.

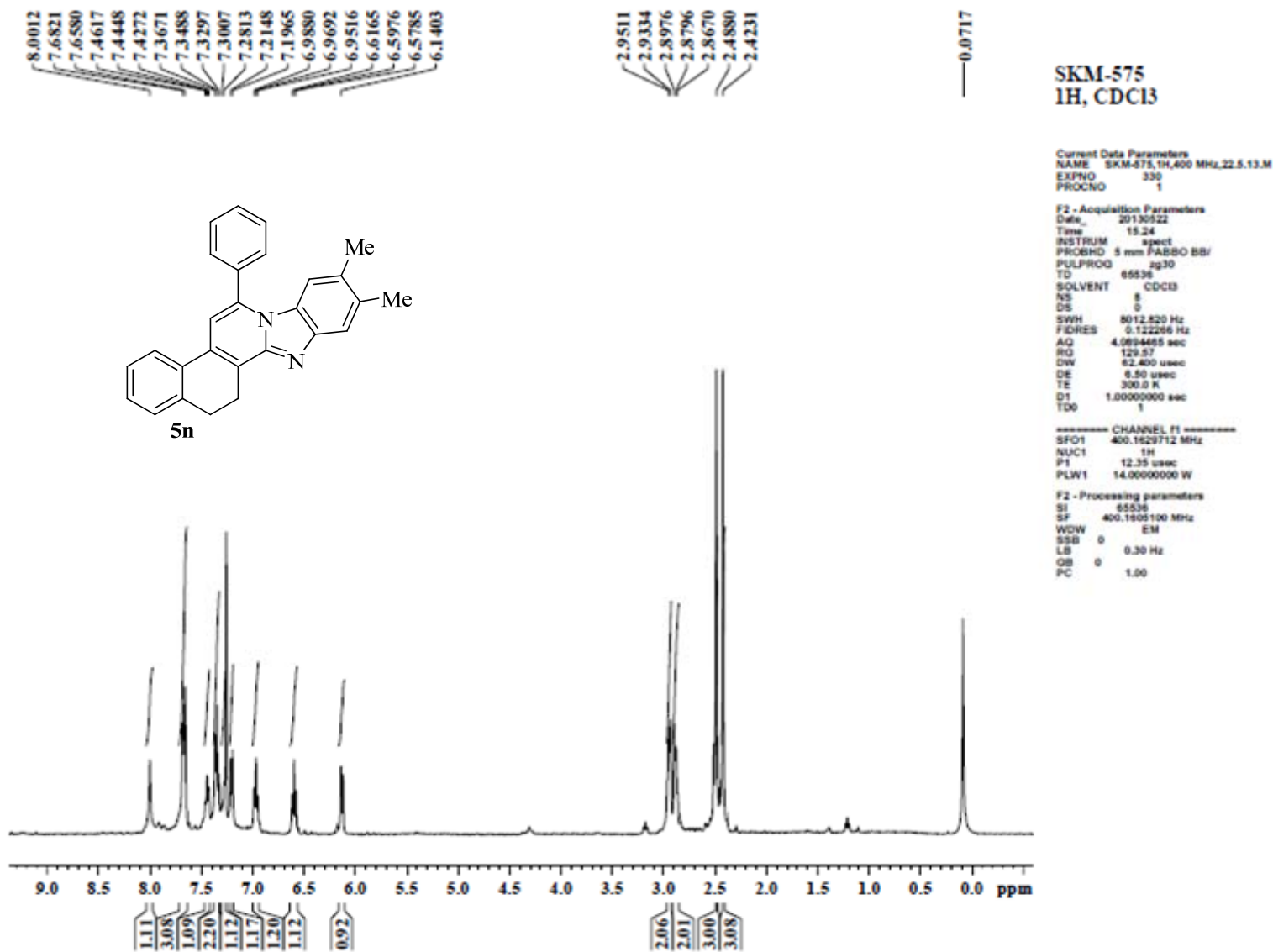


Figure 61: ^1H -NMR Spectrum of **5n**.

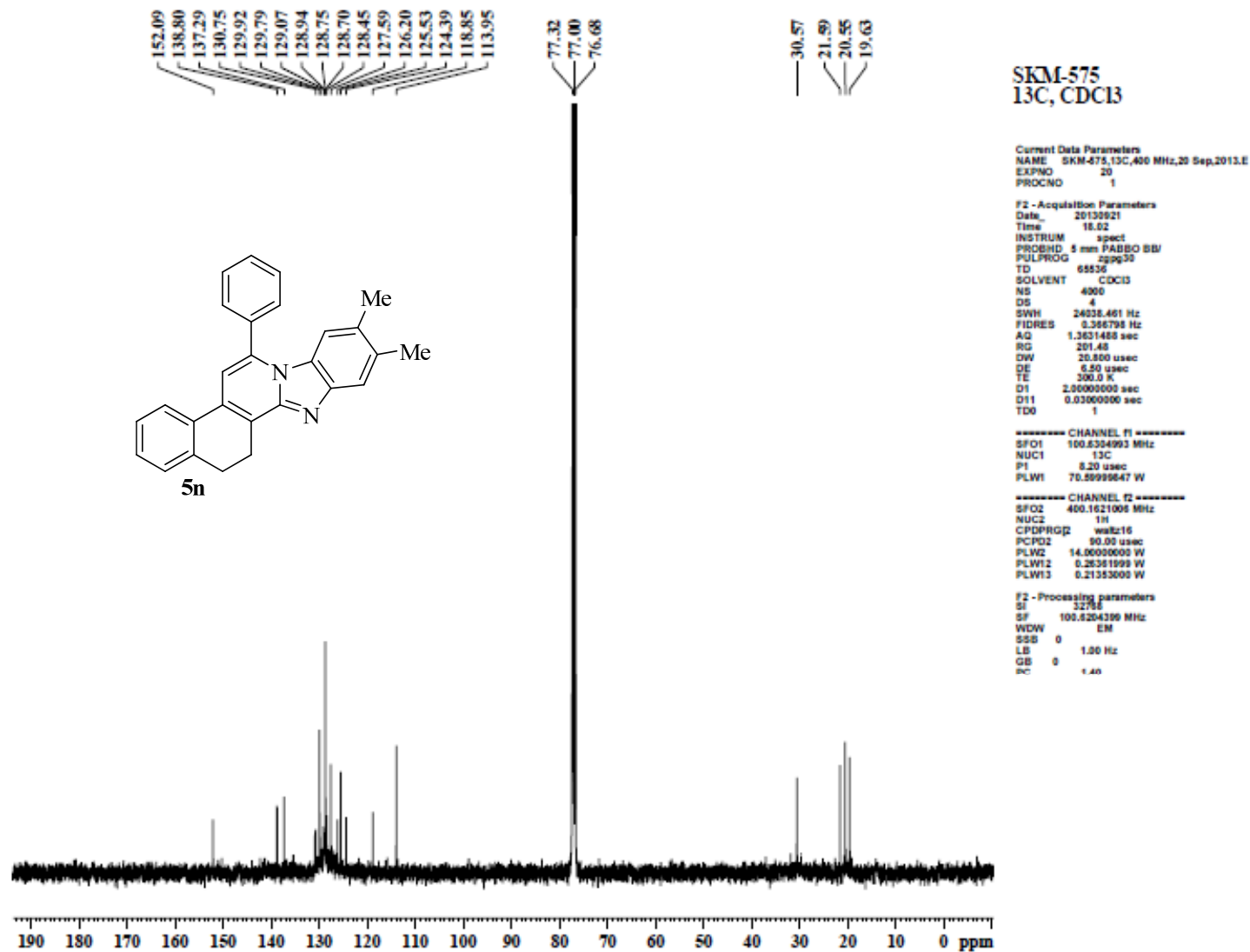


Figure 62: ^{13}C -NMR Spectrum of **5n**.

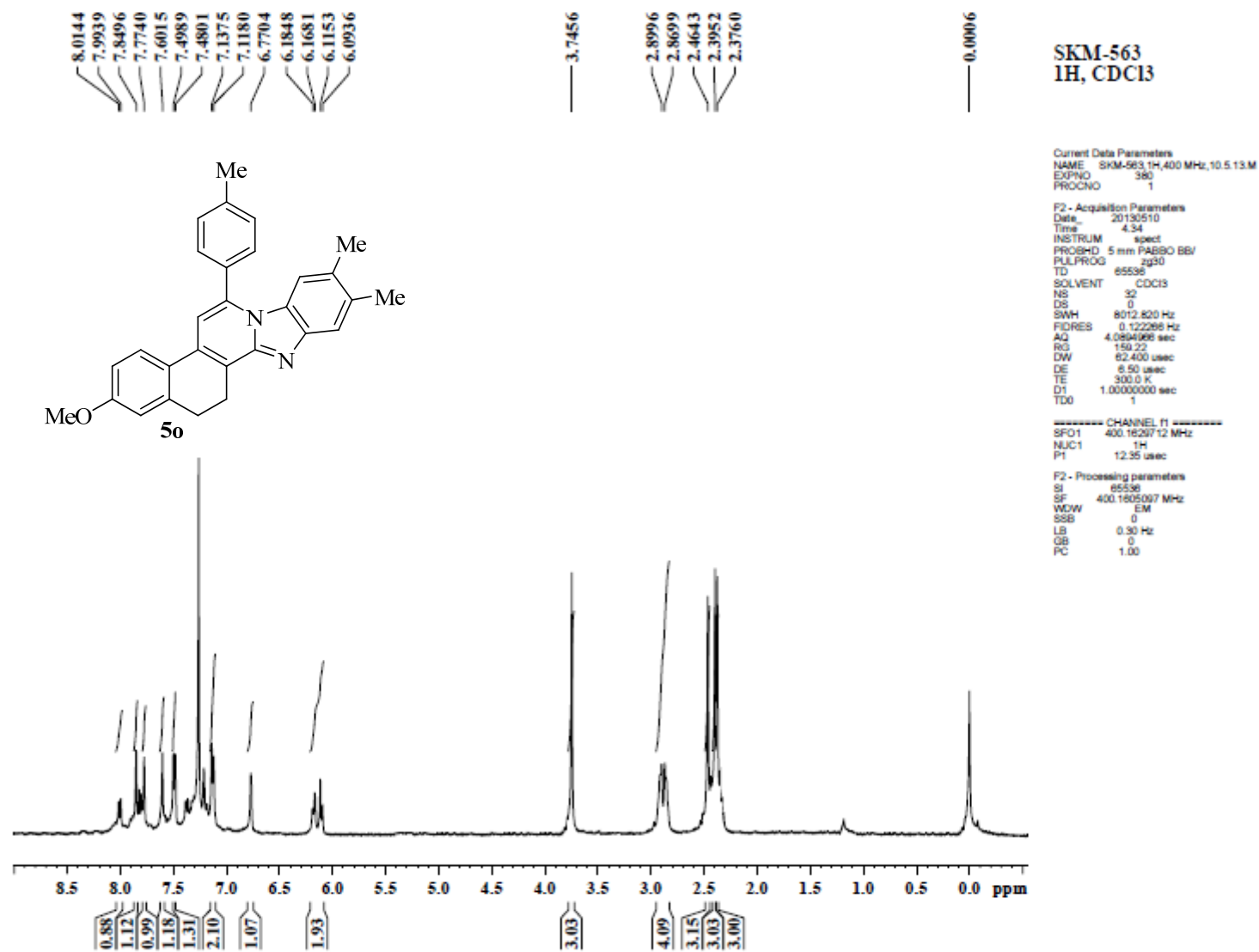


Figure 63: ^1H -NMR Spectrum of **5o**.

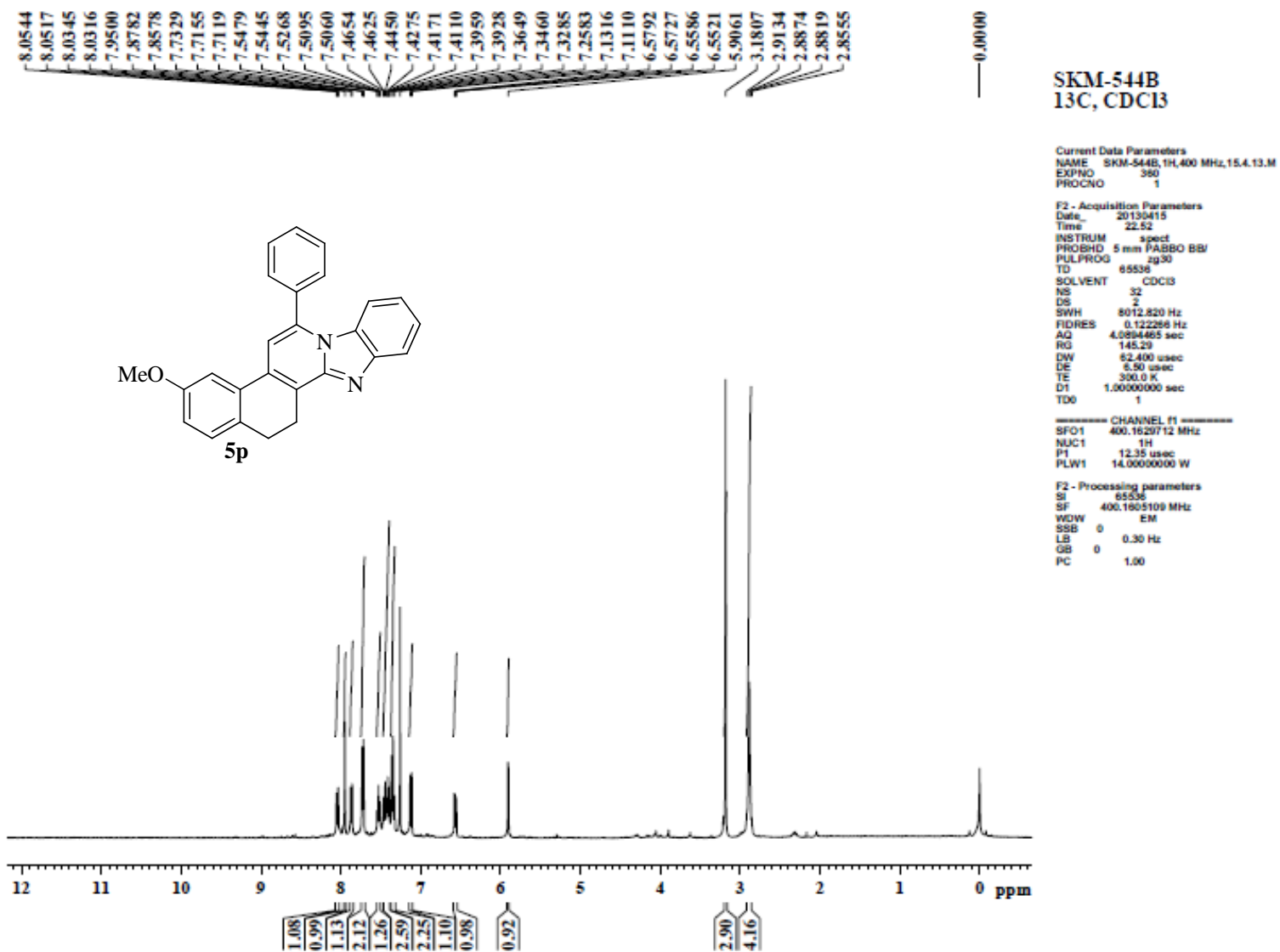


Figure 64: ^1H -NMR Spectrum of **5p**.

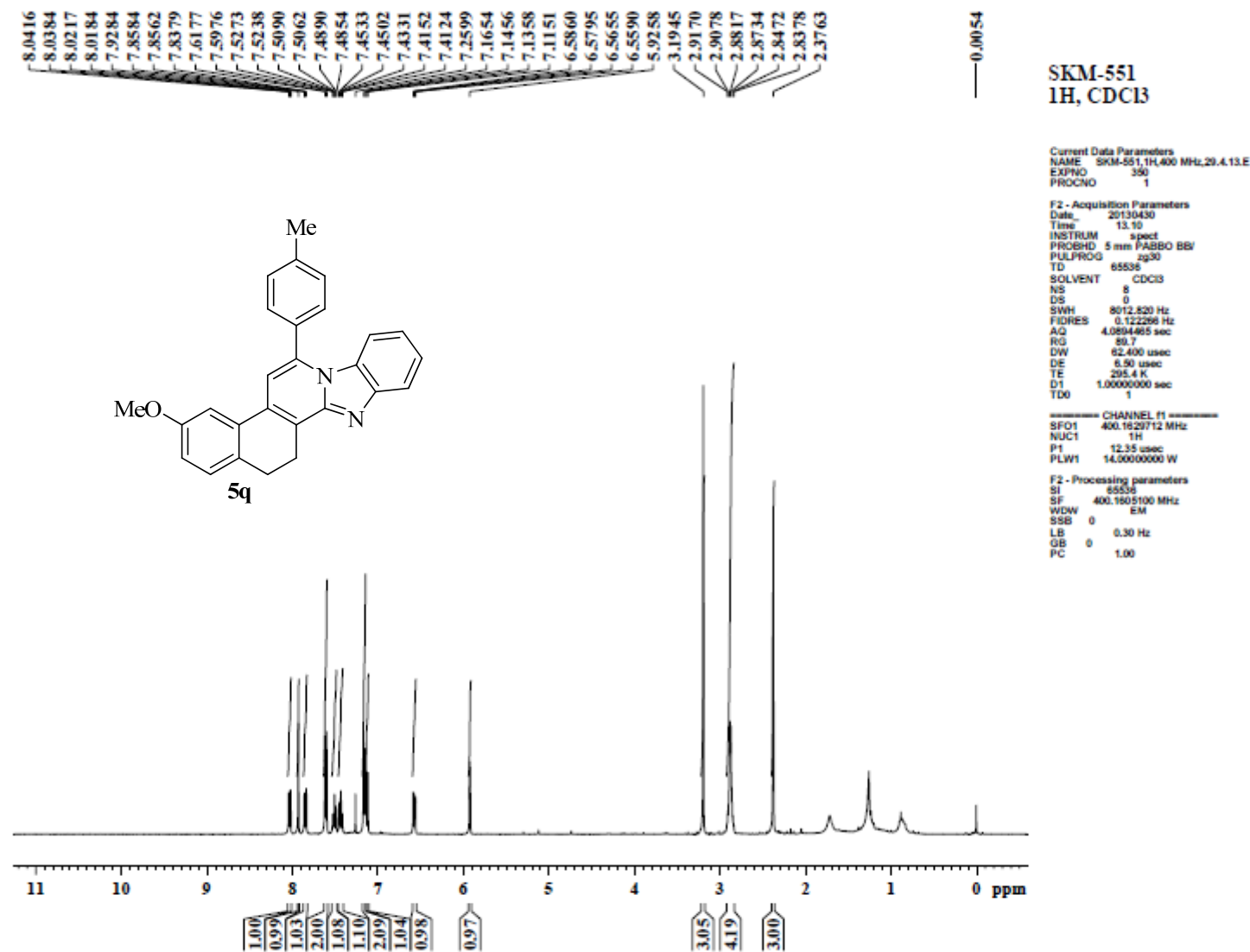


Figure 65: ¹H -NMR Spectrum of 5q.

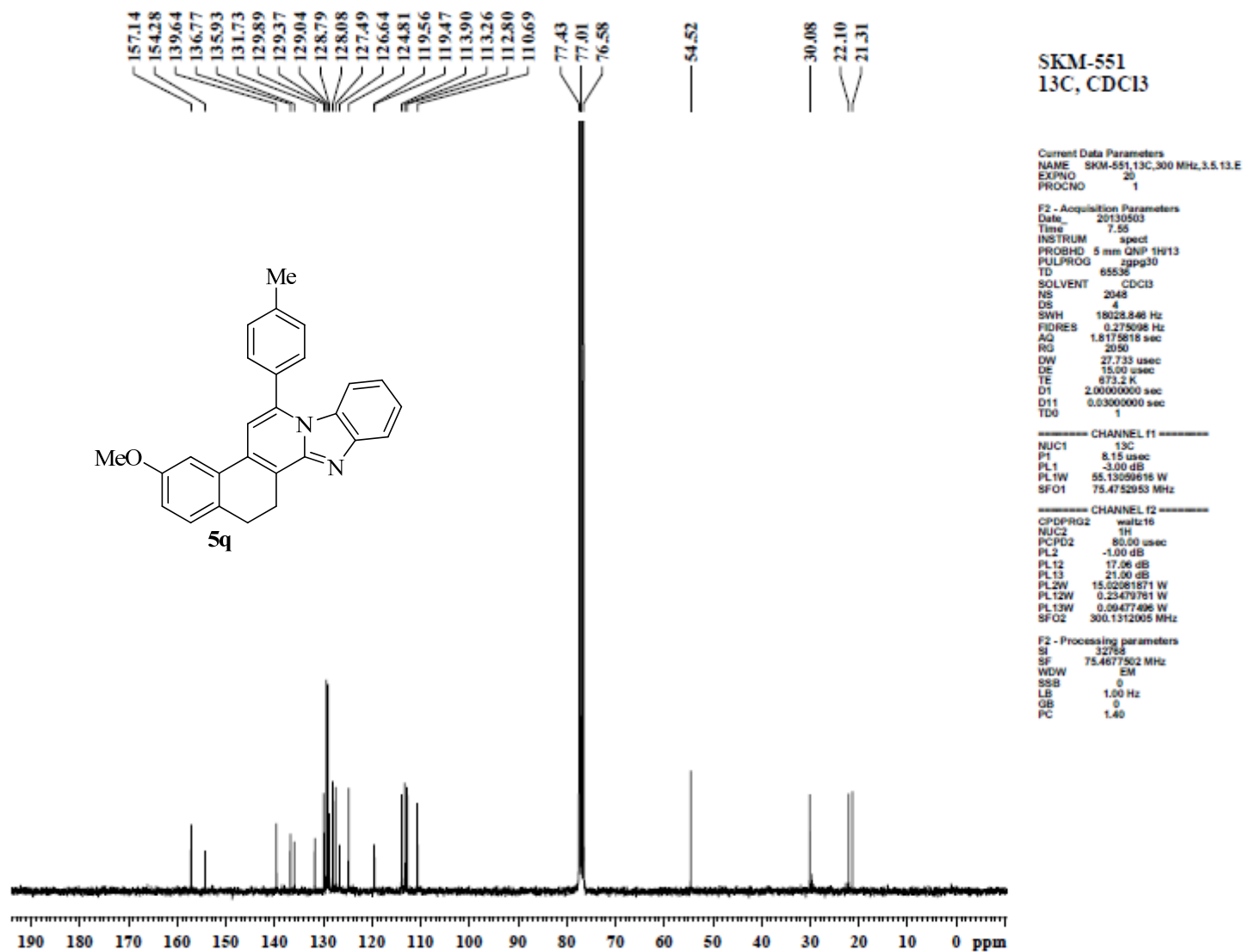


Figure 66: ^{13}C -NMR Spectrum of **5q**.

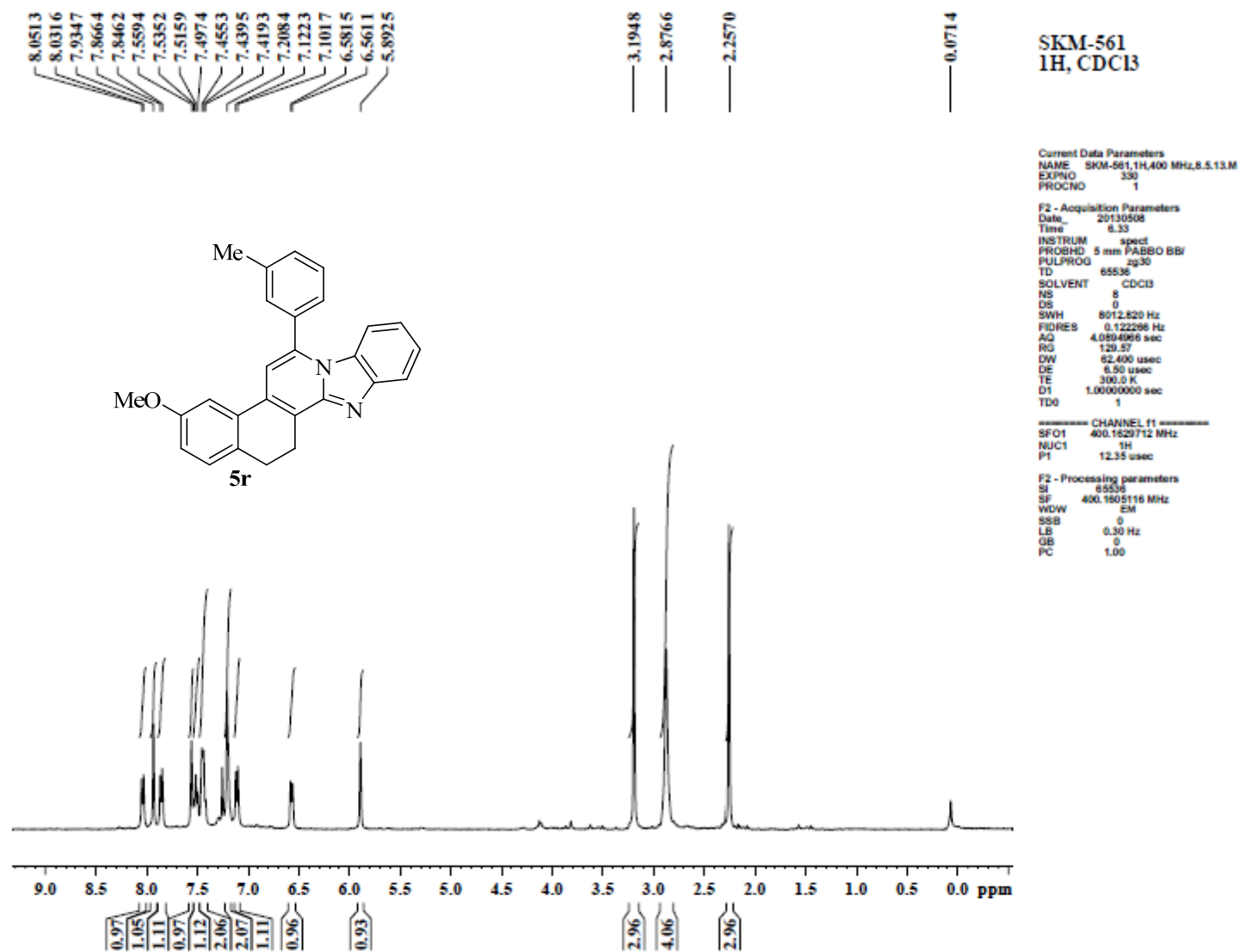


Figure 67: ¹H -NMR Spectrum of **5r**.

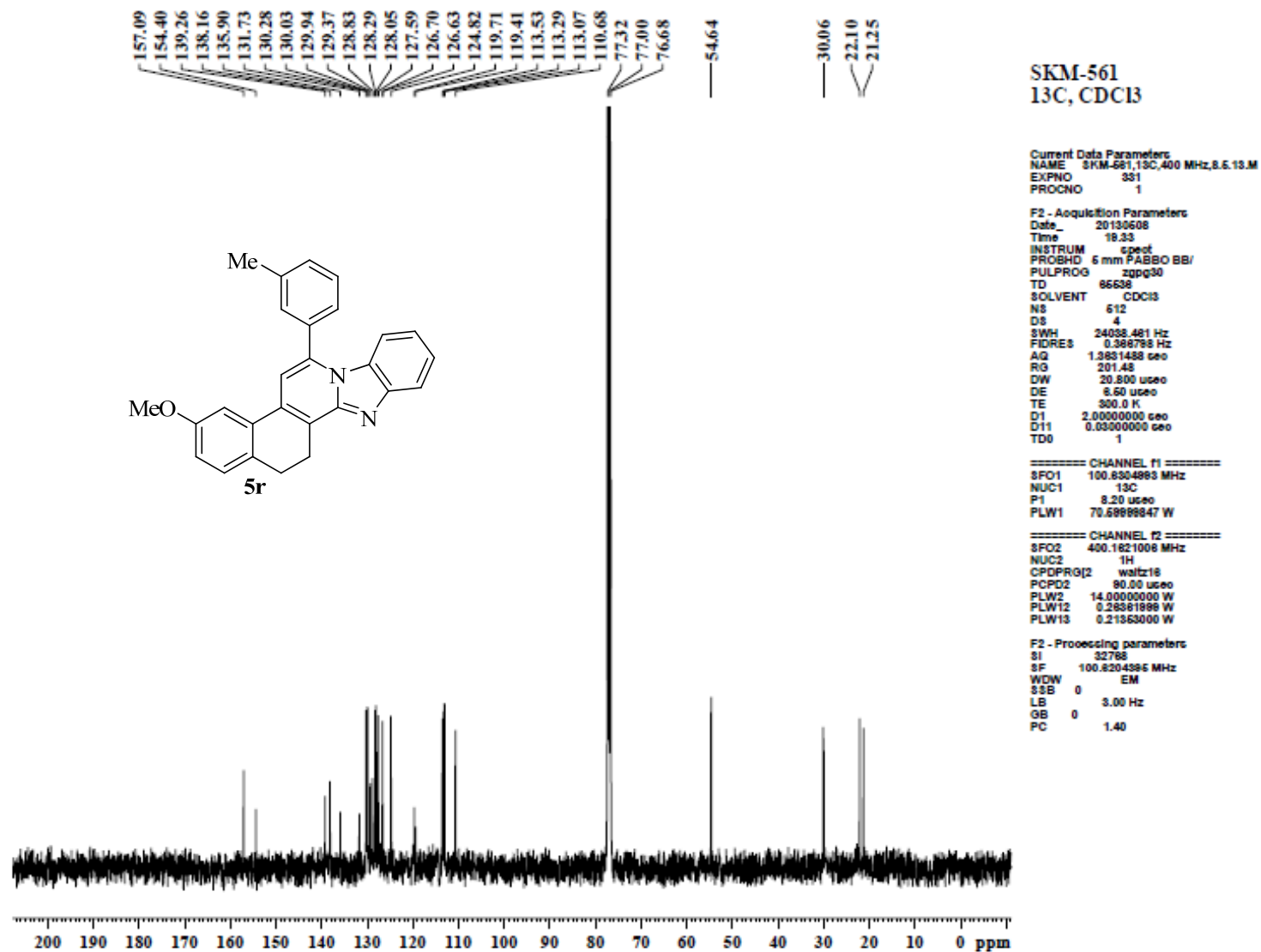


Figure 68: ^{13}C -NMR Spectrum of **5r**.

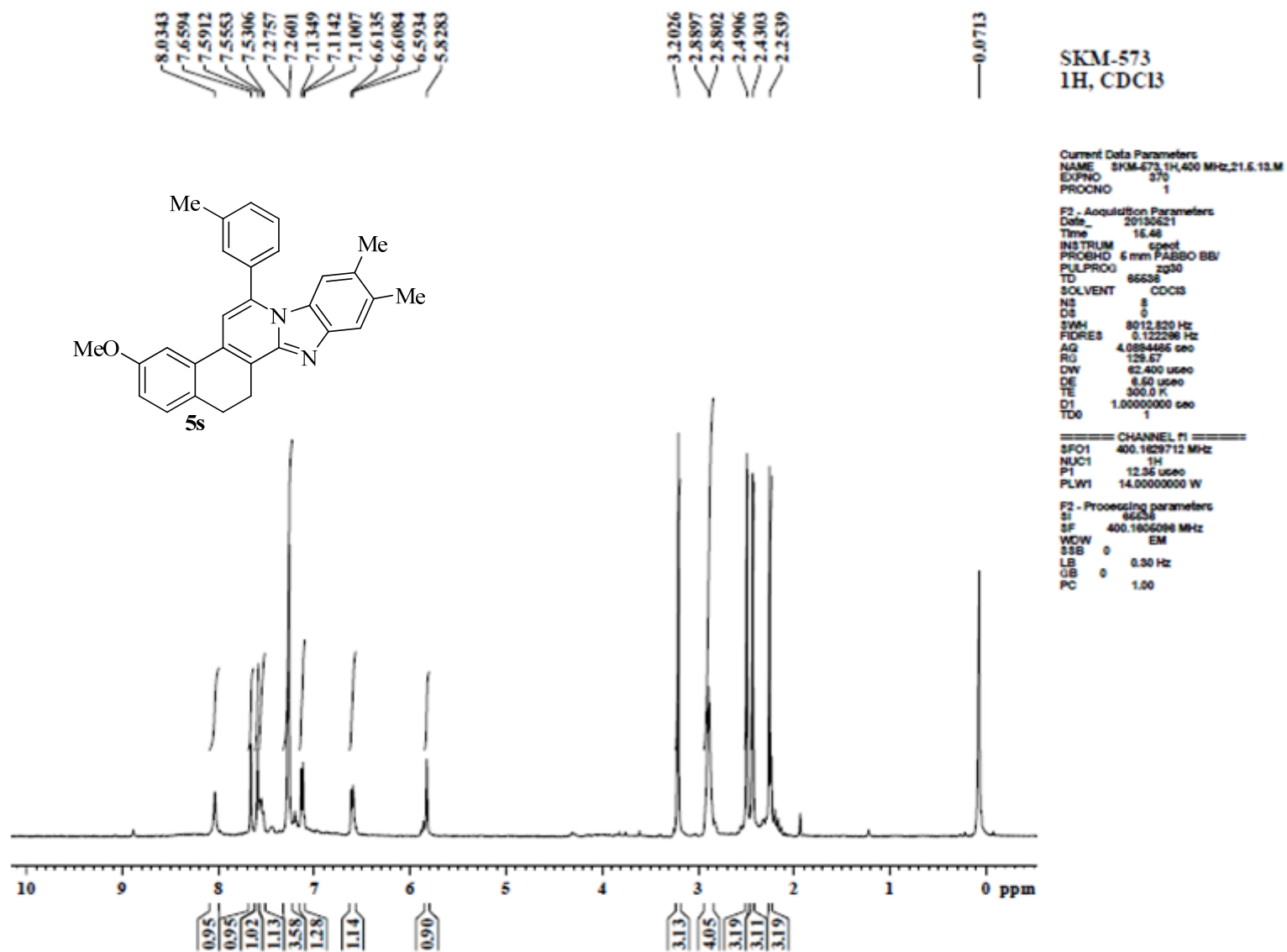
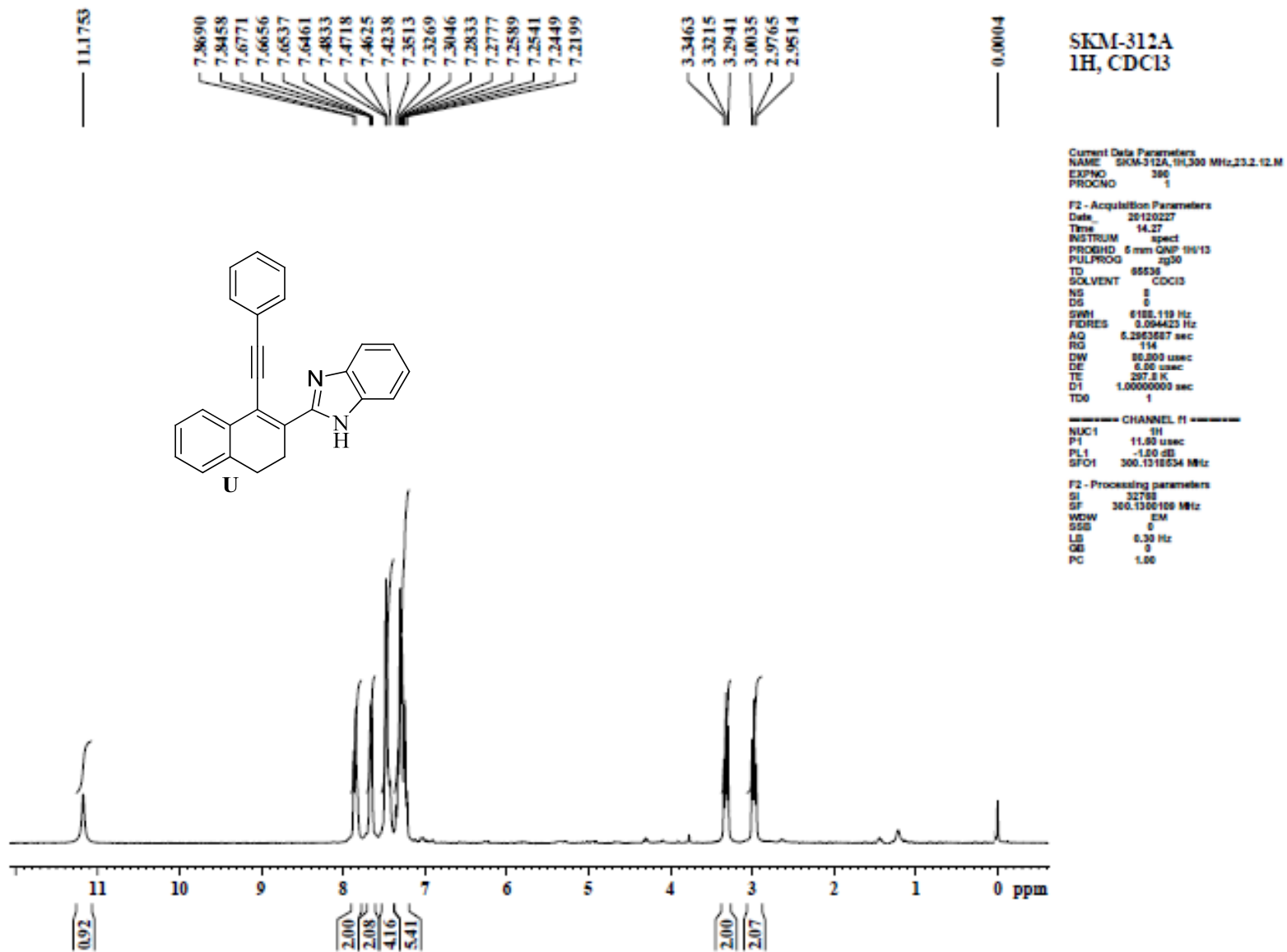


Figure 69: ¹H -NMR Spectrum of **5s**.



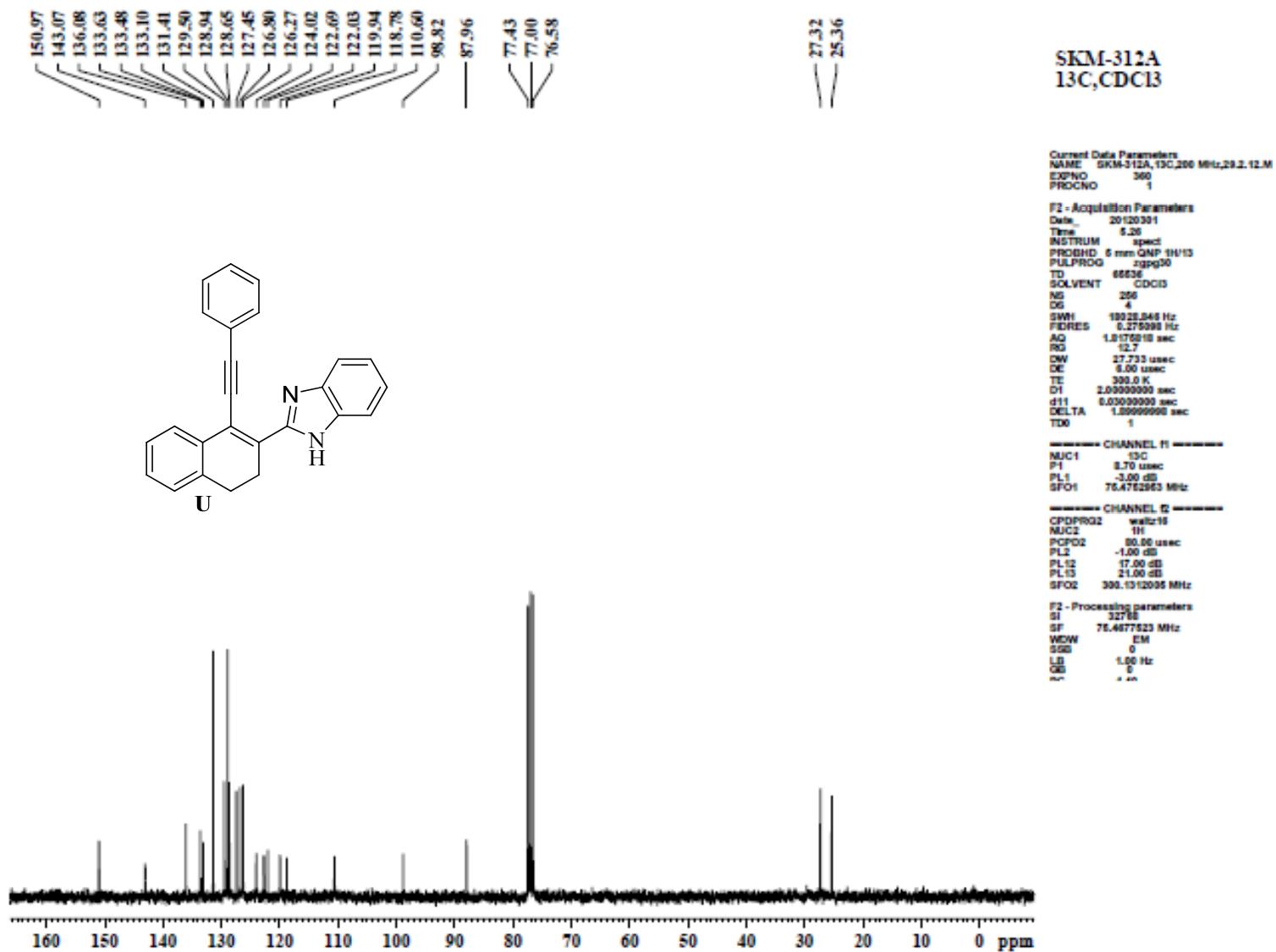


Figure 71: ¹³C -NMR Spectrum of **U**.

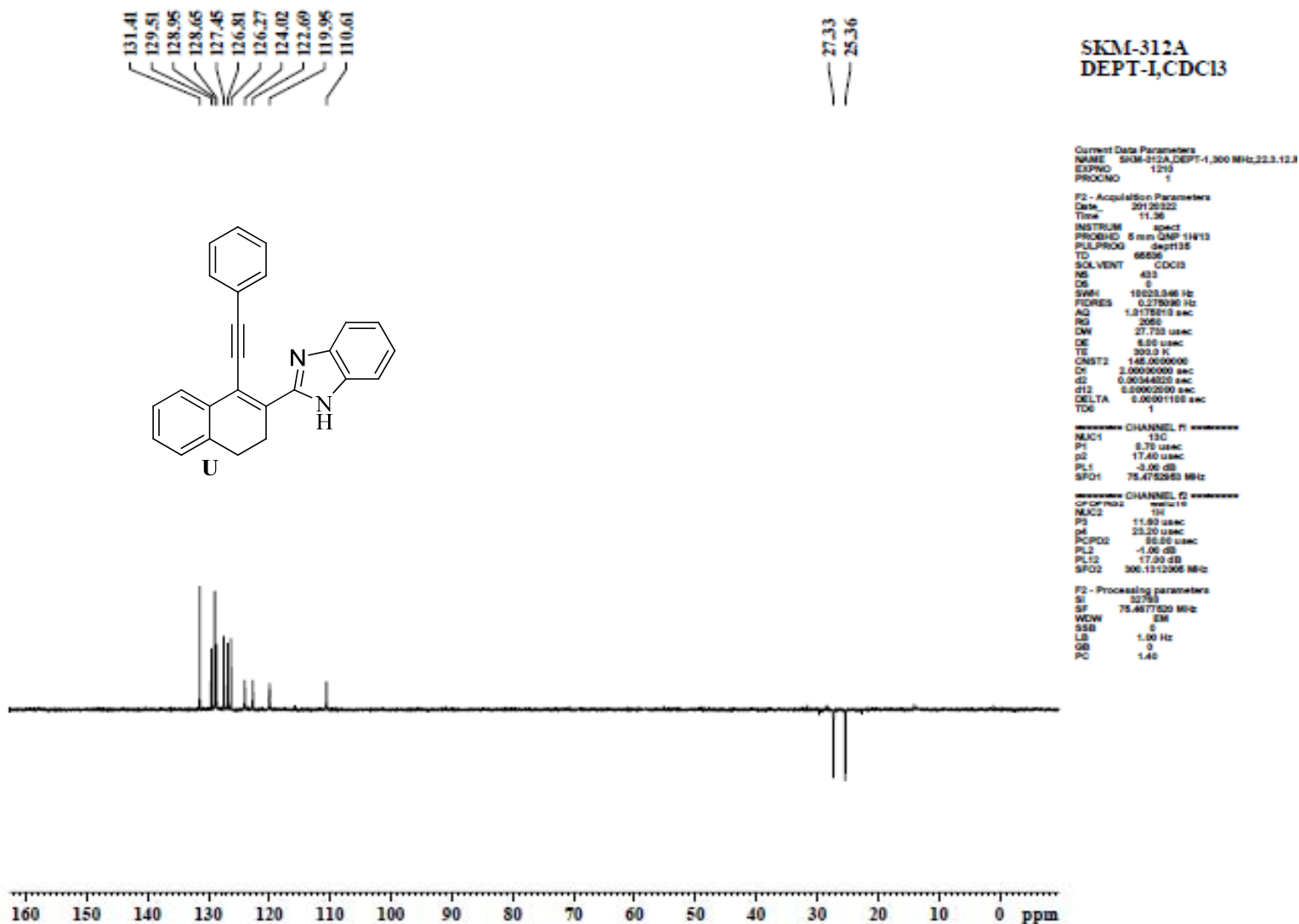
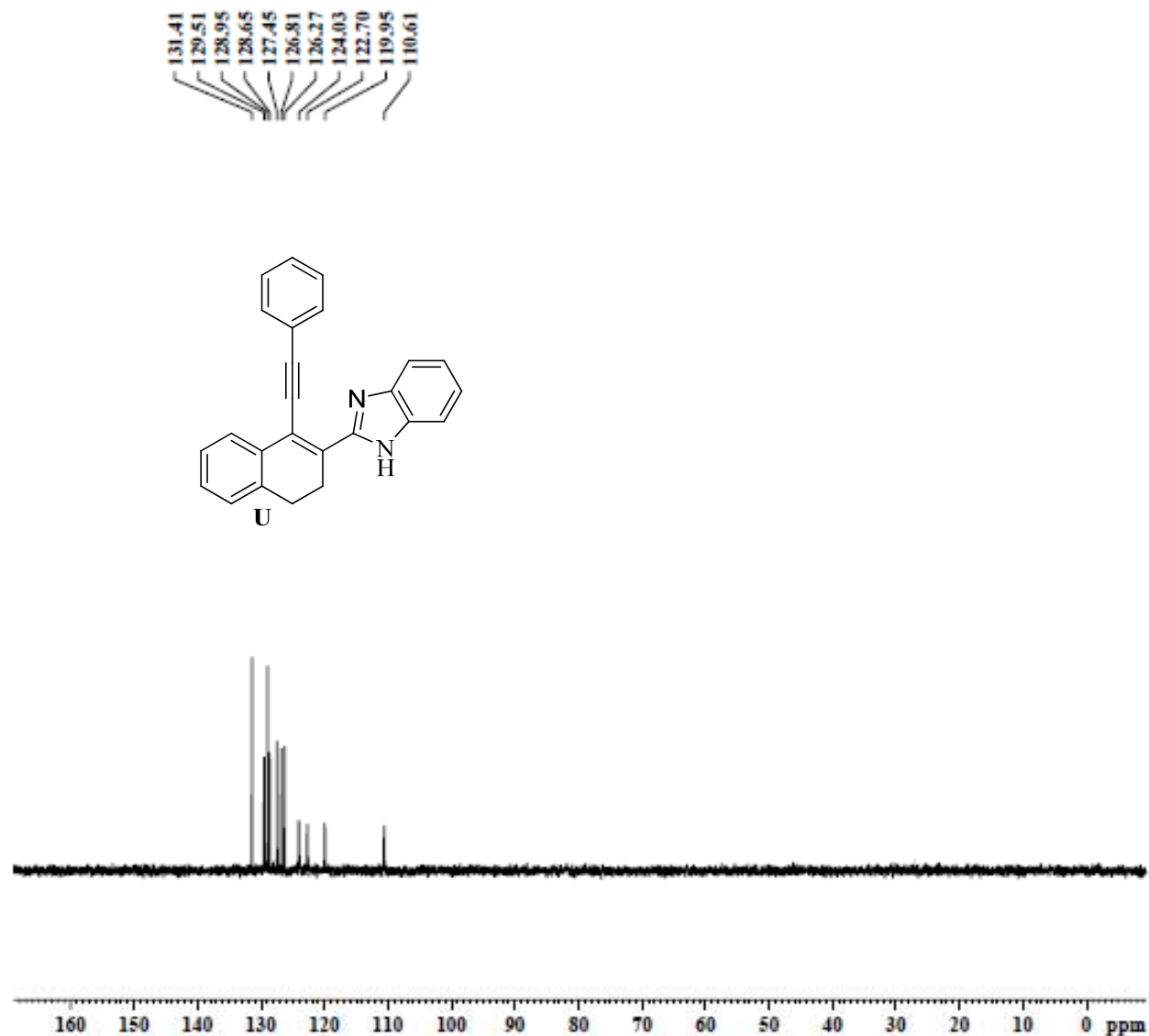


Figure 72: DEPT-I -Spectrum of **U**.



**SKM-312A
DEPT-II,CDC13**

Current Data Parameters
 NAME SKM-312A_DEPT-II,300 MHz,123.12 M
 EXPNO 1211
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120322
 Time 12.54
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG dept90
 TD 65536
 SOLVENT CDC13
 NS 118
 DS 0
 SWH 18028.848 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 6.00 usec
 TE 300.0 K
 CNST2 145.9000000
 D1 2.0000000 sec
 d2 0.00344828 sec
 d12 0.00002000 sec
 DELTA 0.00001100 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.70 usec
 p2 17.40 usec
 PL1 -3.00 dB
 SFO1 75.4782963 MHz

----- CHANNEL f2 -----
 CPDPRG2 waHz16
 NUC2 1H
 P3 11.80 usec
 p4 23.20 usec
 PCPD2 00.00 usec
 PL2 -1.00 dB
 PL2z 17.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677620 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 73: DEPT-II -Spectrum of U.