

Indium triflate catalysed 3-aza-Cope rearrangement of Amino acid derived α,β -unsaturated esters to the alkylidene oxindoles

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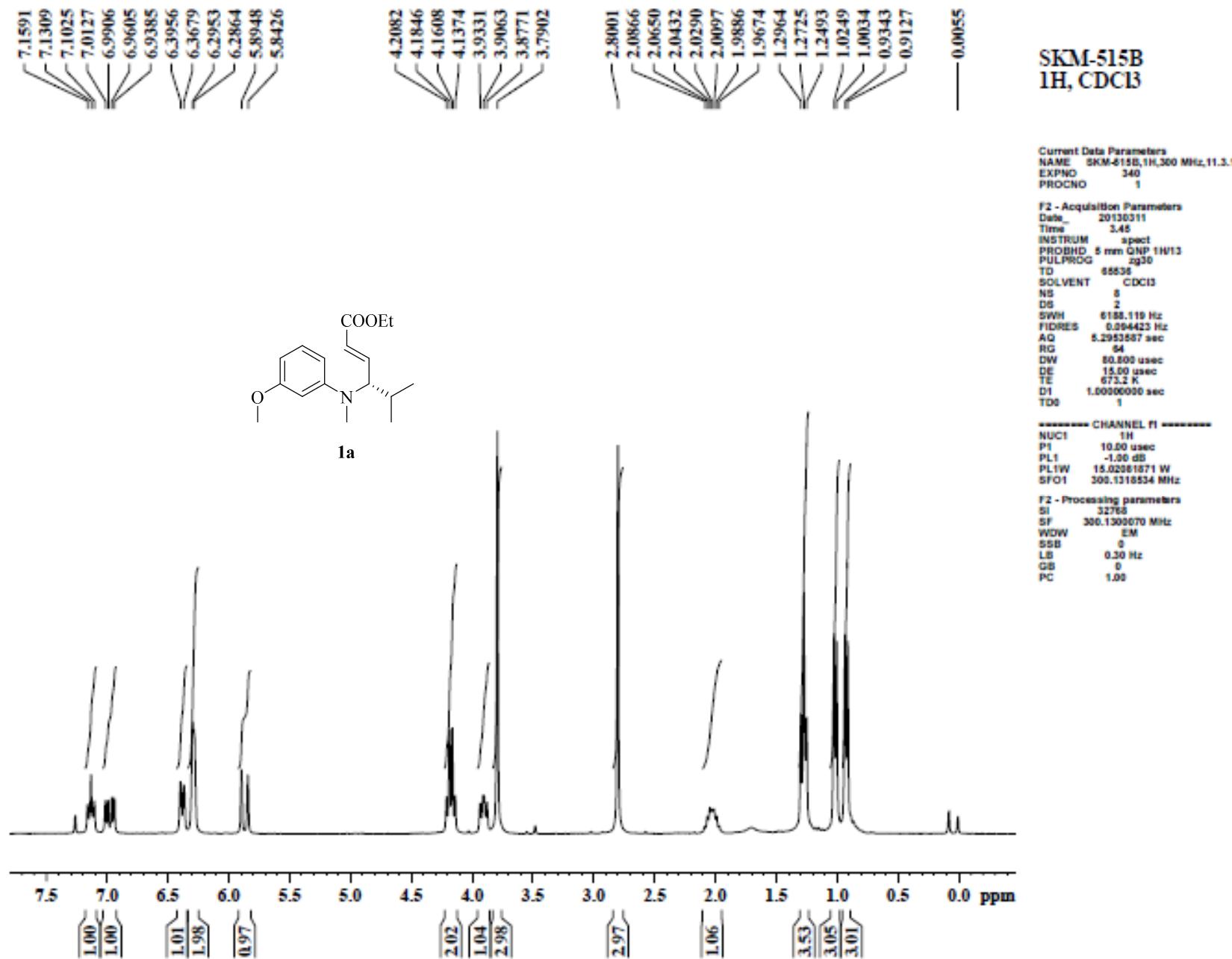
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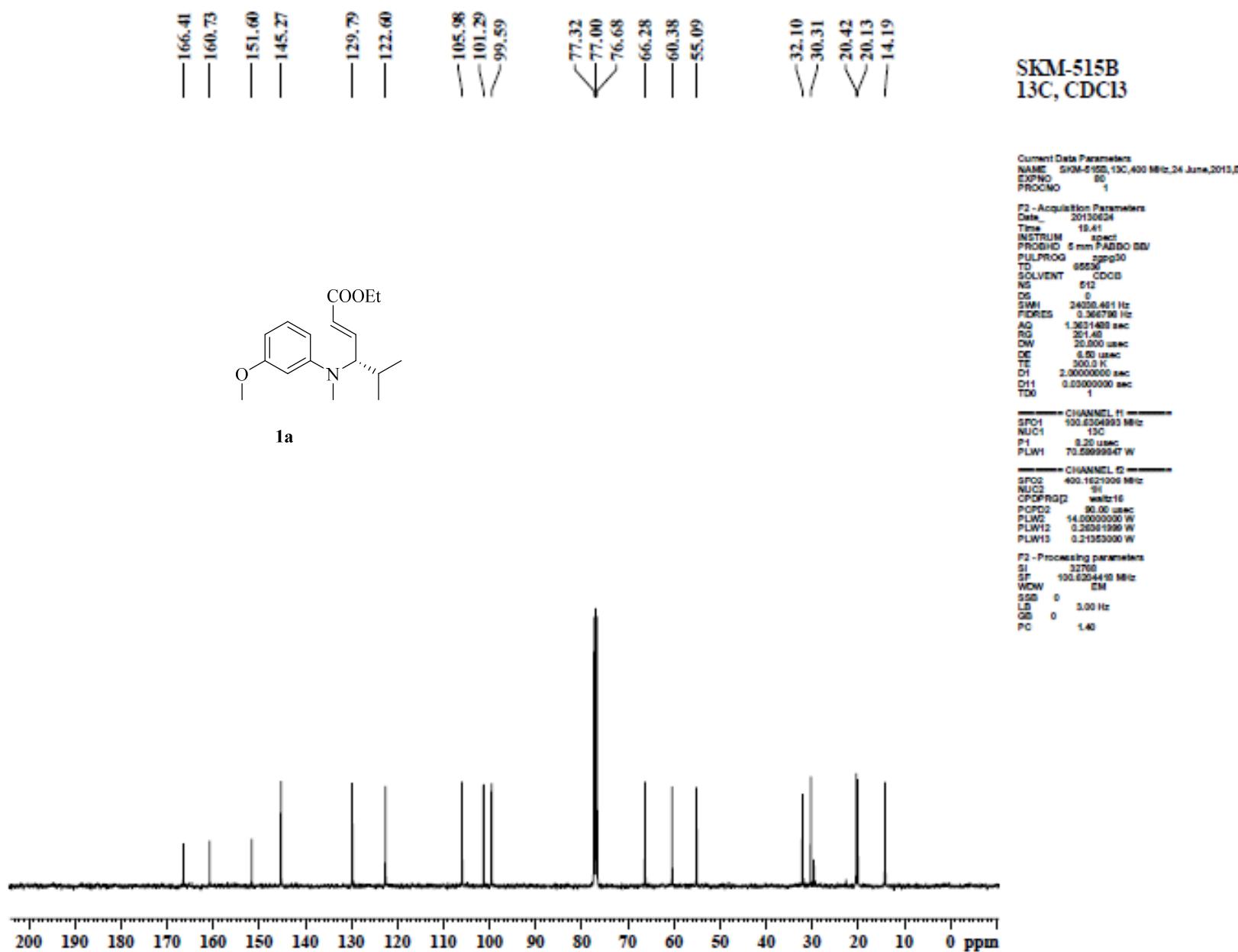
1. Spectra of **1a-1n**
2. Spectra of **2a-2n**

2-27

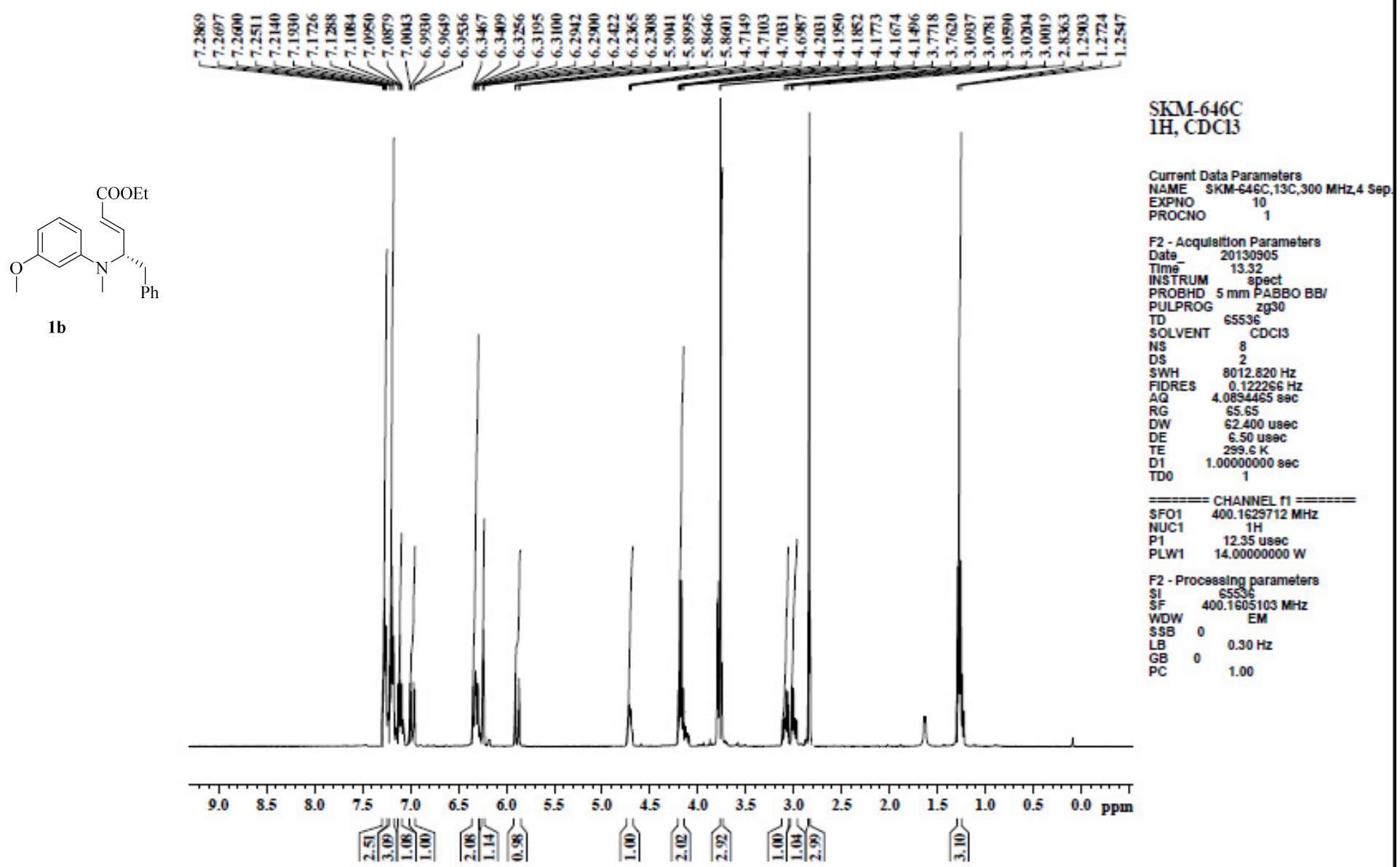
28-55



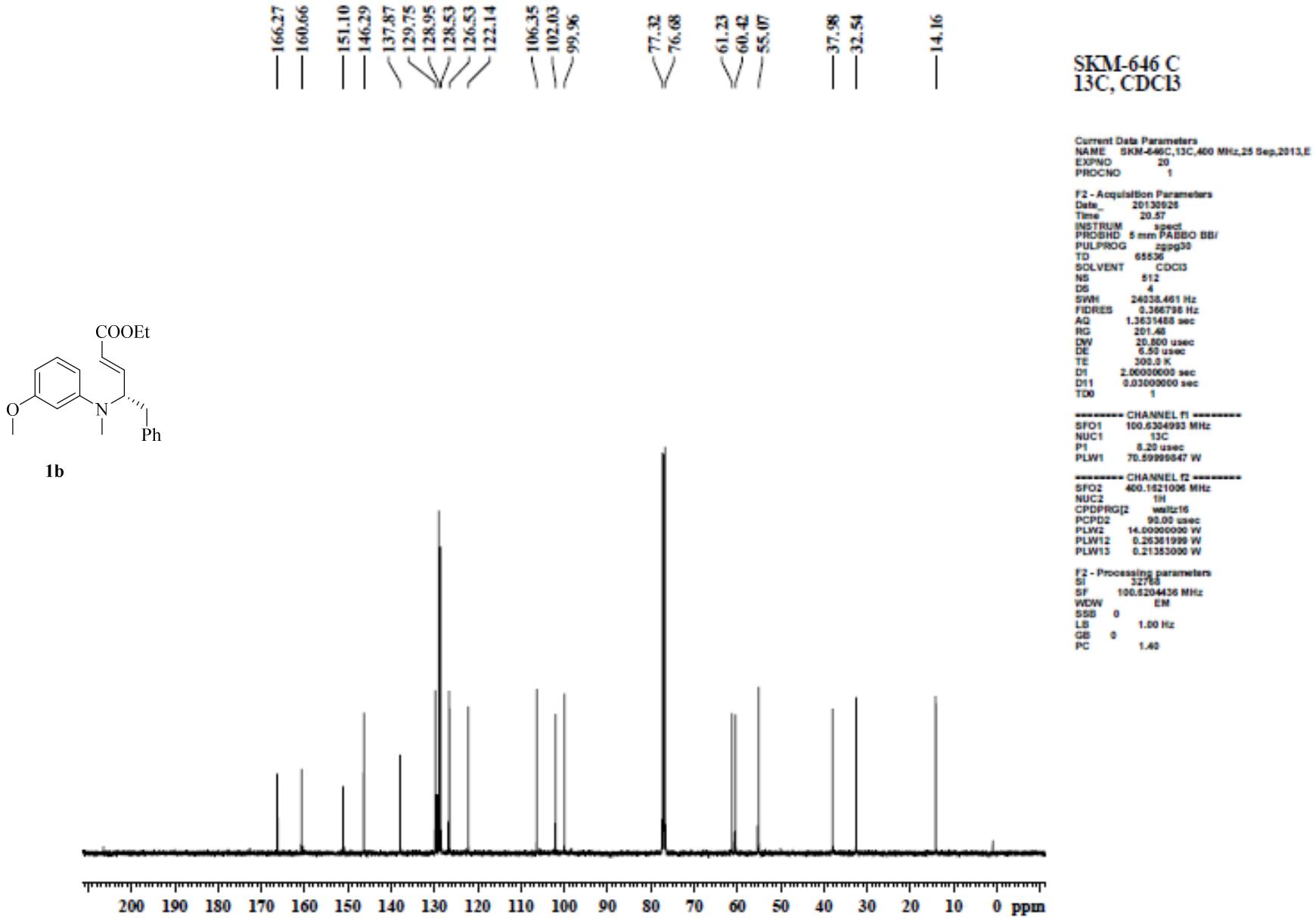
¹H -NMR Spectrum of **1a**



¹³C -NMR Spectrum of **1a**

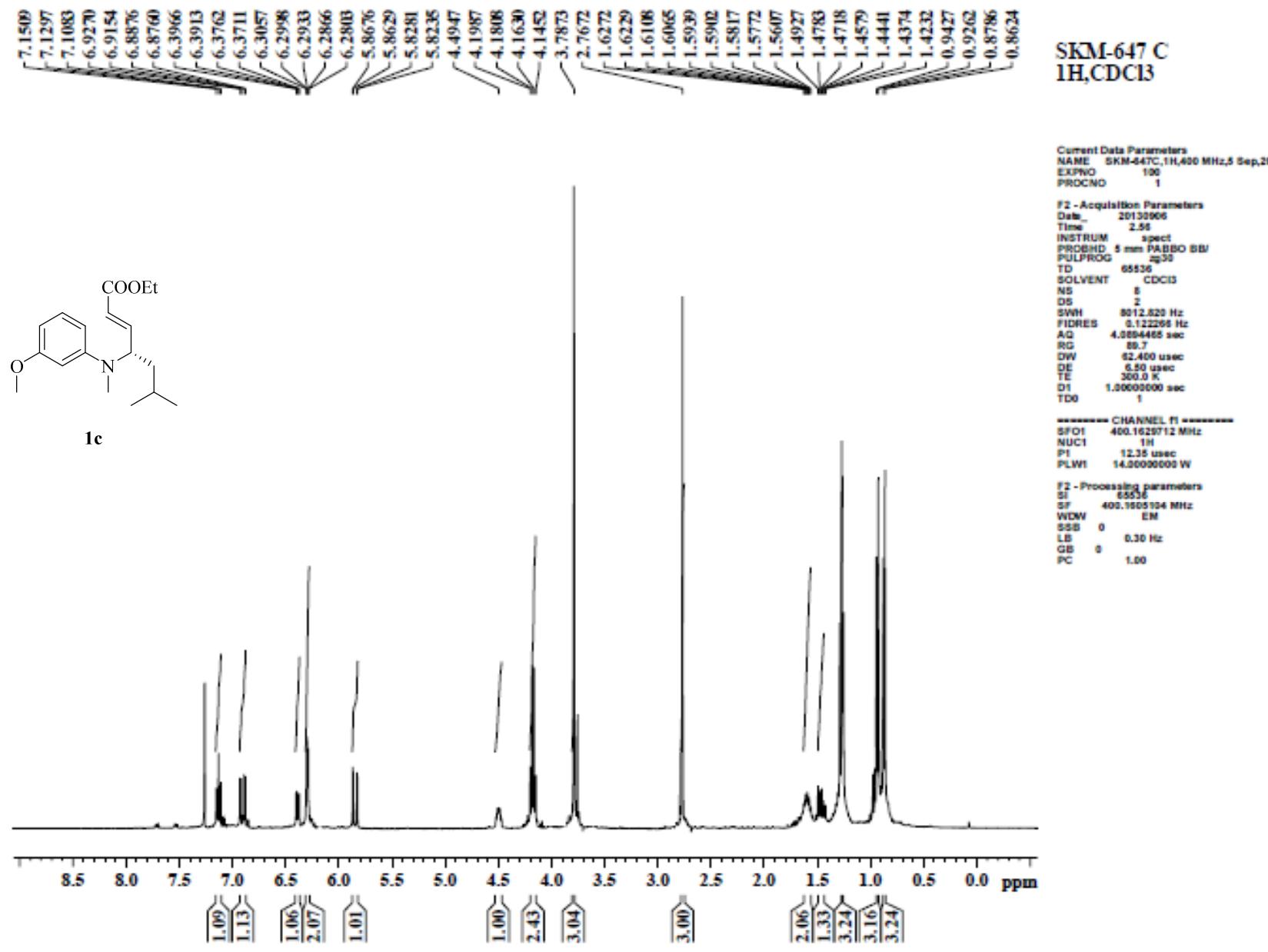


¹H -NMR Spectrum of **1b**

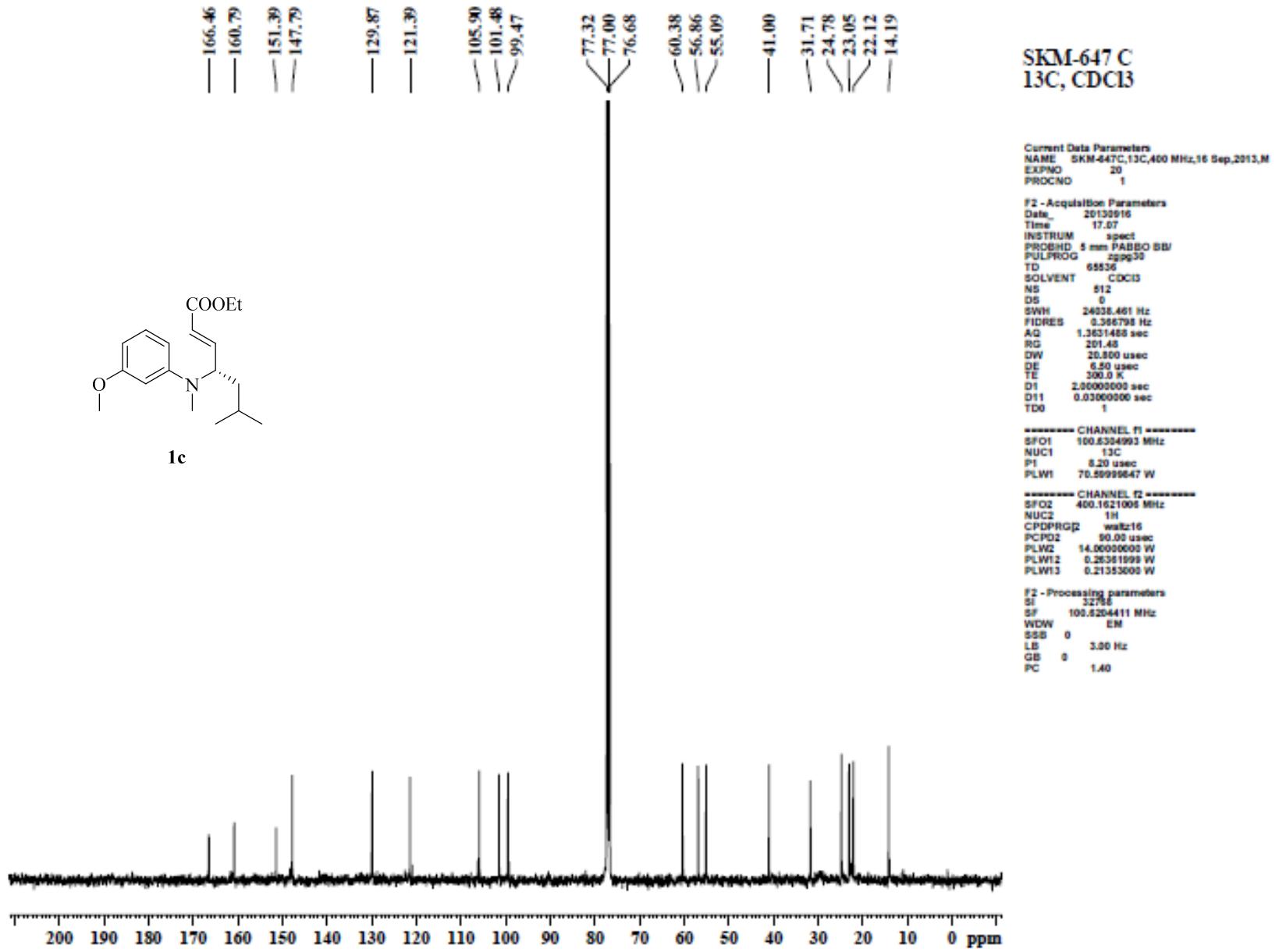


¹³C -NMR Spectrum of **1b**

SKM-647 C
1H, CDCl₃



¹H -NMR Spectrum of 1c





SKM-656A
1H, CDCl₃

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EXPNO 80
PROCNO 1

F2 - Acquisition Parameters

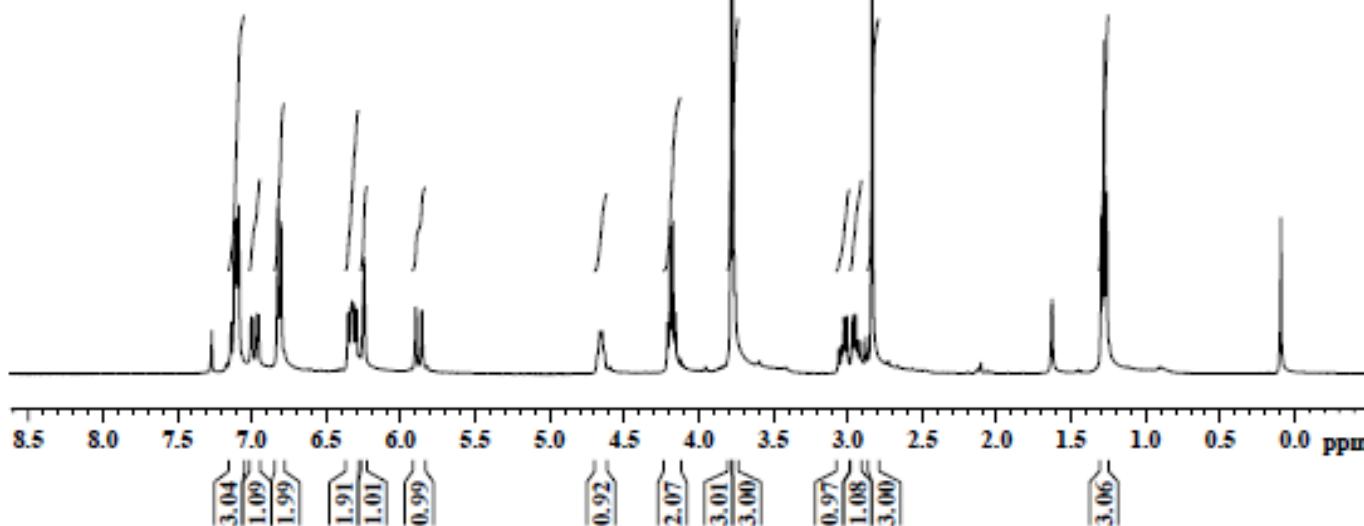
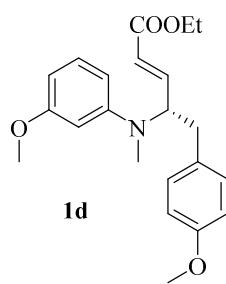
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PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 8
DS 0
SWH 9615.385 Hz
FIDRES 0.146719 Hz
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RG 58.68
DW 52.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TDO 1

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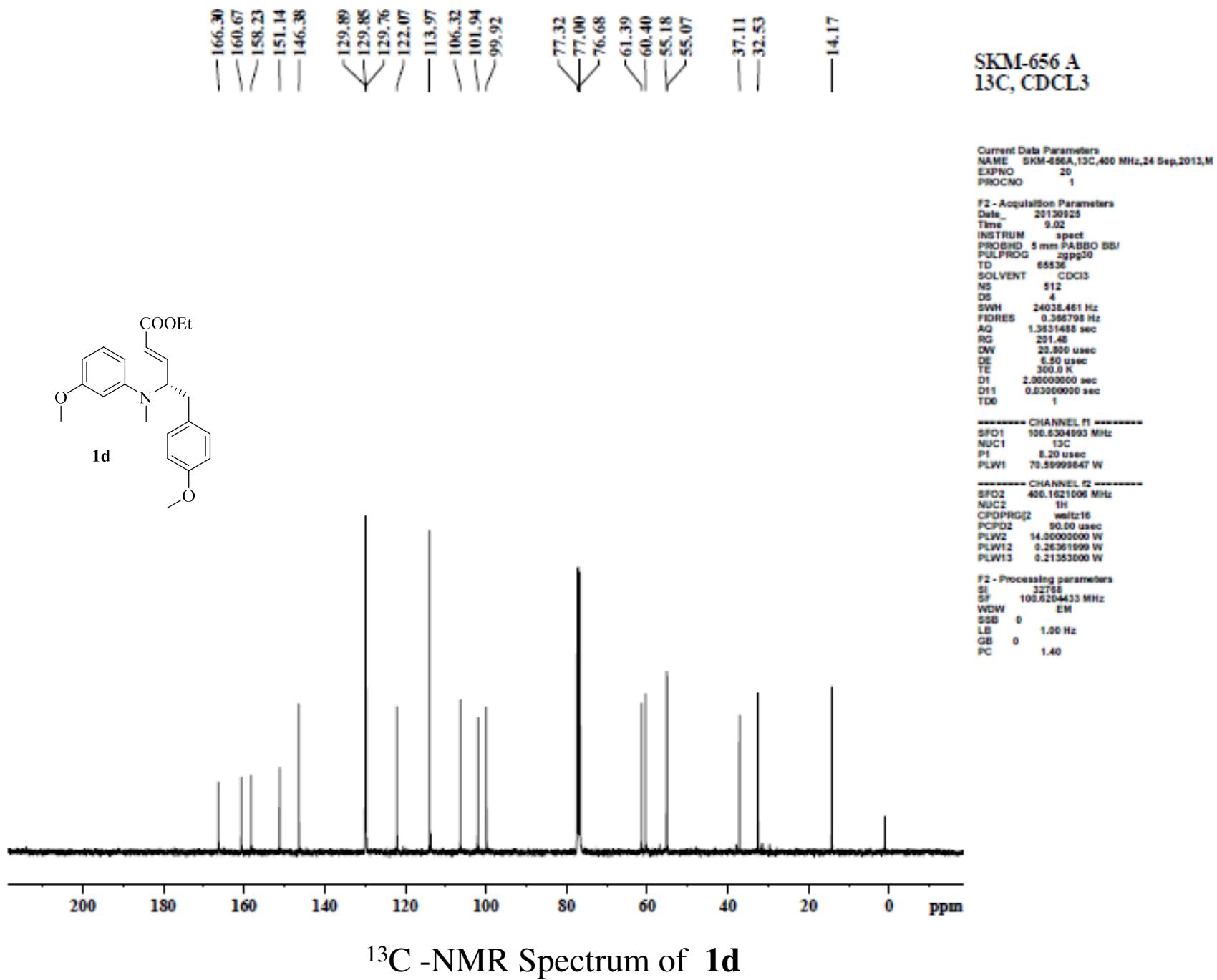
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NUC1 1H
P1 12.35 usec
PLWI 14.0000000 W

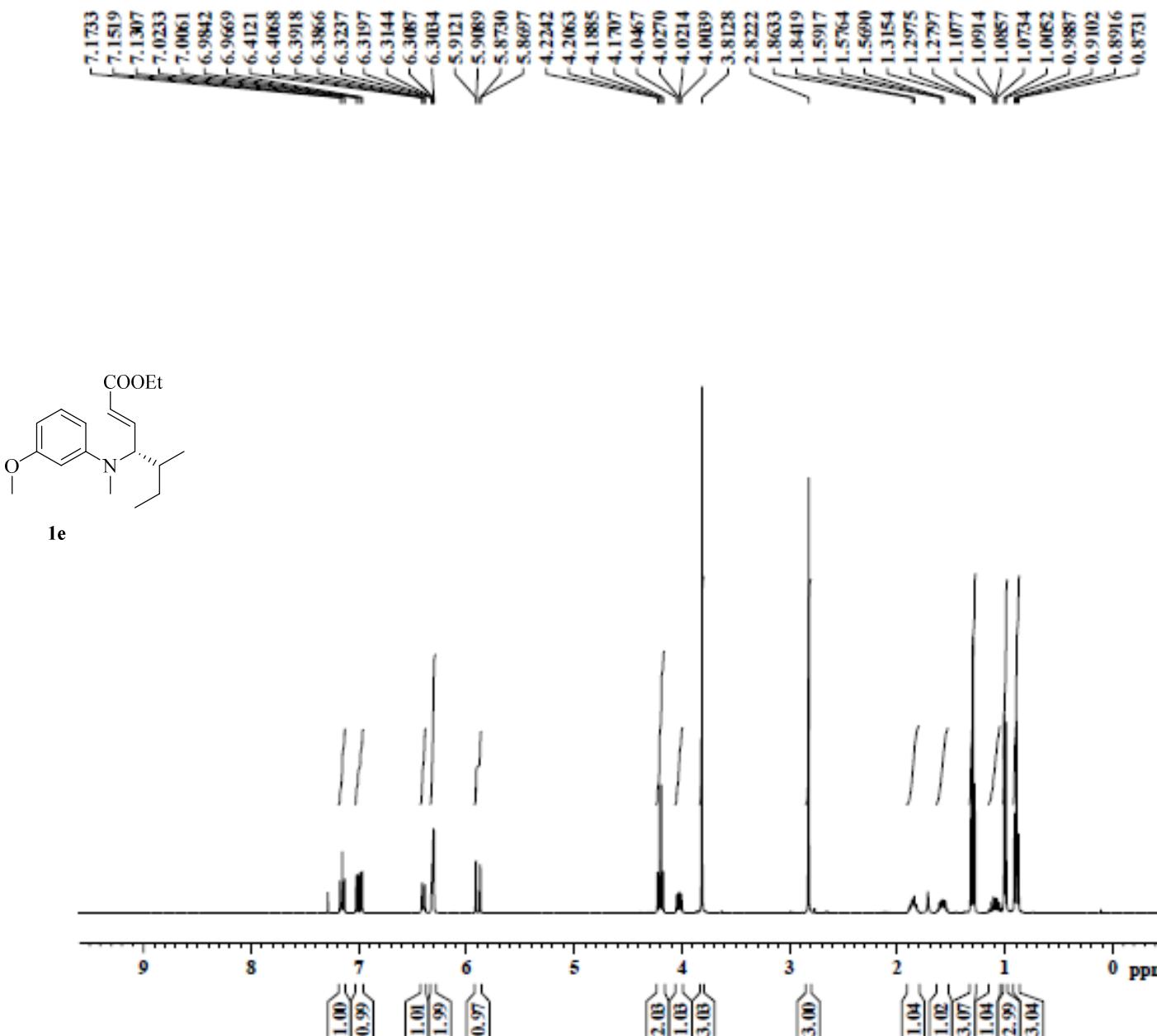
F2 - Processing parameters

SI 65536
SF 400.1605079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H -NMR Spectrum of 1d





SKM-662A
1H, CDCl₃

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EXPNO 50
PROCNO 1

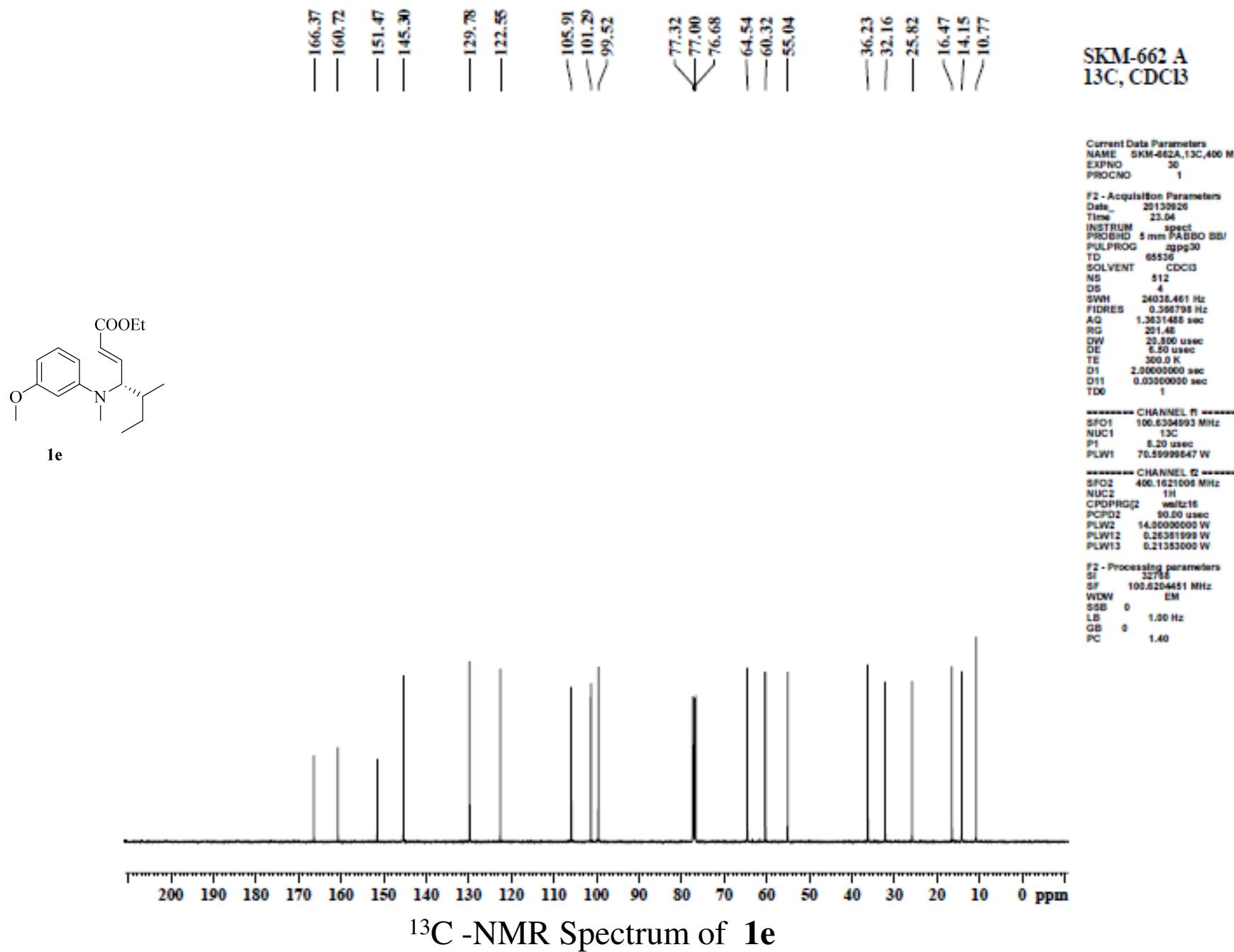
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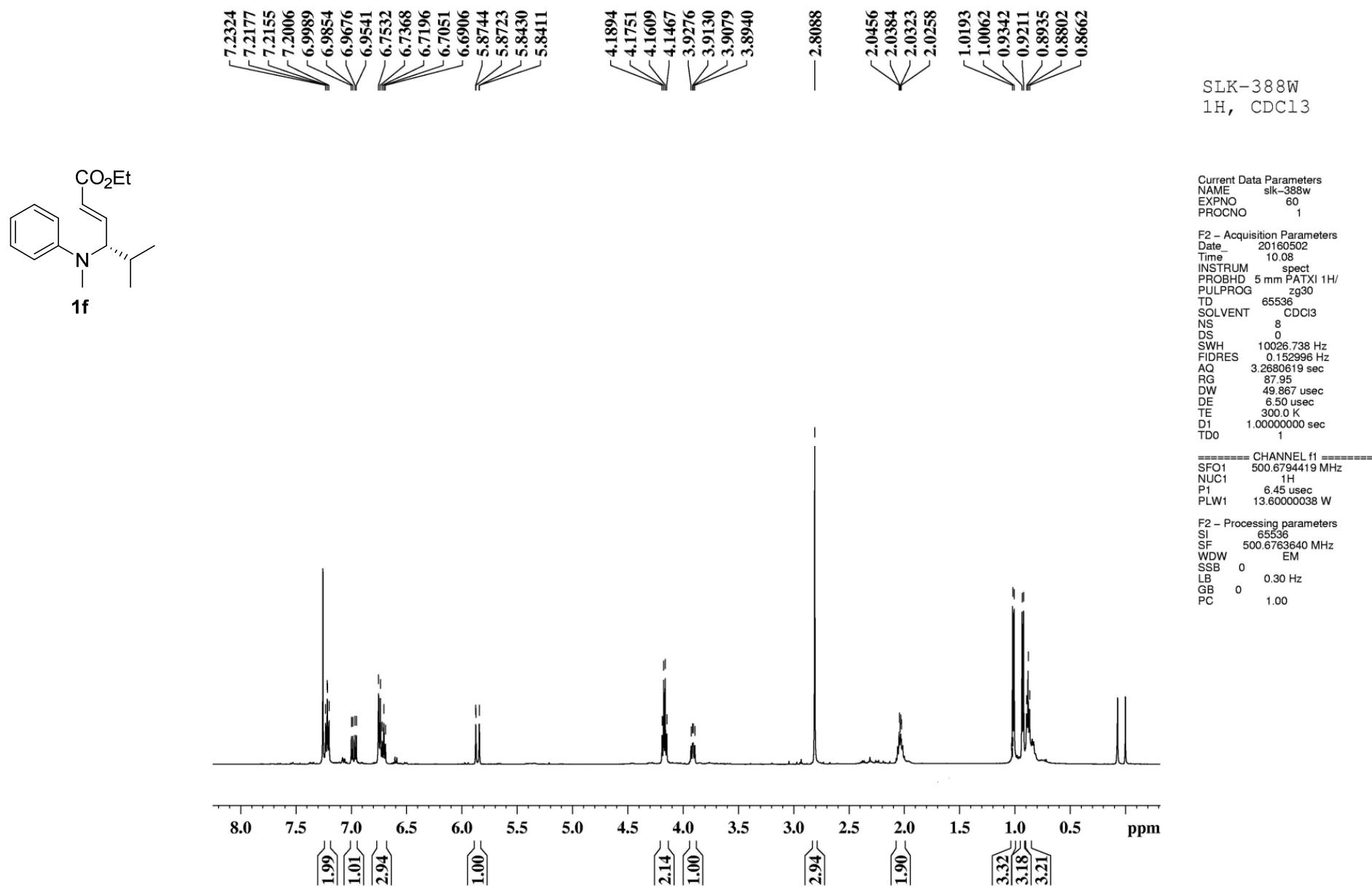
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Time 7.11
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PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122366 Hz
AQ 4.0094465 sec
RG 31.99
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DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TDO 1

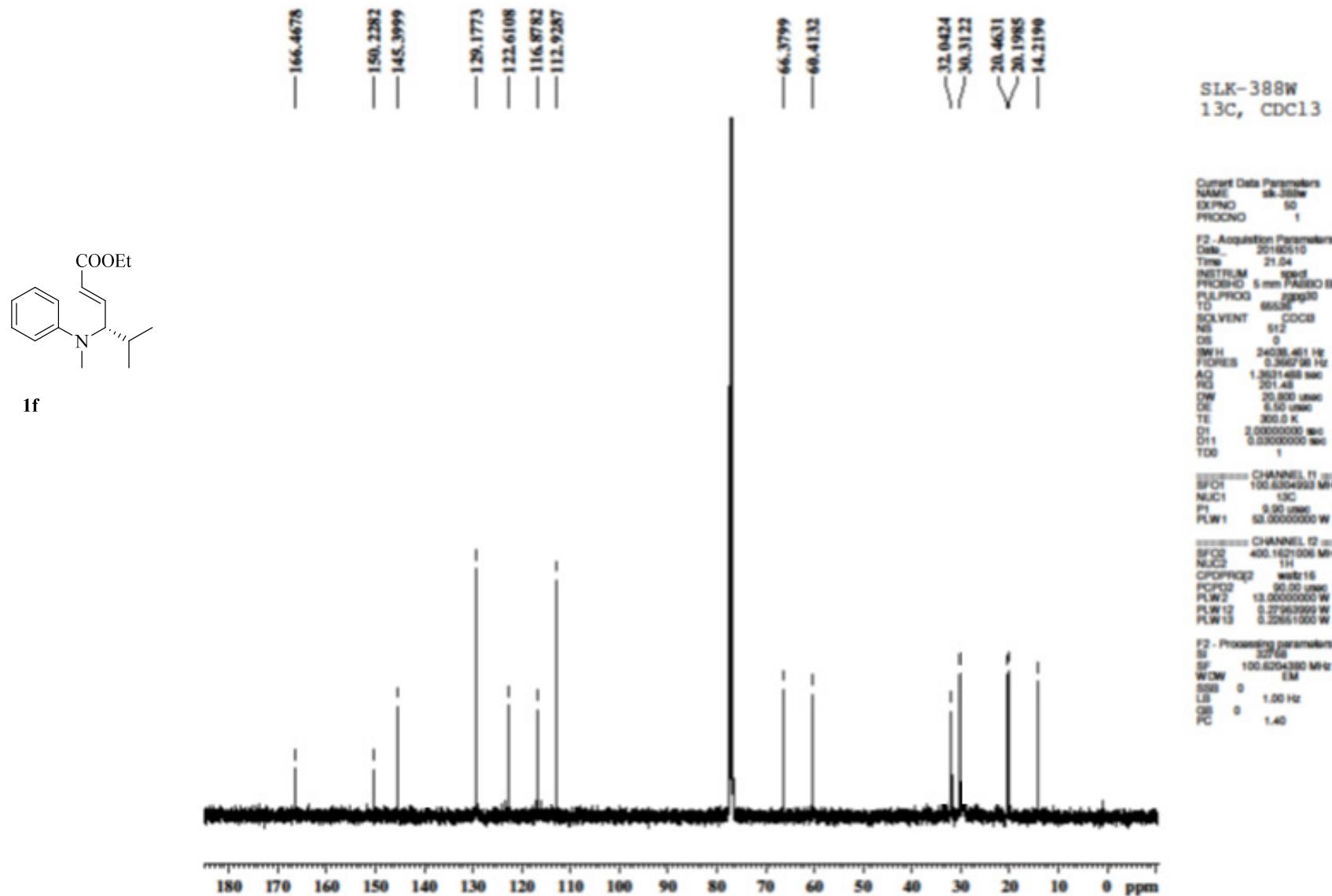
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NUC1 1H
P1 12.35 usec
PLW1 14.0000000 W

F2 - Processing parameters
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SF 400.1605000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

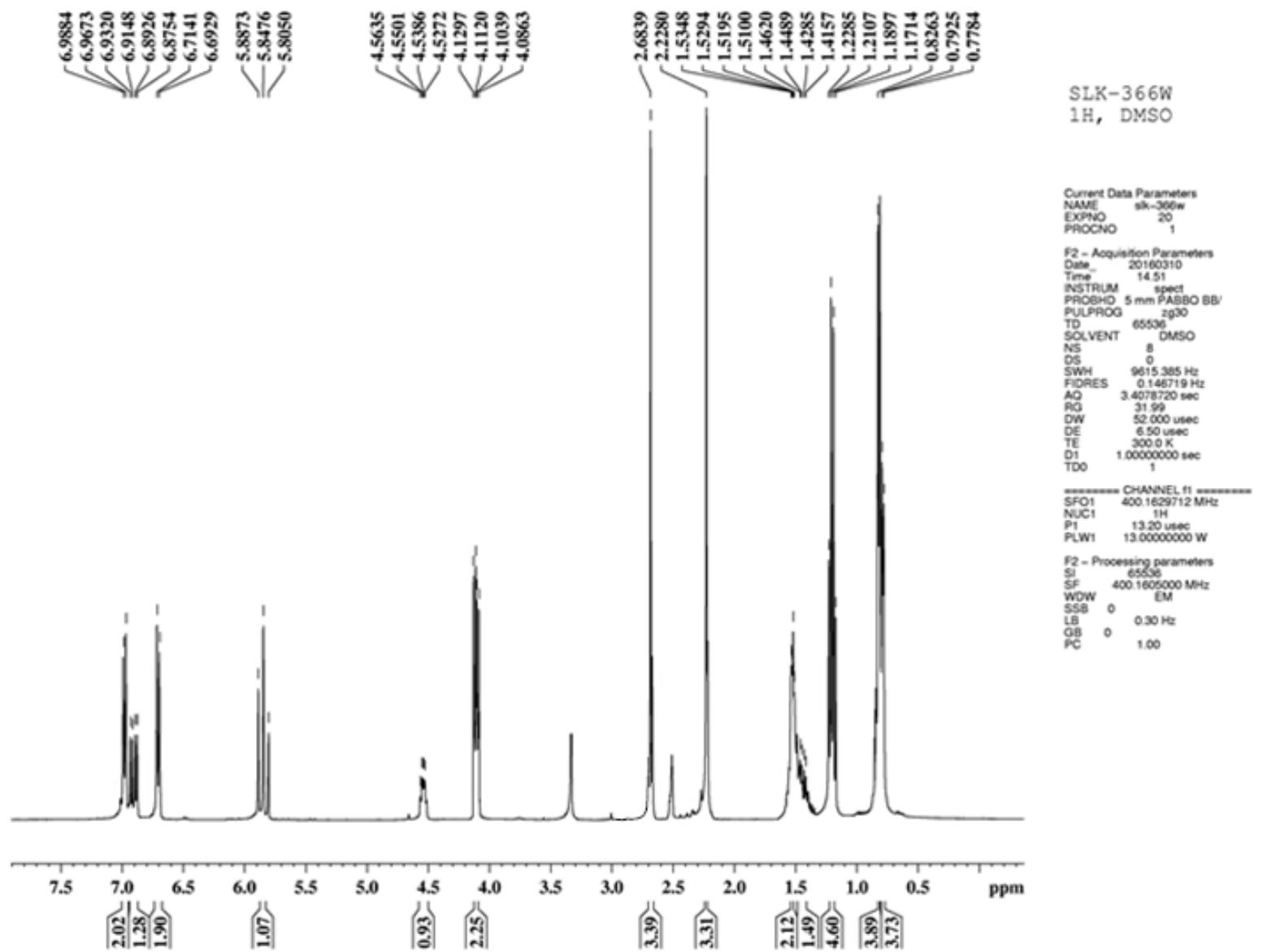
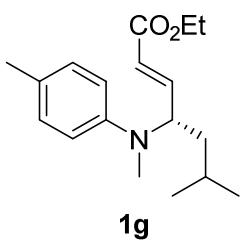
¹H -NMR Spectrum of 1e



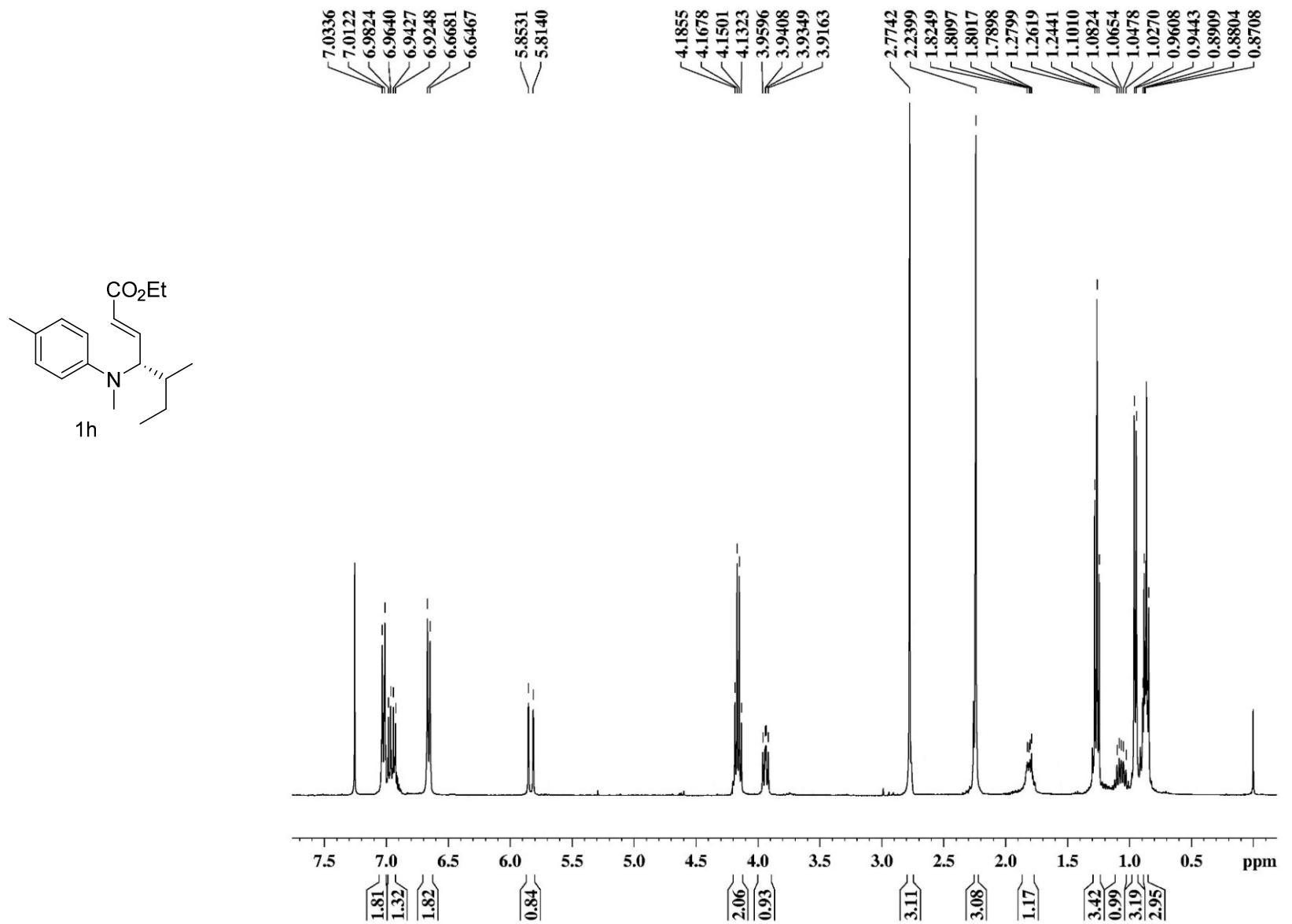




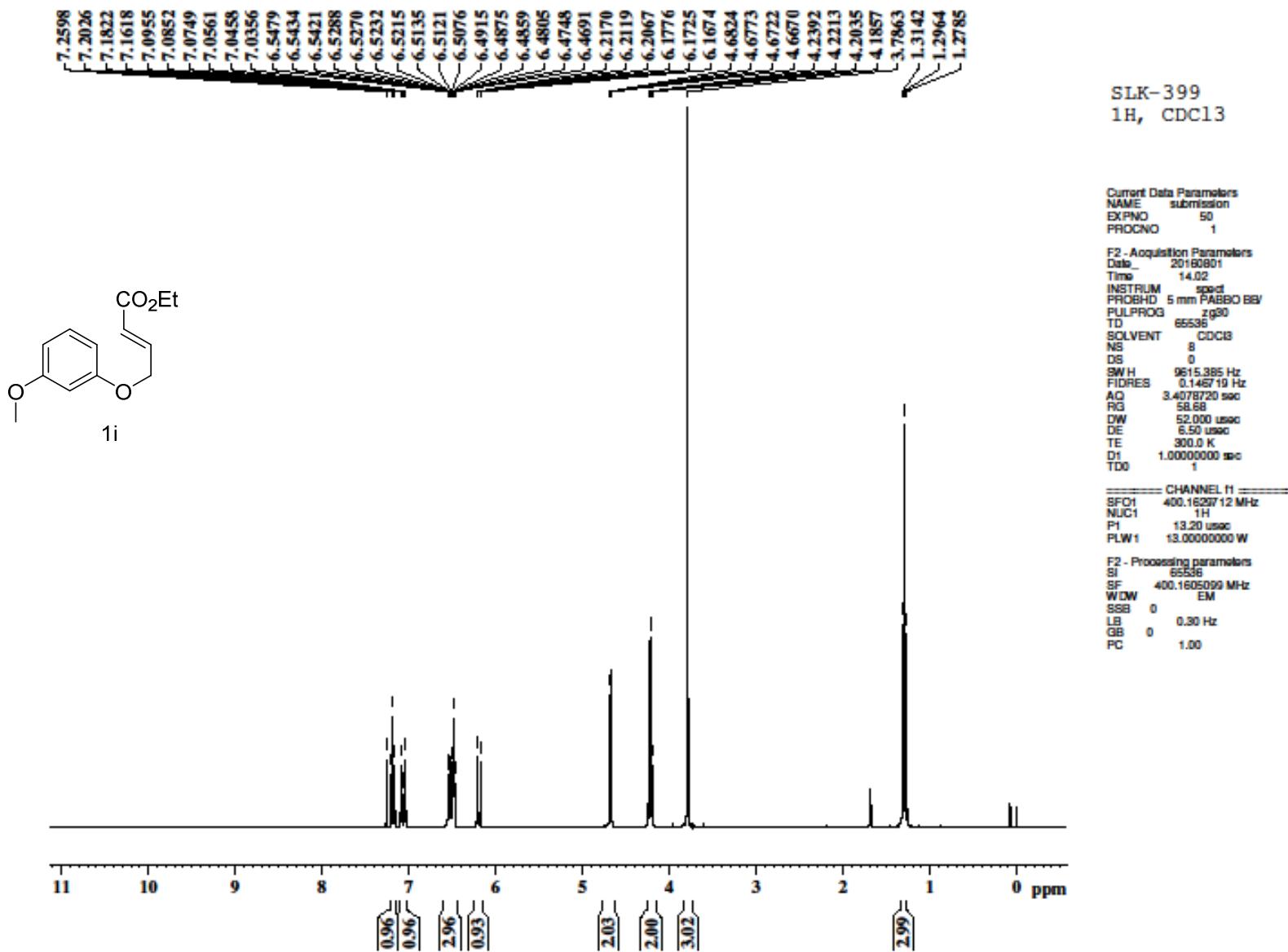
¹³C -NMR Spectrum of **1f**



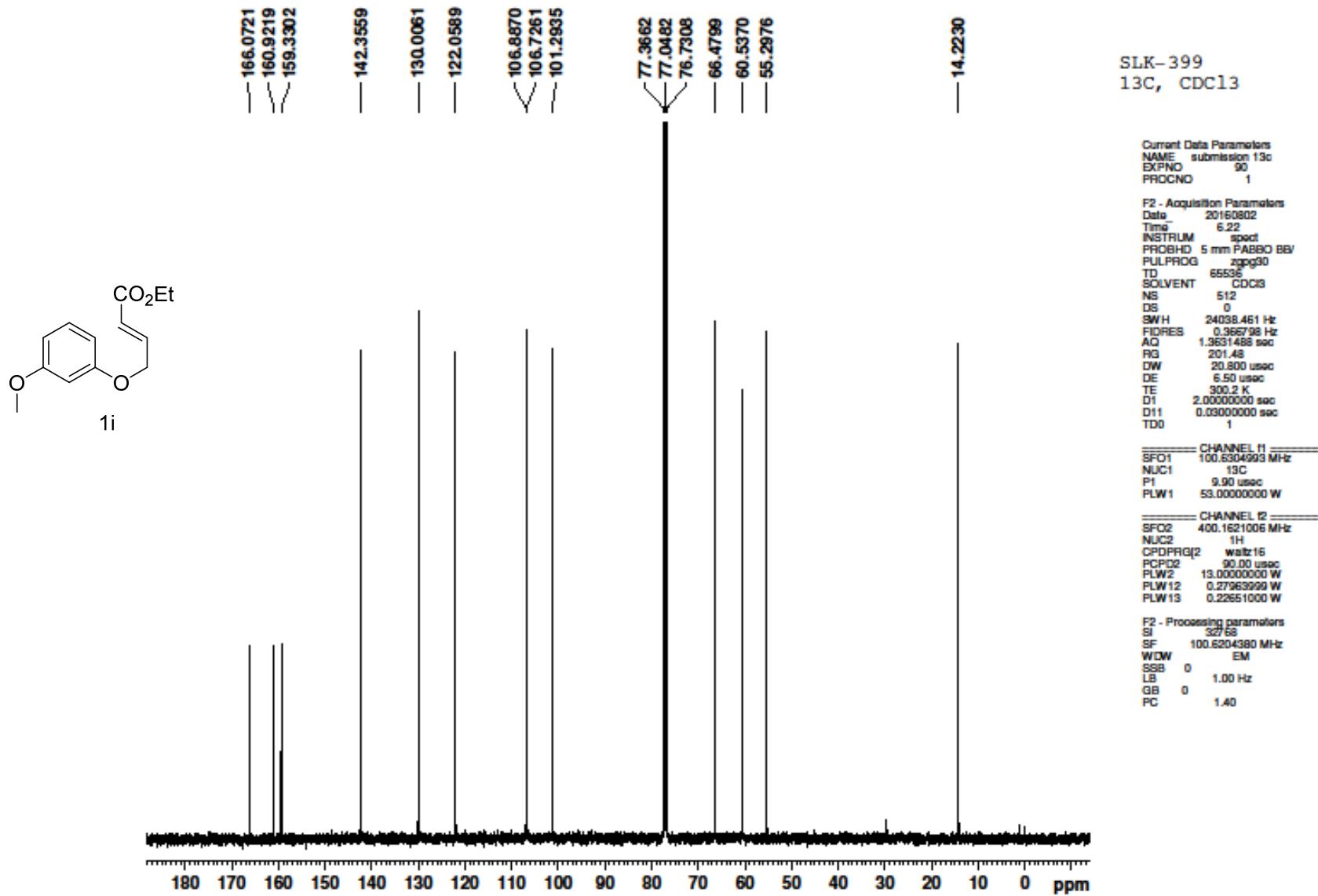
¹H -NMR Spectrum of **1g**



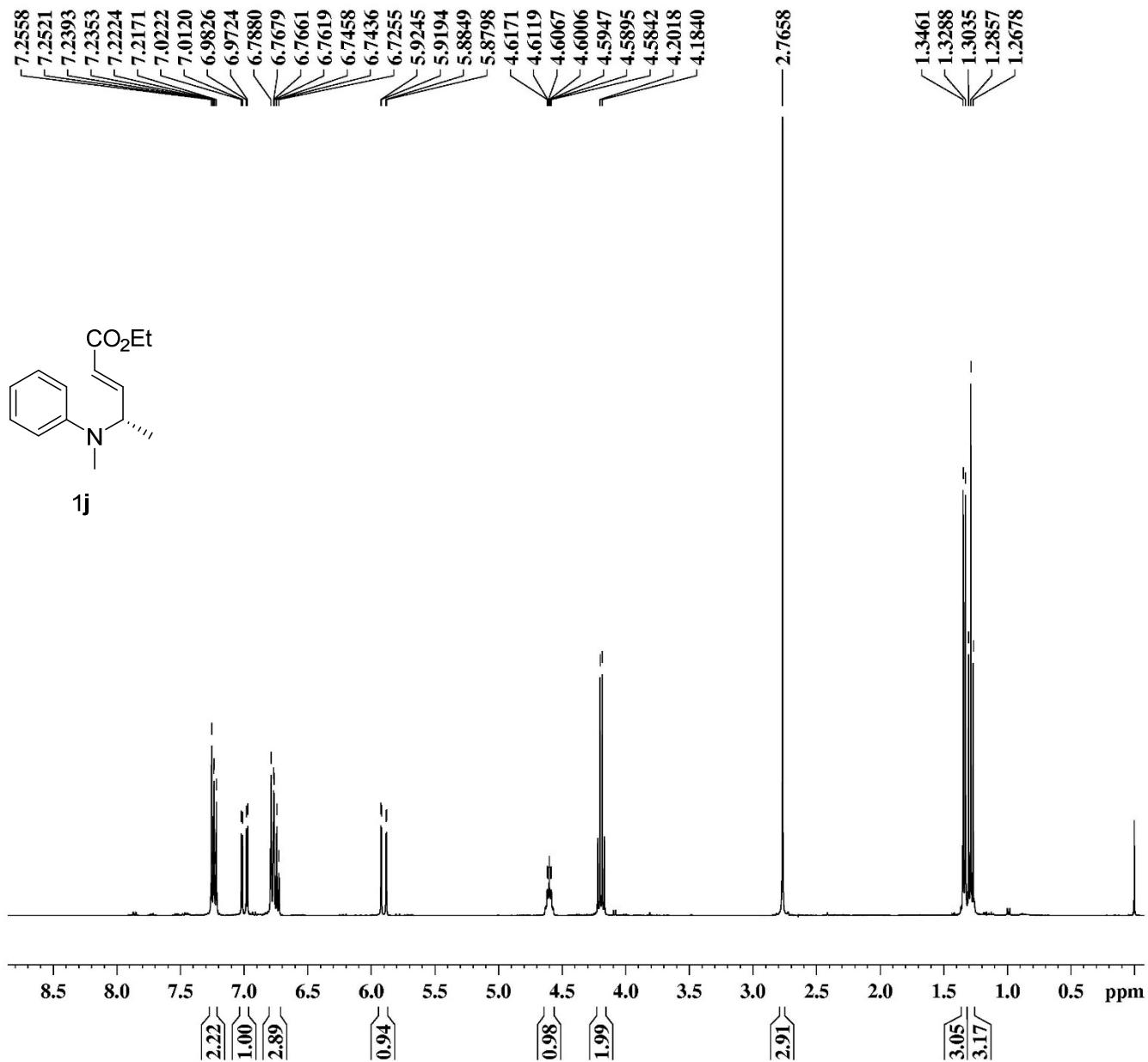
¹H -NMR Spectrum of **1h**



¹H -NMR Spectrum of **1i**



¹³C -NMR Spectrum of **1i**



¹H -NMR Spectrum of **1j**

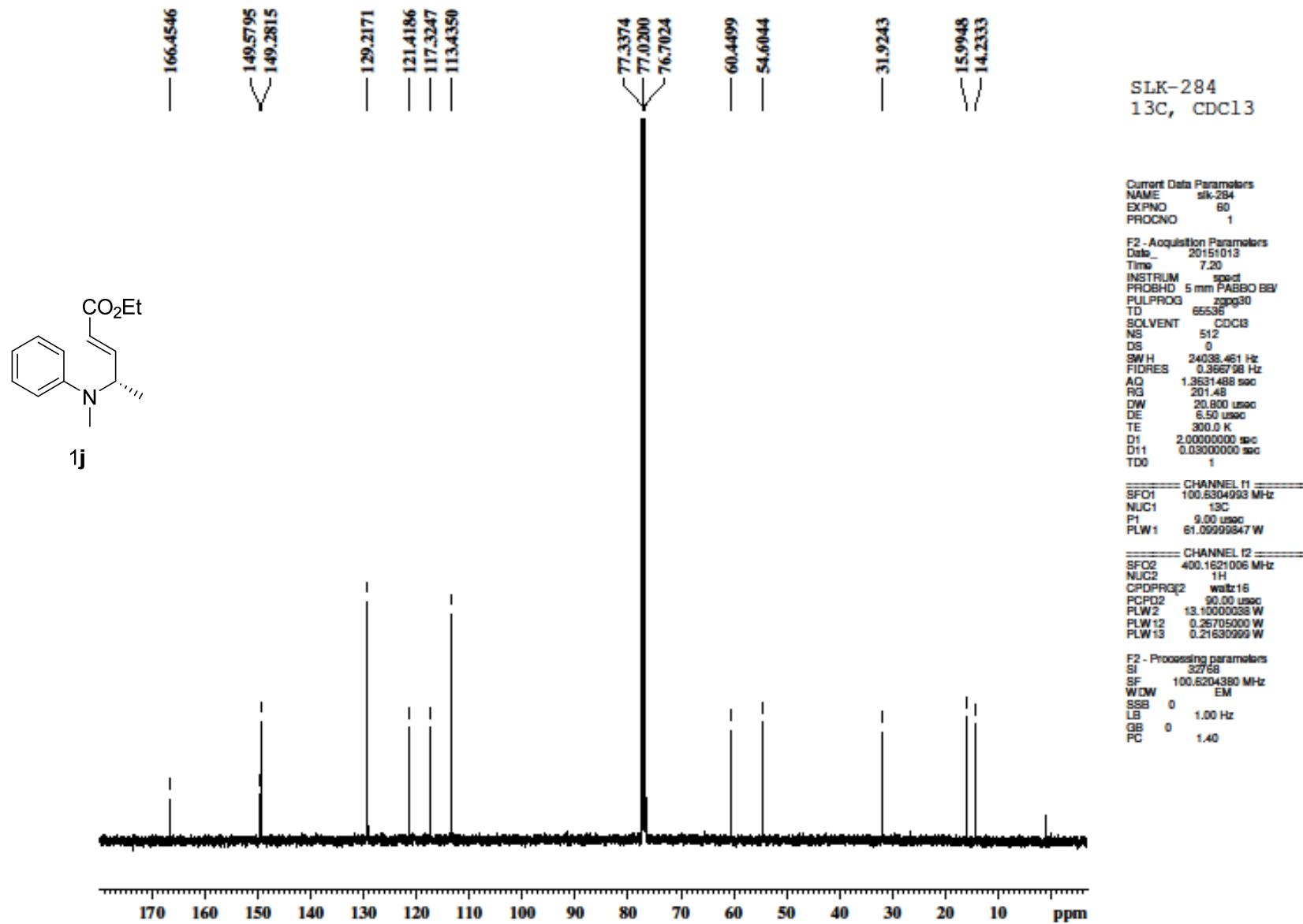
SLK-284
1H, CDCl₃

Current Data Parameters
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EXPNO 10
PROCNO 1

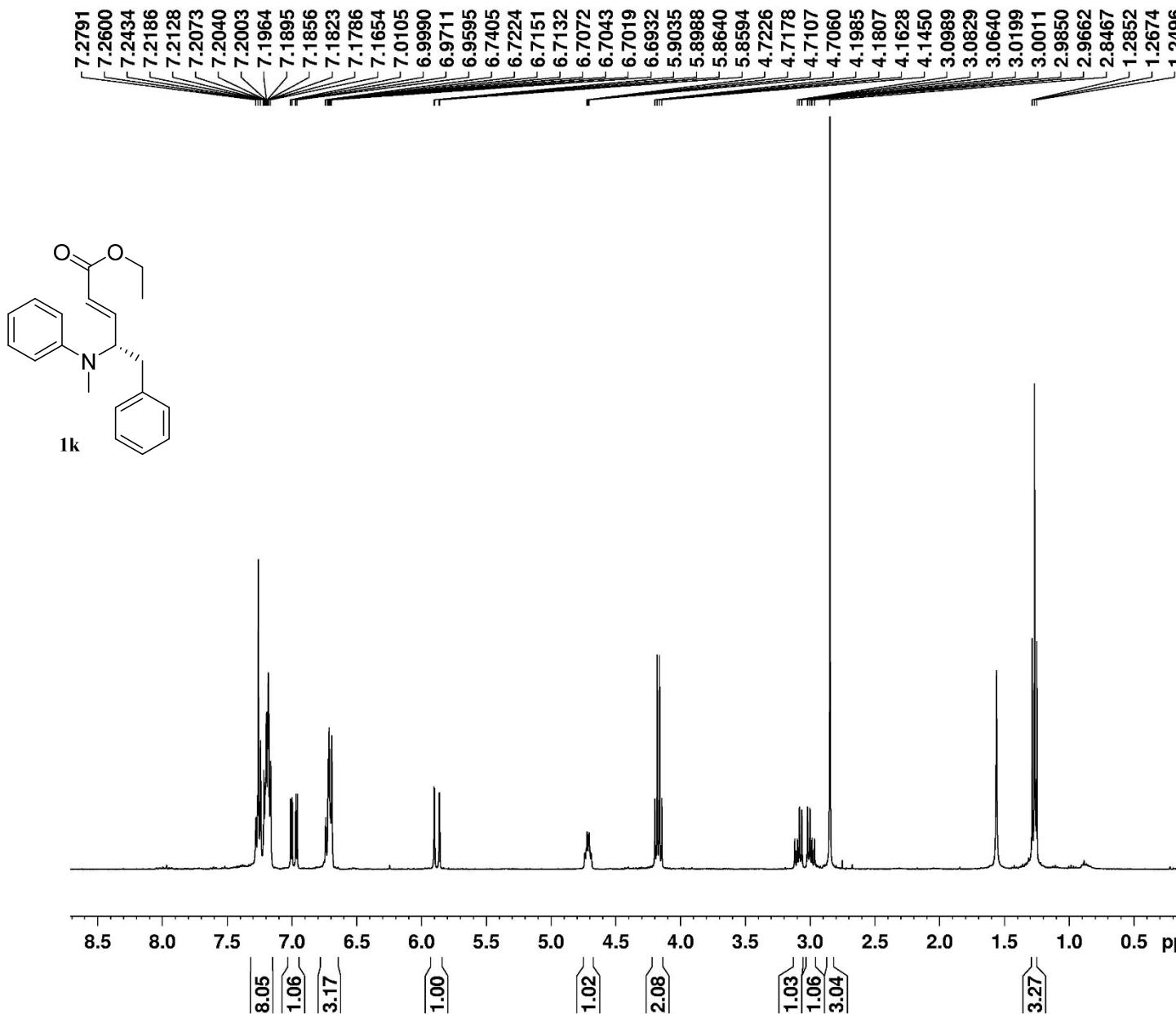
F2 – Acquisition Parameters
Date 20150730
Time 6.04
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 100.41
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1
T0 1

===== CHANNEL f1 =====
SFO1 400.1629712 MHz
NUC1 1H
P1 13.20 usec
PLW1 13.00000000 W

F2 – Processing parameters
SI 65536
SF 400.1605116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C -NMR Spectrum of **1j**



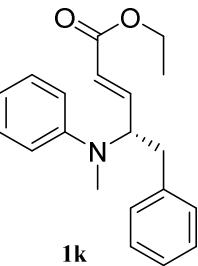
SLK-478W
1H, CDCl₃

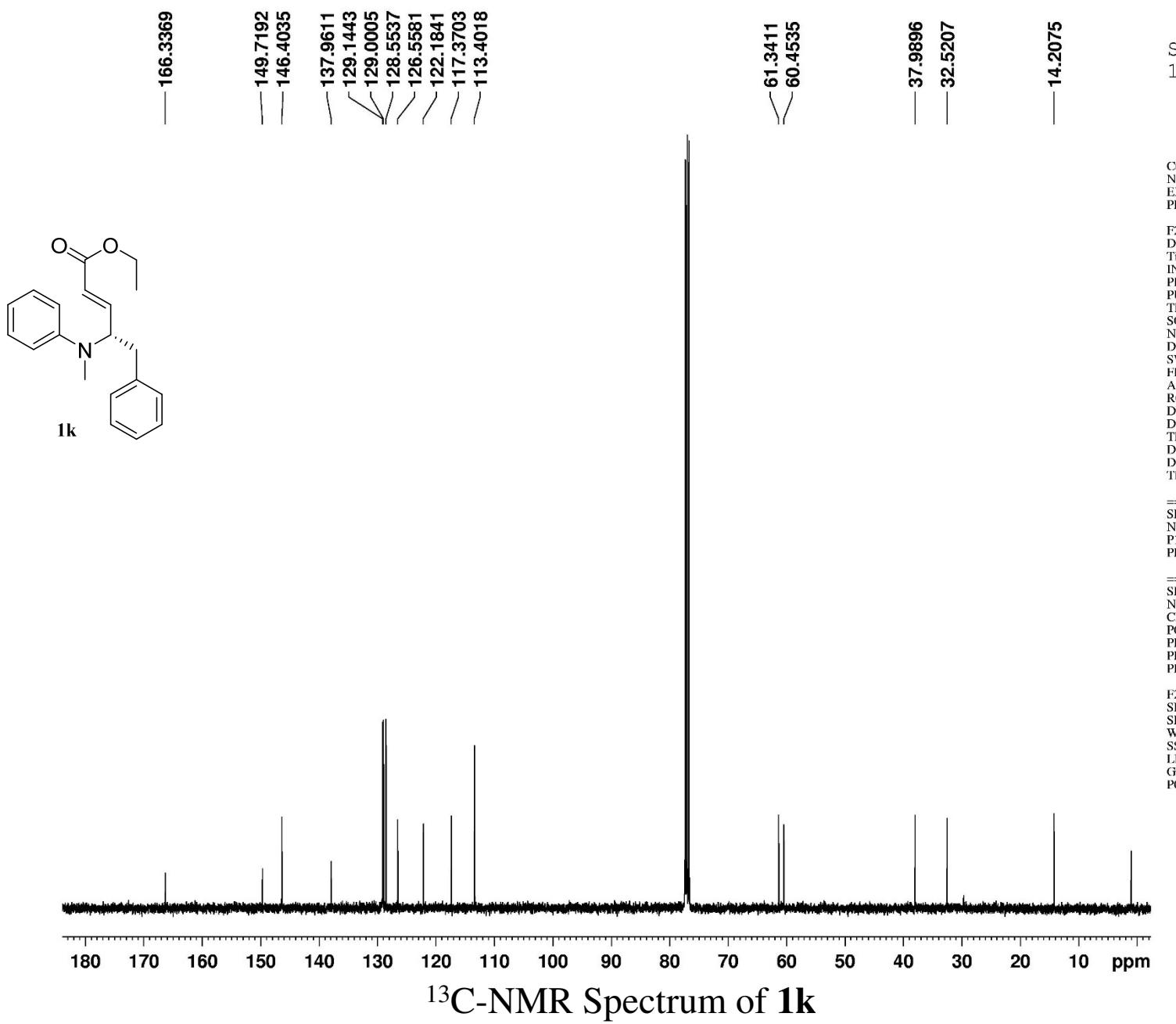
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EXPNO 60
PROCNO 1

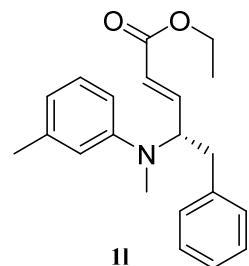
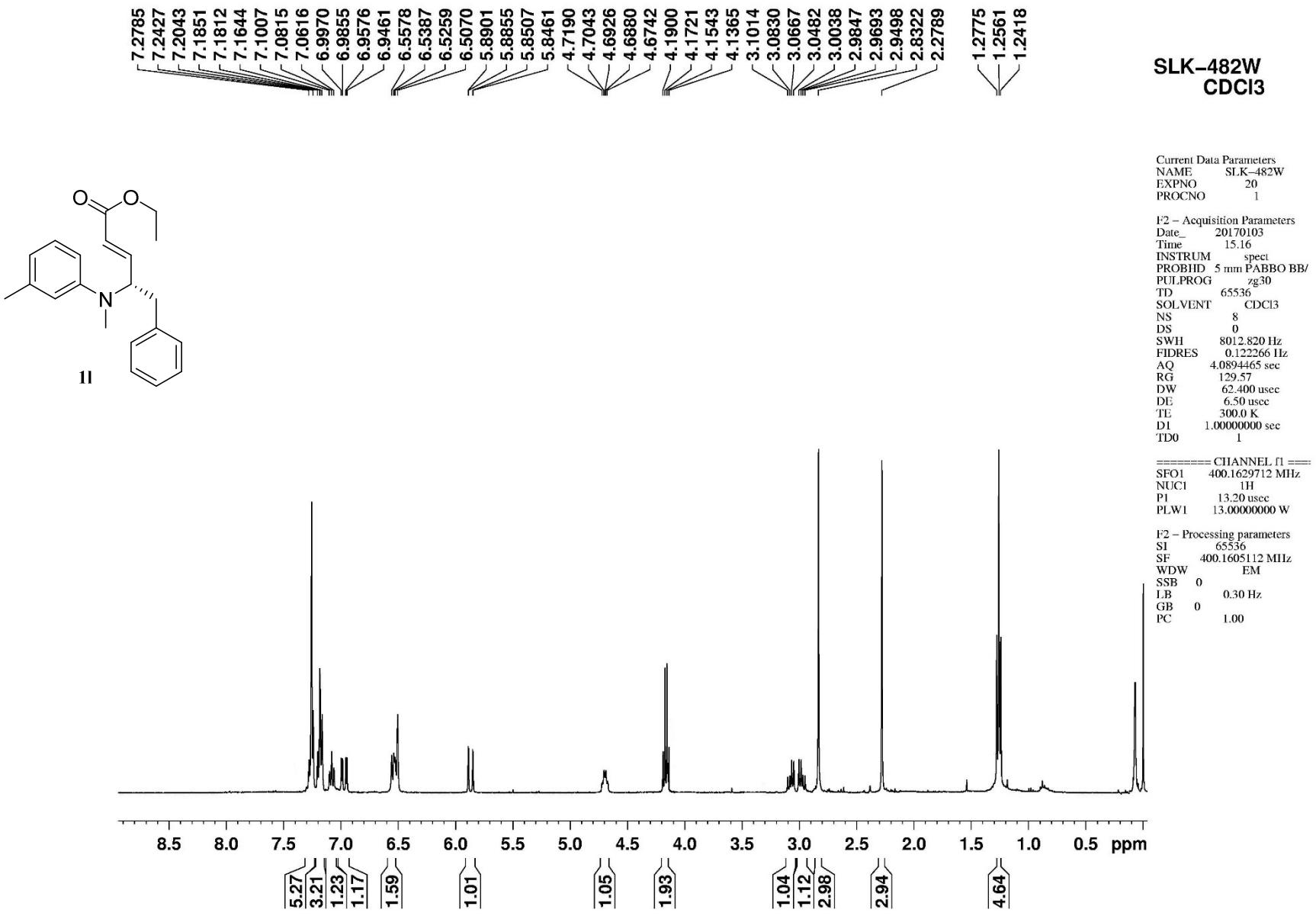
F2 – Acquisition Parameters
Date 20161230
Time 15.40
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PROBHD 5 mm PABBO BB/
PUL.PROG zg30
TD 65536
SOLVENT CDCl₃
NS 8
DS 0
SW1 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 129.57
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1629712 MHz
NUC1 1H
P1 13.20 usec
PLW1 13.00000000 W

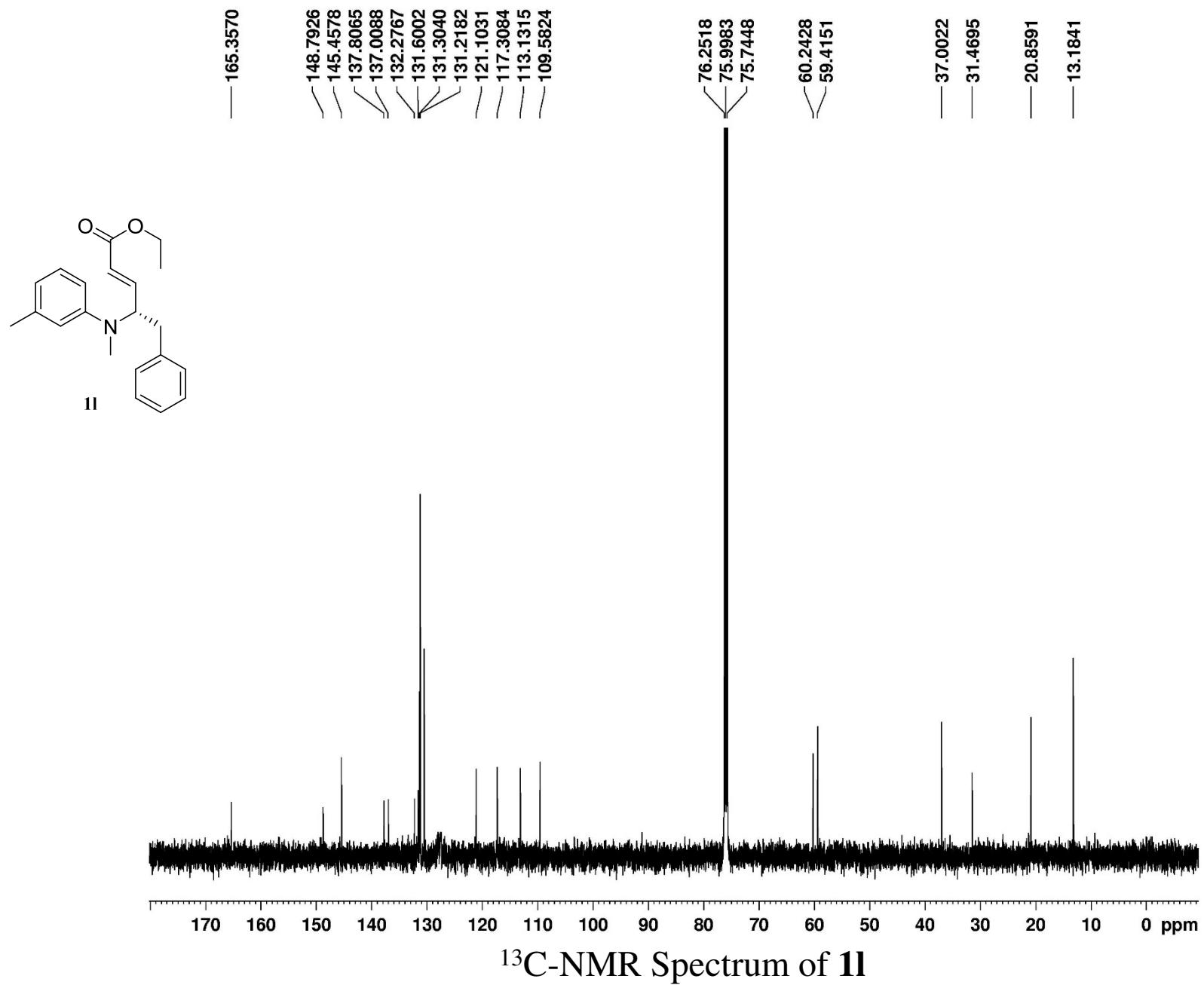
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SF 400.1605095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







¹H-NMR Spectrum of **1l**



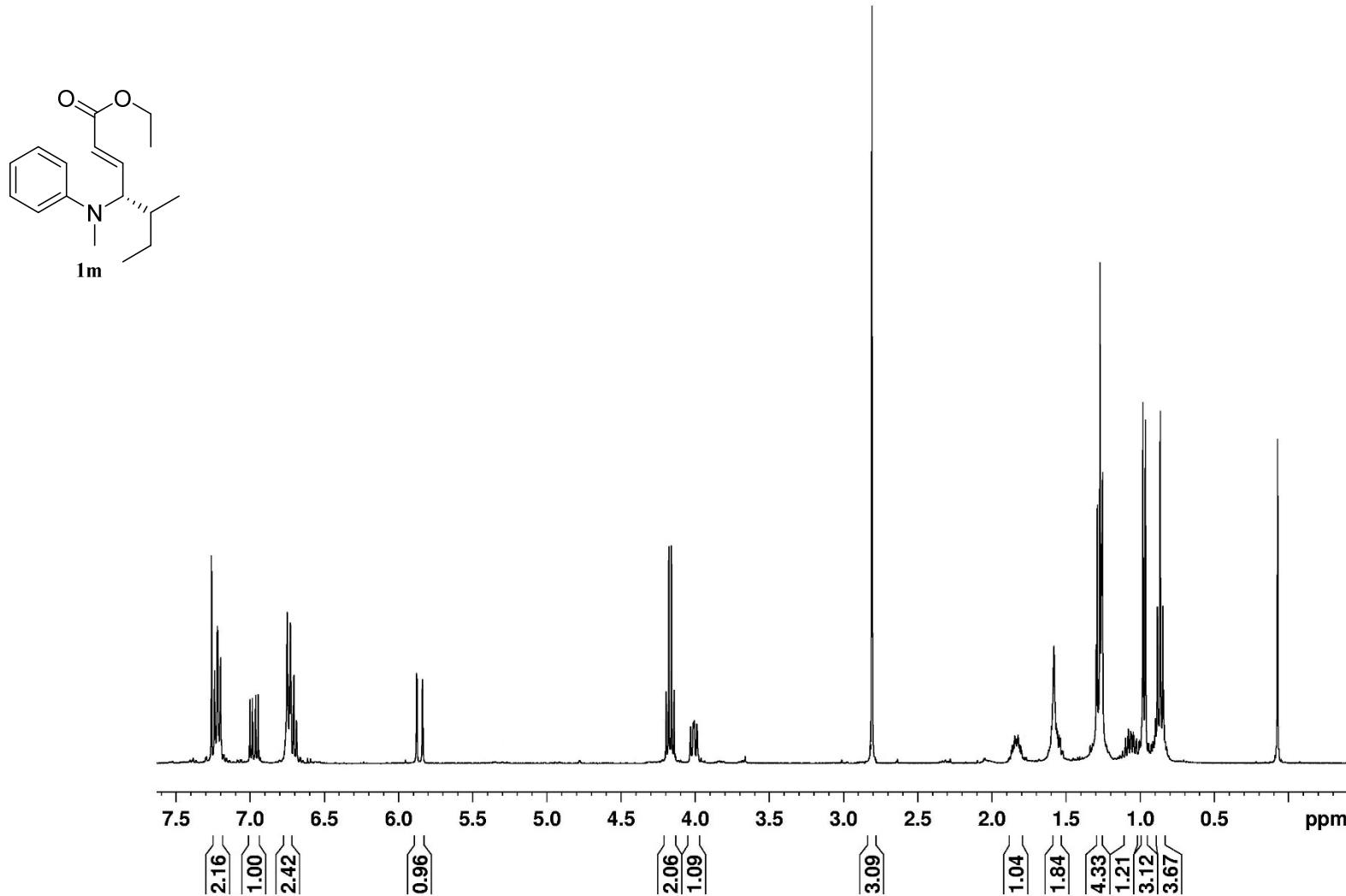
Current Data Parameters
 NAME SLK-482W
 EXPNO 40
 PROCNO 1

F2 – Acquisition Parameters
 Date 20170106
 Time 17.23
 INSTRUM spect
 PROBID 5 mm PAXI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 2048
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.4541311 Hz
 AQ 1.1010048 sec
 RG 38.43
 DW 16.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

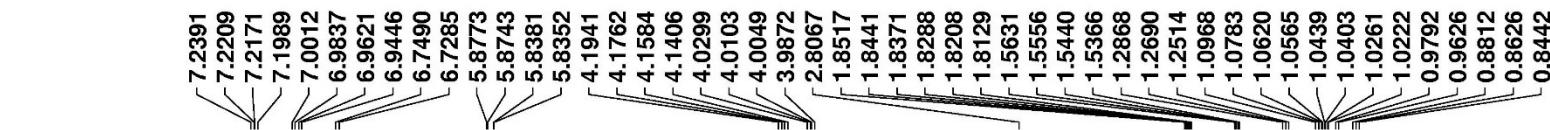
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 SFO1 125.9077573 MHz
 NUC1 ¹³C
 P1 9.23 usec
 PLW1 244.00000000 W

===== CHANNEL f2 =====
 SFO2 500.6783527 MHz
 NUC2 ¹H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.60000038 W
 PLW12 0.08840500 W
 PLW13 0.05657900 W

F2 – Processing parameters
 SI 32768
 SF 125.8952970 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



¹H-NMR Spectrum of **1m**



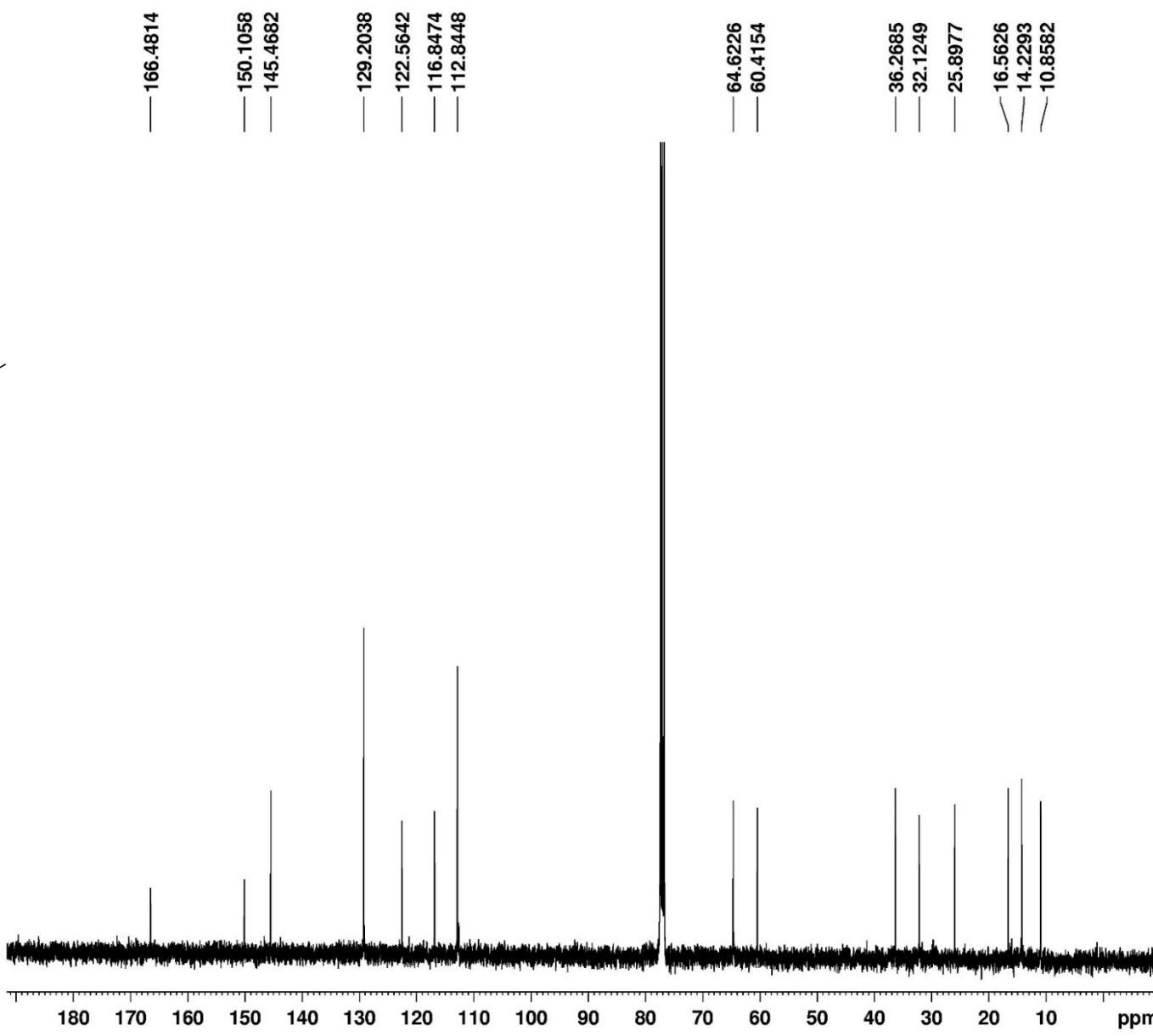
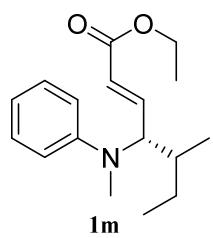
SM-77W,
1H, CDCl₃

Current Data Parameters
 NAME SM-77W
 EXPNO 20
 PROCNO 1

F2 – Acquisition Parameters
 Date 20170105
 Time 22.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 8
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122261 Hz
 AQ 4.0894465 sec
 RG 114.26
 DW 62,400 usec
 DE 6.50 usec
 TE 295.7 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usc
 PLW1 13.00000000 W

F2 – Processing parameters
 SI 65536
 SF 400.1605097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



¹³C-NMR Spectrum of **1m**

SM-77W,
13C, CDCl₃

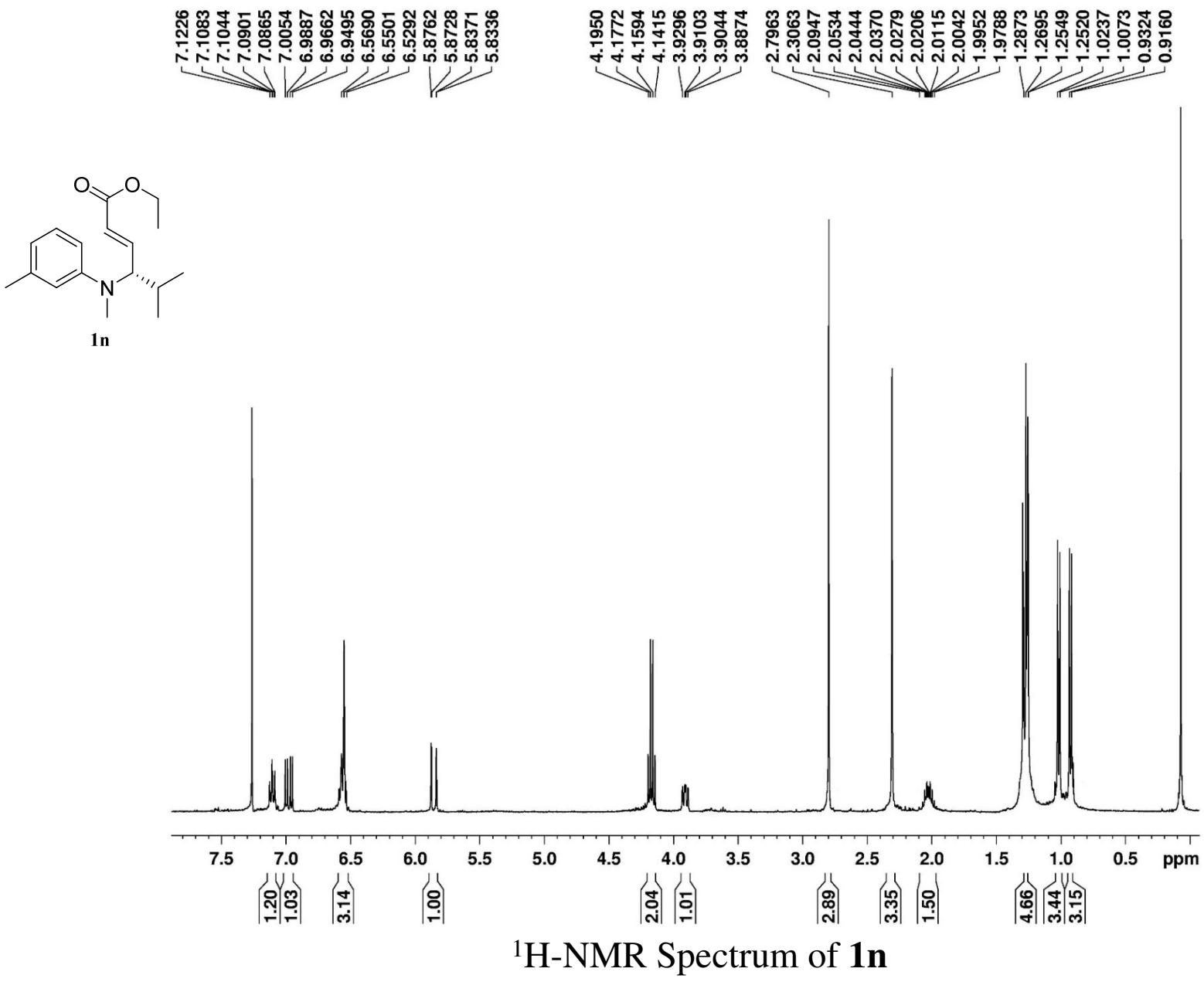
Current Data Parameters
 NAME SM-77WN
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date 20170107
 Time 23.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 512
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 201.48
 DW 20.800 usc
 DE 6.50 usc
 TE 296.7 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6304993 MHz
 NUC1 ¹³C
 P1 9.90 usc
 PLW1 53.0000000 W

===== CHANNEL f2 =====
 SFO2 400.1621006 MHz
 NUC2 ¹H
 CPDPRG[2] waltz16
 PCPD2 90.00 usc
 PLW2 13.00000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
 SI 32768
 SF 100.6204380 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

7.1226
7.1083
7.1044
7.0901
7.0865
7.0054
6.9887
6.9662
6.9495
6.5690
6.5501
6.5292
5.8762
5.8728
5.8371
5.8336

4.1950
4.1772
4.1594
4.1415
3.9296
3.9103
3.9044
3.8874

2.7963
2.3063
2.0947
2.0534
2.0444
2.0370
2.0279
2.0206
2.0115
2.0042
1.9952
1.9788
1.2873
1.2695
1.2549
1.2520
1.0237
1.0073
0.9324
0.9160

1.20
1.03
3.14
1.00
2.04
1.01
2.89
3.35
1.50
4.66
3.44
3.15

¹H-NMR Spectrum of **1n**

SM-80W,
13C, CDCl₃

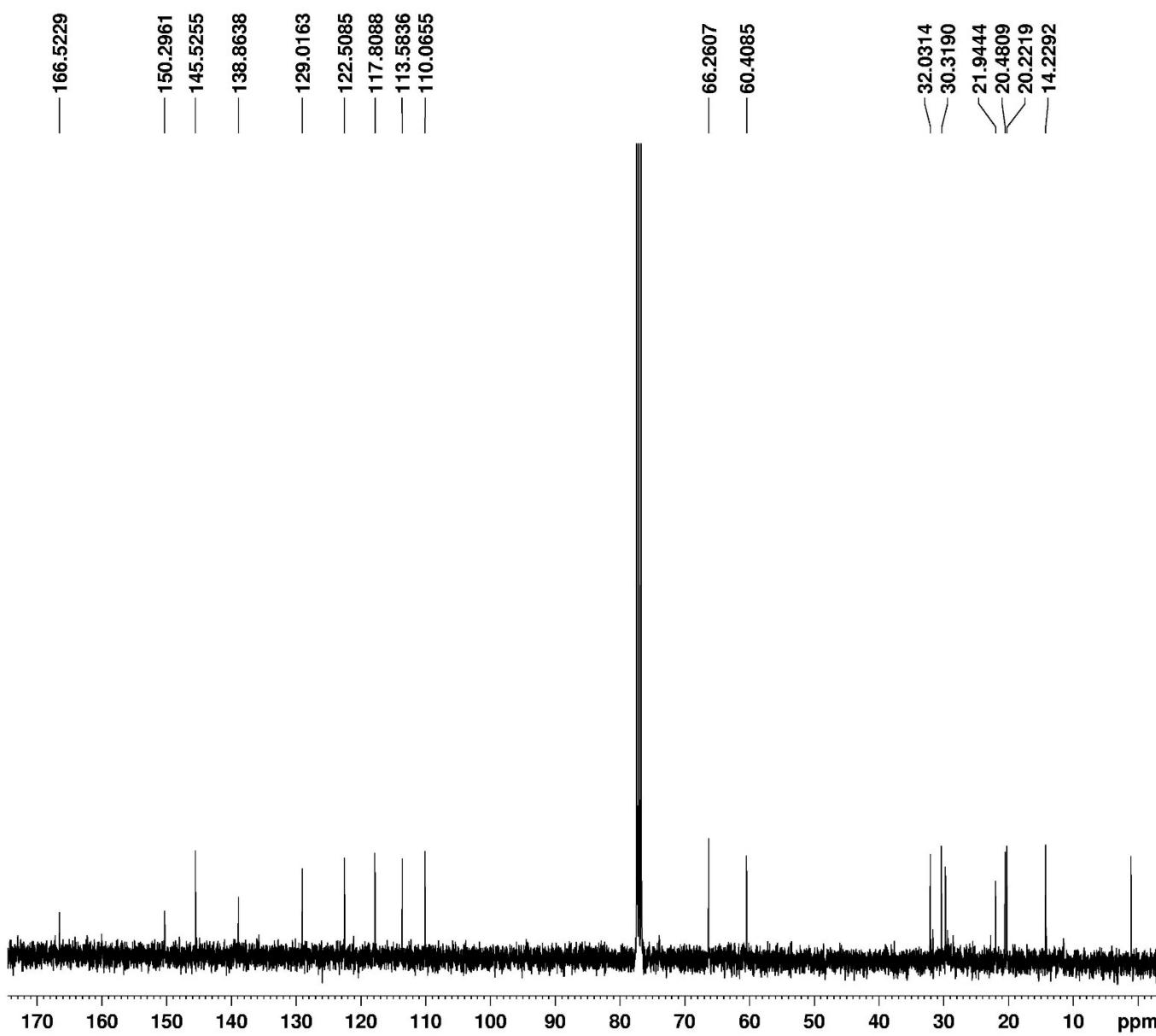
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 EXPNO 30
 PROCNO 1

F2 – Acquisition Parameters
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 Time 23.44
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 PROBHD 5 mm PABBO BB/
 PULPROG zpg30
 TD 65536
 SOLVENT CDCl₃
 NS 512
 DS 0
 SW1 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
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 DE 6.50 usec
 TE 296.8 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TDO 1

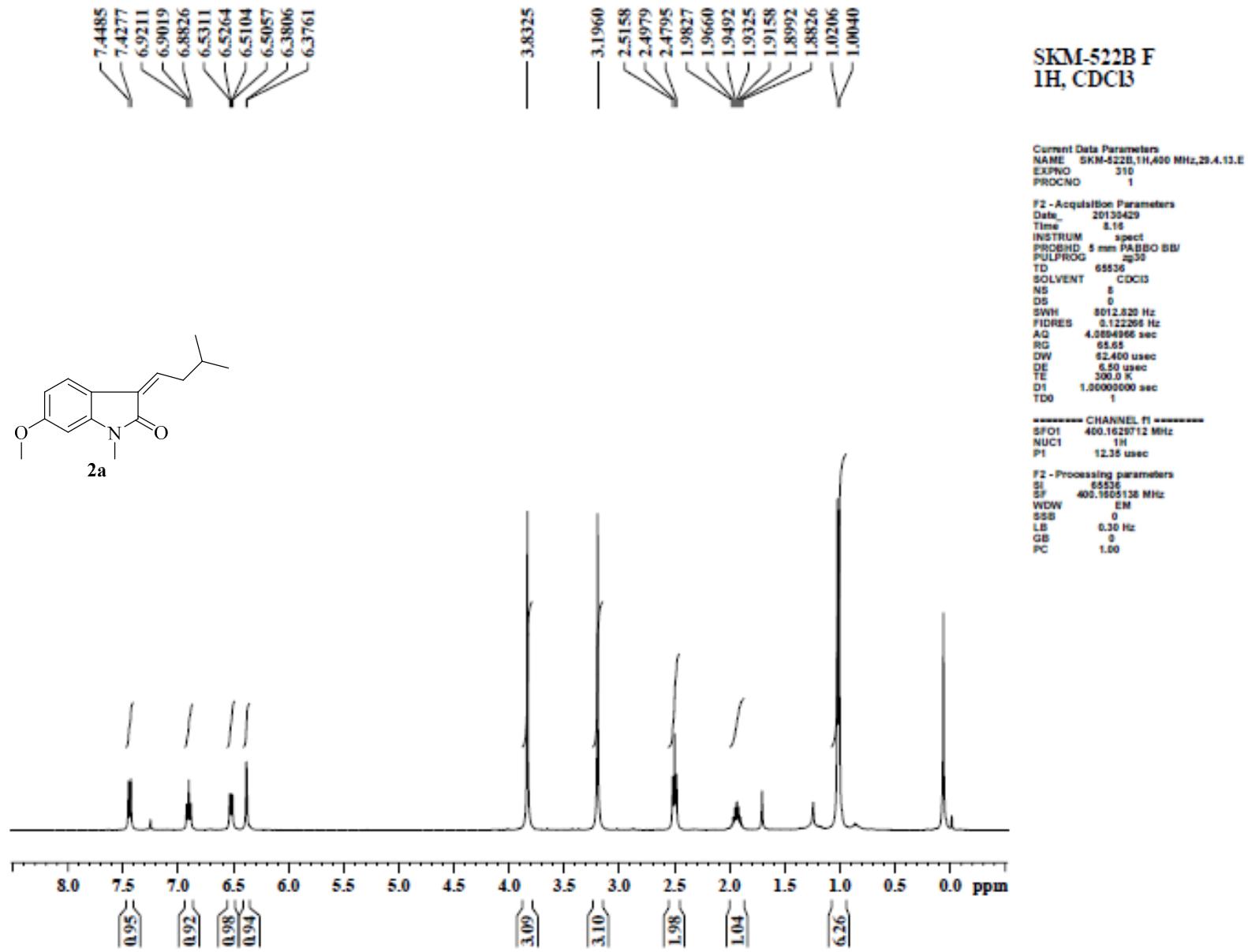
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 SFO1 100.6304993 MHz
 NUC1 ¹³C
 PI 9.90 usec
 PLW1 53.0000000 W

===== CHANNEL f2 =====
 SFO2 400.1621006 MHz
 NUC2 ¹H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 13.0000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

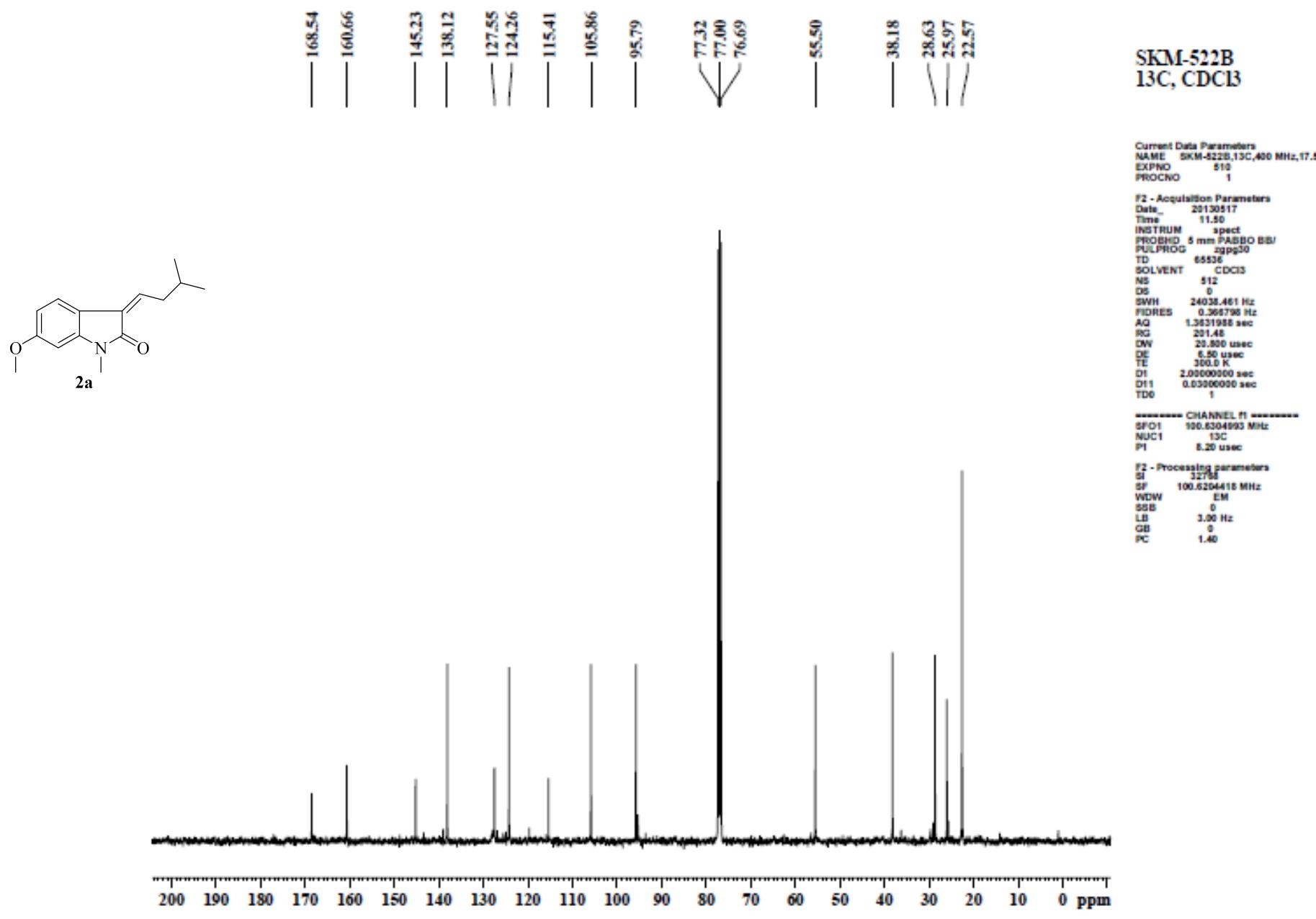
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 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



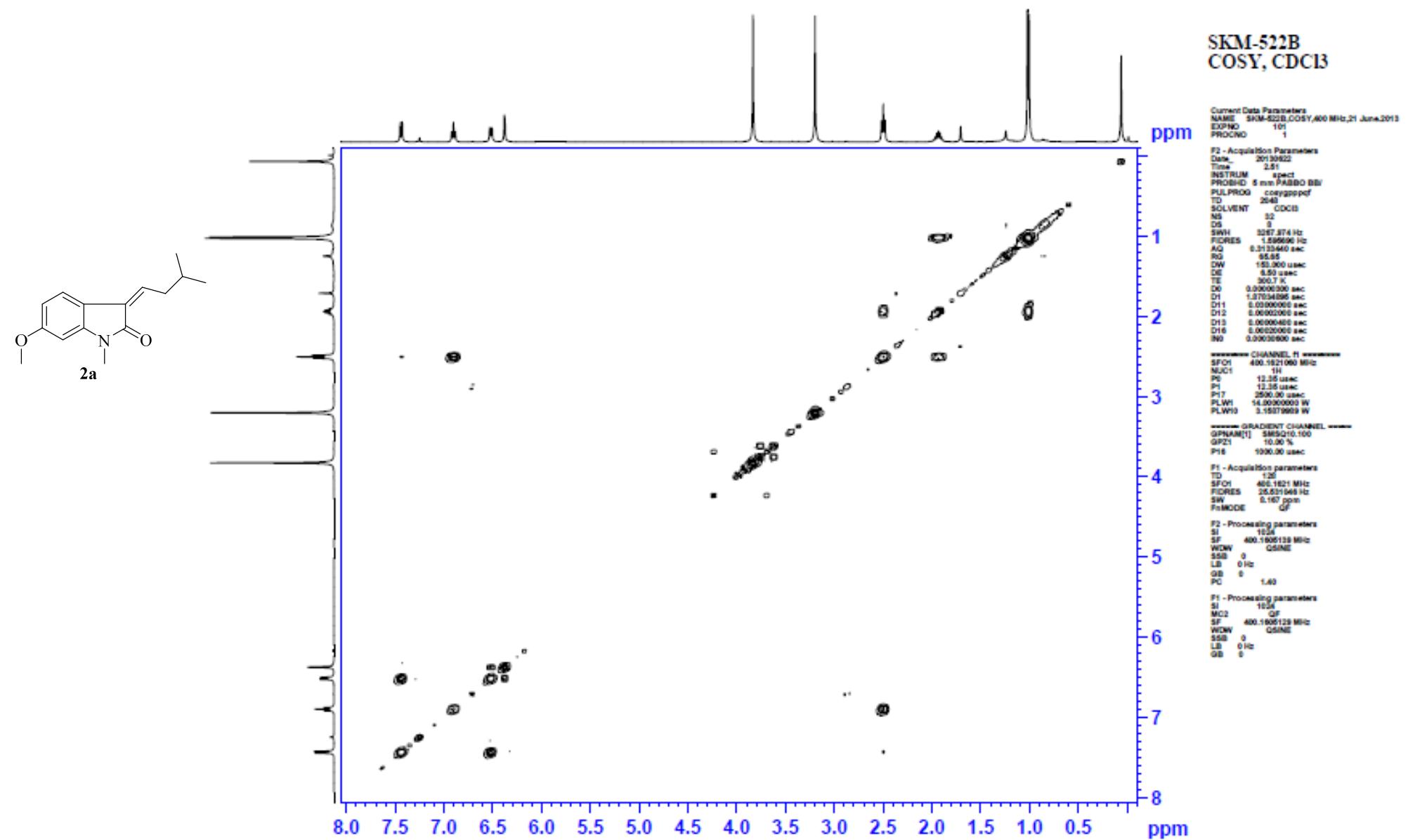
¹³C-NMR Spectrum of **1n**



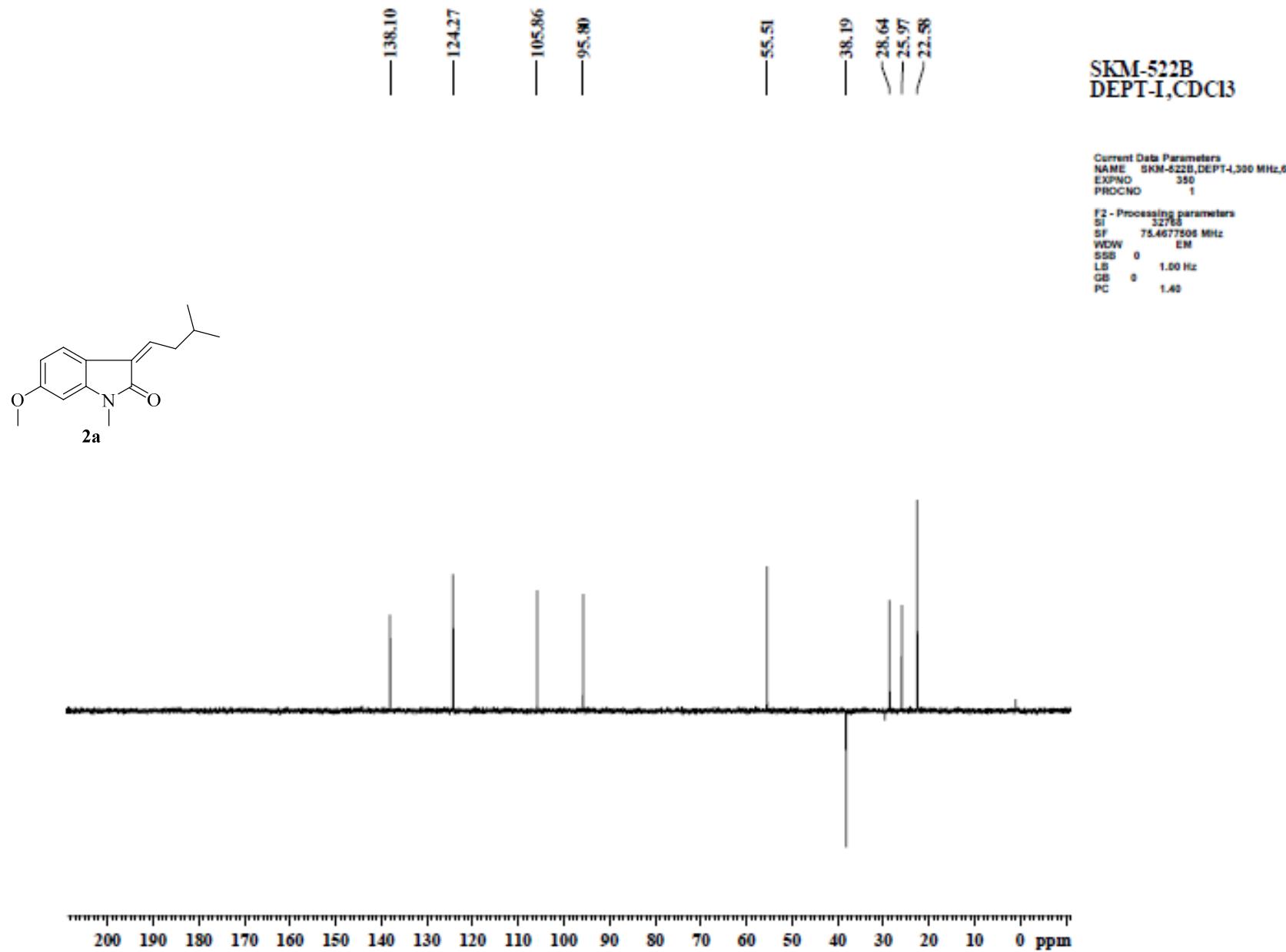
¹H -NMR Spectrum of **2a**



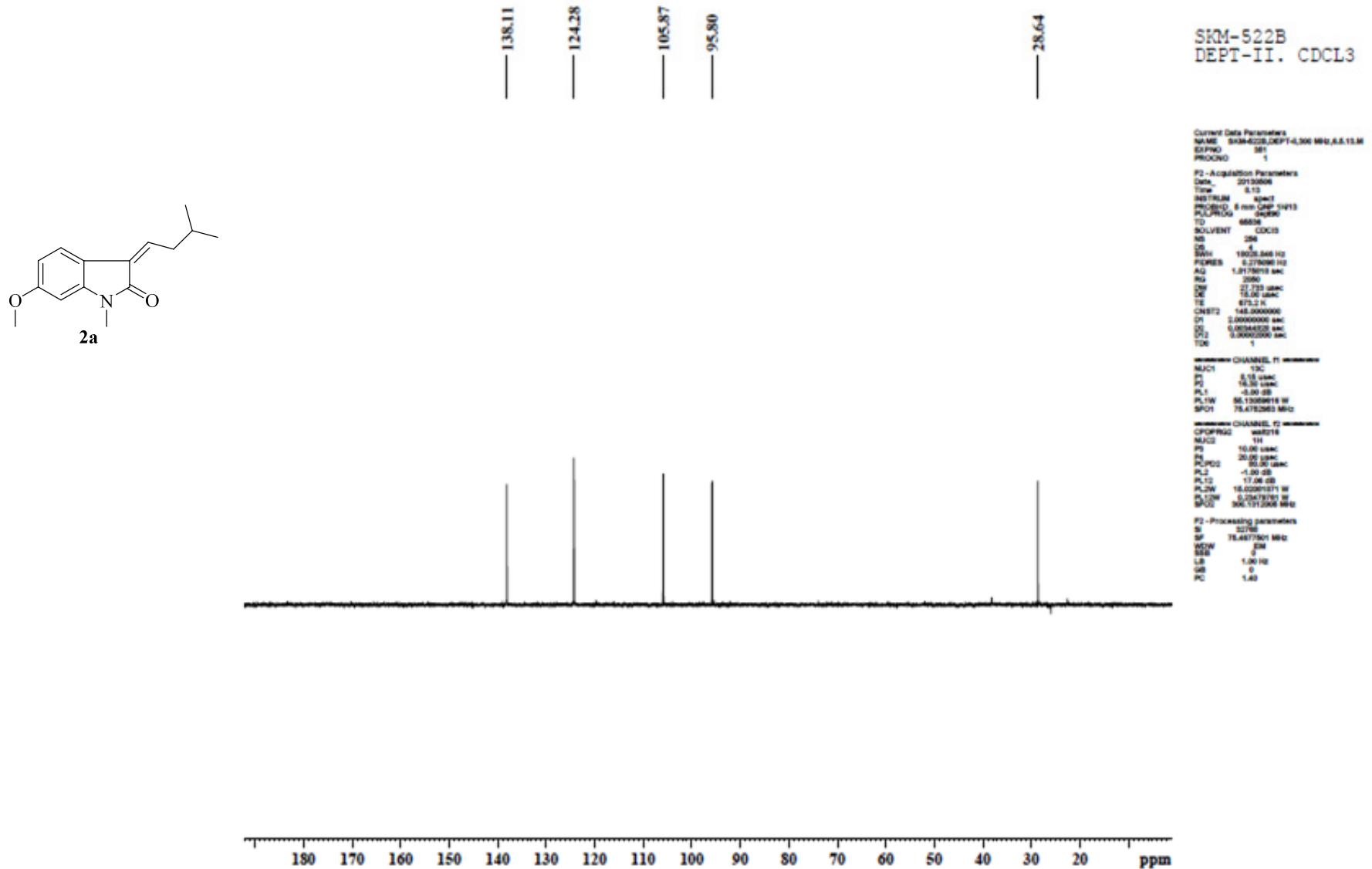
SKM-522B
COSY, CDCl₃



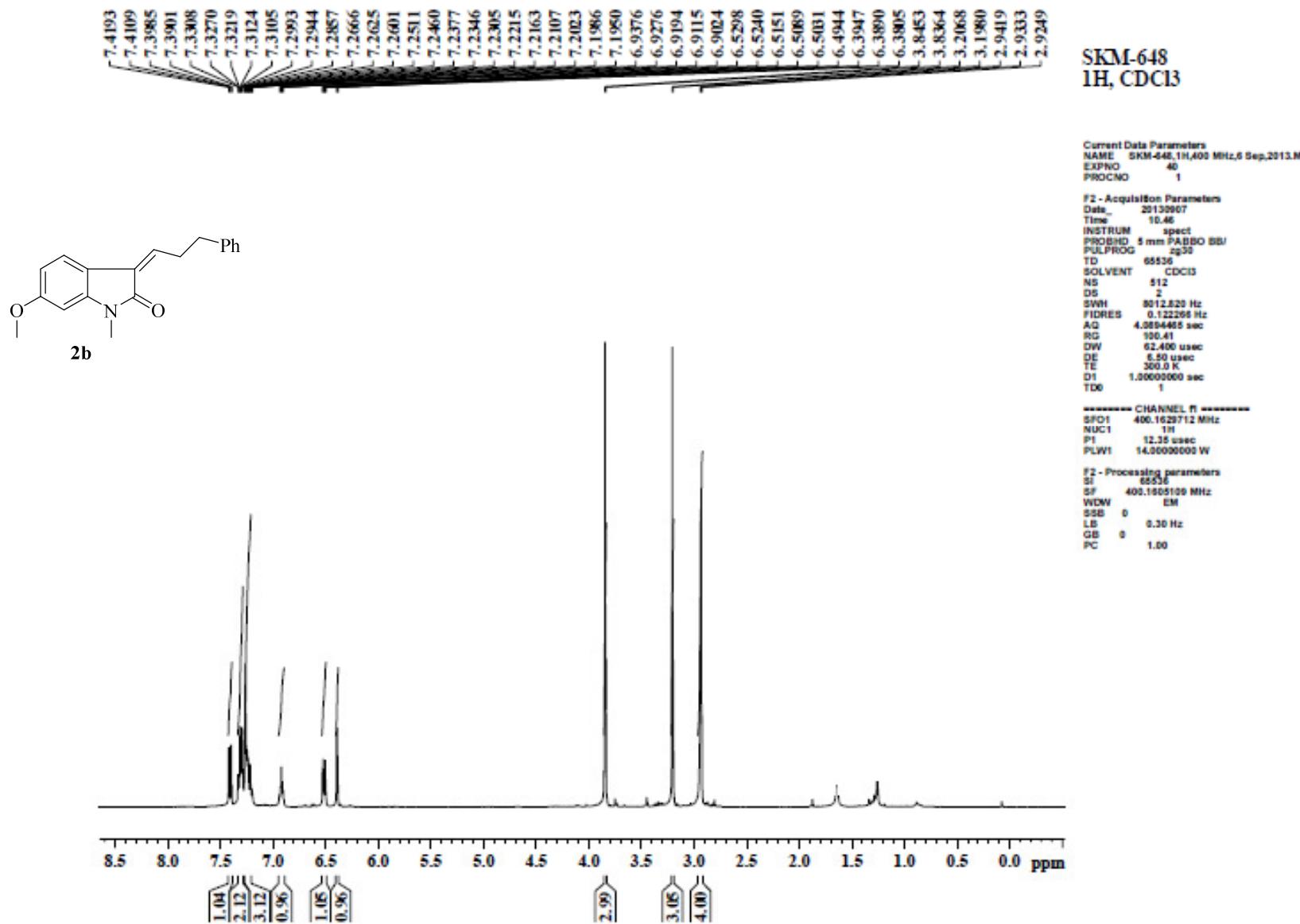
COSY Spectrum of **2a**



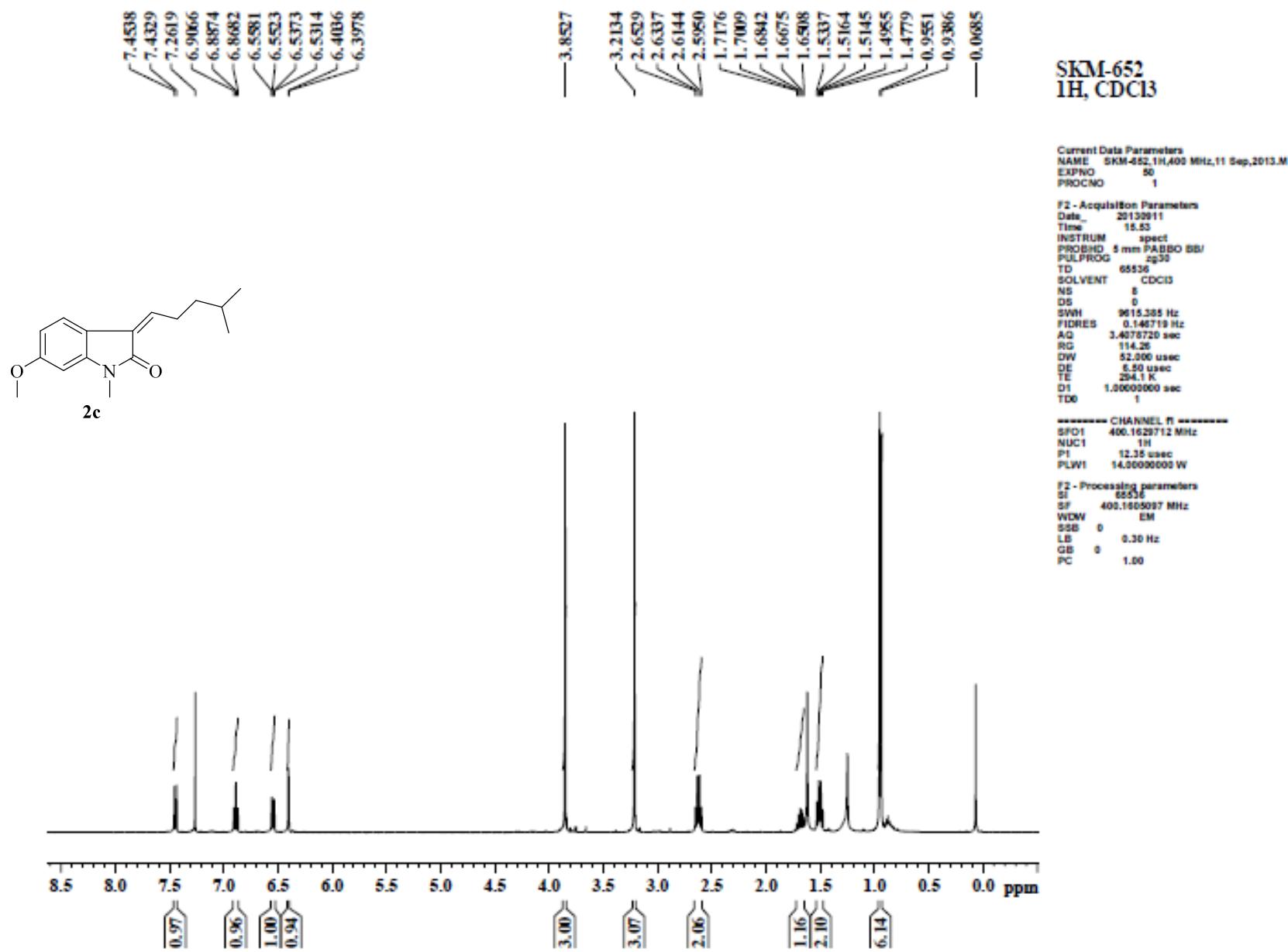
DEPT-I Spectrum of **2a**



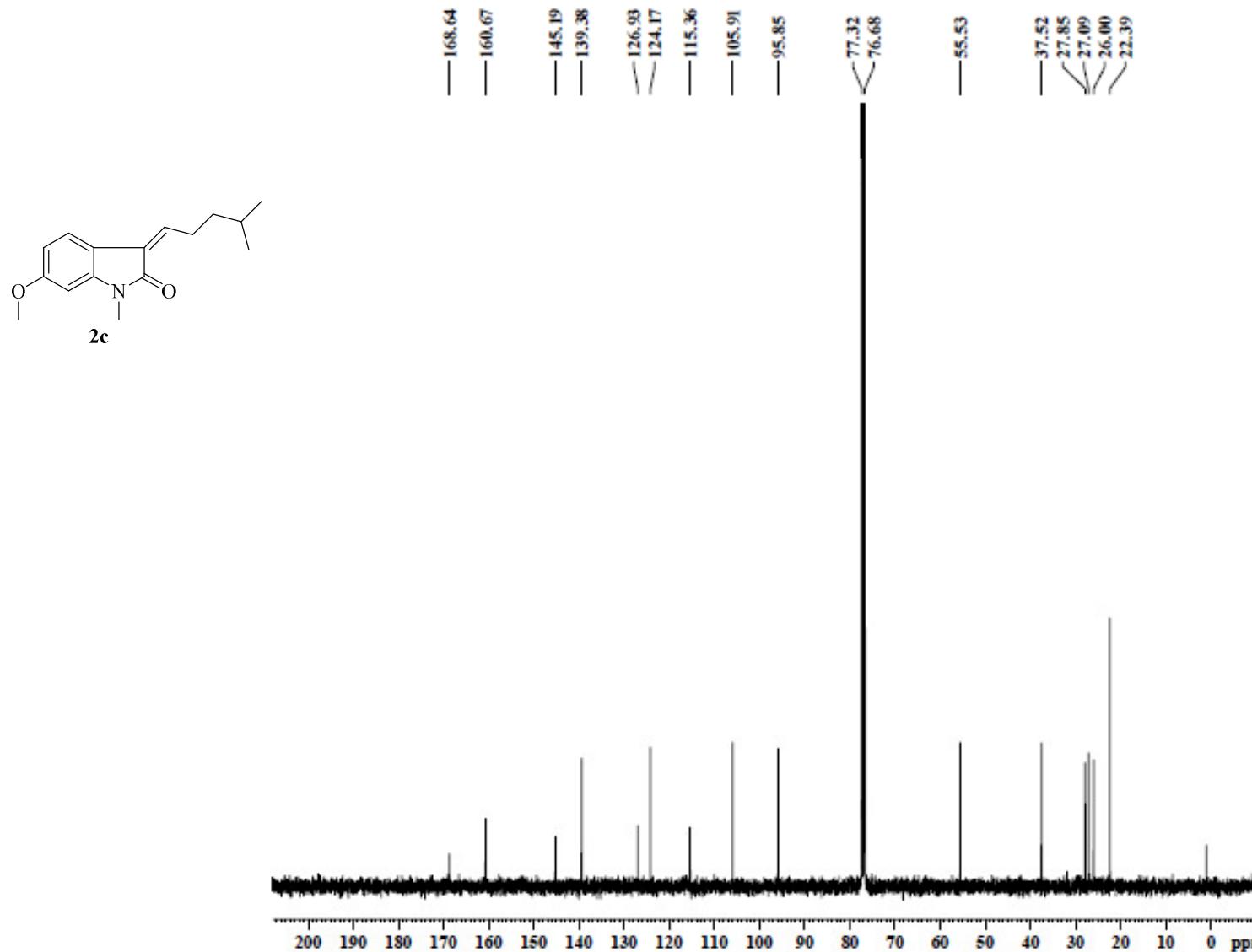
DEPT-II Spectrum of 2a



¹H -NMR Spectrum of **2b**



¹H -NMR Spectrum of **2c**



SKM-652
13C, CDCl₃

Current Data Parameters
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EXPNO 30
PROCNO 1

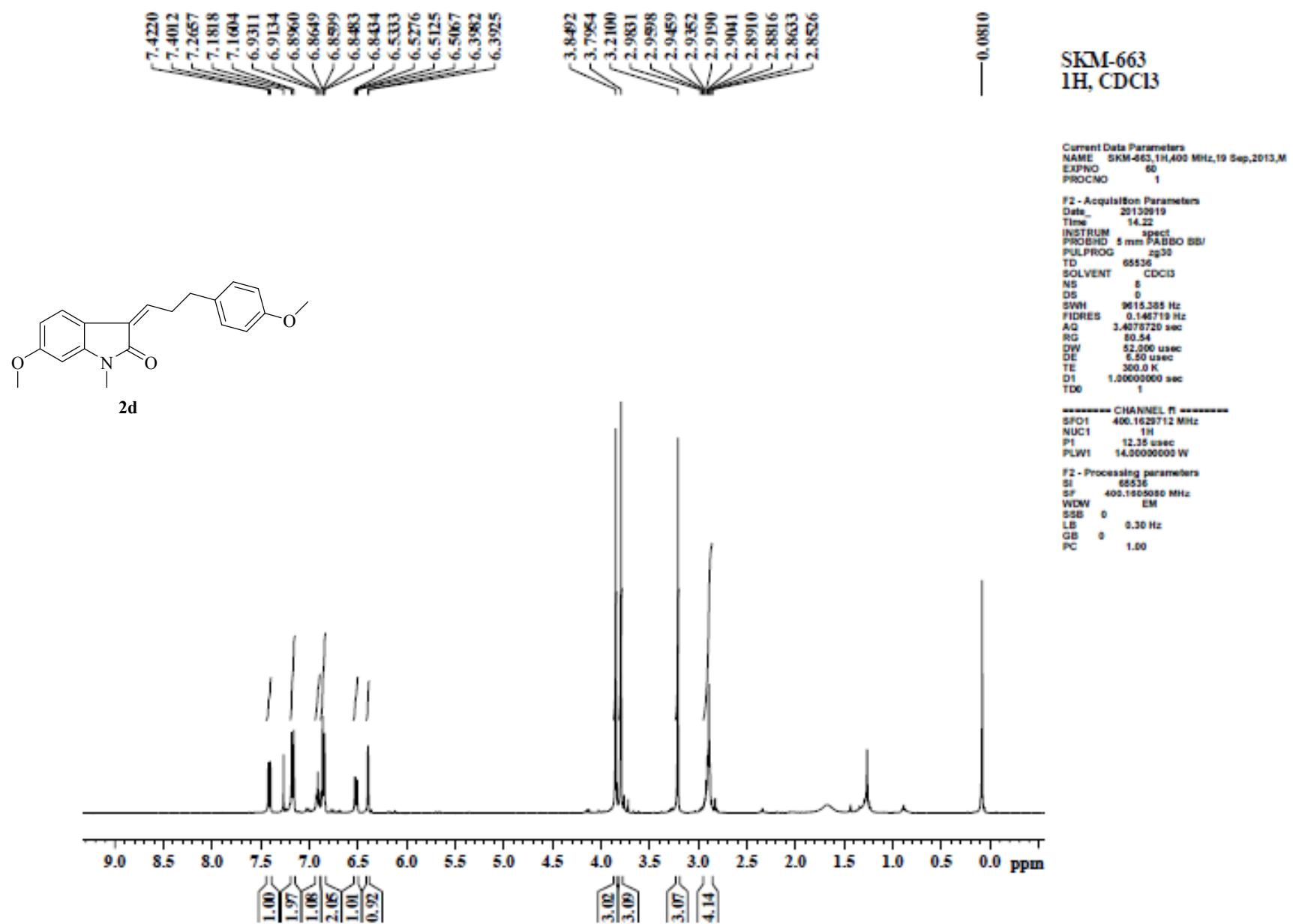
F2 - Acquisition Parameters
Date 20130913
Time 13.22
INSTRUM spect
PROBHD 5 mm PABBO BB1
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 512
DS 4
SWH 2435.461 Hz
FIDRES 0.385795 Hz
AQ 1.383148 sec
RG 201.48
DW 20.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL F1 -----
SFO1 100.6304993 MHz
NUC1 13C
P1 8.20 usec
PLW1 70.59998647 W

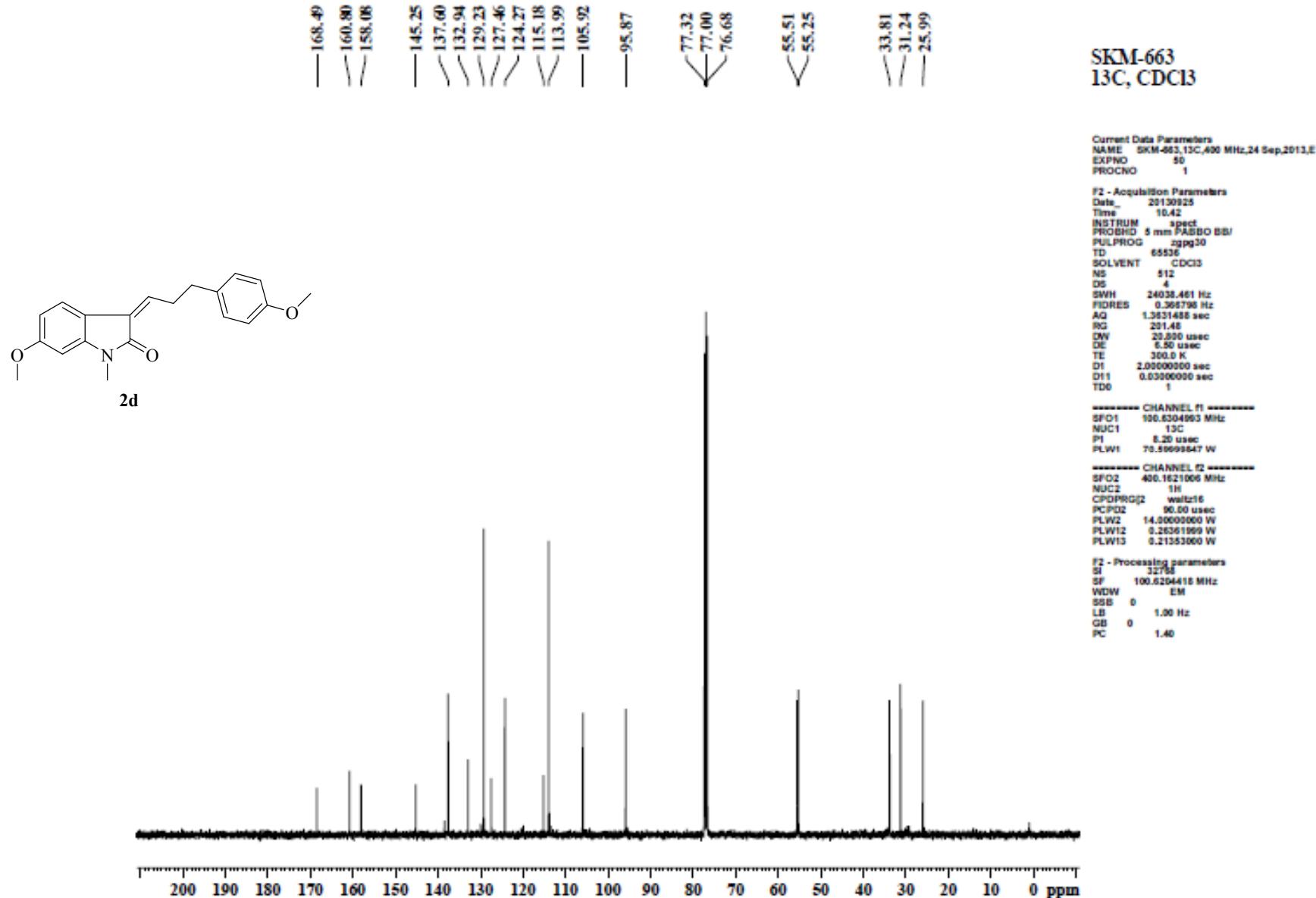
----- CHANNEL Q2 -----
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPDQ2 90.00 usec
PLW2 14.00000000 W
PLW12 0.25361999 W
PLW13 0.21353300 W

F2 - Processing parameters
SF 32768
SF 100.6304996 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

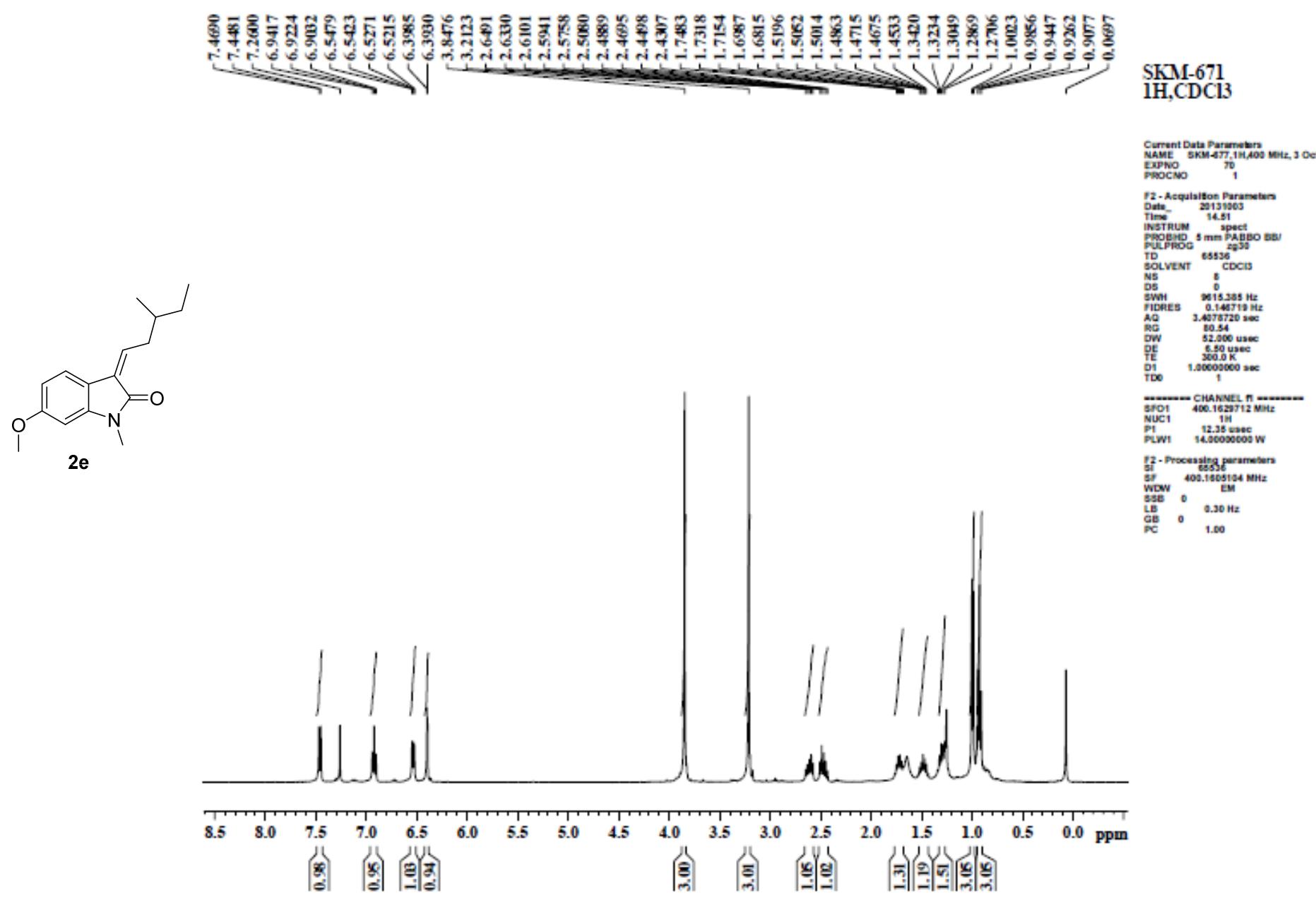
¹³C -NMR Spectrum of **2c**

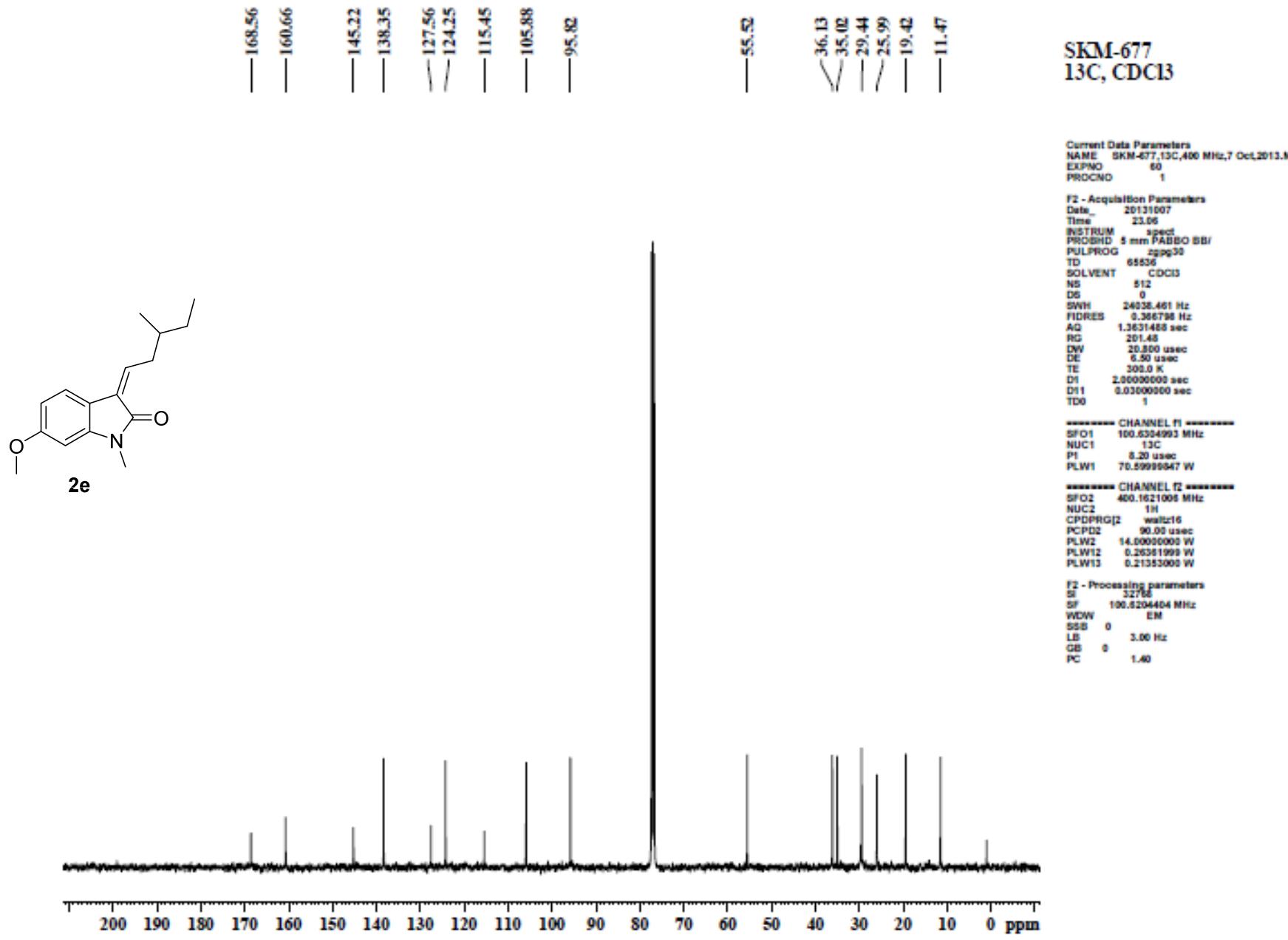


¹H -NMR Spectrum of **2d**

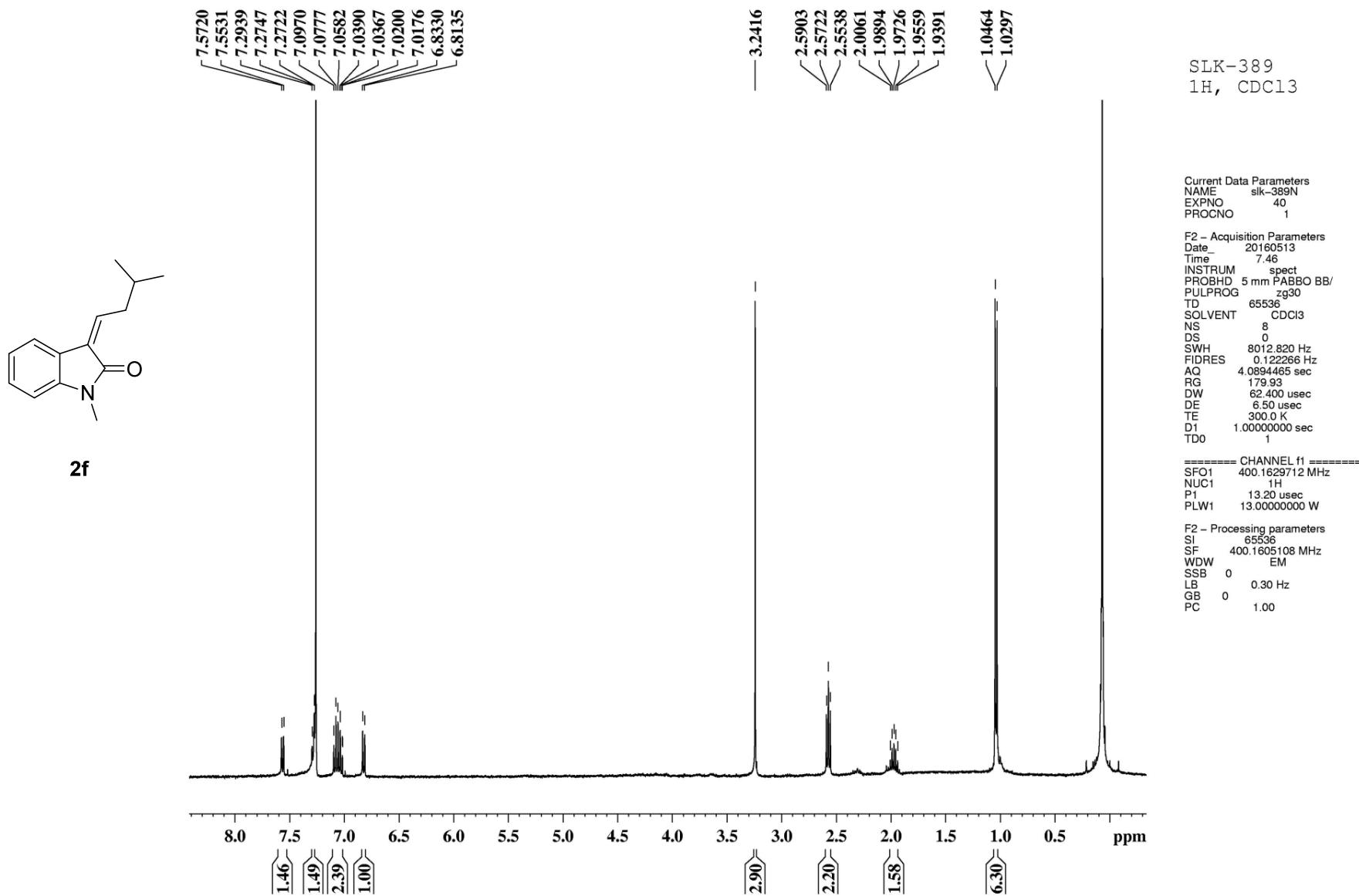


¹³C -NMR Spectrum of **2d**

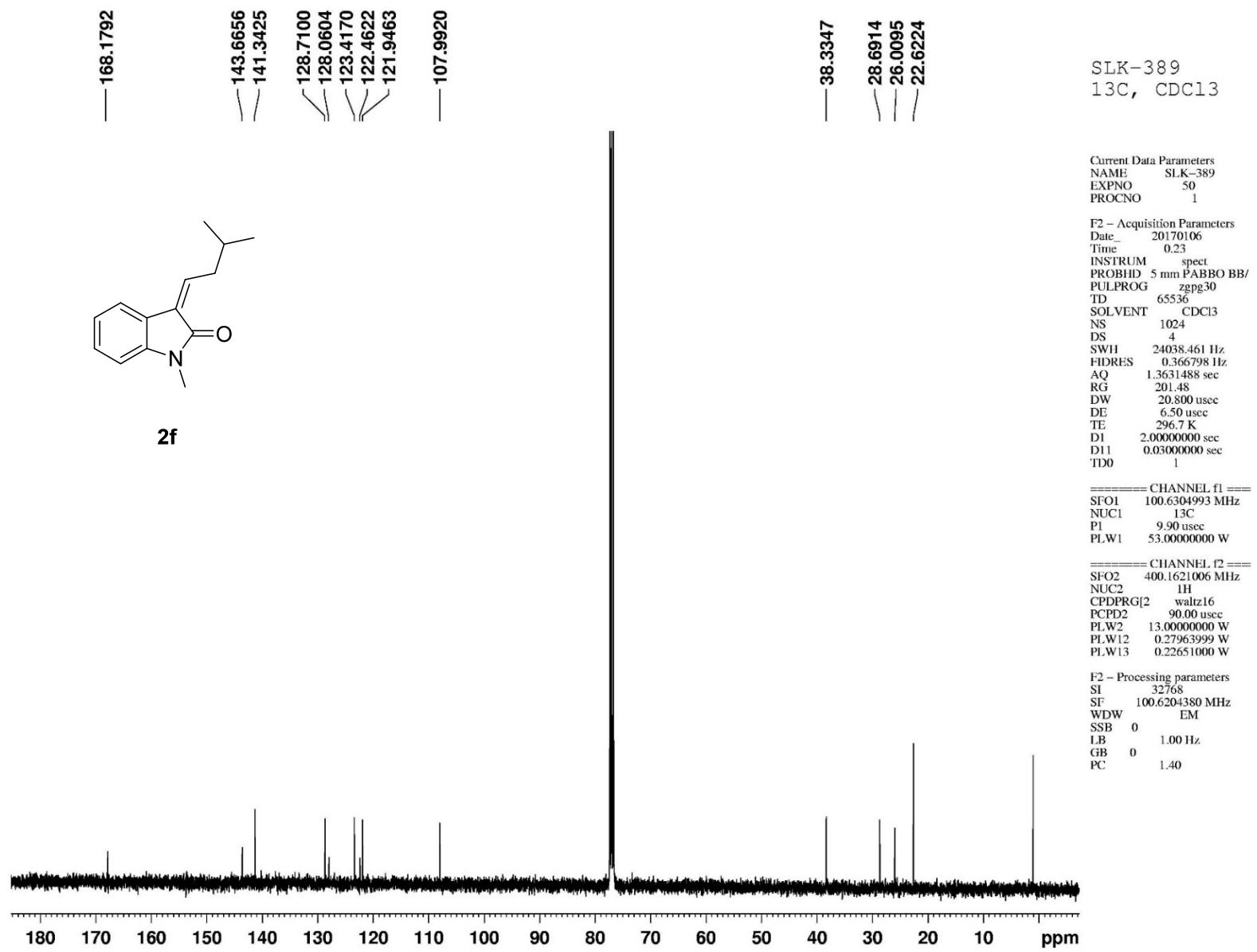




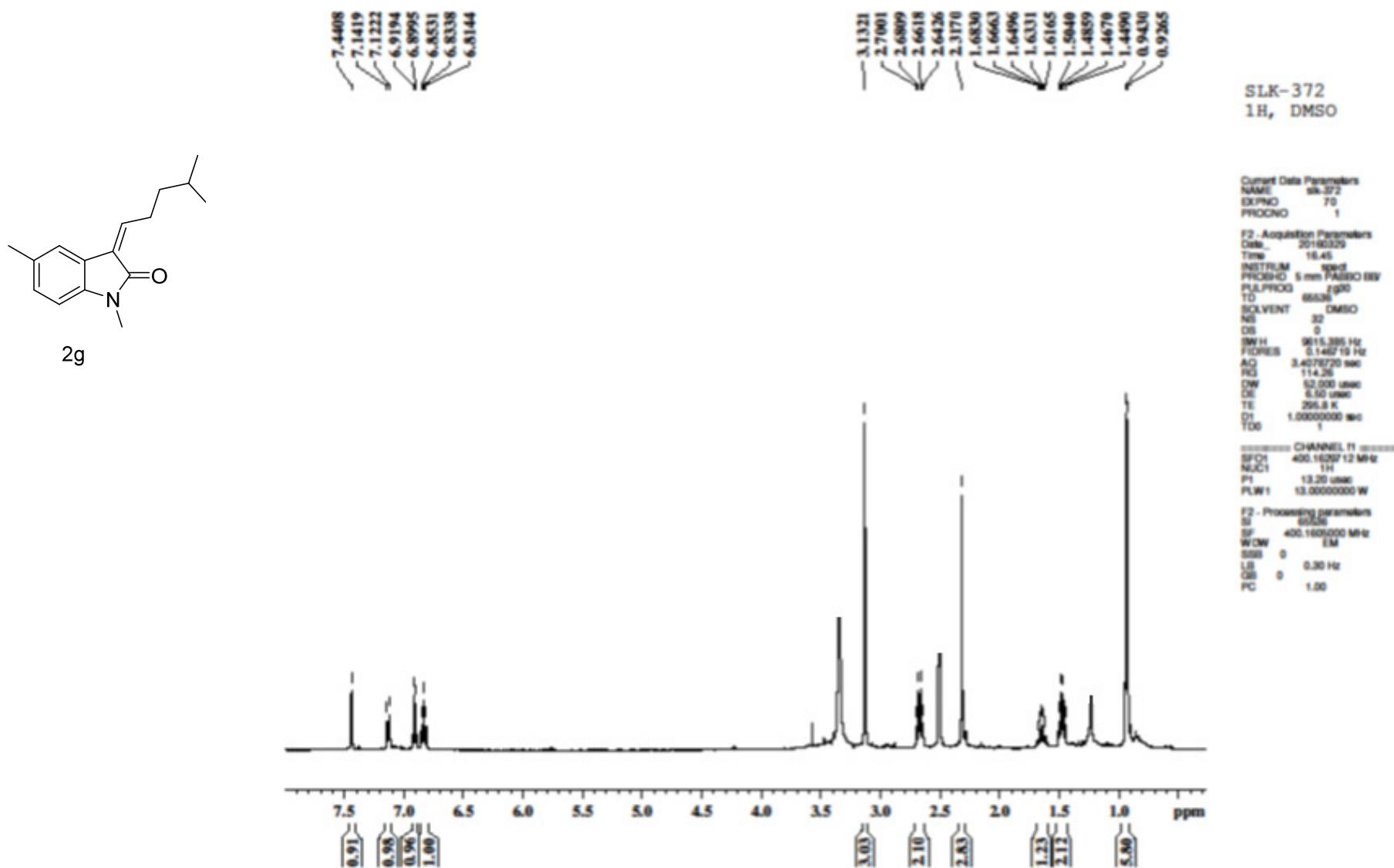
¹³C -NMR Spectrum of 2e



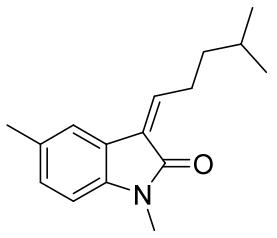
¹H -NMR Spectrum of **2f**



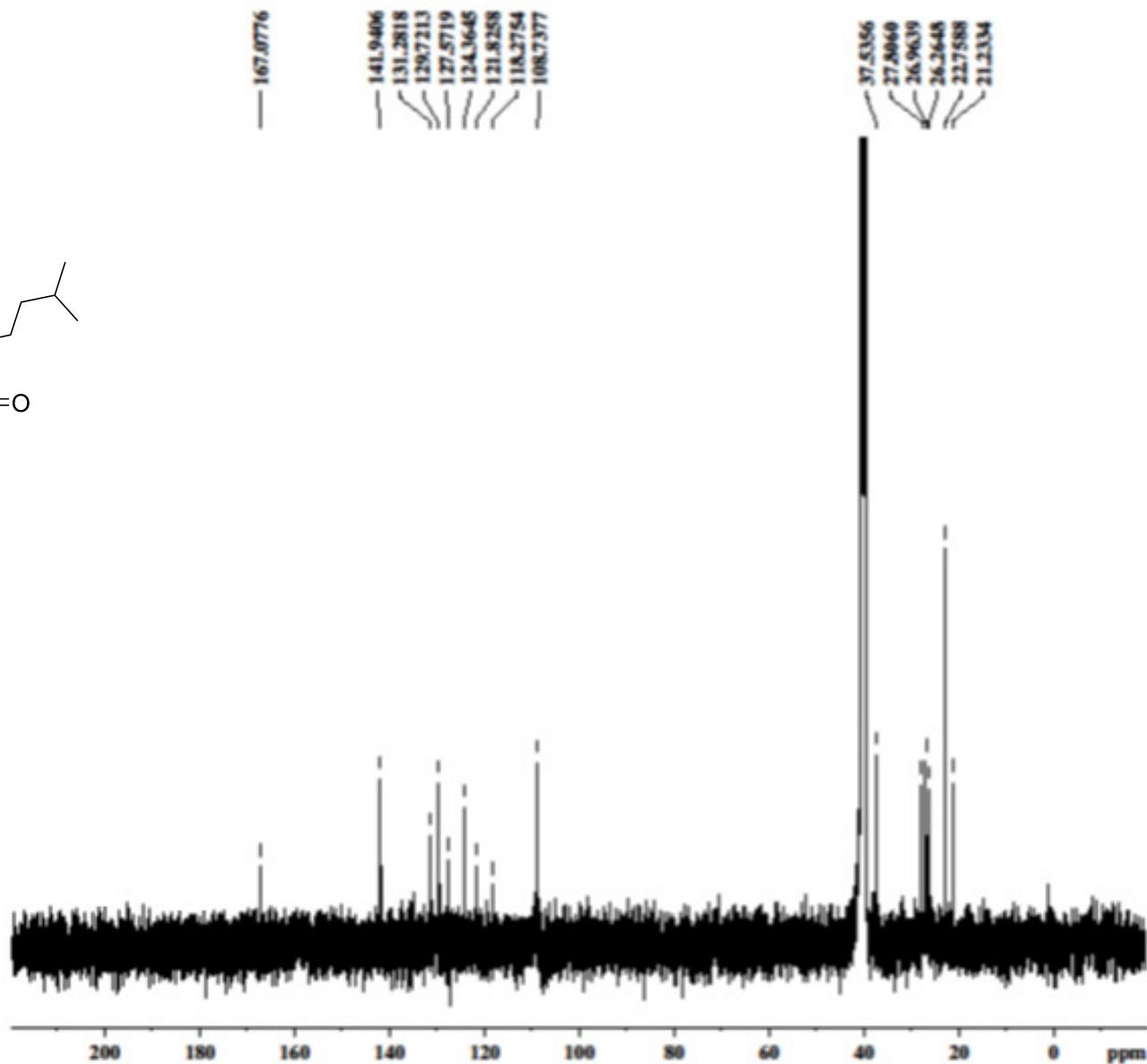
¹³C -NMR Spectrum of **2f**



^1H -NMR Spectrum of **2g**



2g



SLK-372
13C, CDCl₃

Current Data Parameters
NAME: SLK-372
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date: 20160403
Time: 1.54
INSTRUM: spect
PROBHD: 5 mm TBISSO BBV
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 1024
DS: 0
SWH: 24038.461 Hz
FIDRES: 0.386798 Hz
AQ: 1.3631468 sec
RG: 201.48
DW: 20.000 usec
DE: 6.50 usec
TE: 300.0 K
D1: 2.0000000 sec
D11: 0.03000000 sec
TDD: 1

===== CHANNEL 1 ======
SF01: 100.6304993 MHz
NUC1: 13C
P1: 9.00 usec
PLW1: 50.0000000 W

===== CHANNEL 02 ======
SF02: 400.1621006 MHz
NUC2: 1H
CPDP02: wsb16
PCP02: 90.00 usec
PLW2: 13.00000000 W
PLW12: 0.27952999 W
PLW13: 0.22661000 W

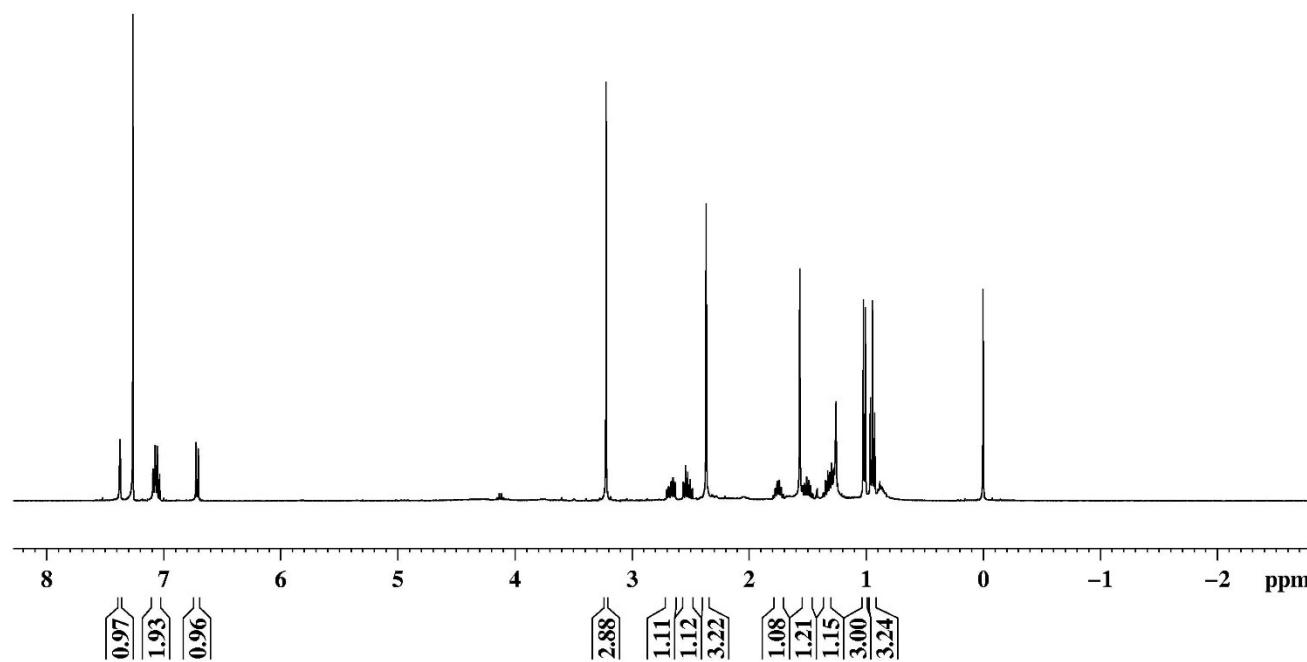
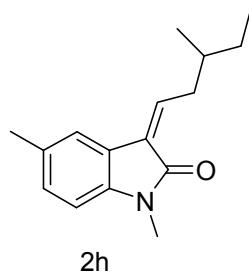
F2 - Processing parameters
SI: 32768
SF: 100.6204380 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
QSI: 0.140

¹³C -NMR Spectrum of 2g

7.3705
 7.0869
 7.0694
 7.0508
 7.0316
 6.7206
 6.7008

3.2186
 2.7018
 2.6861
 2.6673
 2.6624
 2.6467
 2.6284
 2.5590
 2.5400
 2.5205
 2.5005
 2.4815
 2.3637
 1.7892
 1.7727
 1.7563
 1.7397
 1.7232
 1.7067
 1.6765
 1.5641
 1.5388
 1.5243
 1.5203
 1.5053
 1.4908
 1.4865
 1.4722
 1.3448
 1.3262
 1.3073
 1.2926
 1.0211
 1.0044
 0.9613
 0.9429
 0.9243

SLK-375
1H, CDCl₃



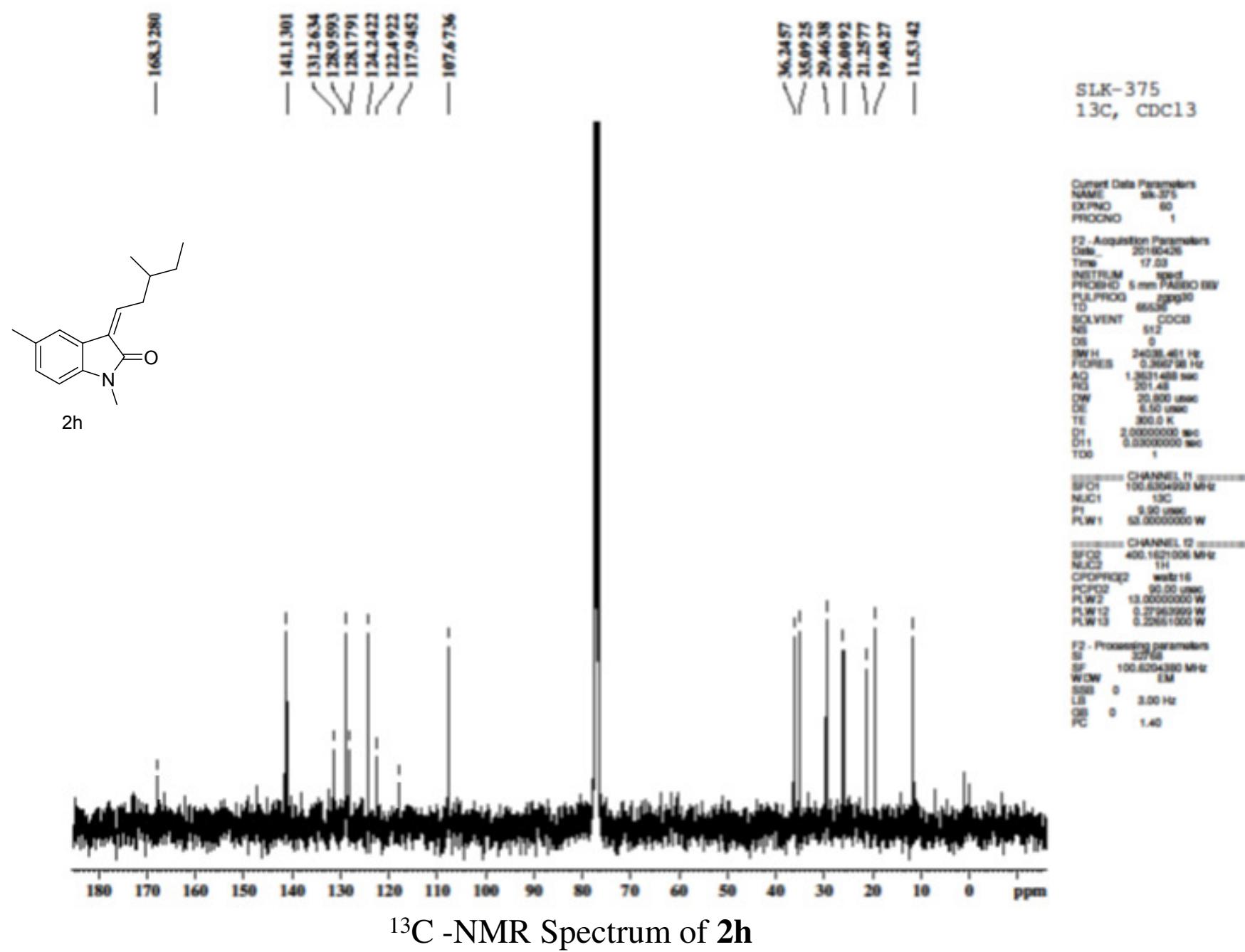
¹H -NMR Spectrum of 2h

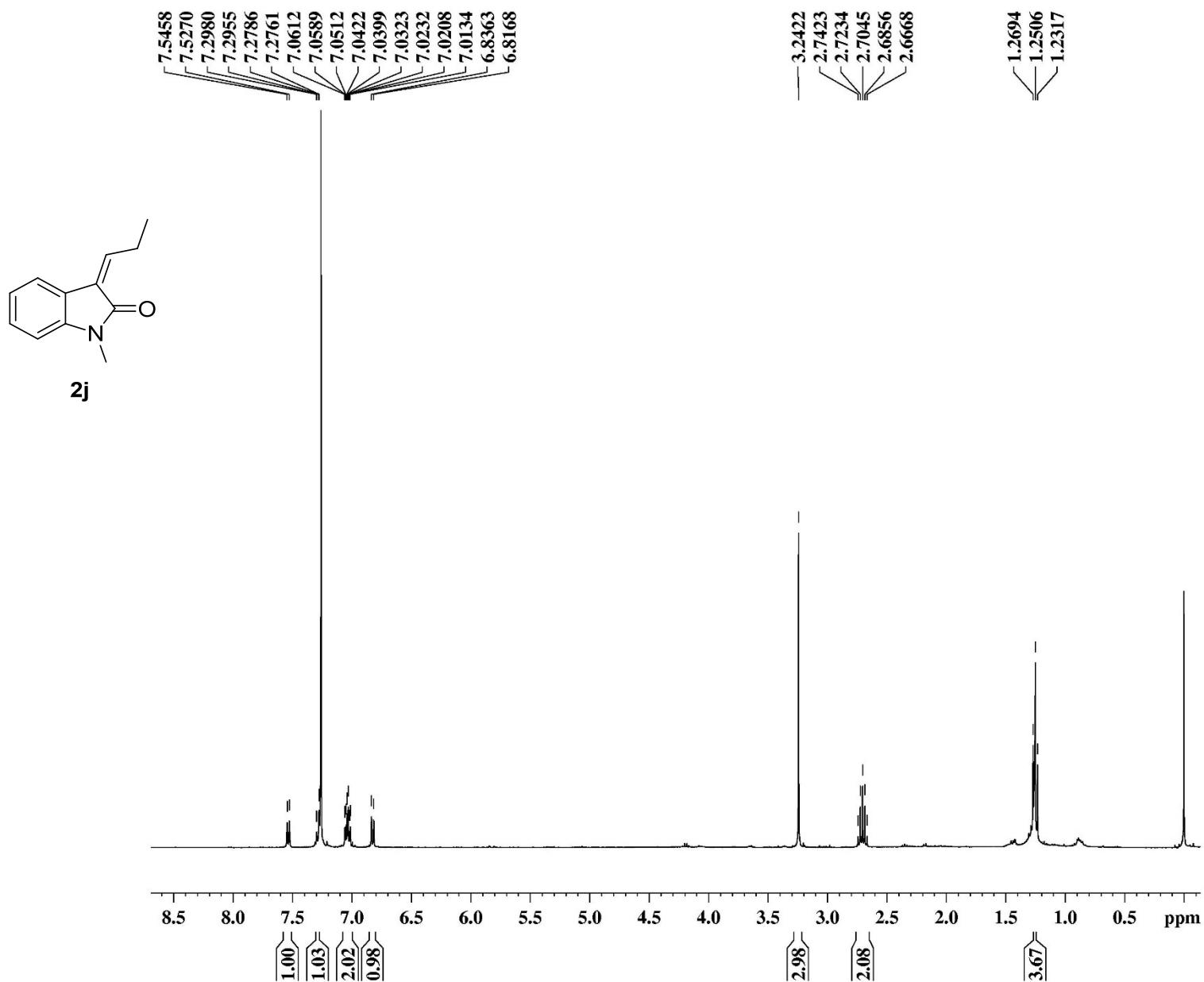
Current Data Parameters
NAME slk-375
EXPNO 160
PROCNO 1

F2 – Acquisition Parameters
Date 20160412
Time 3.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 8
DS 0
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4078720 sec
RG 129.57
DW 52.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1629712 MHz
NUC1 1H
P1 13.20 usec
PLW1 13.00000000 W

F2 – Processing parameters
SI 65536
SF 400.1605099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



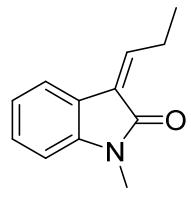


Current Data Parameters
 NAME slk-285
 EXPNO 30
 PROCNO 1

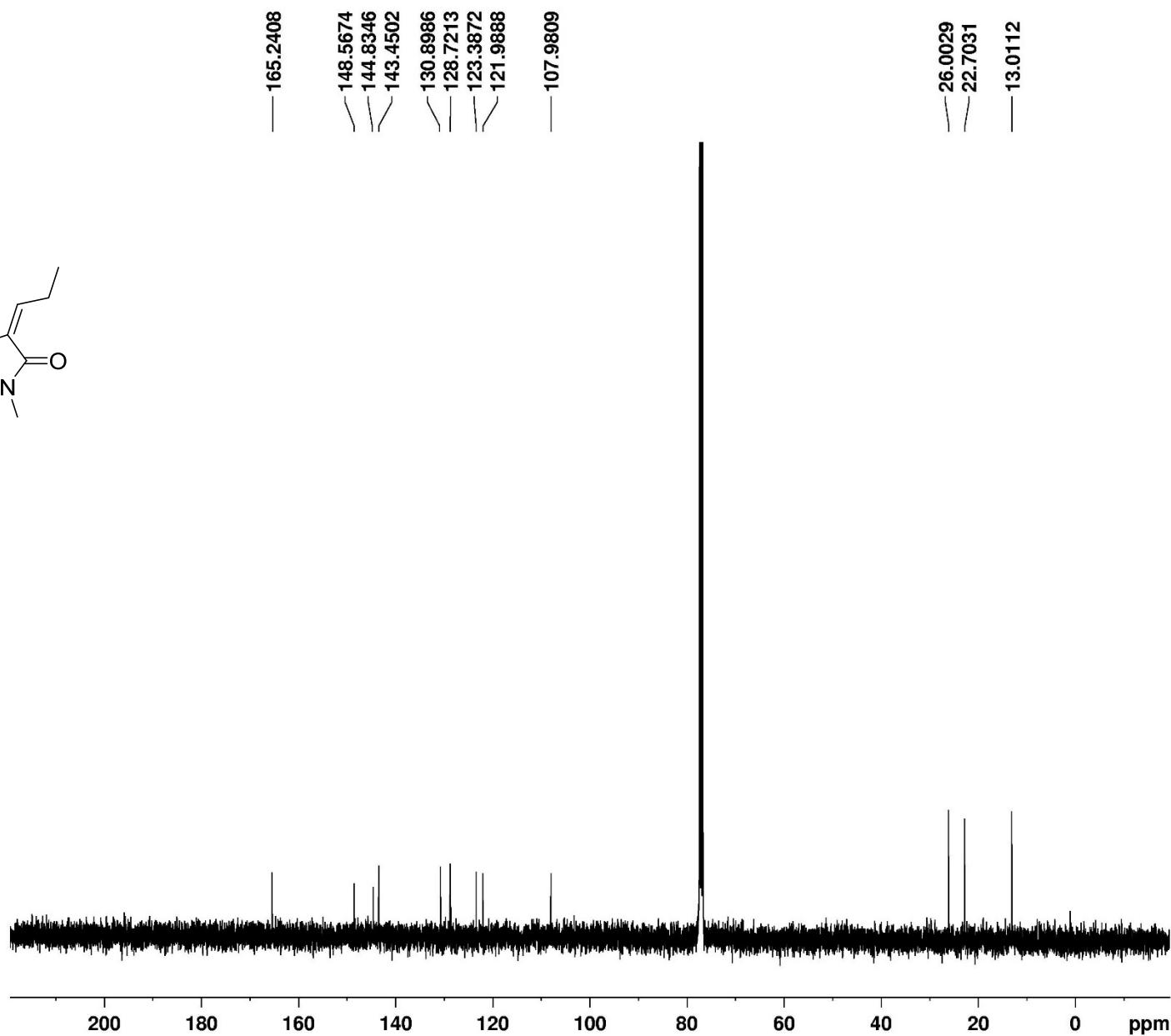
F2 – Acquisition Parameters
 Date 20160805
 Time 14.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 64
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 159.22
 DW 52.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1629712 MHz
 NUC1 ¹H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 – Processing parameters
 SI 65536
 SF 400.1605096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



2j



¹³C -NMR Spectrum of 2j

SLK-285
13C, CDCl₃

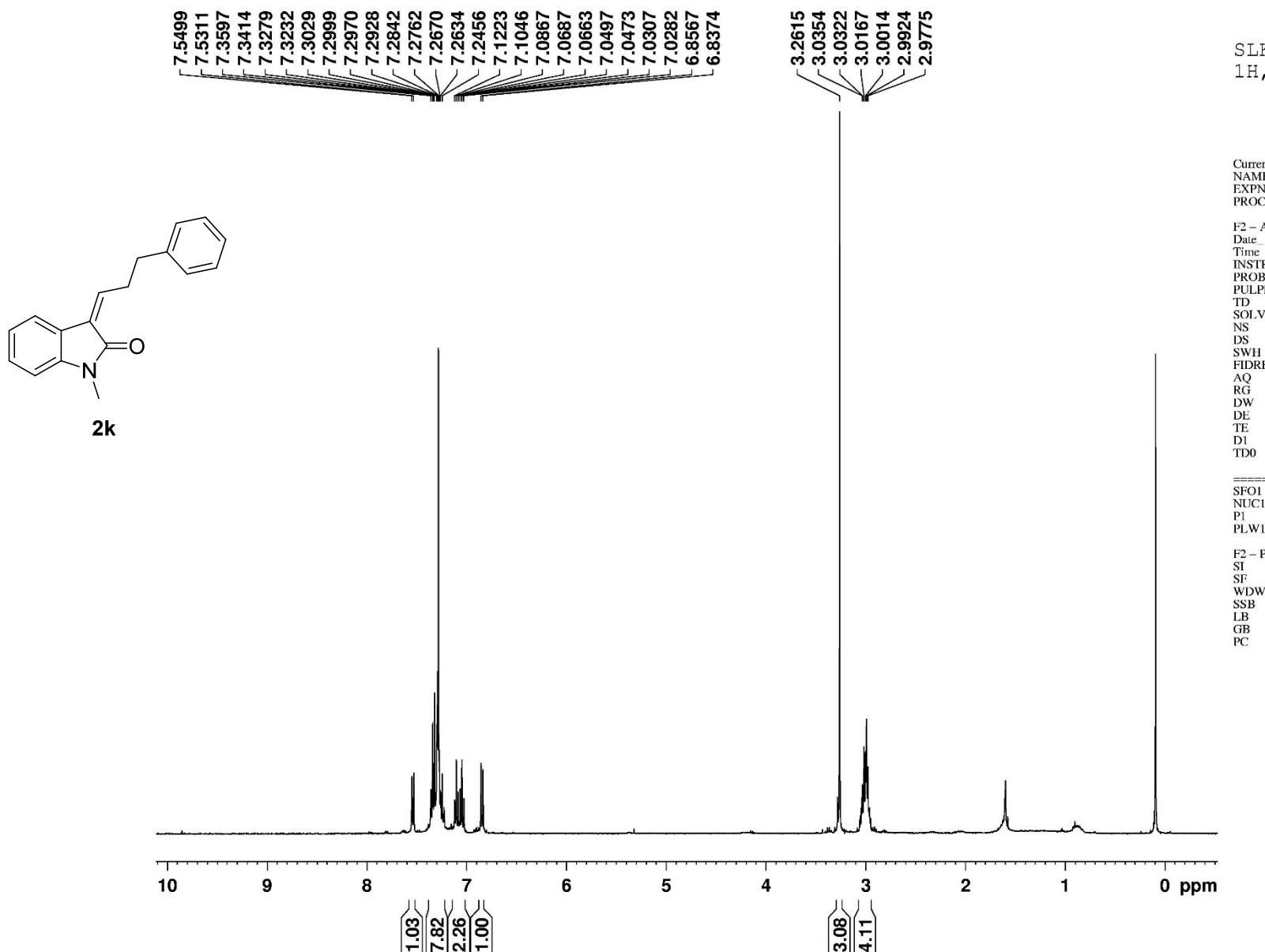
Current Data Parameters
NAME synergy
EXPNO 70
PROCNO 1

F2 – Acquisition Parameters
Date 20160807
Time 12.33
INSTRUM spect
PROBID 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 512
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 201.48
DW 20.800 usec
DE 6.50 usec
TE 301.4 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

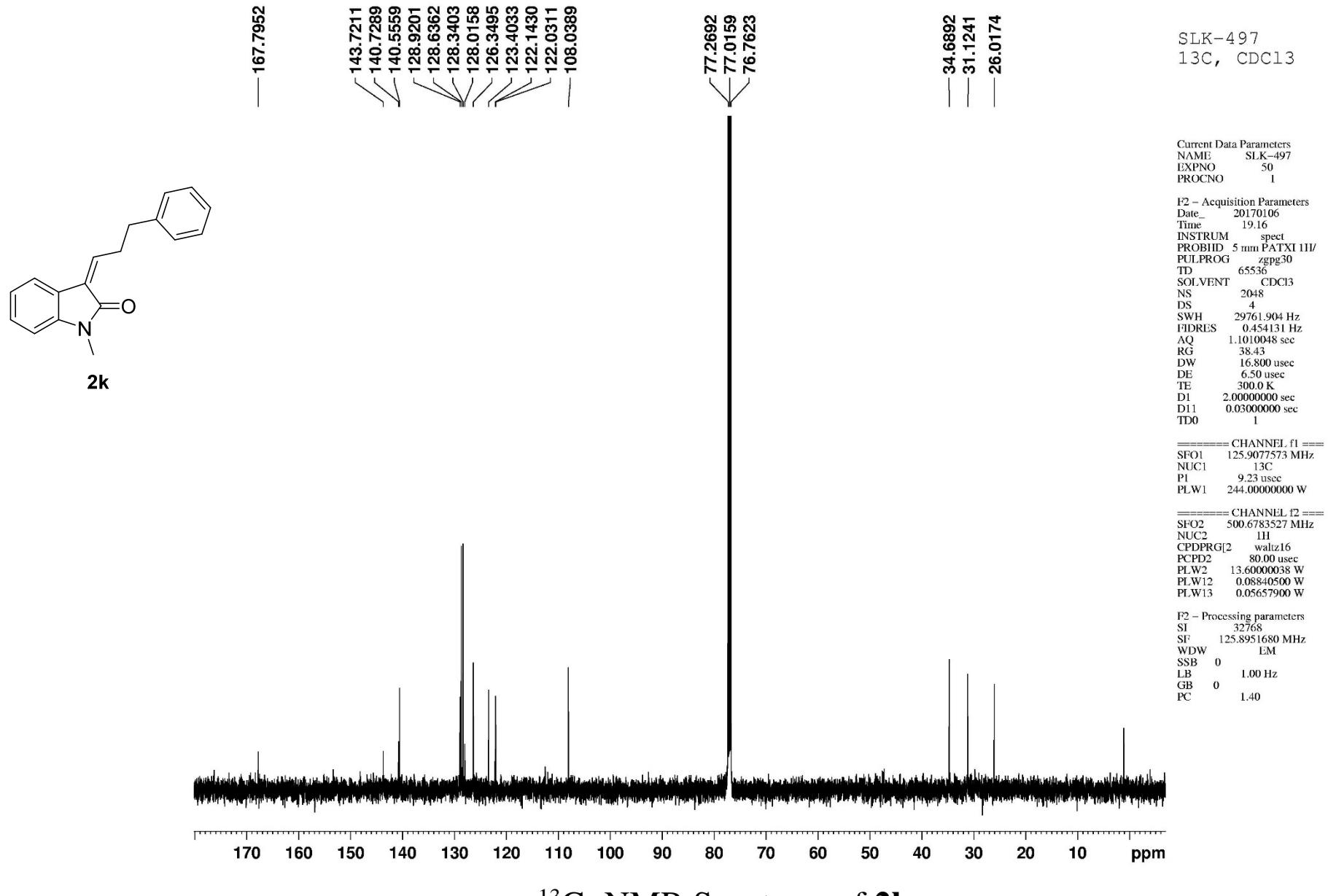
===== CHANNEL f1 =====
SFO1 100.6304993 MHz
NUC1 ¹³C
P1 9.90 usec
PLW1 53.00000000 W

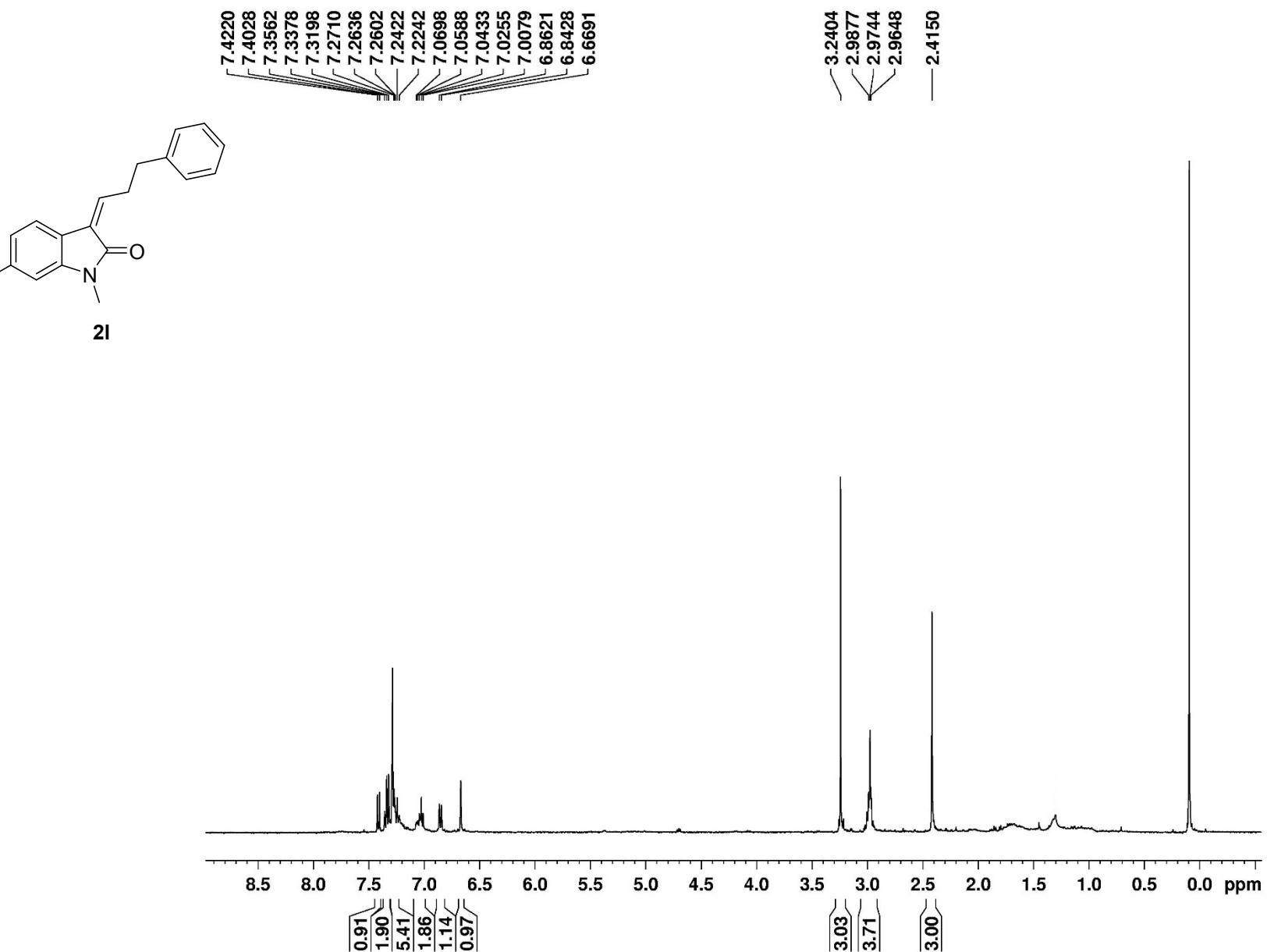
===== CHANNEL f2 =====
SFO2 400.1621006 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.27963999 W
PLW13 0.22651000 W

F2 – Processing parameters
SI 32768
SF 100.6204380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

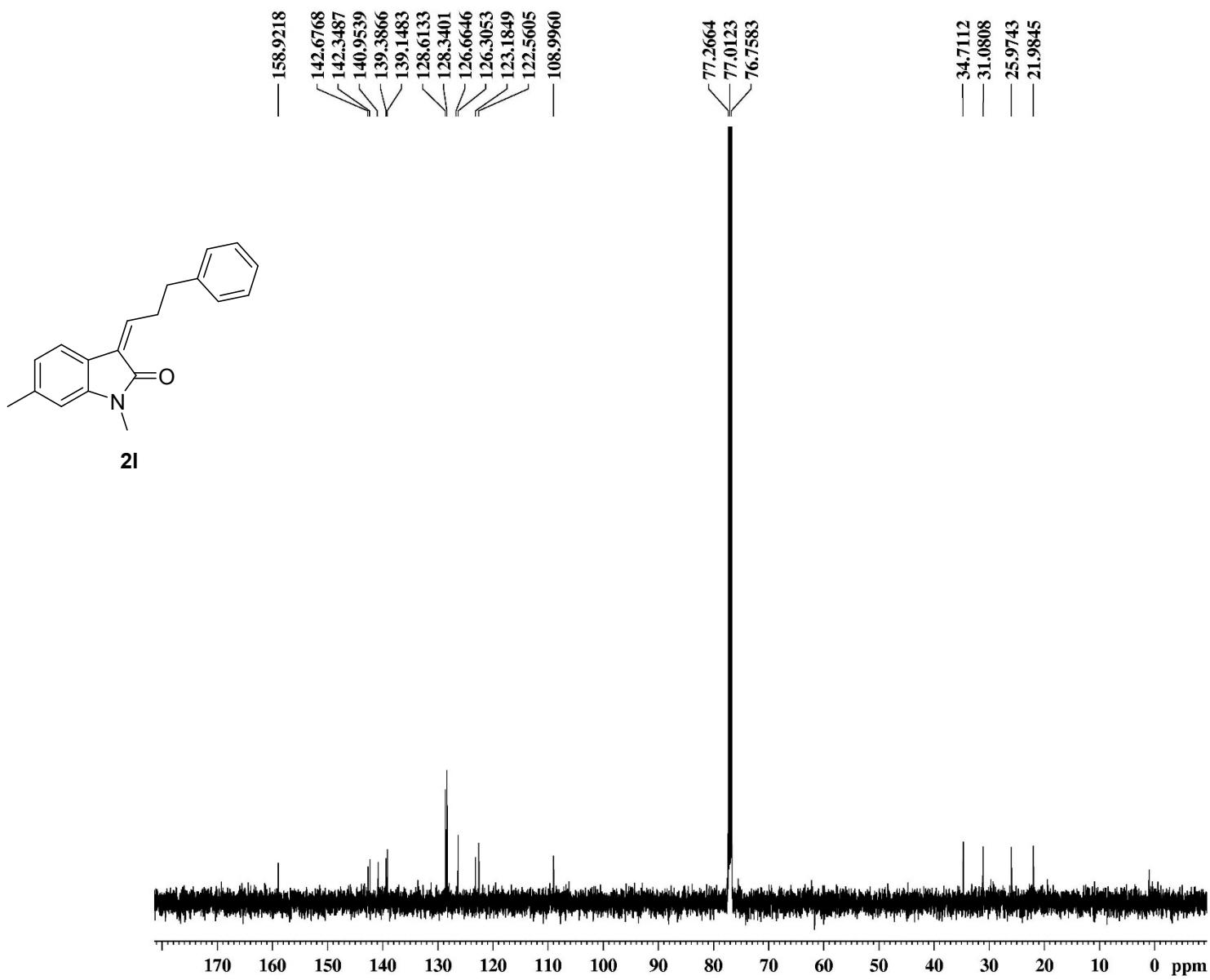


^1H -NMR Spectrum of **2k**





¹H -NMR Spectrum of **2l**



^{13}C -NMR Spectrum of **2l**

SLK-498
13C, CDCl₃

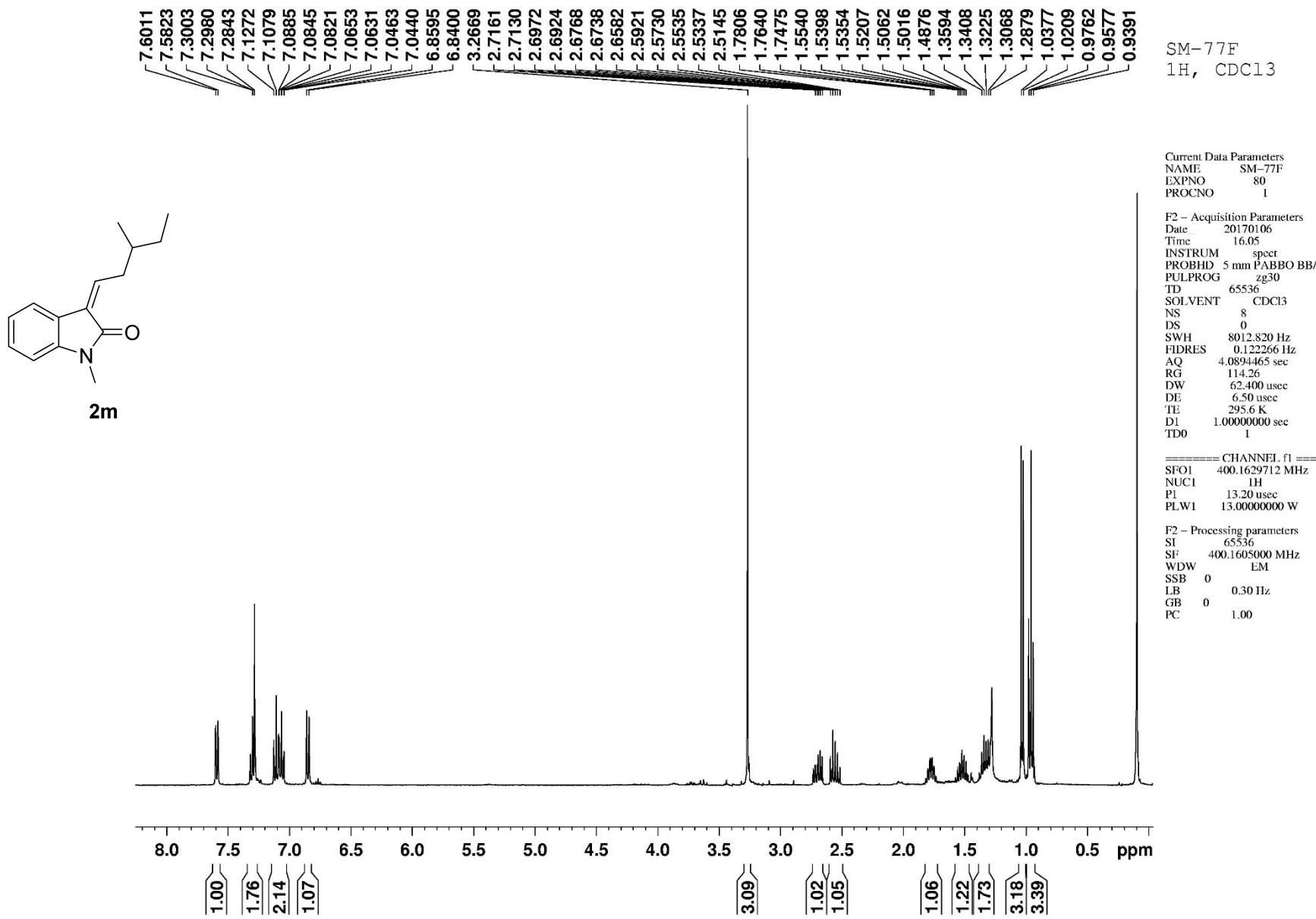
Current Data Parameters
NAME SLK-498F
EXPNO 60
PROCNO 1

F2 – Acquisition Parameters
Date_ 20170106
Time 21.09
INSTRUM spect
PROBID_ 5 mm PABXI III/
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 2048
DS 4
SW1 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 38.43
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TDD 1

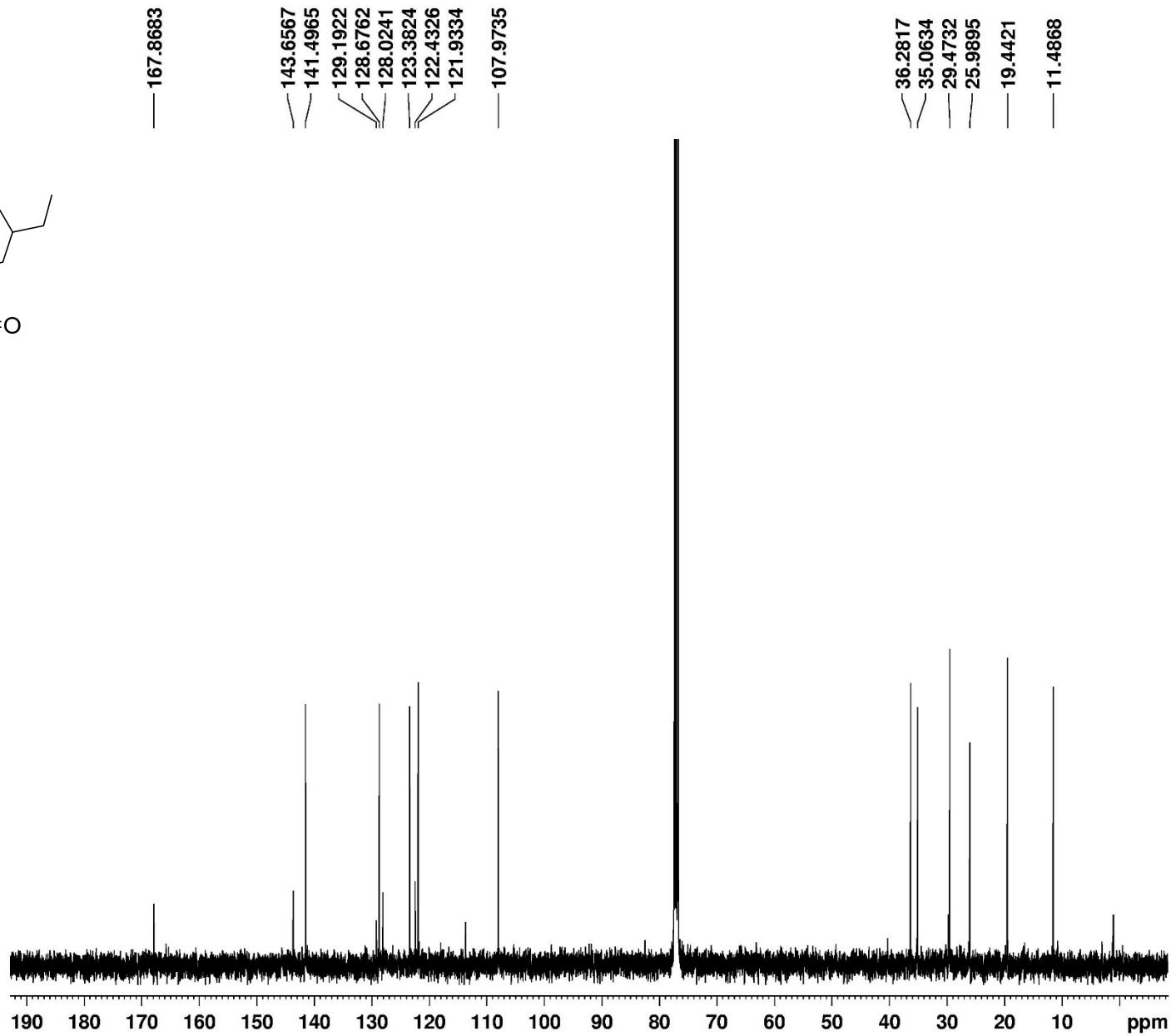
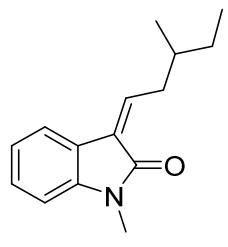
===== CHANNEL f1 =====
SFO1 125.907573 MHz
NUC1 ¹³C
P1 9.23 usec
PLW1 244.0000000 W

===== CHANNEL f2 =====
SFO2 500.6783527 MHz
NUC2 ¹³I
CPDRG[2 waltz16
FCPD2 80.00 usec
PLW2 13.60000038 W
PLW12 0.08840500 W
PLW13 0.05657900 W

F2 – Processing parameters
SI 32768
SF 125.8951680 MHz
WDW BM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹H -NMR Spectrum of 2m



SLK-77F
13C, CDCl₃

Current Data Parameters
NAME 13C
EXPNO 80
PROCNO 1

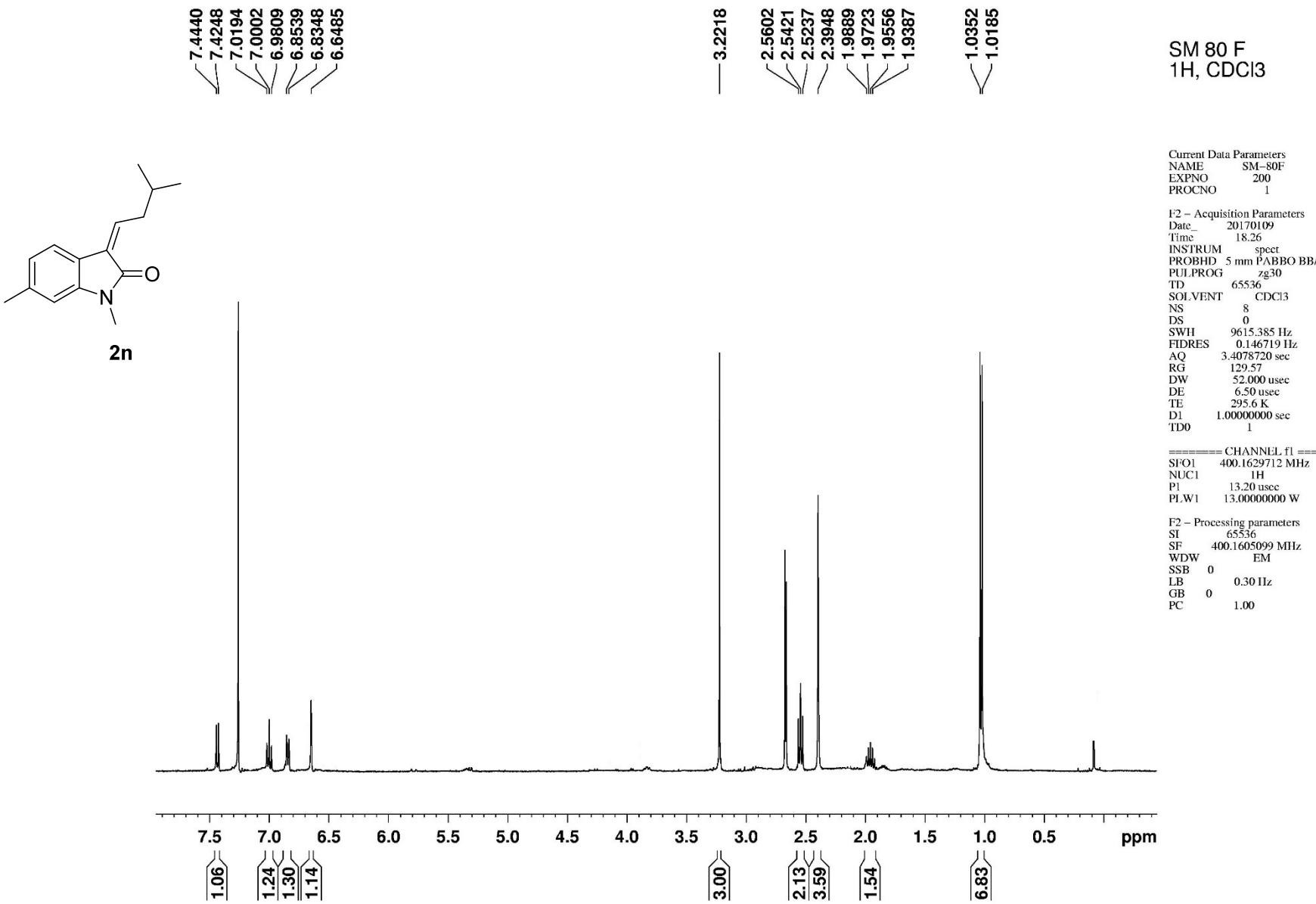
F2 – Acquisition Parameters
Date 20170110
Time 4.16
INSTRUM spect
PROBID 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 512
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 201.48
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

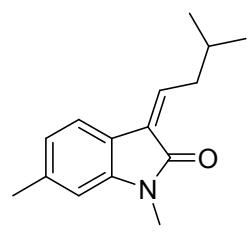
===== CHANNEL f1 =====
SFO1 100.6304993 MHz
NUC1 13C
P1 9.90 usec
PLW1 53.00000000 W

===== CHANNEL f2 =====
SFO2 400.1621006 MHz
NUC2 1H
CPDPGRG[2] waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.27963999 W
PLW13 0.22651000 W

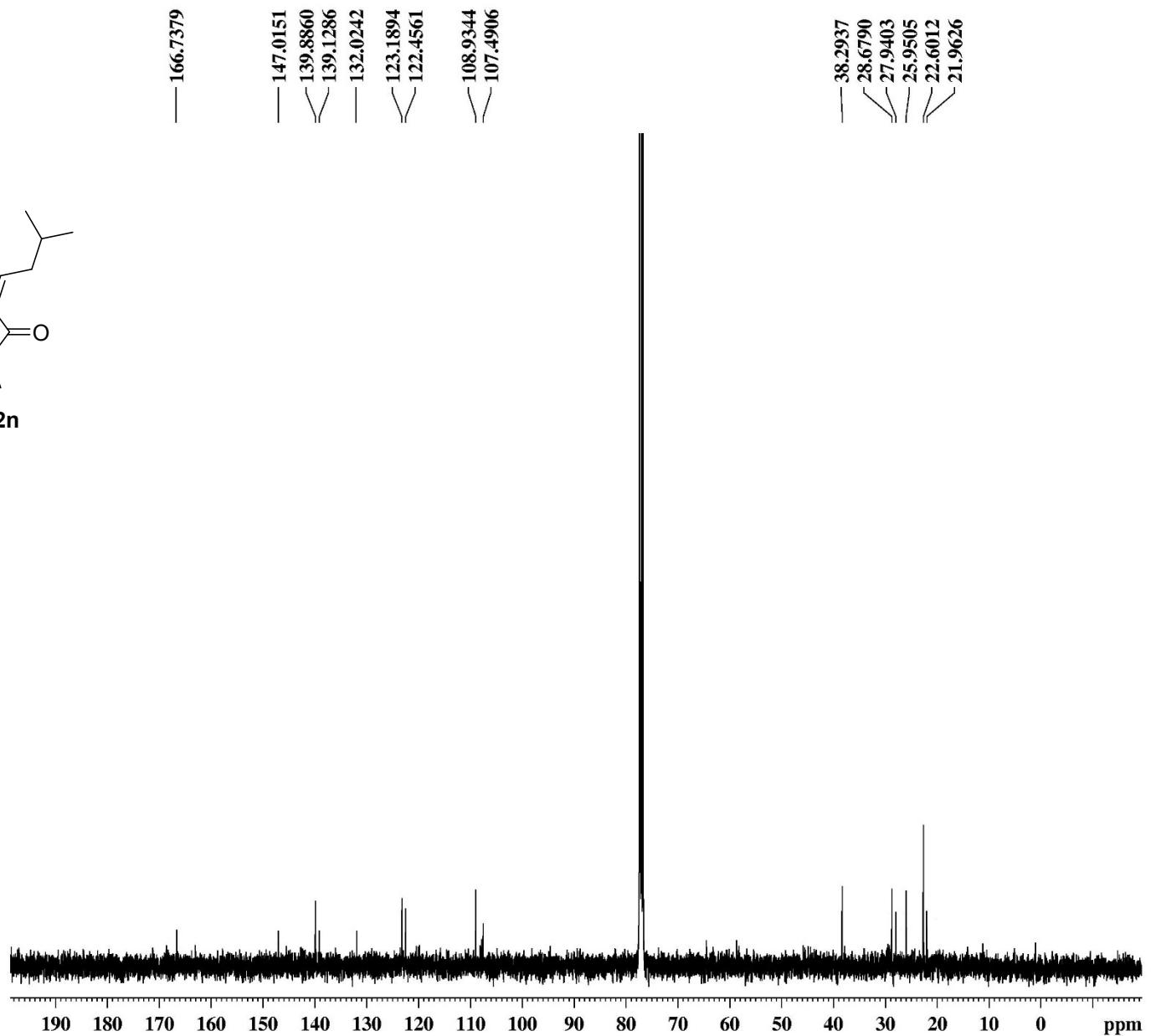
F2 – Processing parameters
SI 32768
SF 100.6204380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13C -NMR Spectrum of **2m**





2n



Current Data Parameters
NAME: SM-80F
EXPNO: 120
PROCNO: 1

F2 - Acquisition Parameters
Date: 20170110
Time: 22:35
INSTRUM: spect
PROBHD: 5 mm PABBO BB/
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 1024
DS: 0
SWH: 24038.461 Hz
FIDRES: 0.366798 Hz
AQ: 1.3631488 sec
RG: 201.48
DW: 20.800 usec
DE: 6.50 usec
TE: 300.0 K
D1: 2.0000000 sec
D11: 0.0300000 sec
TD0: 1

===== CHANNEL f1 ======
SFO1: 100.6304993 MHz
NUC1: ¹³C
P1: 9.90 usec
PLW1: 53.0000000 W

===== CHANNEL f2 ======
SFO2: 400.1621006 MHz
NUC2: ¹H
CPDPG[2]: waltz16
PCPD2: 90.00 usec
PLW2: 13.0000000 W
PLW12: 0.27963999 W
PLW13: 0.22651000 W

F2 - Processing parameters
SI: 32768
SF: 100.6204380 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

¹³C -NMR Spectrum of **2n**