

Supplementary materials for

Discovery of Novel diphenyl acrylonitrile derivatives that Promote Adult Rats' Hippocampal Neurogenesis

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100081, China

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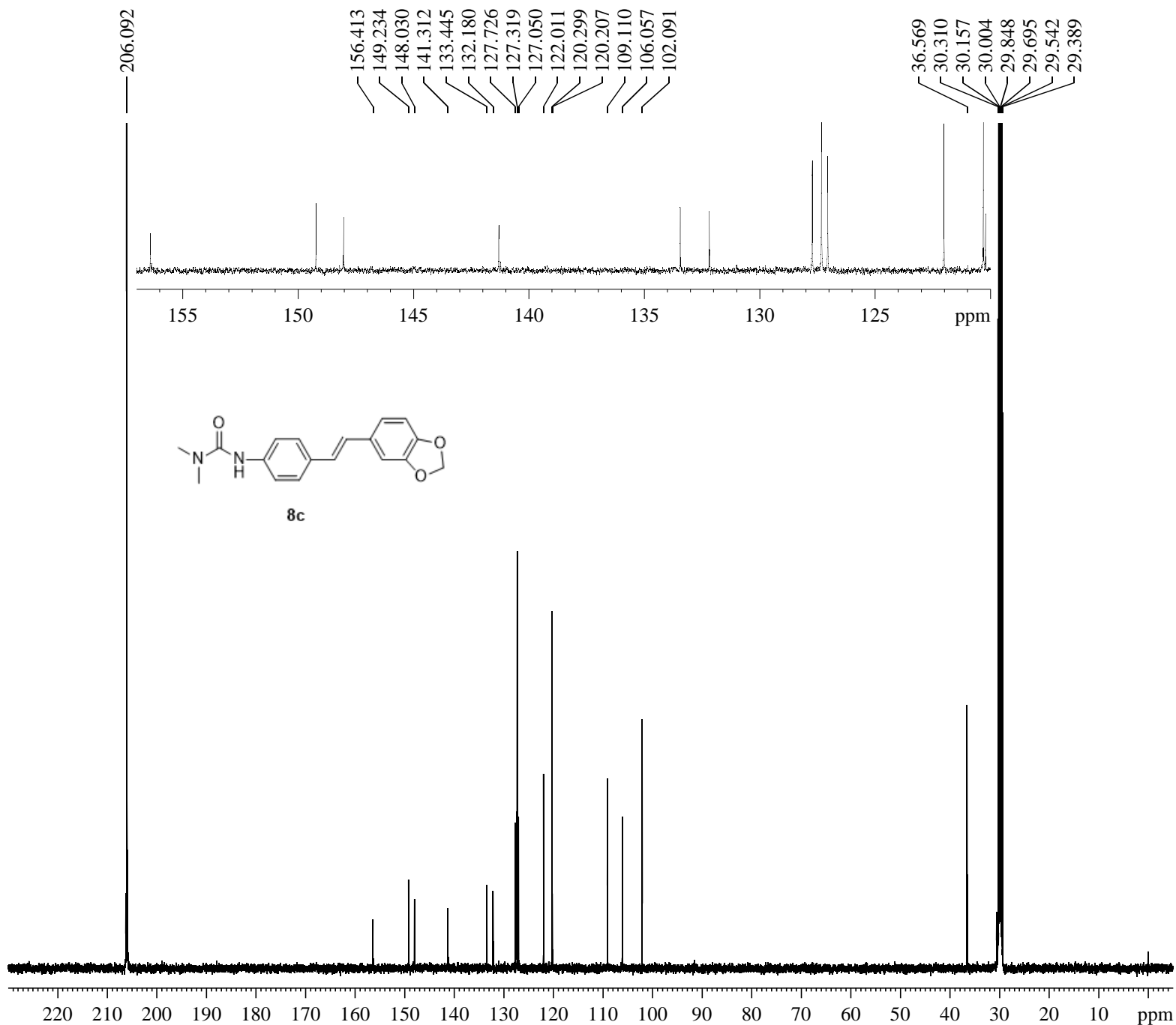
* Correspondence: hqing@bit.edu.cn(H.Q.); ljhbit@bit.edu.cn(J.-H.L.)

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Table S1. NMR spectra checklist for the target compounds.

Compounds	¹ H NMR	¹³ C NMR	HRMS
8c	√	√	√
8d	√	√	√
8e	√	√	√
8g	√	√	√
8h	√	√	√
8j	√	√	√
8k	√	√	√
8l	√	√	√
9b	√	√	√
12f	√	√	√
18b	√	√	√
23b	√	√	√
23i	√	√	√
24b	√	√	√
29a	√	√	√
29b	√	√	√
32a	√	√	√
32b	√	√	√
36a	√	√	√
39b	√	√	√
42b	√	√	√



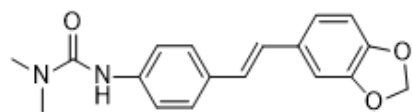
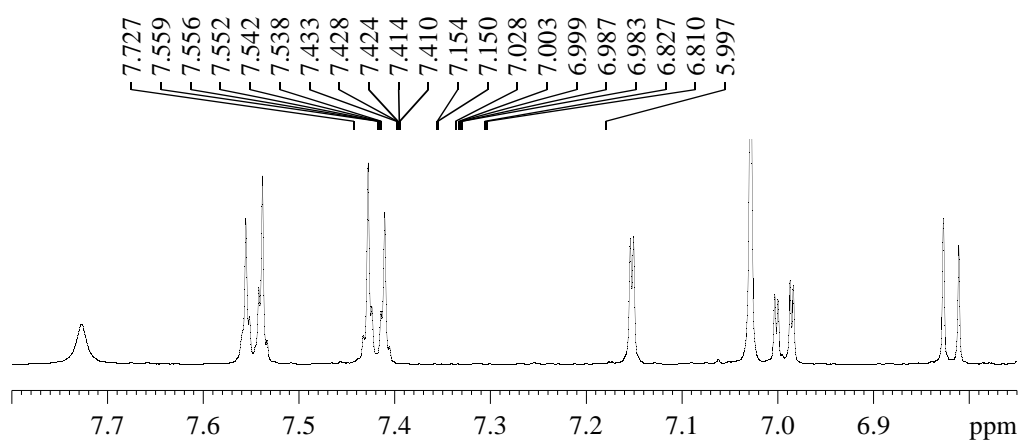
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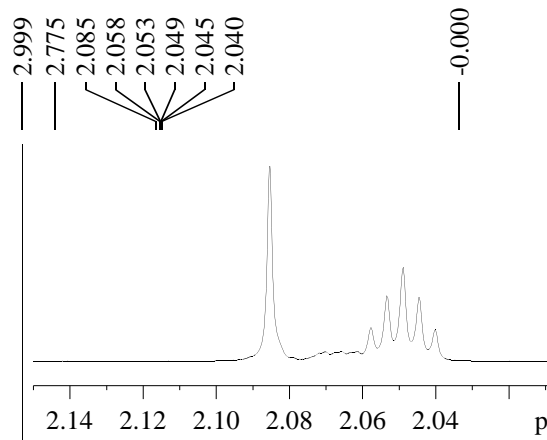
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8c

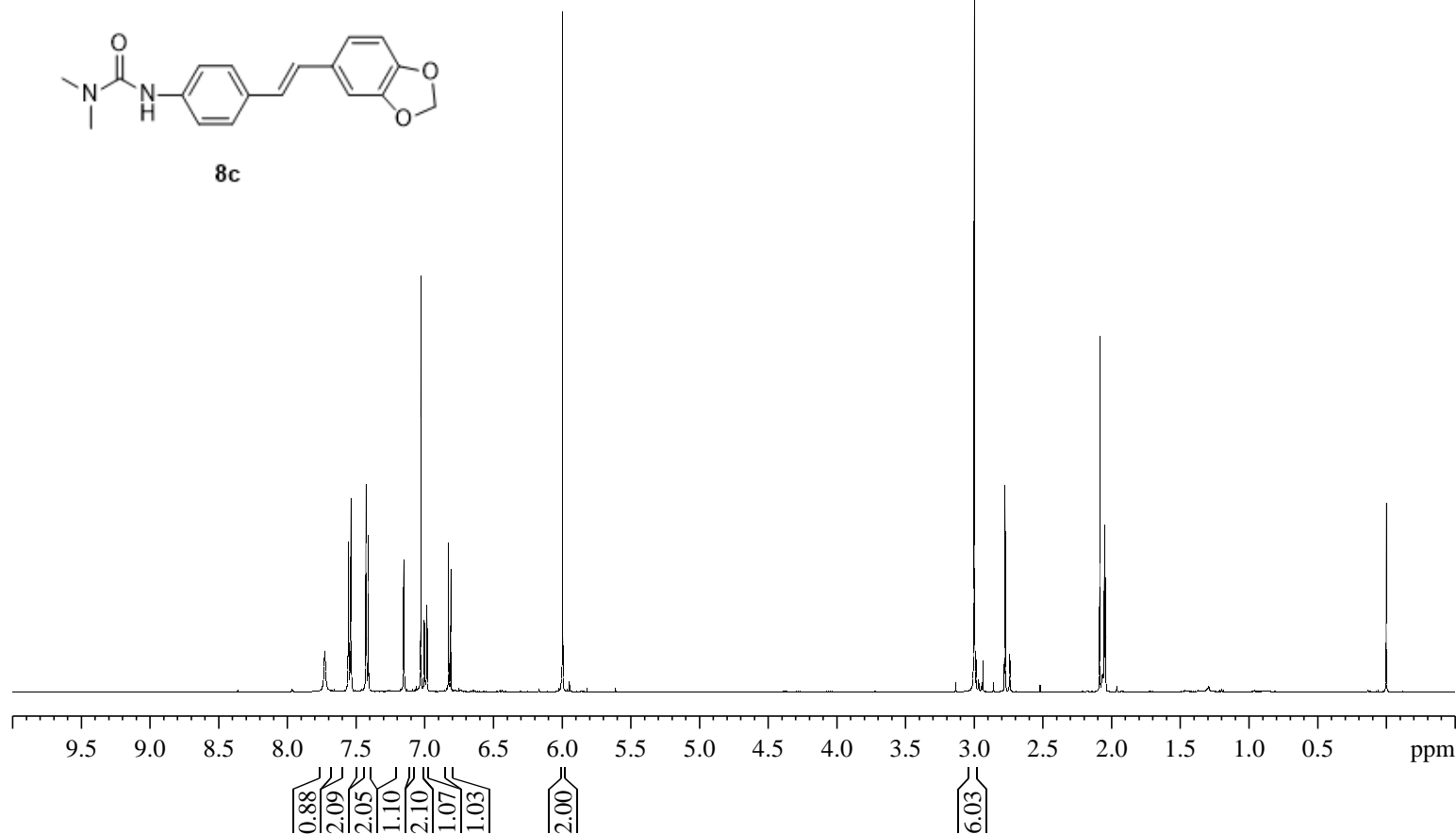


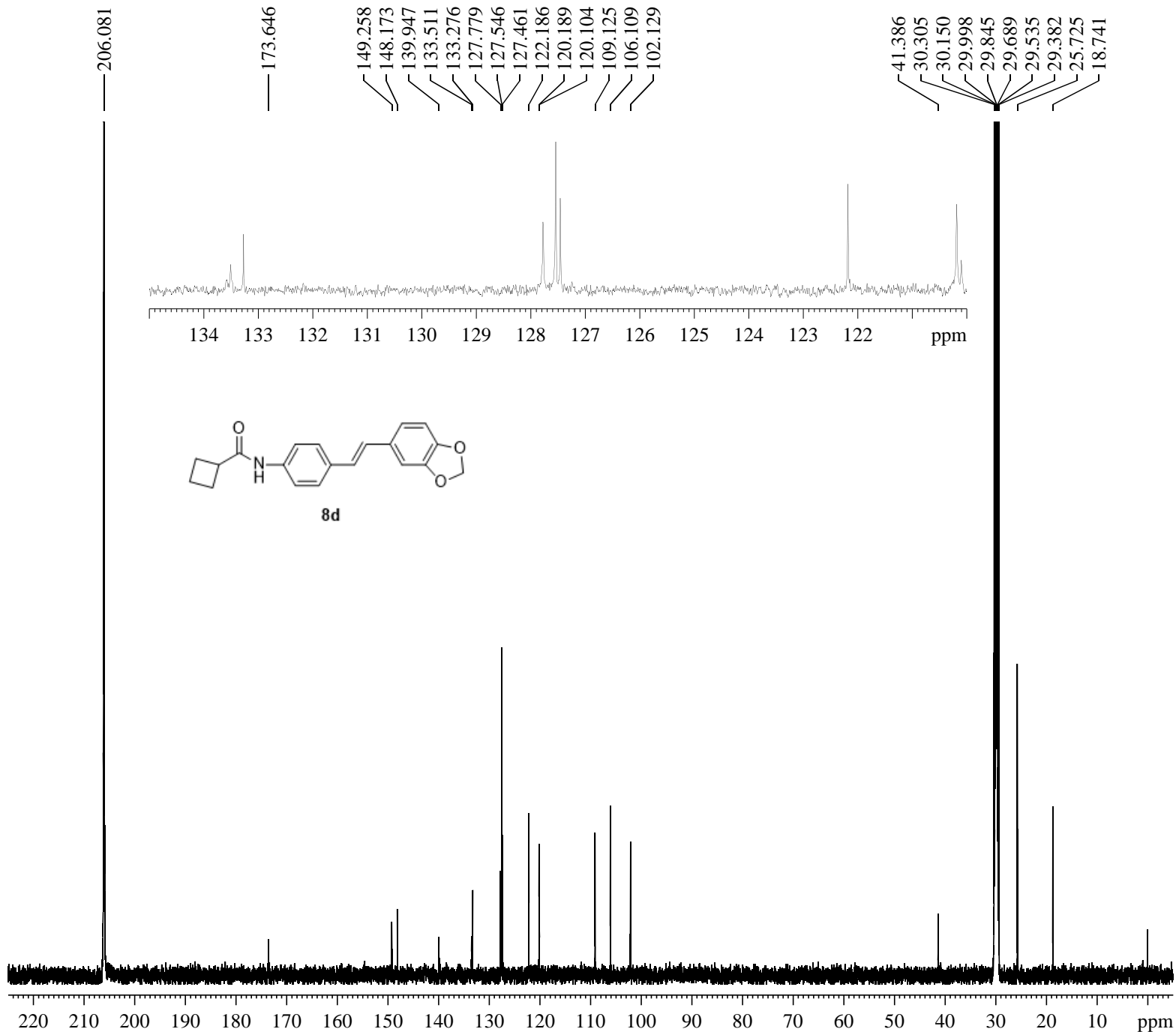
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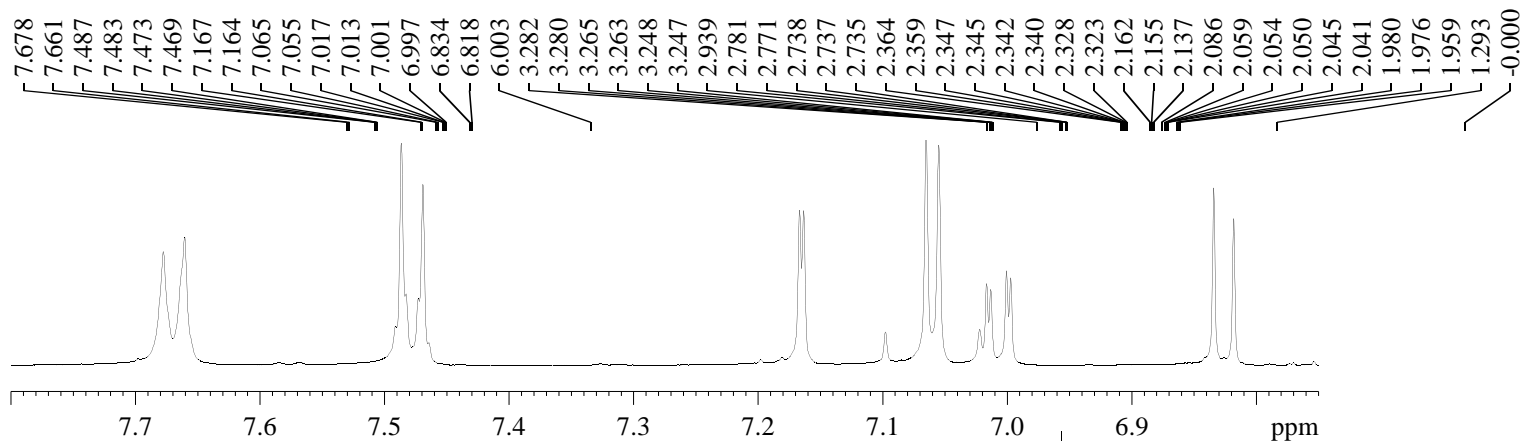
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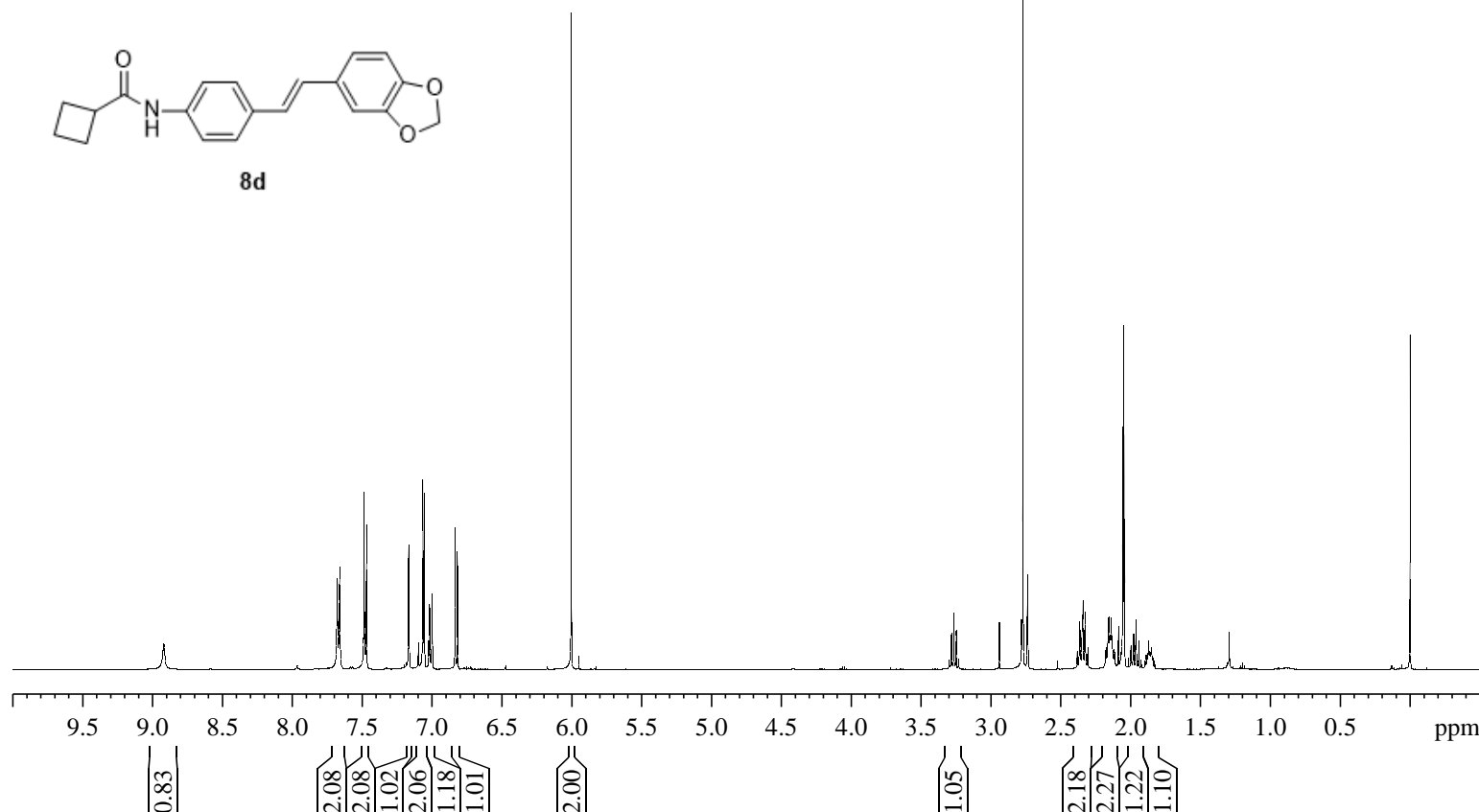
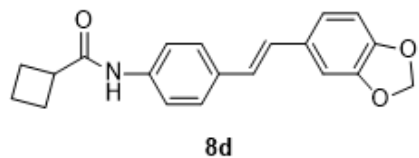


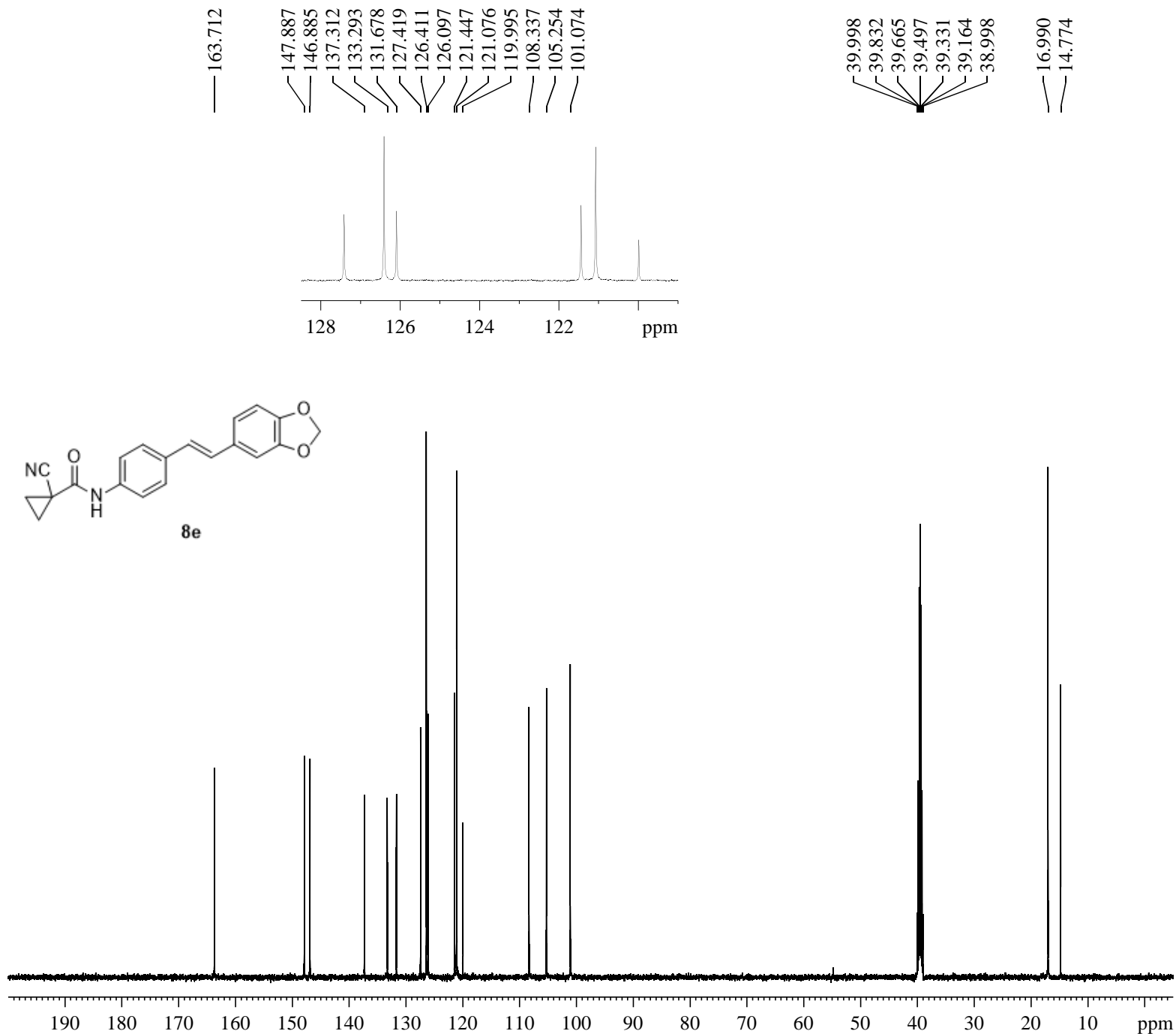
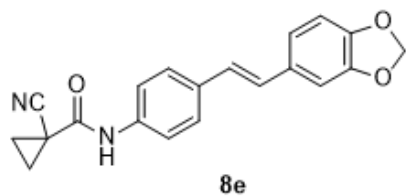
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 P1 11.26 usec
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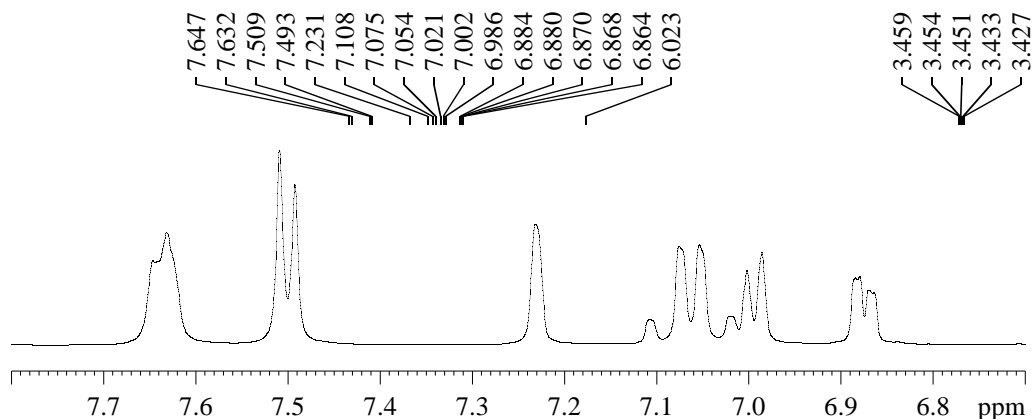
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 TD0 1

===== CHANNEL f1 =====
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 NUC1 13C
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===== CHANNEL f2 =====
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 NUC2 1H
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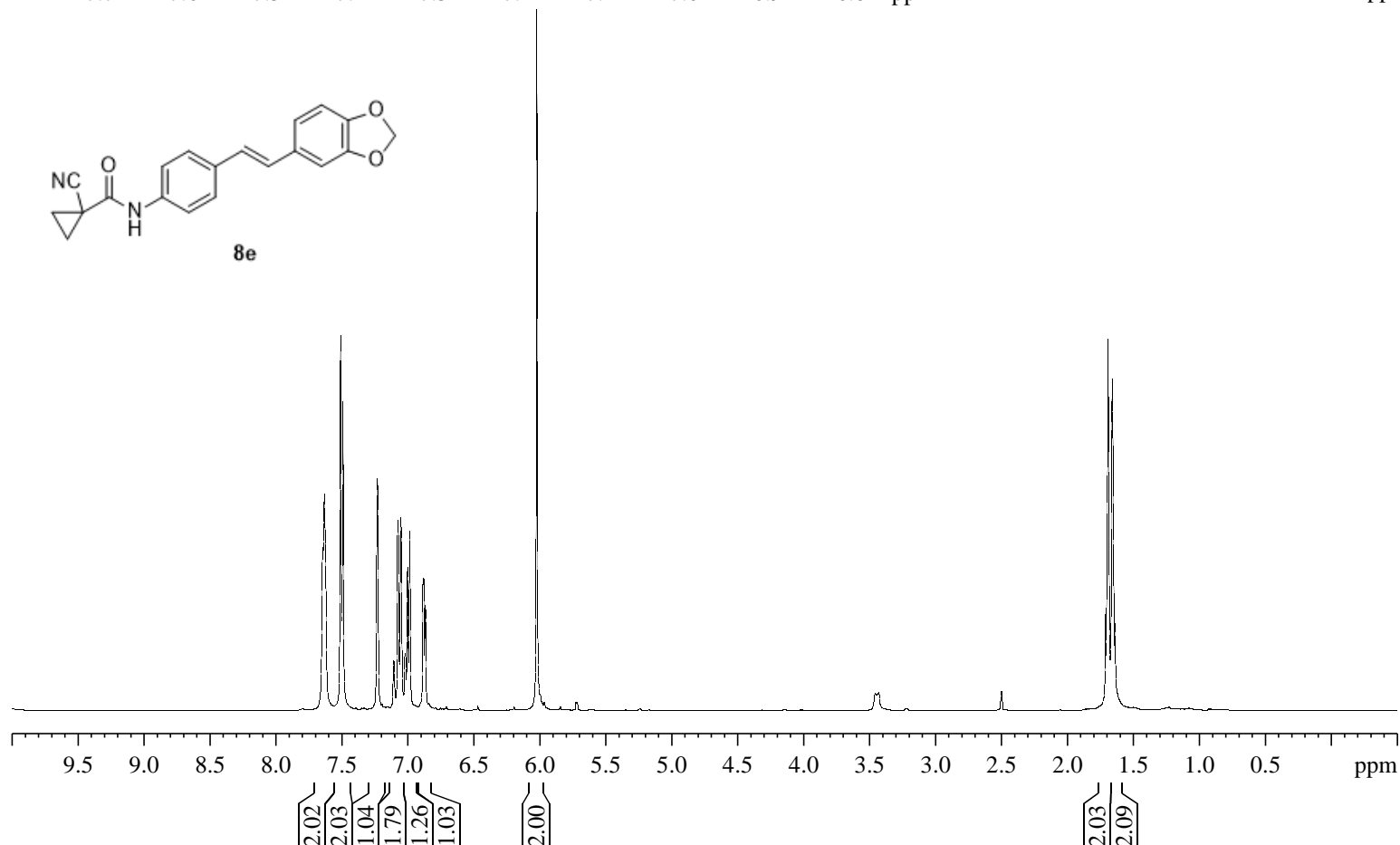
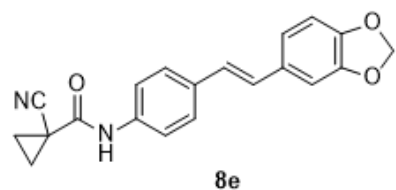


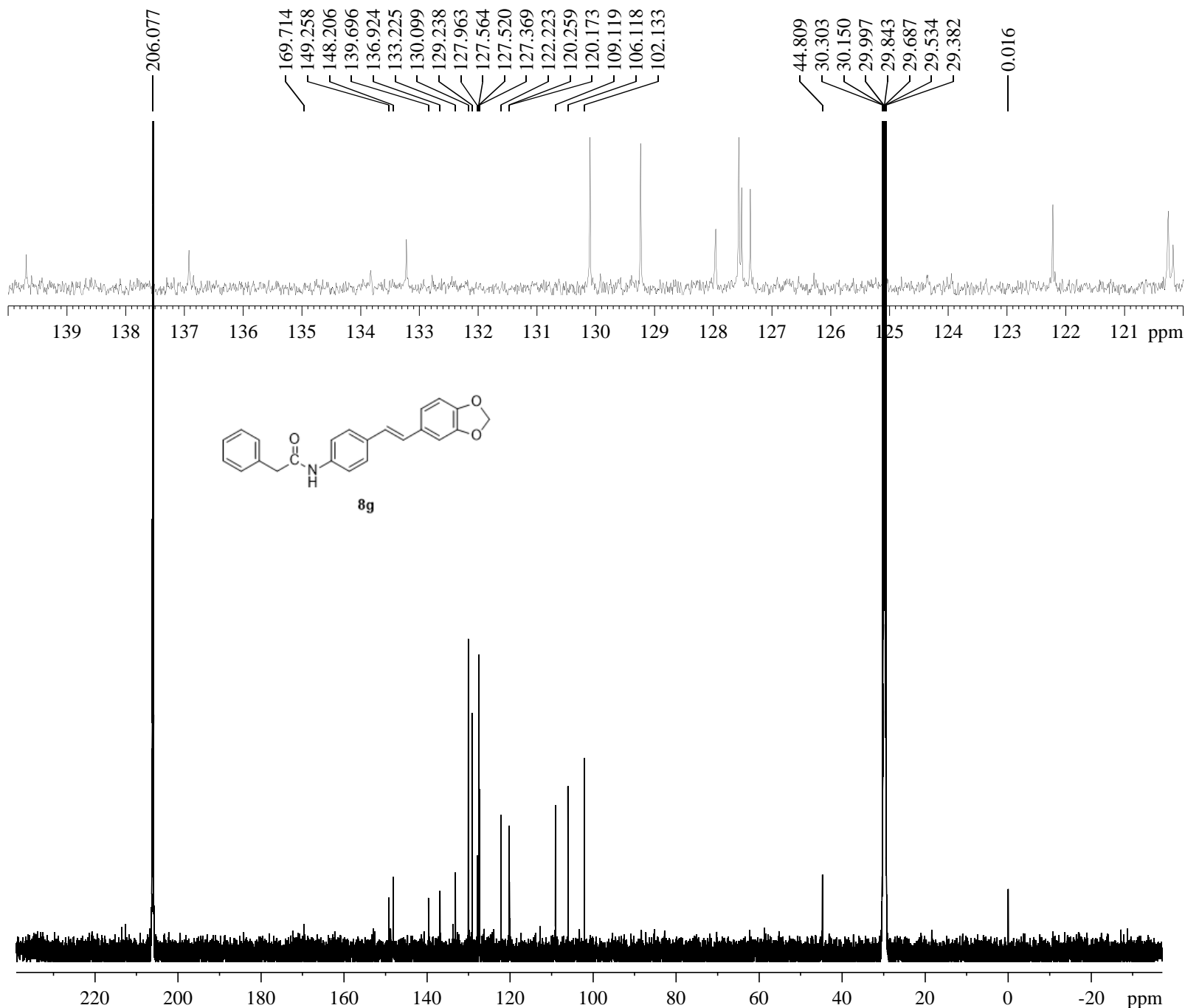
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 AQ 3.2767999 sec
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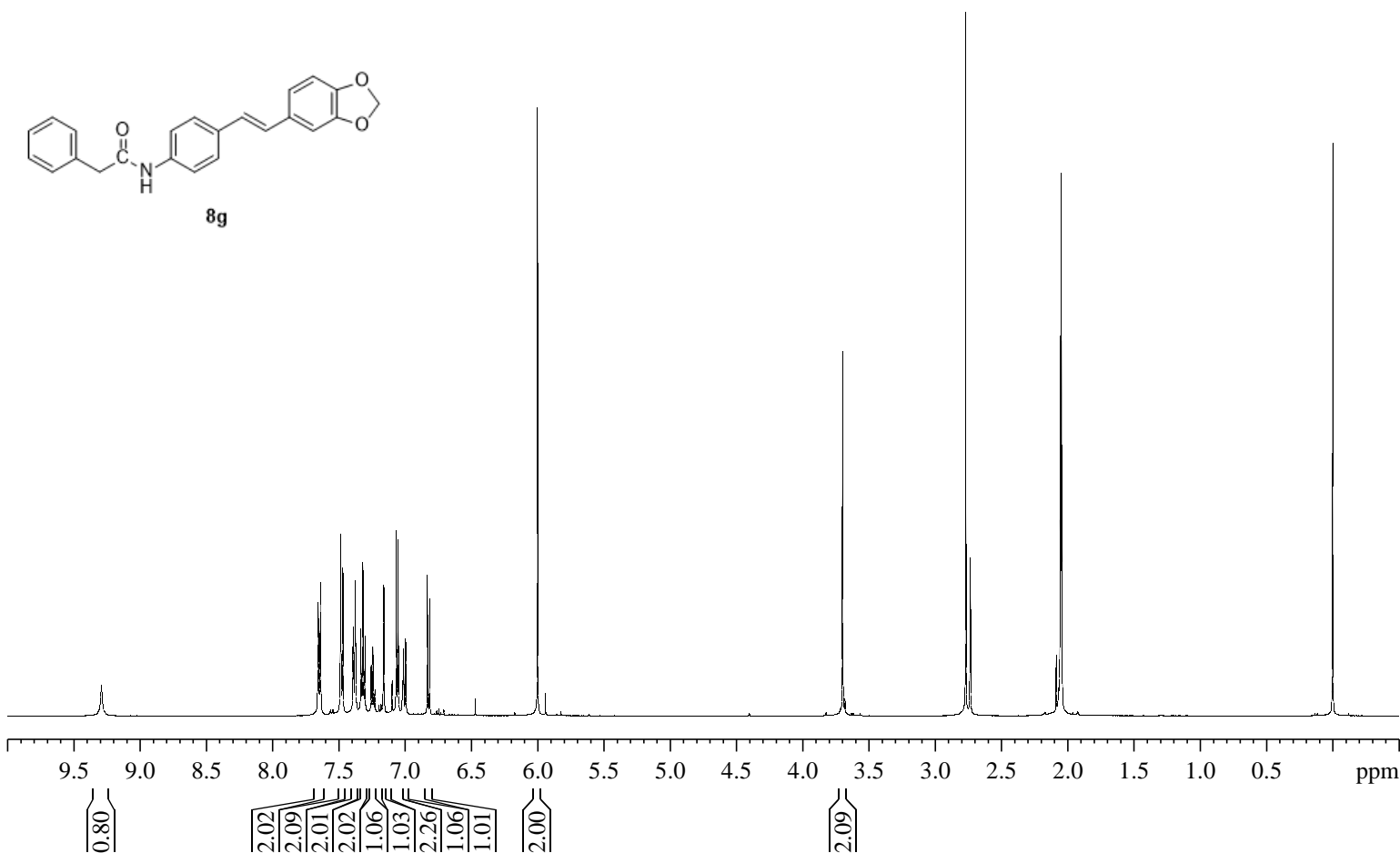
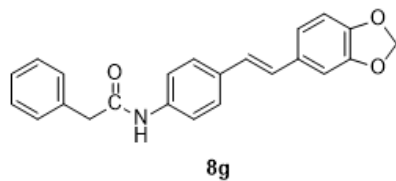
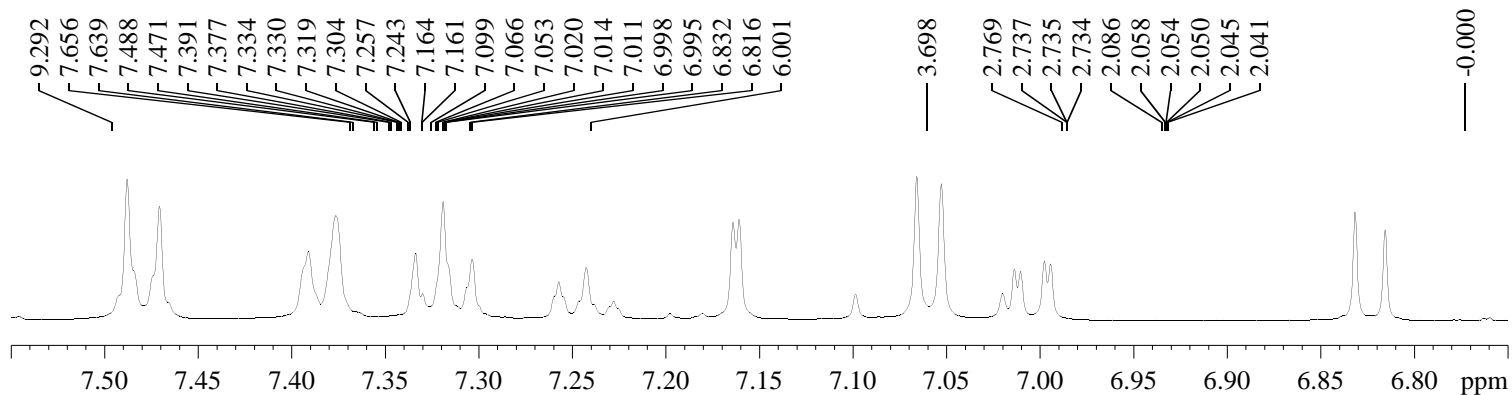
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 D11 0.03000000 sec
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===== CHANNEL f1 =====
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 NUC1 13C
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 PLW1 125.88999939 W

===== CHANNEL f2 =====
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 NUC2 1H
 CPDPRG[2] waltz16
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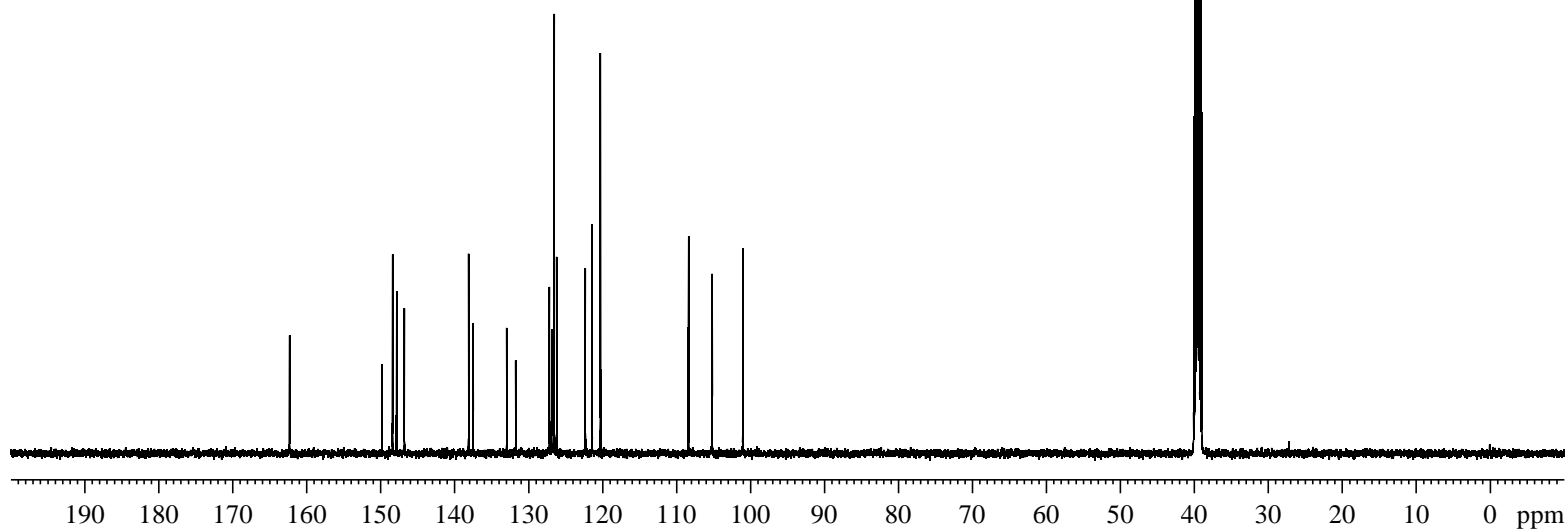
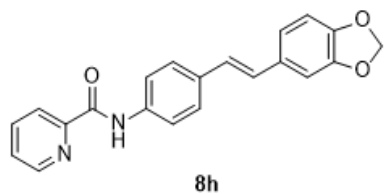
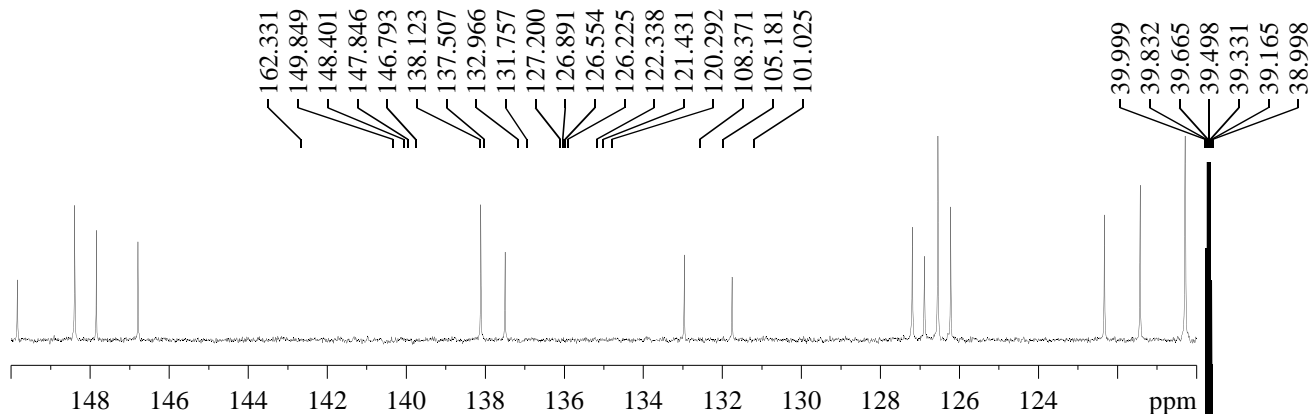


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 RG 198.55
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 DE 6.50 usec
 TE 303.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
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 NUC1 1H
 P1 11.26 usec
 PLW1 19.95299911 W

F2 - Processing parameters
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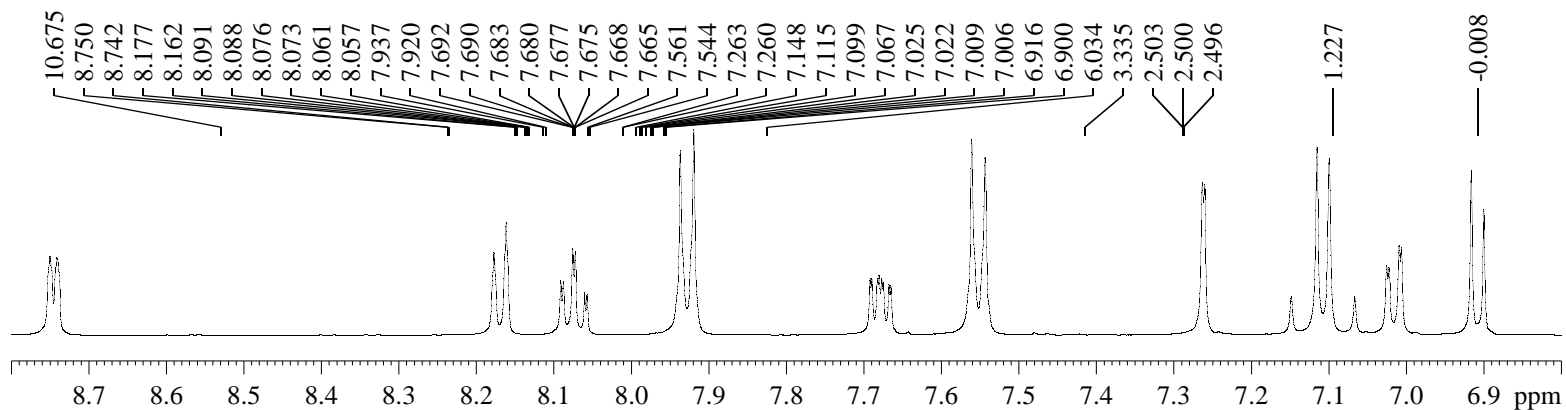
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 SOLVENT DMSO
 NS 1024
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 FIDRES 0.529819 Hz
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 RG 198.55
 DW 14.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

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 NUC1 13C
 P1 8.99 usec
 PLW1 125.88999939 W

===== CHANNEL f2 =====
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 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.39528000 W
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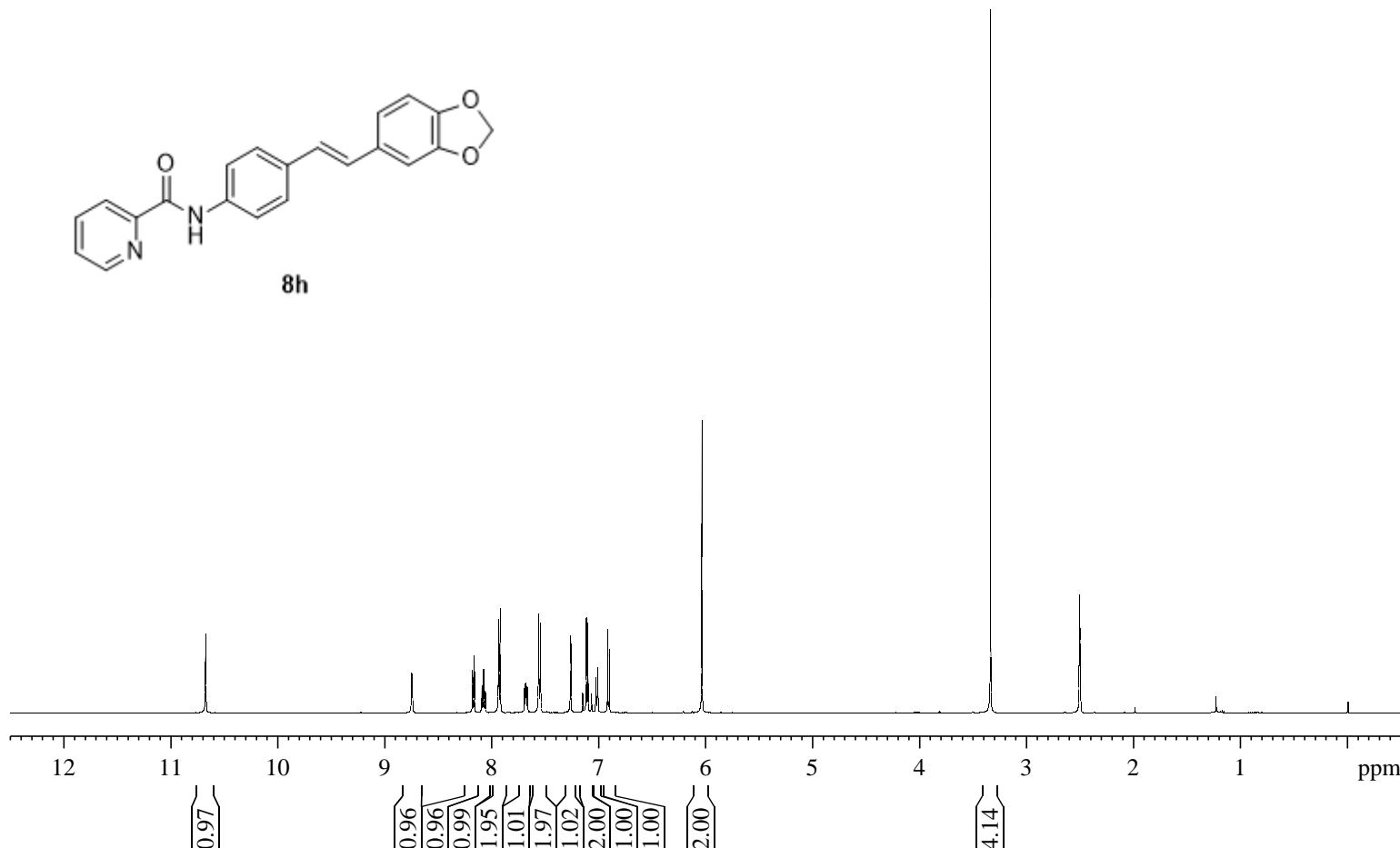
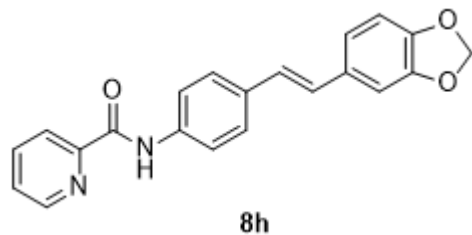


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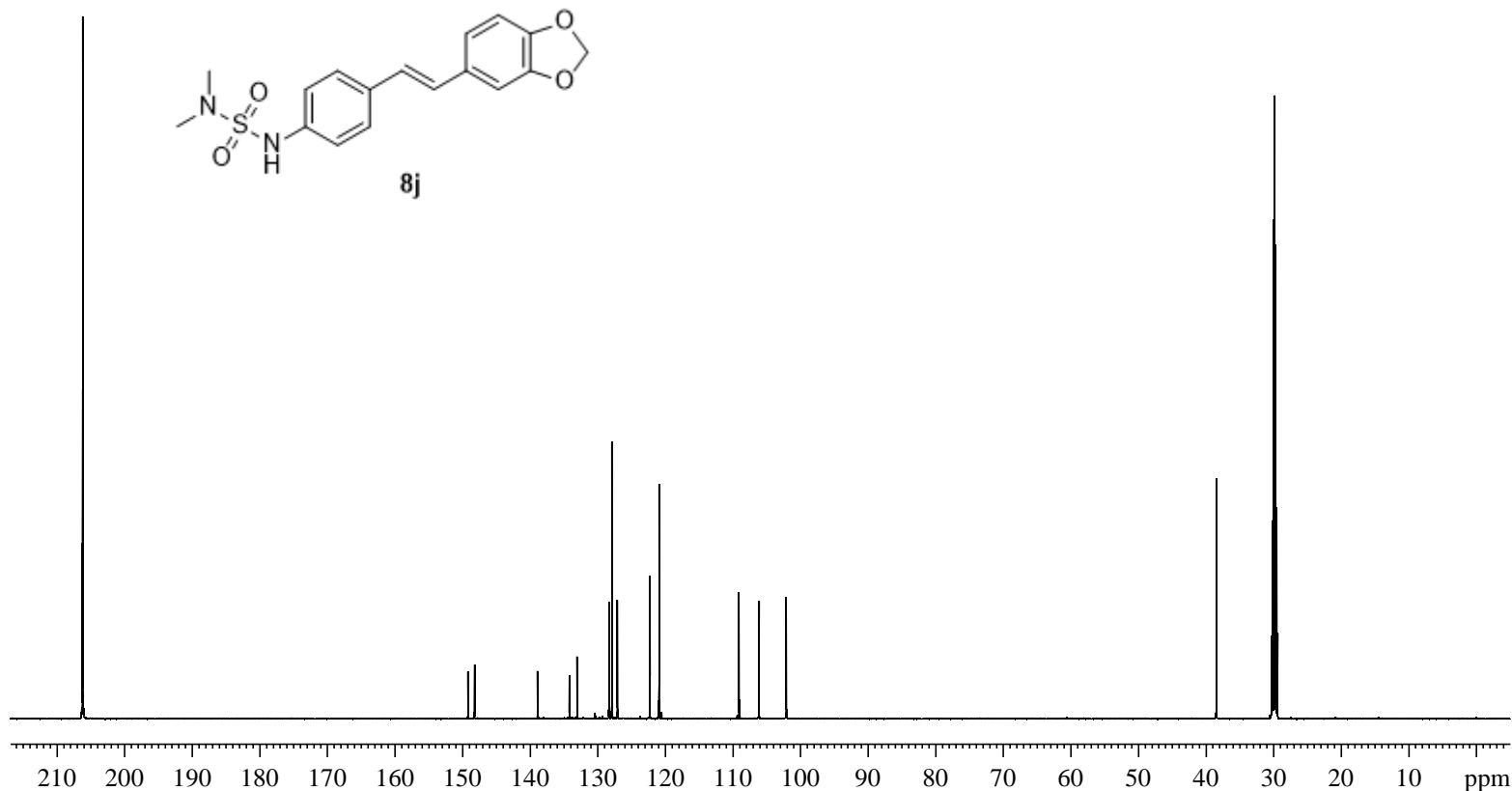
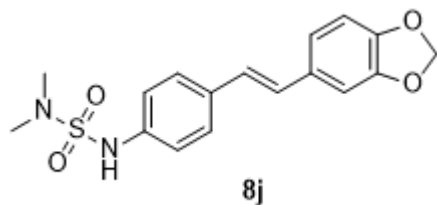
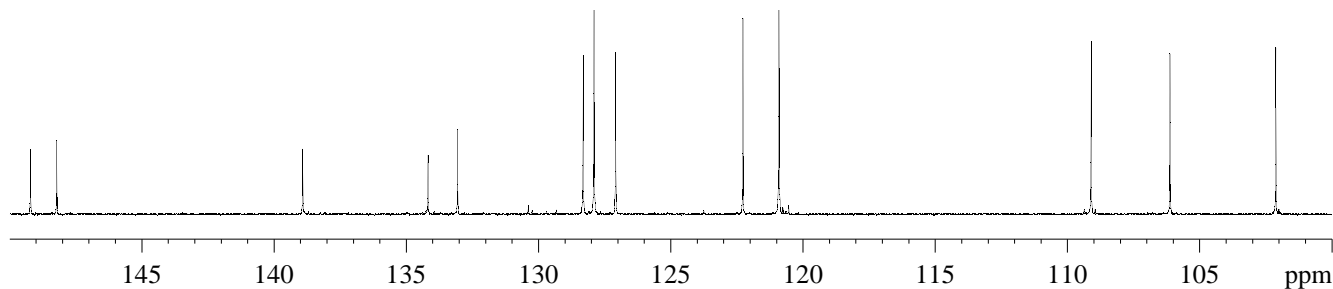
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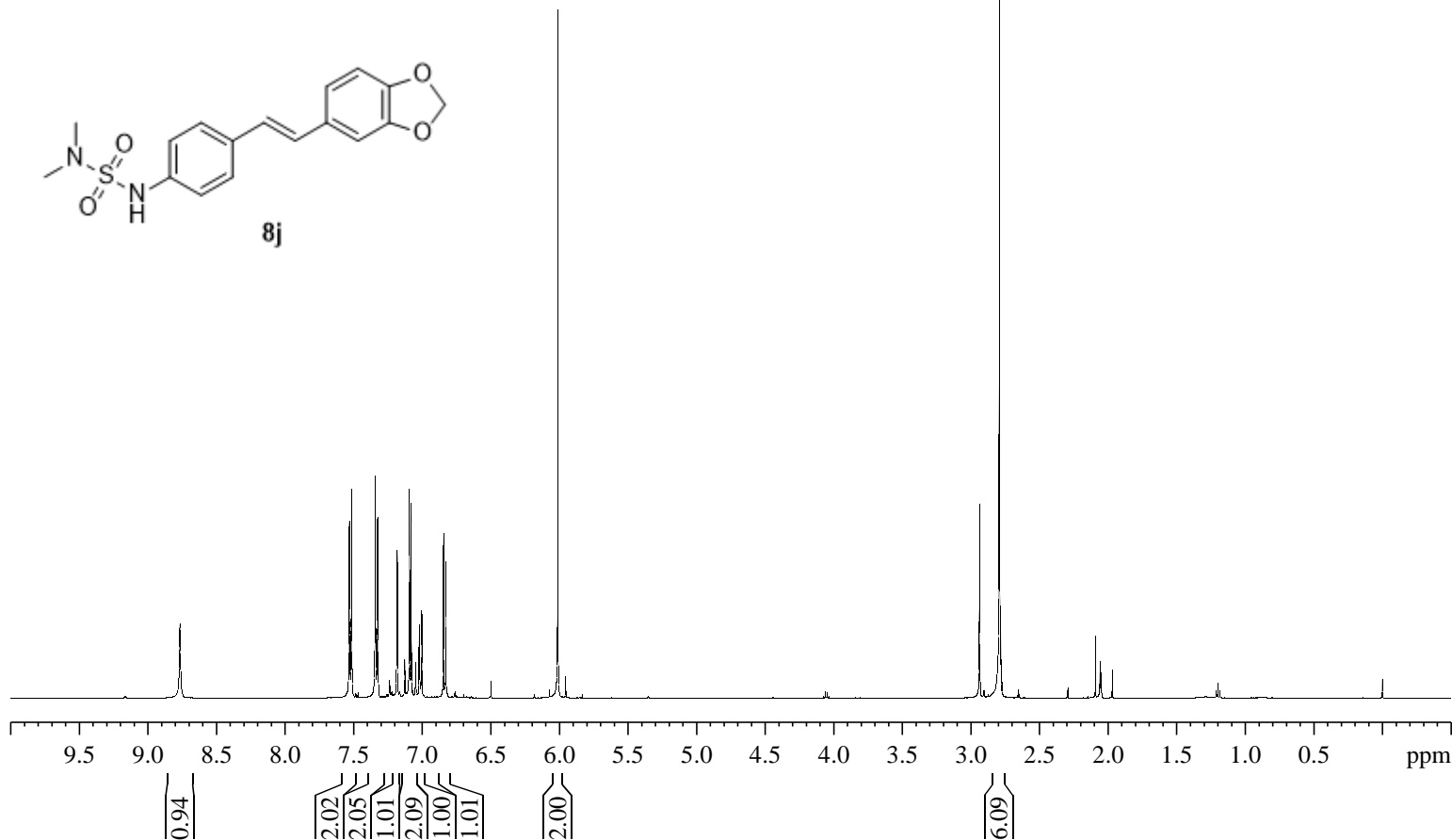
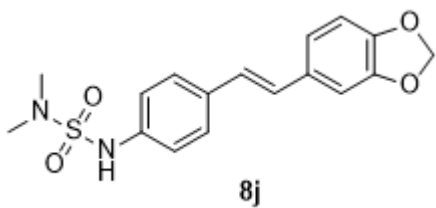
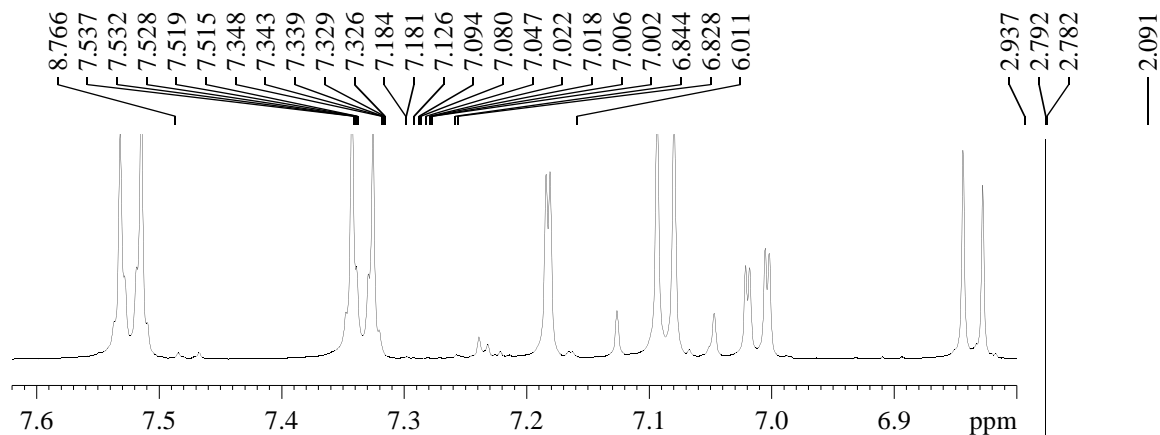
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RG 198.55
DW 14.400 usec
DE 6.50 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 8.99 usec
PLW1 125.88999939 W

===== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 19.95299911 W
PLW12 0.39528000 W
PLW13 0.25297999 W

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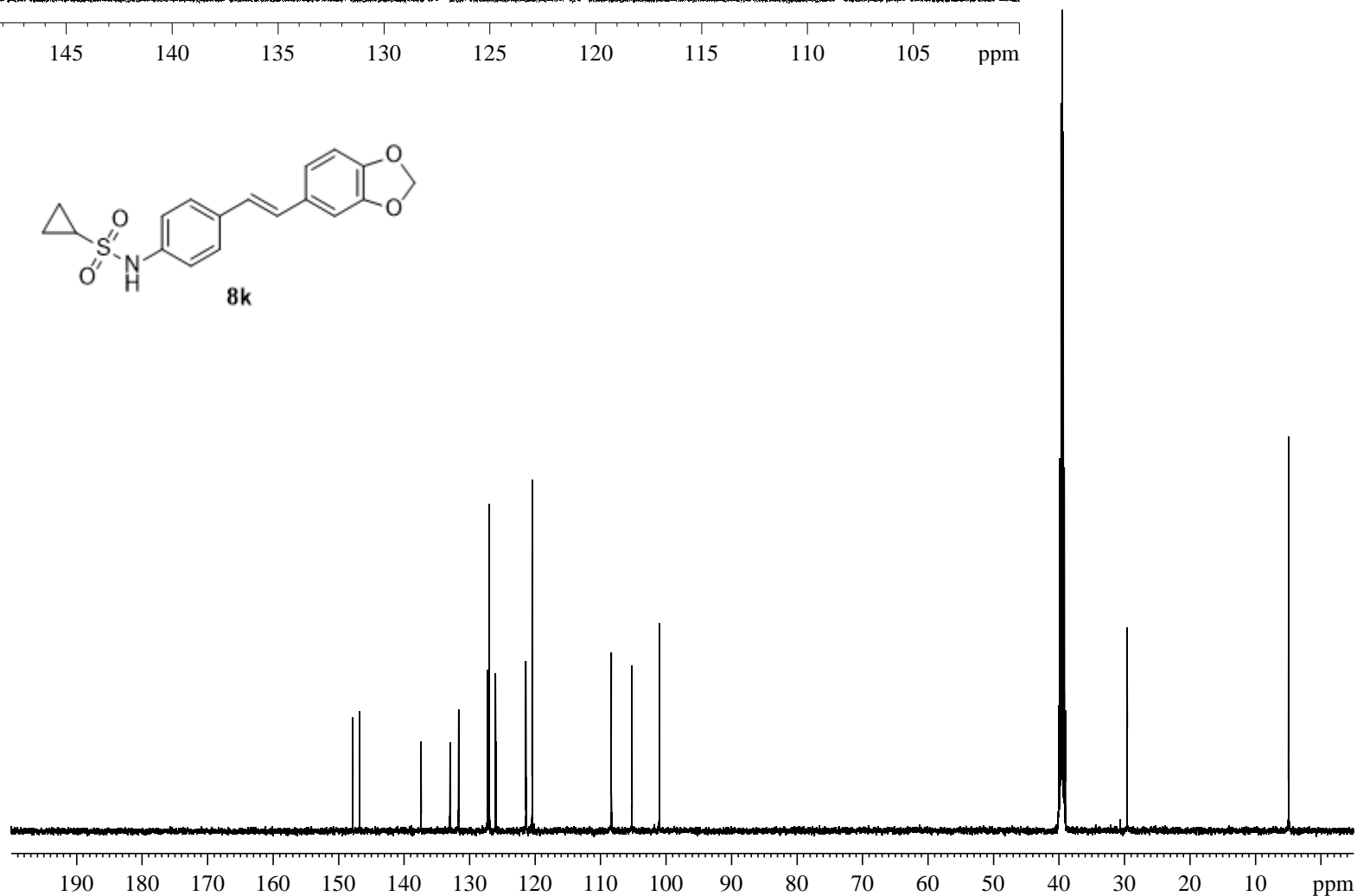
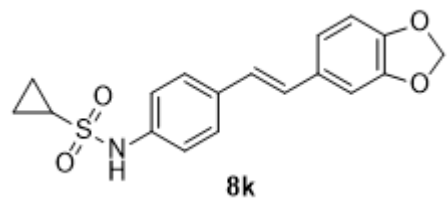
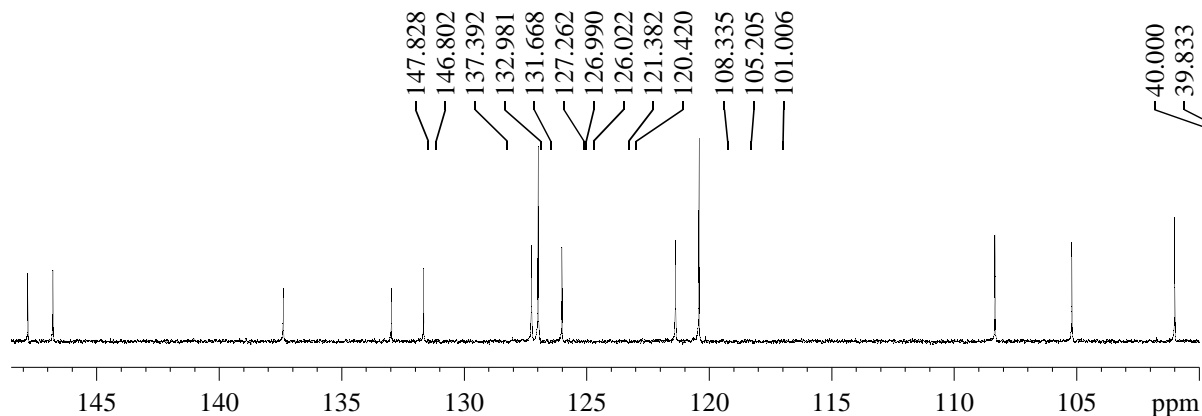


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 NUC1 1H
 P1 11.26 usec
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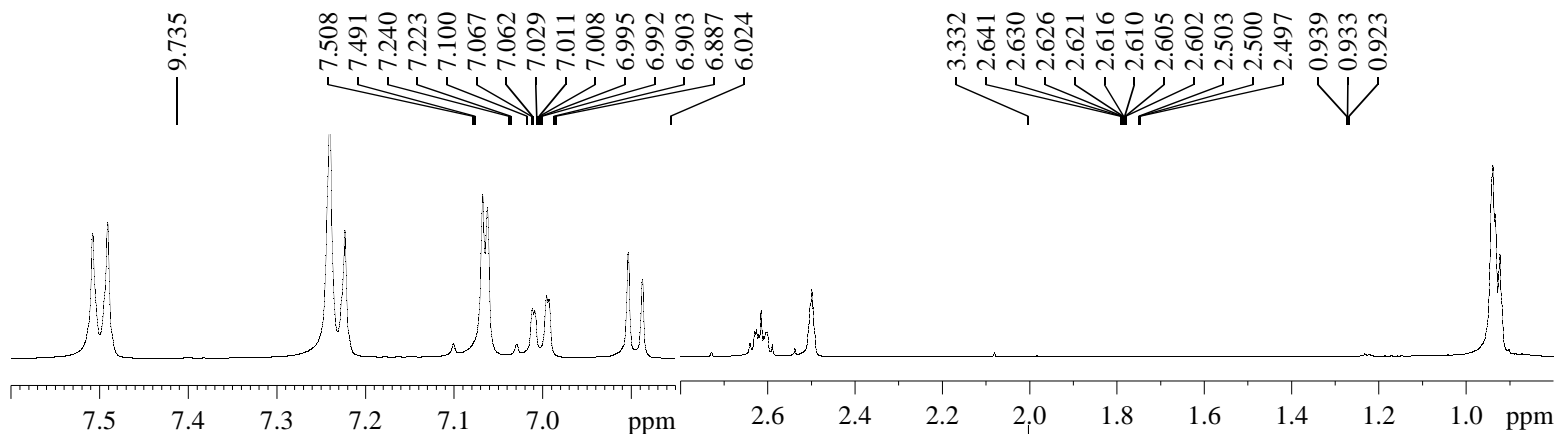
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RG 198.55
DW 14.400 usec
DE 6.50 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 8.99 usec
PLW1 125.88999939 W

===== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 19.95299911 W
PLW12 0.39528000 W
PLW13 0.25297999 W

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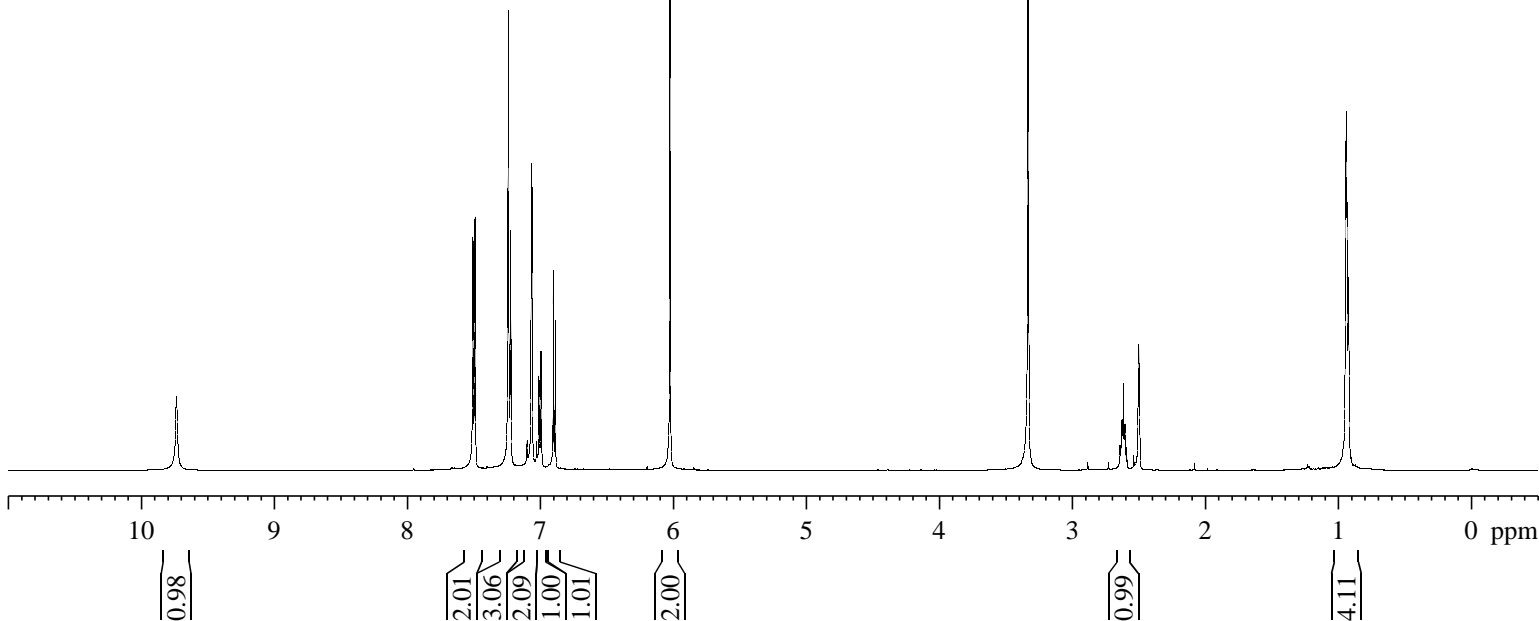
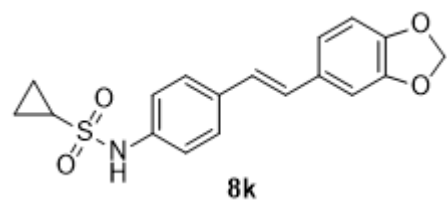


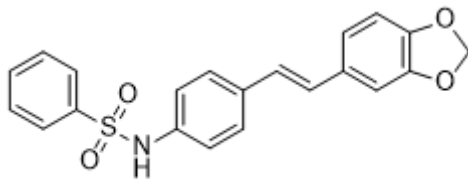
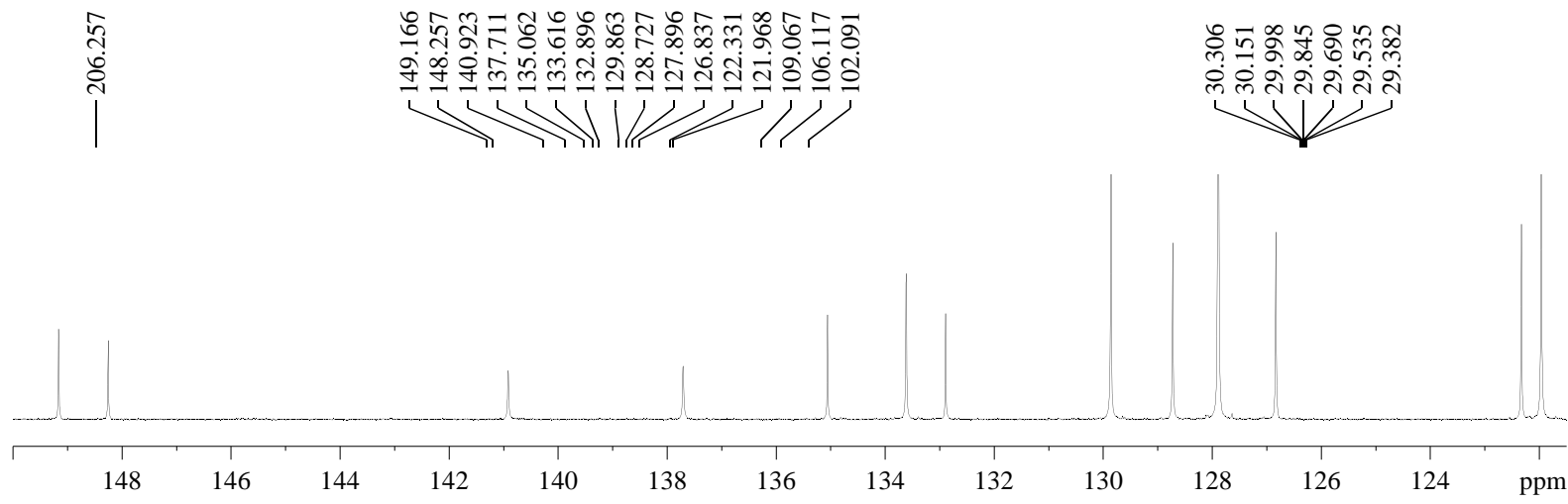
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 TD0 1

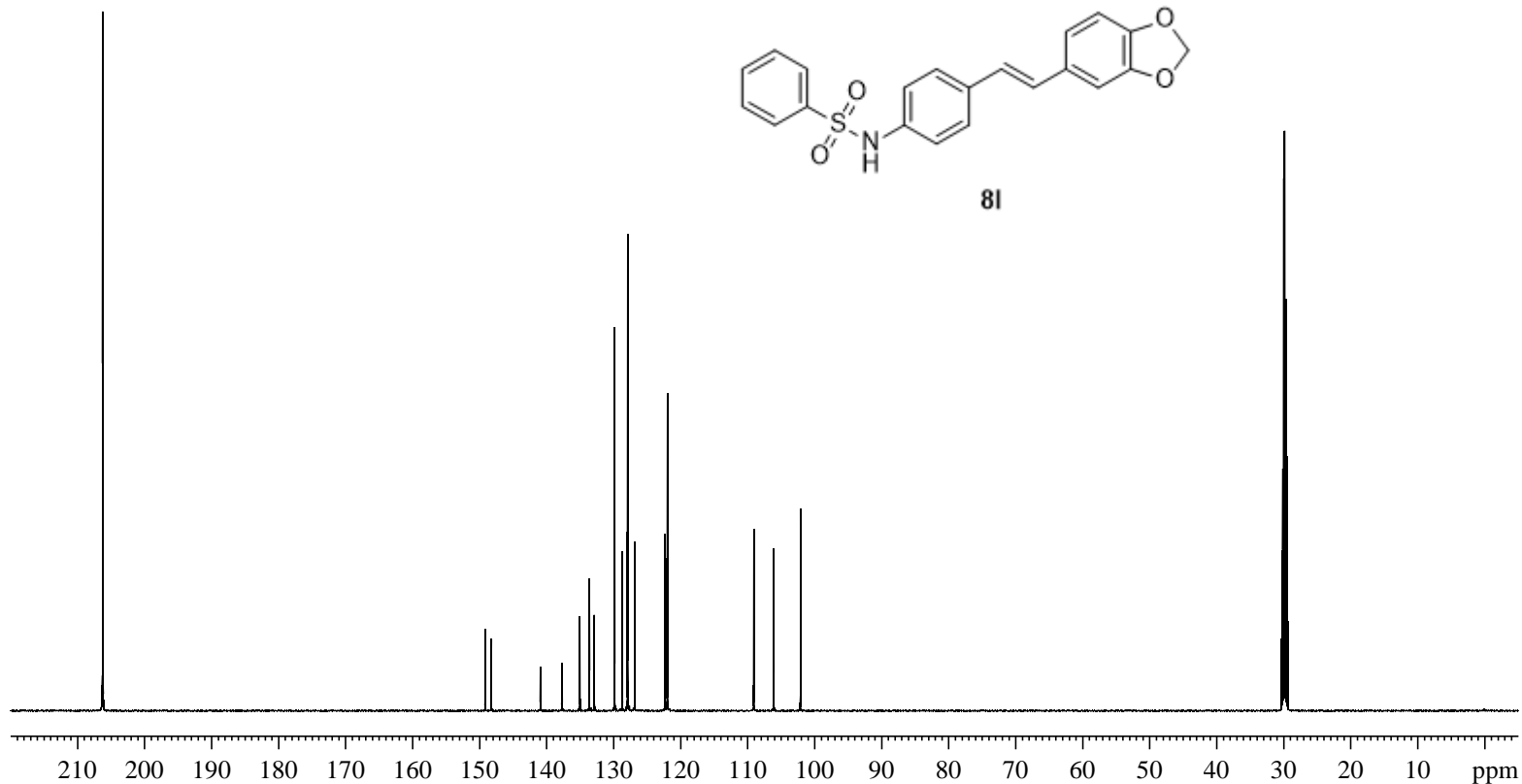
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 LB 0.30 Hz
 GB 0
 PC 1.00





8l



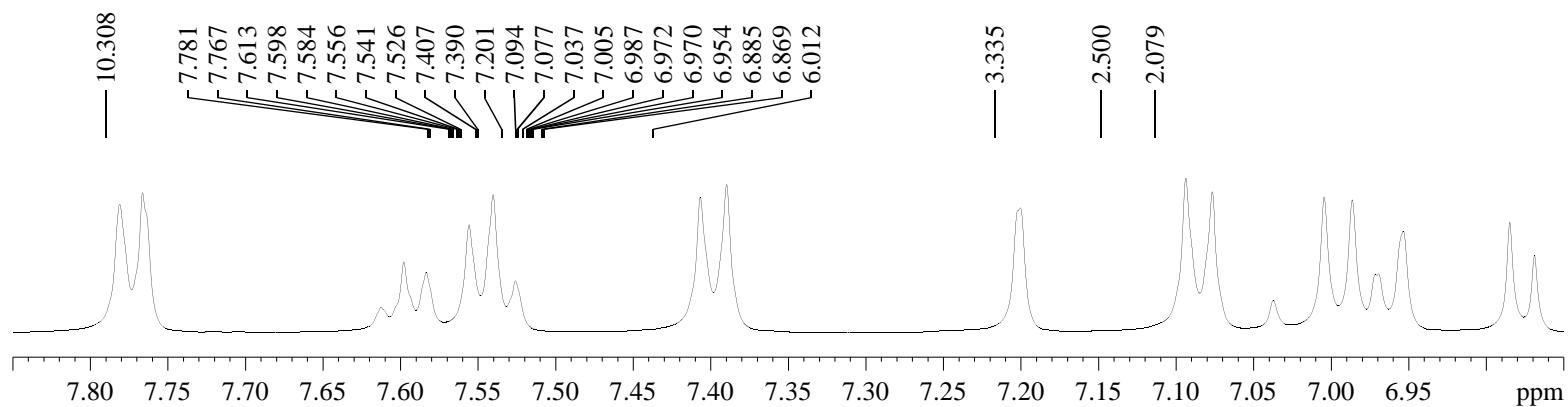
Current Data Parameters
 NAME NMR15110068-Iss-12
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20151110
 Time 1.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1200
 DS 4
 SWH 34722.223 Hz
 FIDRES 0.529819 Hz
 AQ 0.9437184 sec
 RG 198.55
 DW 14.400 usec
 DE 6.50 usec
 TE 303.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.99 usec
 PLW1 125.88999939 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.39528000 W
 PLW13 0.25297999 W

F2 - Processing parameters
 SI 32768
 SF 125.7576824 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

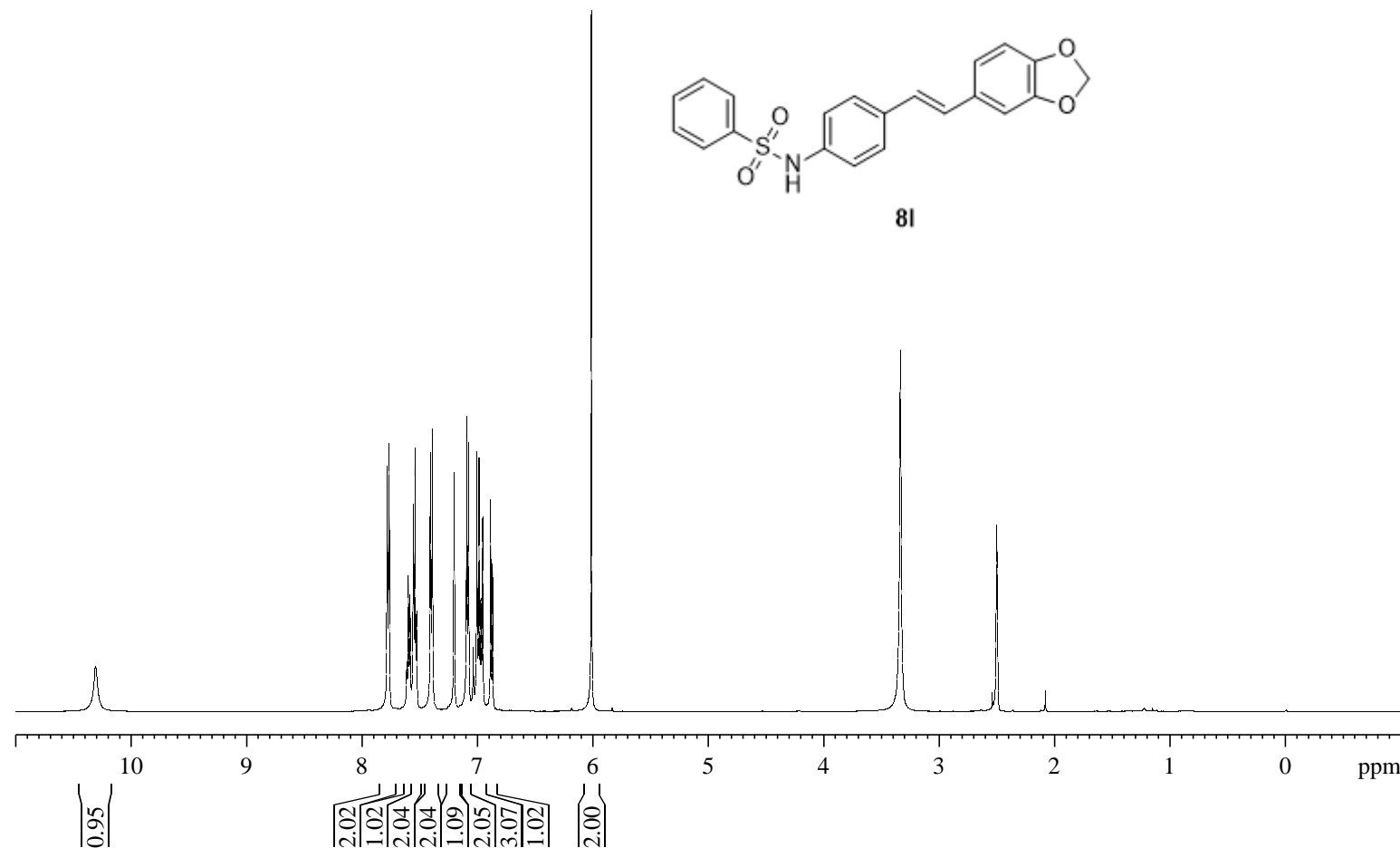


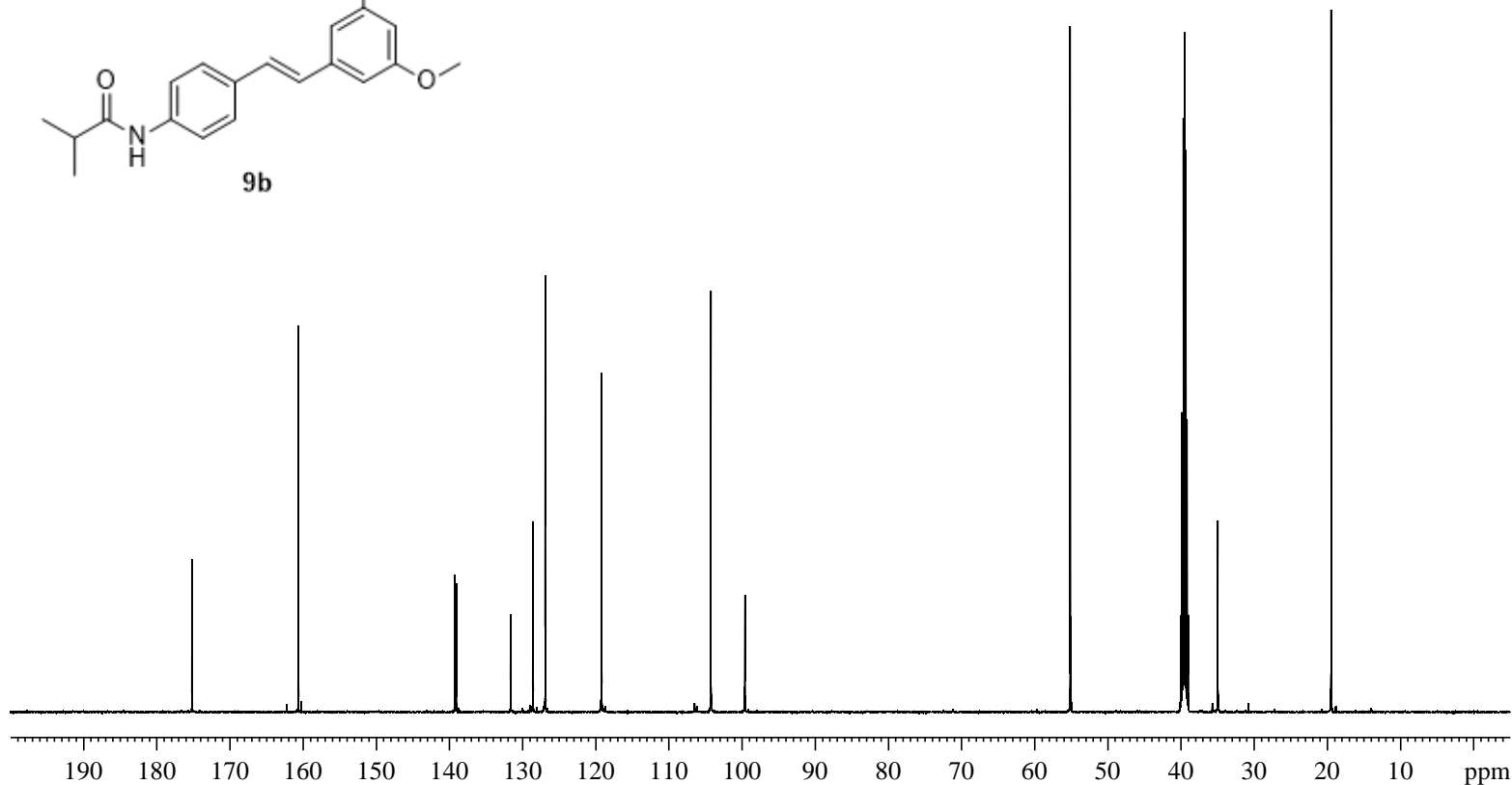
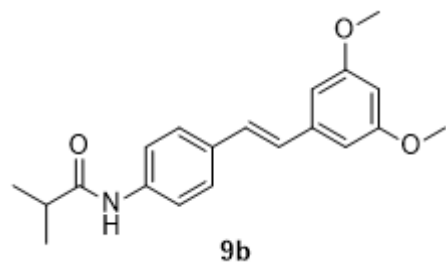
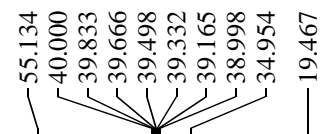
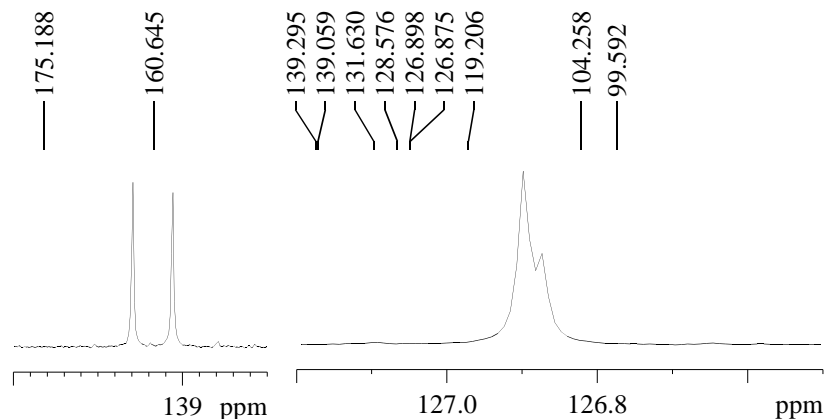
Current Data Parameters
 NAME NMR15110068-lss-12
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20151116
 Time 10.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 90.46
 DW 50.000 usec
 DE 6.50 usec
 TE 303.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.26 usec
 PLW1 19.95299911 W

F2 - Processing parameters
 SI 65536
 SF 500.1300047 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00





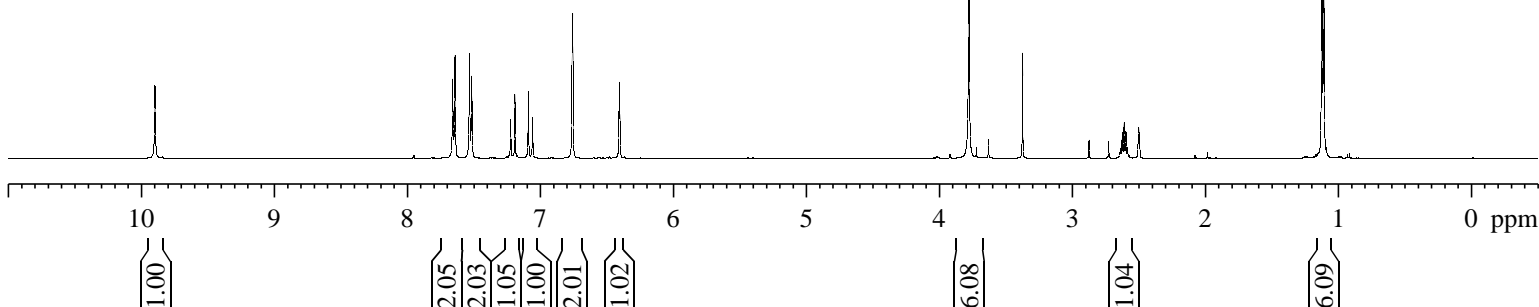
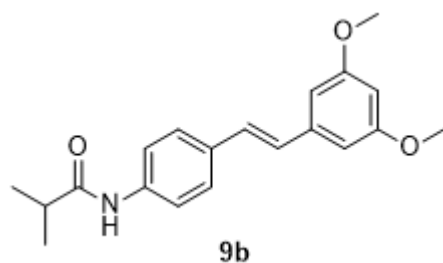
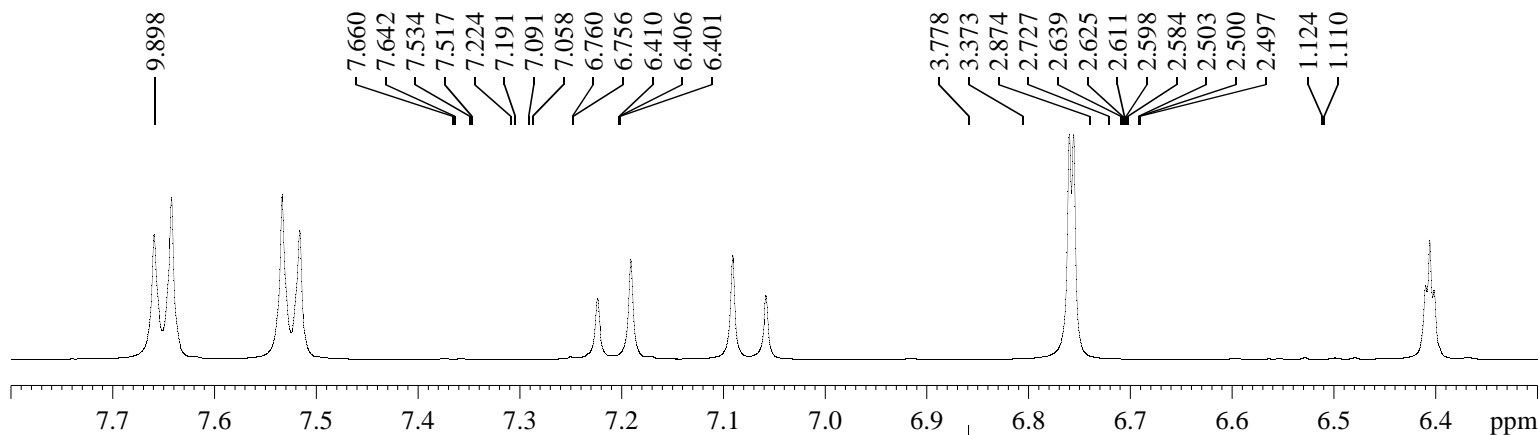
Current Data Parameters
 NAME NMR16020154-LSS-21
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160227
 Time 4.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 34722.223 Hz
 FIDRES 0.529819 Hz
 AQ 0.9437184 sec
 RG 198.55
 DW 14.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.99 usec
 PLW1 125.88999939 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.39528000 W
 PLW13 0.25297999 W

F2 - Processing parameters
 SI 32768
 SF 125.7578506 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

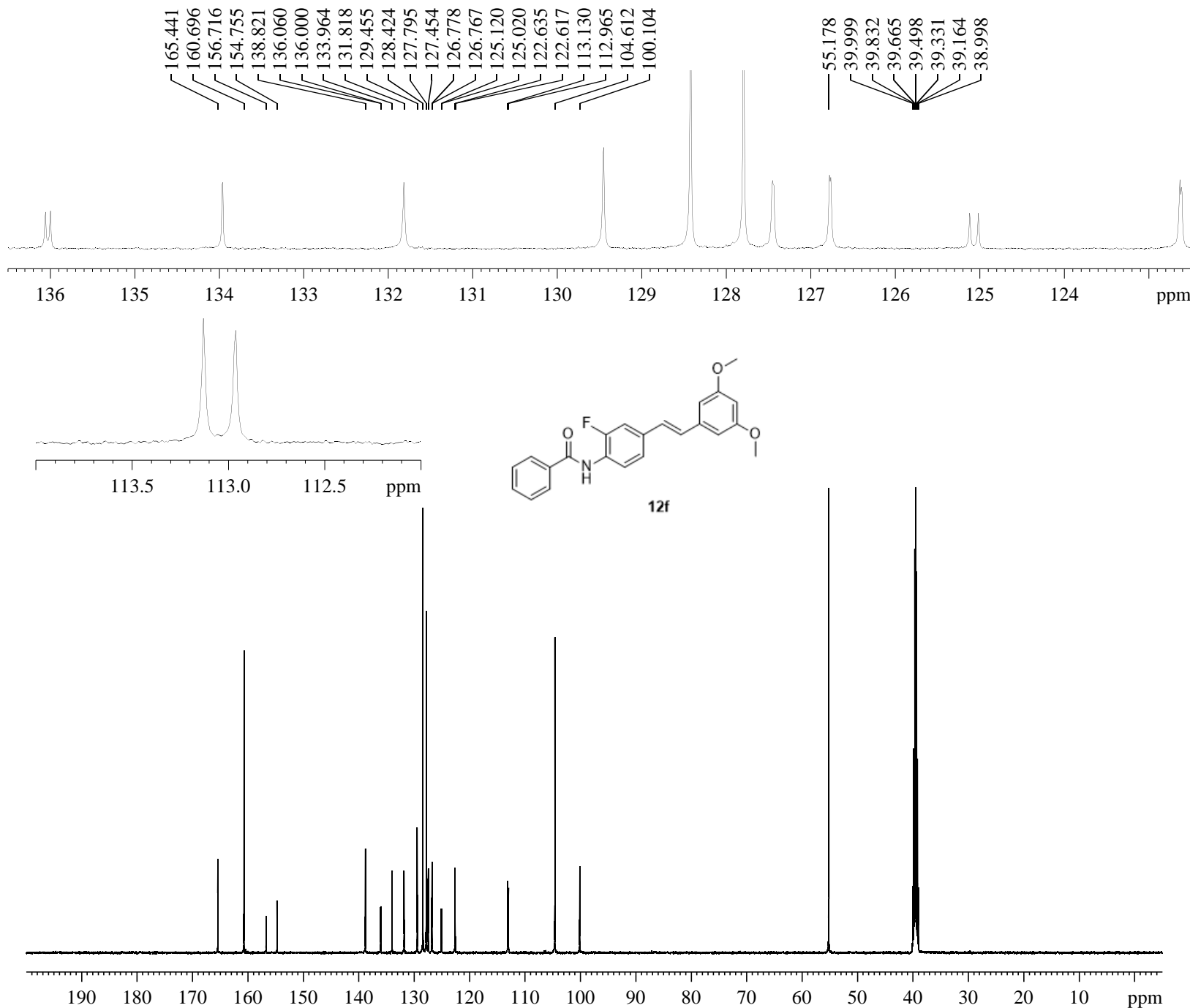


Current Data Parameters
 NAME NMR16020154-LSS-21
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160225
 Time 11.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 128
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 32.04
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 ¹H
 P1 11.26 usec
 PLW1 19.95299911 W

F2 - Processing parameters
 SI 65536
 SF 500.1300038 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



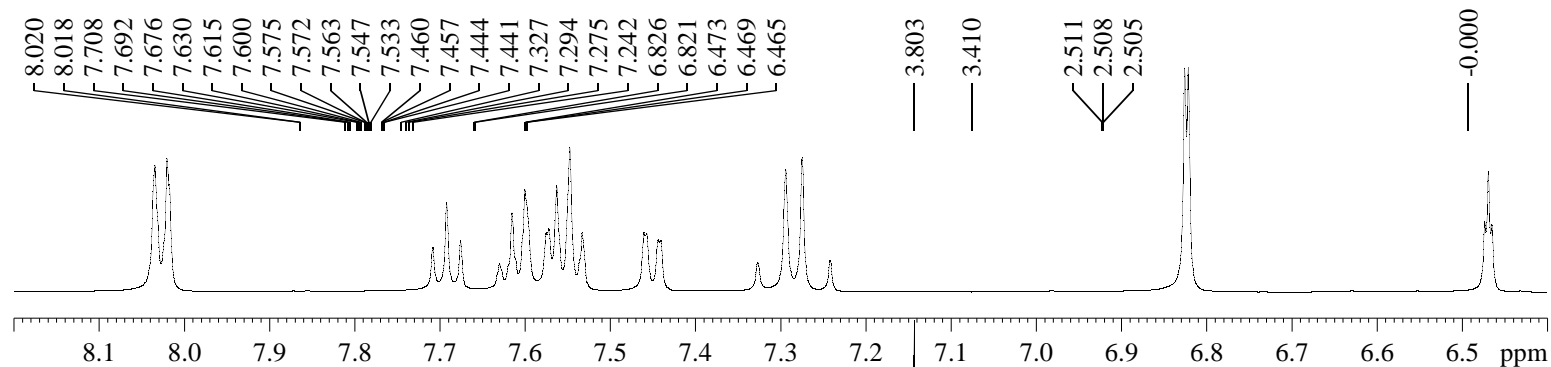
Current Data Parameters
 NAME NMR16031134-LSS-31
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160330
 Time 8.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 600
 DS 4
 SWH 34722.223 Hz
 FIDRES 0.529819 Hz
 AQ 0.9437184 sec
 RG 198.55
 DW 14.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.99 usec
 PLW1 125.88999939 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.39528000 W
 PLW13 0.25297999 W

F2 - Processing parameters
 SI 32768
 SF 125.7578496 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

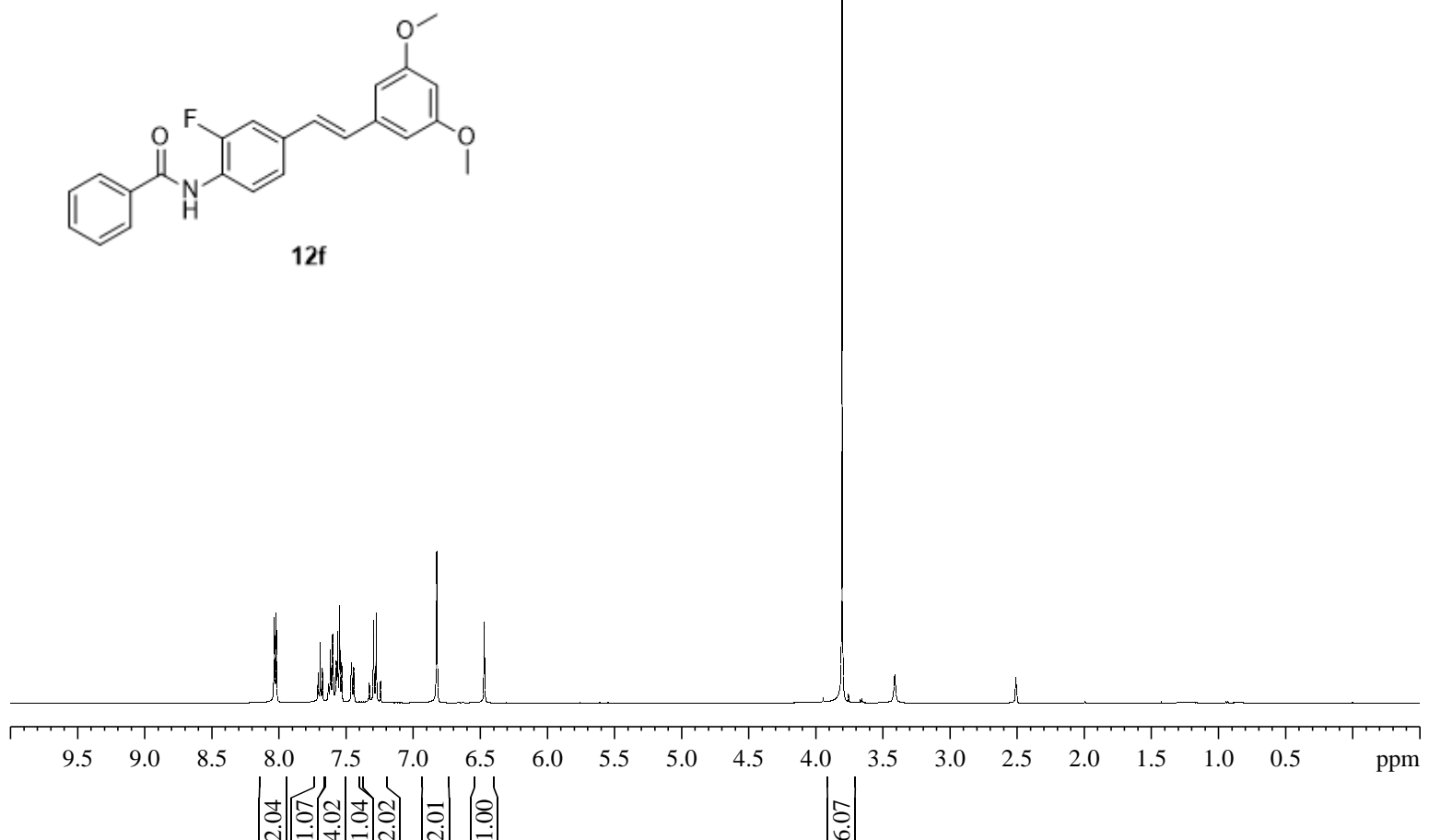


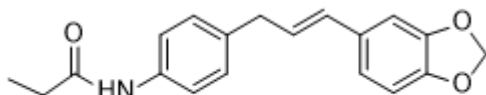
Current Data Parameters
 NAME NMR16031134-LSS-31
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160328
 Time 11.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 32.04
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

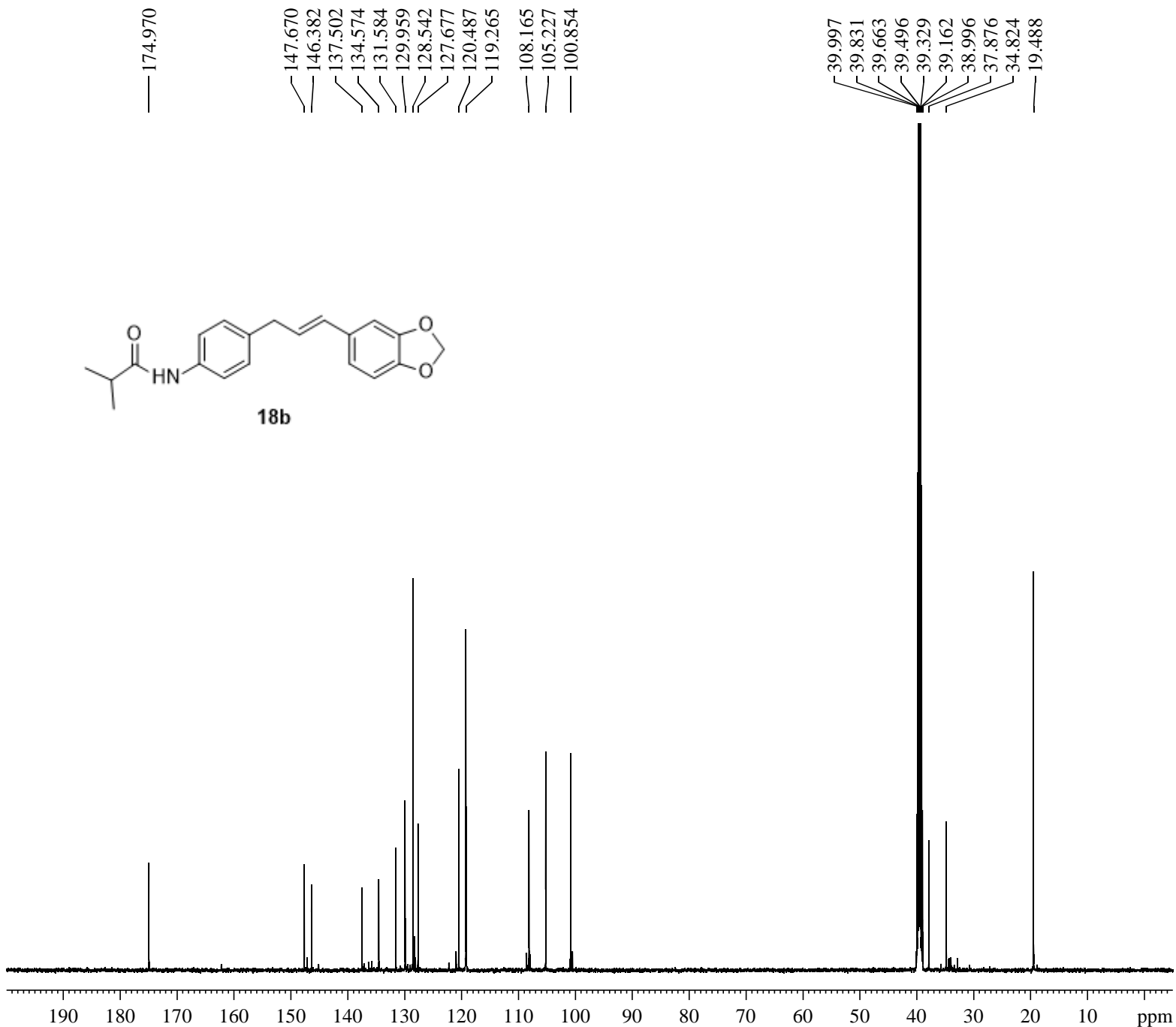
===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.26 usec
 PLW1 19.95299911 W

F2 - Processing parameters
 SI 65536
 SF 500.1300004 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





18b



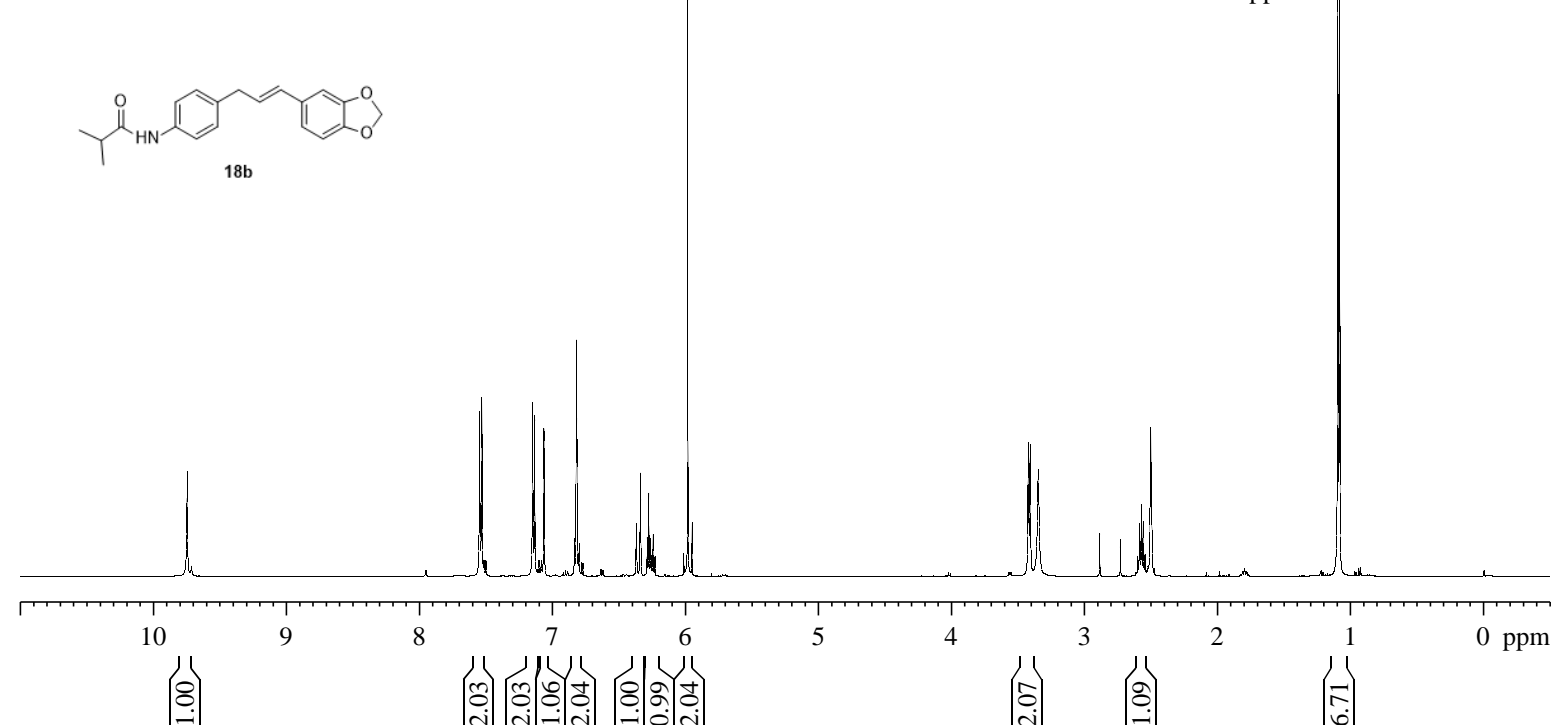
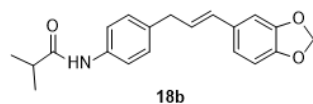
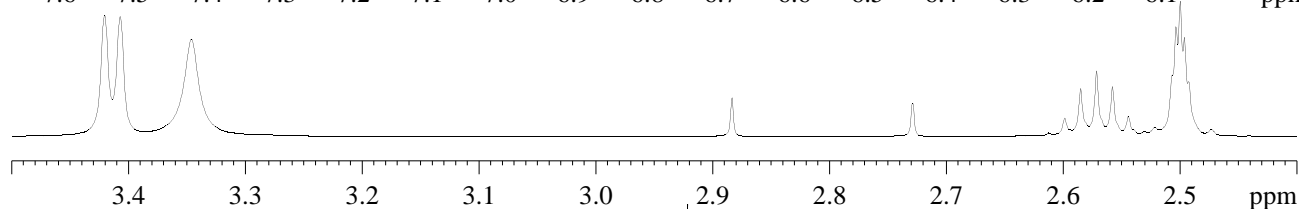
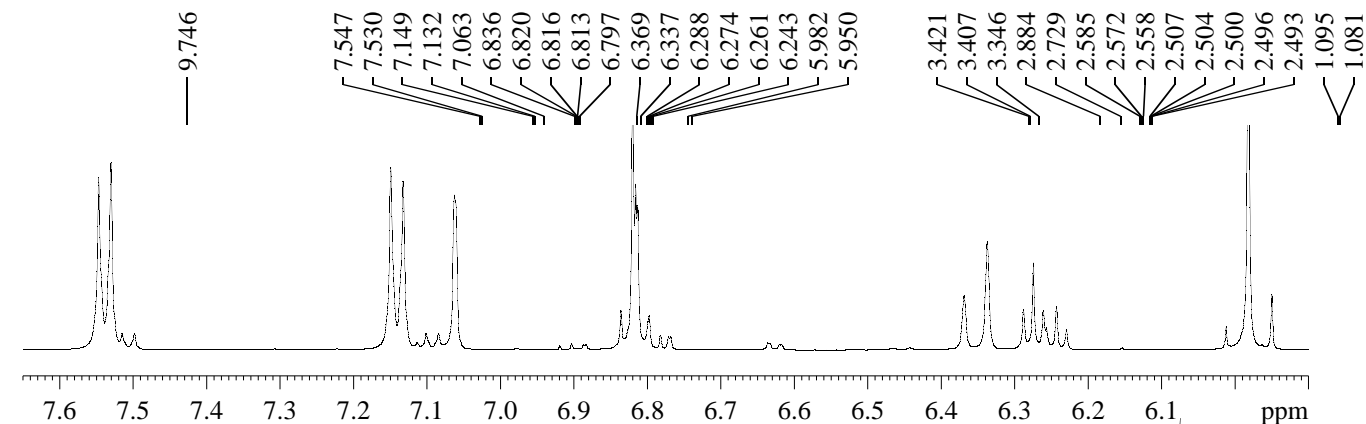
Current Data Parameters
 NAME NMR16020155-LSS-22
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160227
 Time 5.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 34722.223 Hz
 FIDRES 0.529819 Hz
 AQ 0.9437184 sec
 RG 198.55
 DW 14.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.99 usec
 PLW1 125.88999939 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.39528000 W
 PLW13 0.25297999 W

F2 - Processing parameters
 SI 32768
 SF 125.7578517 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

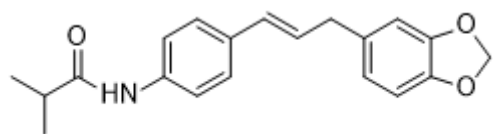


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 NAME NMR16020155-LSS-22
 EXPNO 10
 PROCNO 1

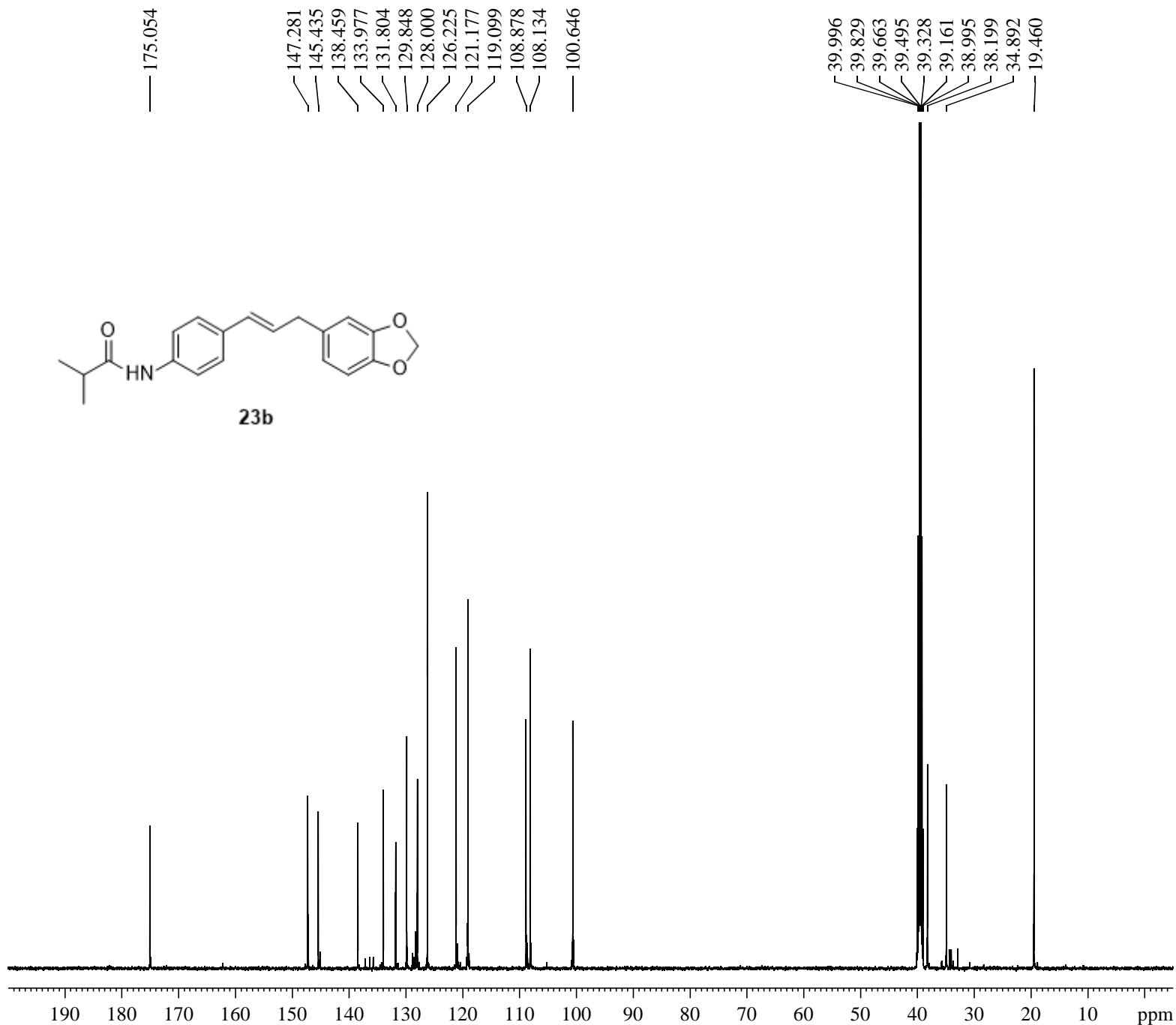
F2 - Acquisition Parameters
 Date_ 20160225
 Time 12.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 128
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 80.16
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.26 usec
 PLW1 19.95299911 W

F2 - Processing parameters
 SI 65536
 SF 500.1300039 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



23b



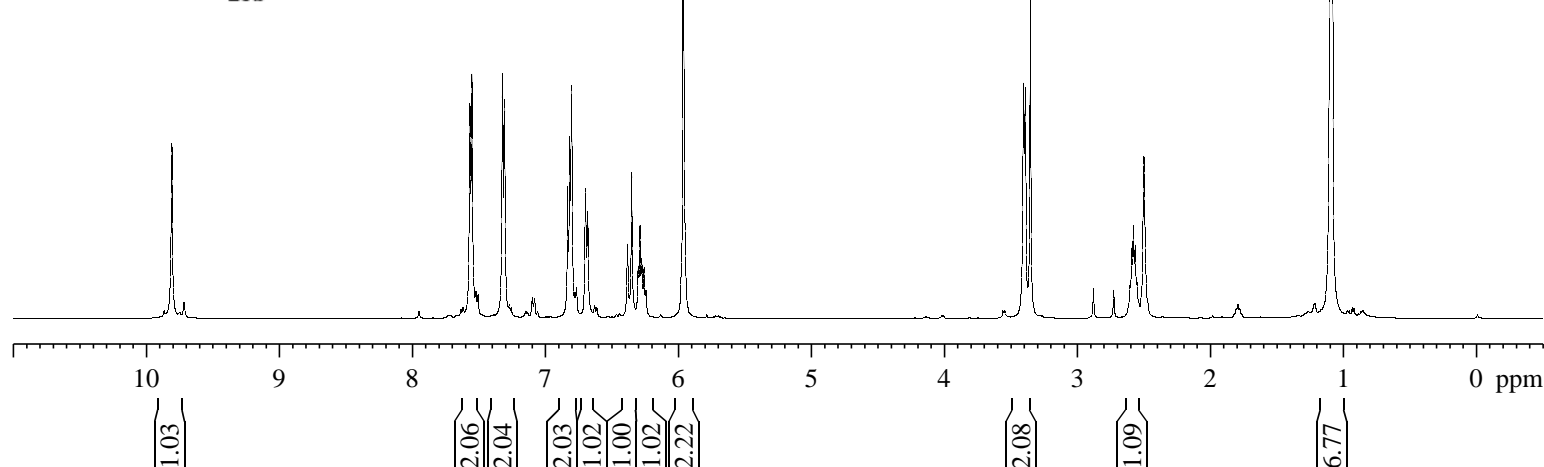
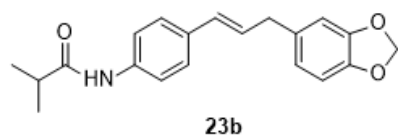
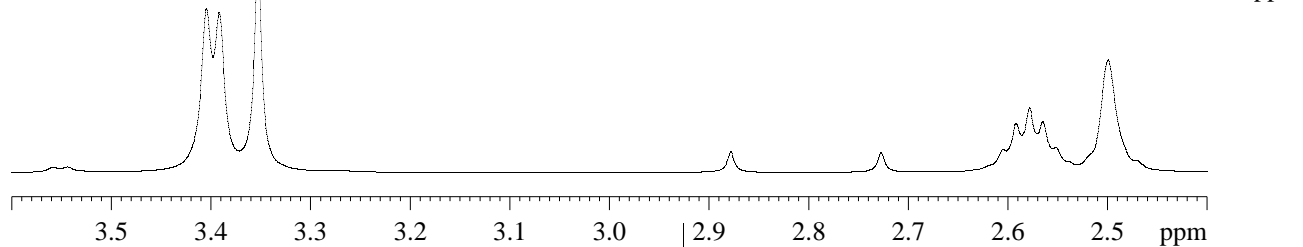
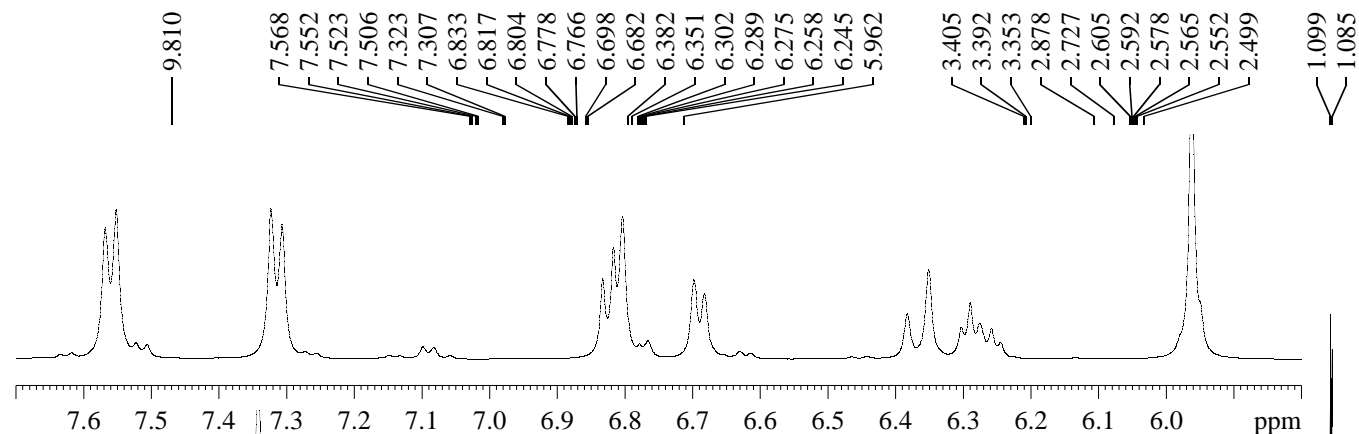
Current Data Parameters
 NAME NMR16020156-LSS-23
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160227
 Time 6.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 34722.223 Hz
 FIDRES 0.529819 Hz
 AQ 0.9437184 sec
 RG 198.55
 DW 14.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.99 usec
 PLW1 125.88999939 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.39528000 W
 PLW13 0.25297999 W

F2 - Processing parameters
 SI 32768
 SF 125.7578517 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

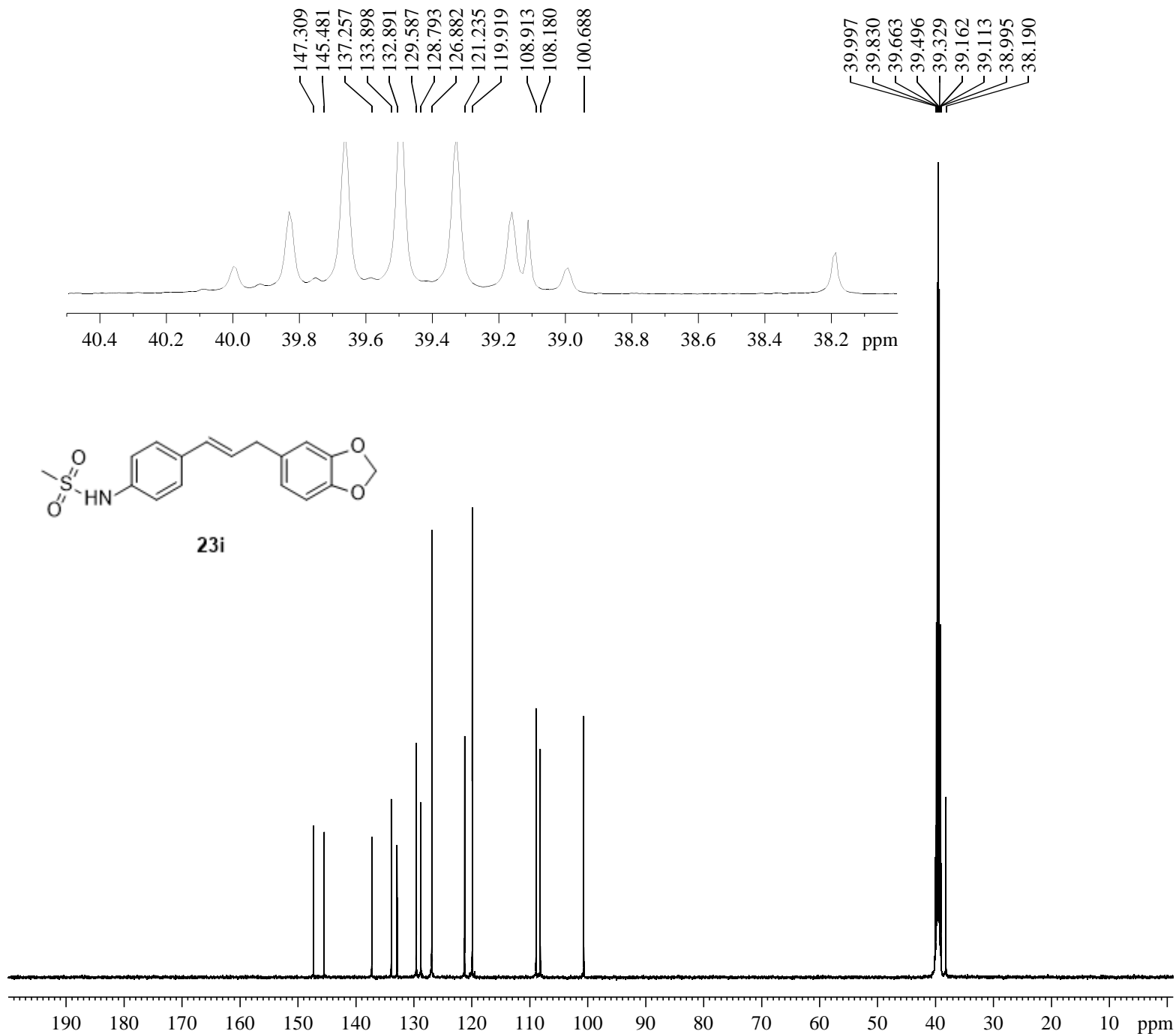


Current Data Parameters
 NAME NMR16020156-LSS-23
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160225
 Time 12.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 128
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 56.83
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.26 usec
 PLW1 19.95299911 W

F2 - Processing parameters
 SI 65536
 SF 500.1300043 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



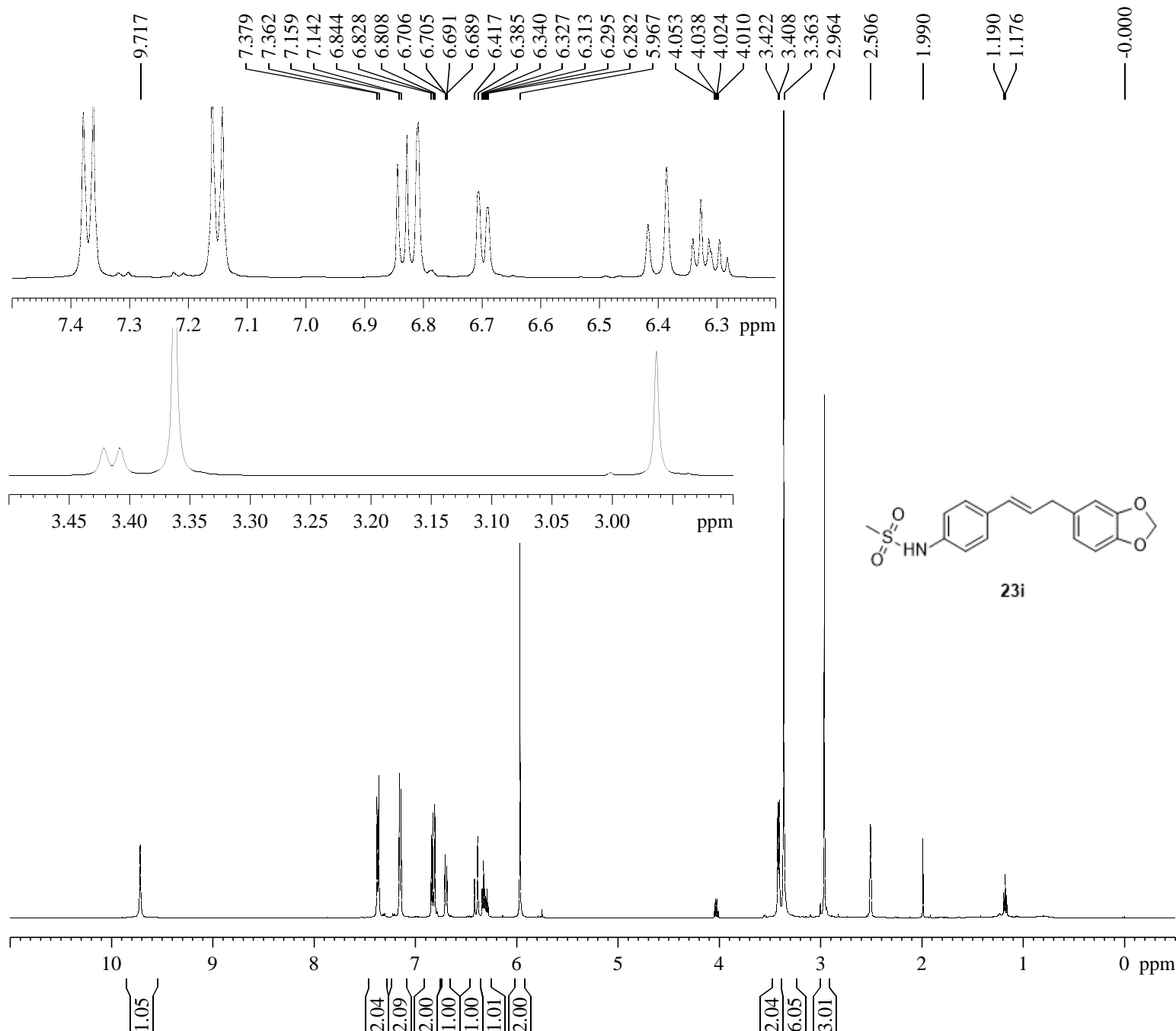
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 NAME NMR16040130-LSS-32-C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160407
 Time 5.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 32894.738 Hz
 FIDRES 0.501934 Hz
 AQ 0.9961472 sec
 RG 198.55
 DW 15.200 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 ¹³C
 P1 8.99 usec
 PLW1 125.88999939 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 ¹H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.39528000 W
 PLW13 0.25297999 W

F2 - Processing parameters
 SI 32768
 SF 125.7578482 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



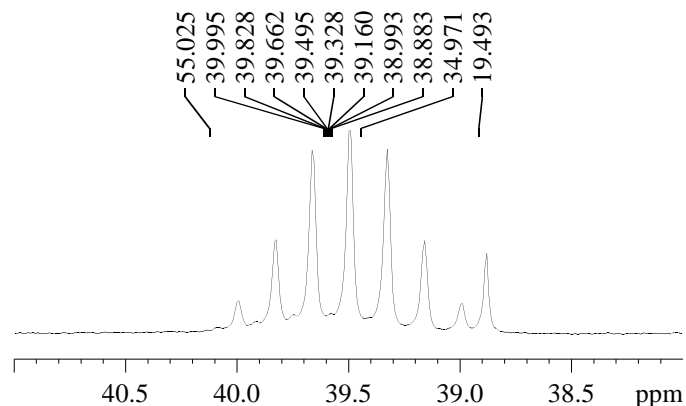
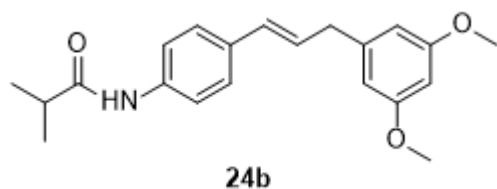
Current Data Parameters
 NAME NMR16031257-LSS-32
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160330
 Time 16.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 72.71
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.26 usec
 PLW1 19.95299911 W

F2 - Processing parameters
 SI 65536
 SF 500.1300013 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

— 175.155 — 160.568 — 142.624 — 138.543 — 131.879 — 130.149 — 127.543 — 126.294 — 119.198 — 106.505 — 97.864



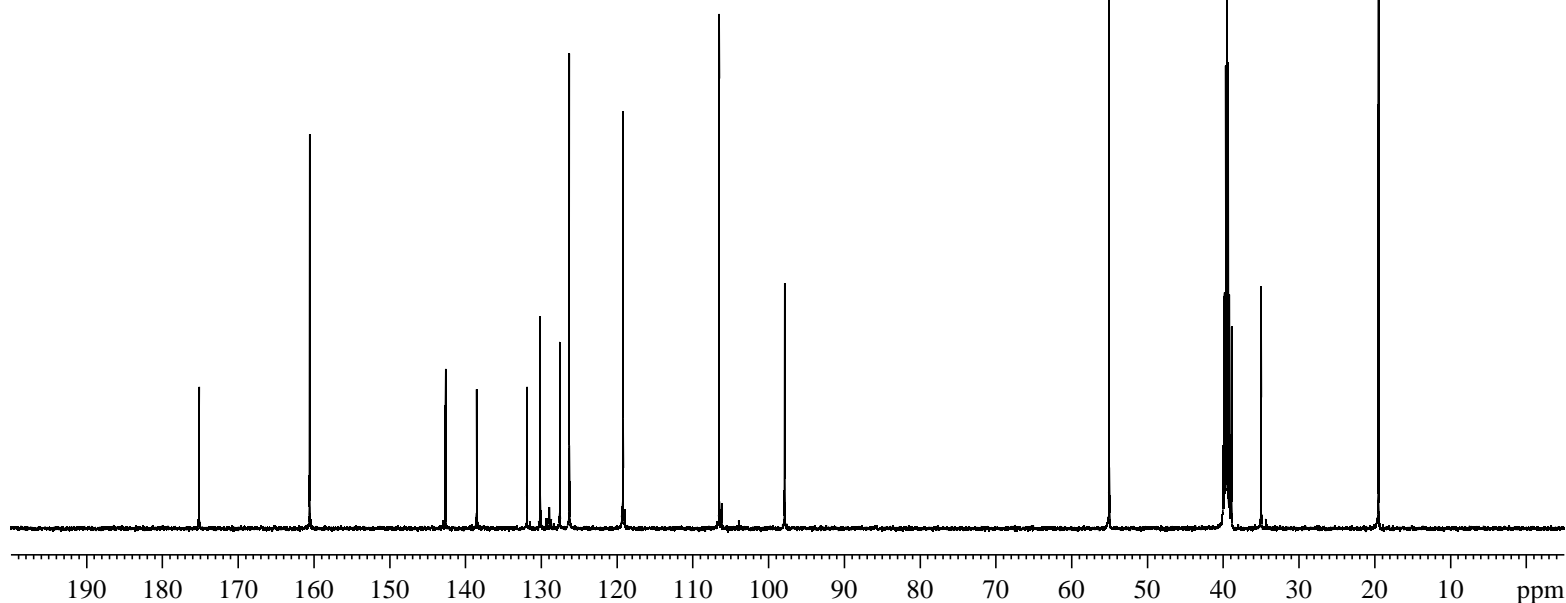
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 EXPNO 2
 PROCNO 1

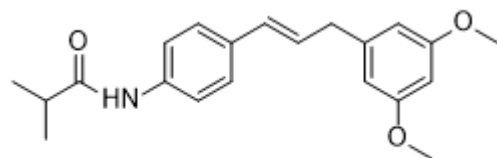
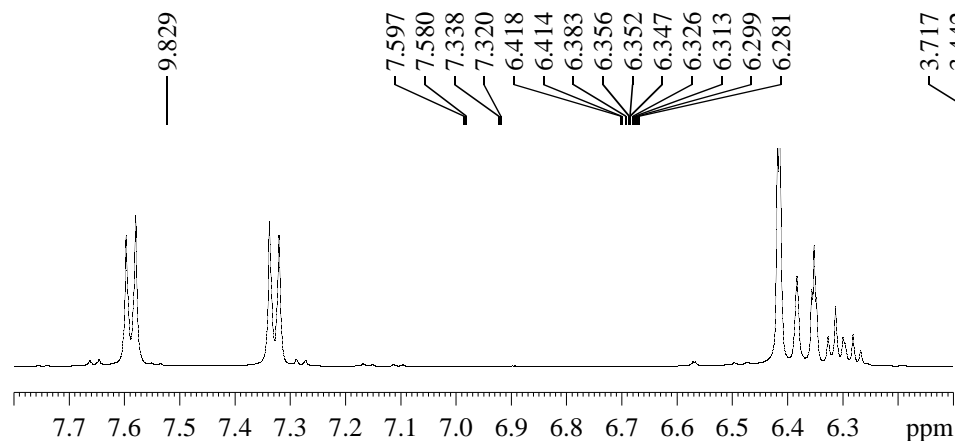
F2 - Acquisition Parameters
 Date_ 20160706
 Time 10.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 256
 DS 4
 SWH 34722.223 Hz
 FIDRES 0.529819 Hz
 AQ 0.9437184 sec
 RG 198.55
 DW 14.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.12 usec
 PLW1 125.88999939 W

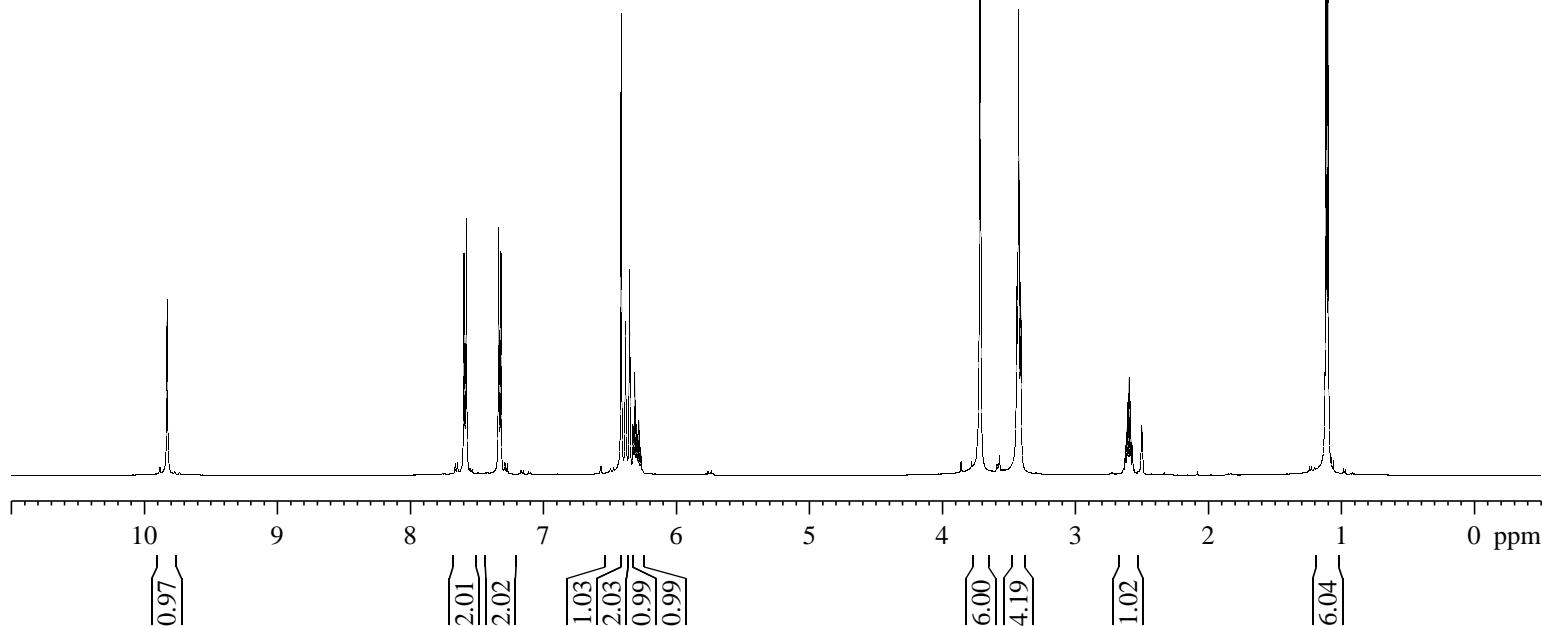
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.41303000 W
 PLW13 0.26434001 W

F2 - Processing parameters
 SI 32768
 SF 125.7578453 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





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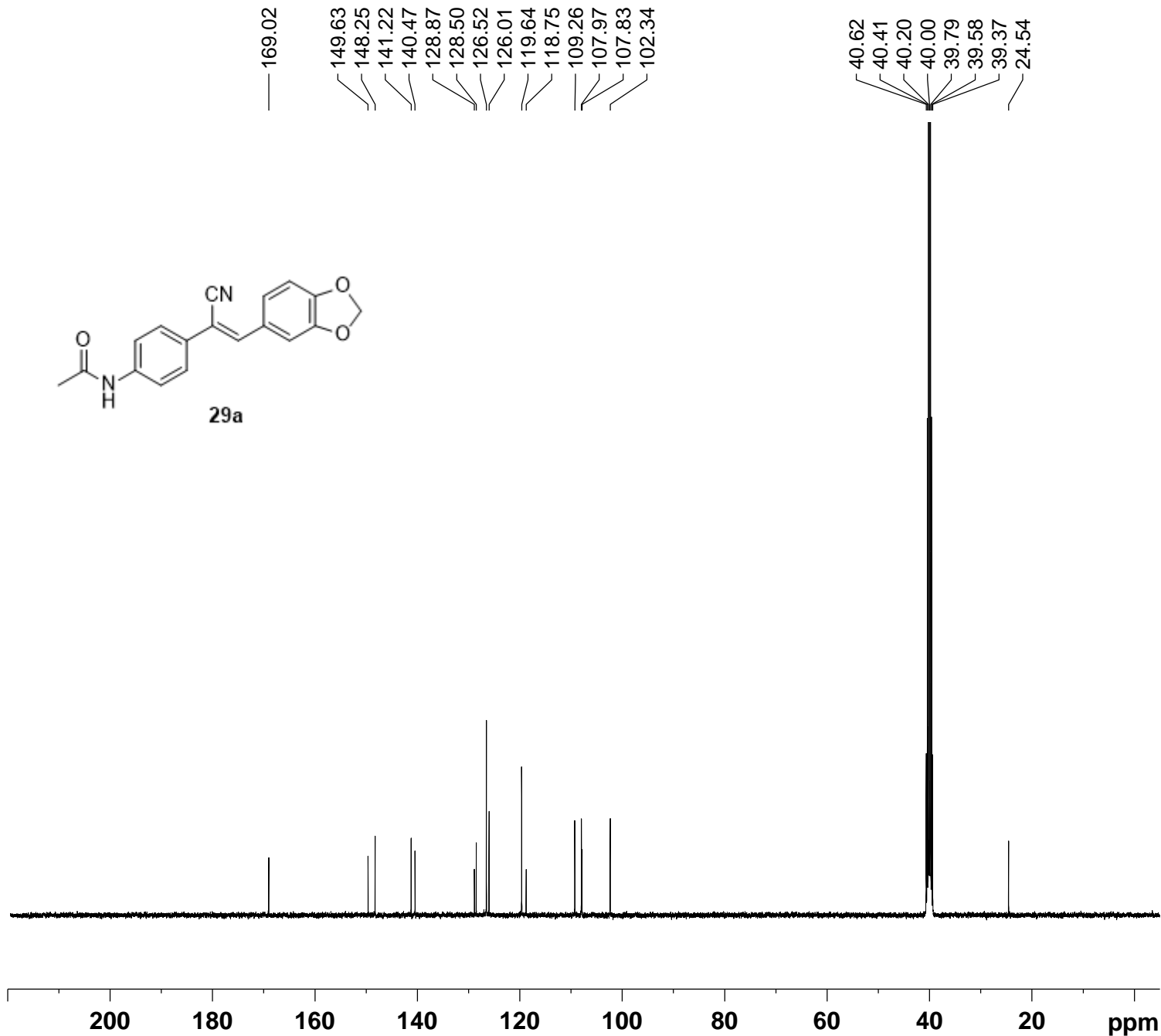
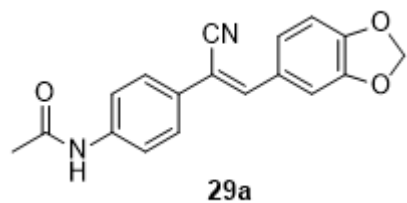
Current Data Parameters
 NAME NMR16070013-LSS-40
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160705
 Time 11.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 32.04
 DW 50.000 usec
 DE 6.50 usec
 TE 299.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1325007 MHz
 NUC1 1H
 P1 11.51 usec
 PLW1 19.95299911 W

F2 - Processing parameters
 SI 65536
 SF 500.1300044 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

MCX

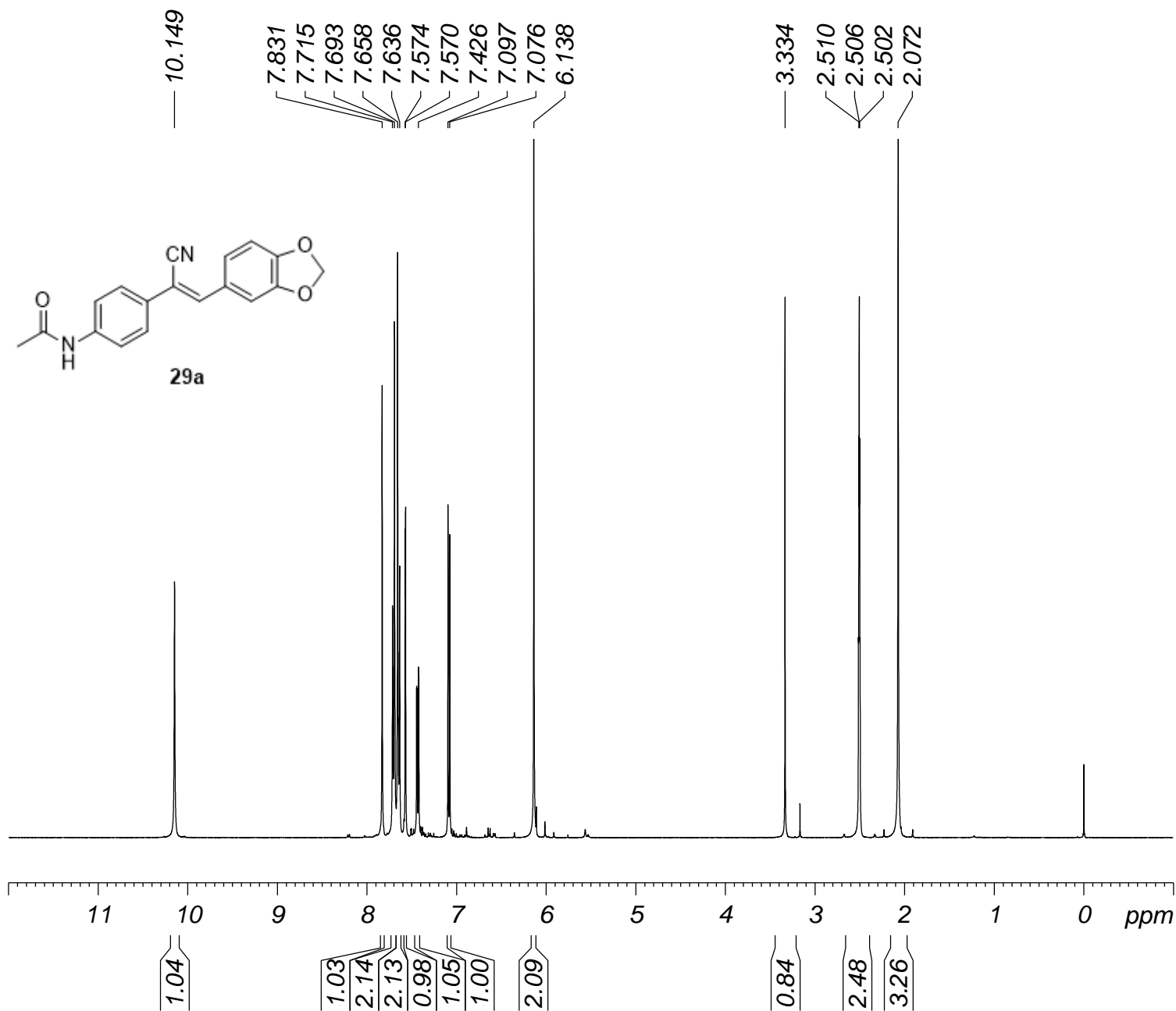


Current Data Parameters
NAME MCX-70
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190225
Time 15.00 h
INSTRUM spect
PROBHD Z116098_0436 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.03199768 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.00300026 W
PLW12 0.20275000 W
PLW13 0.10182000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

MCX



Current Data Parameters

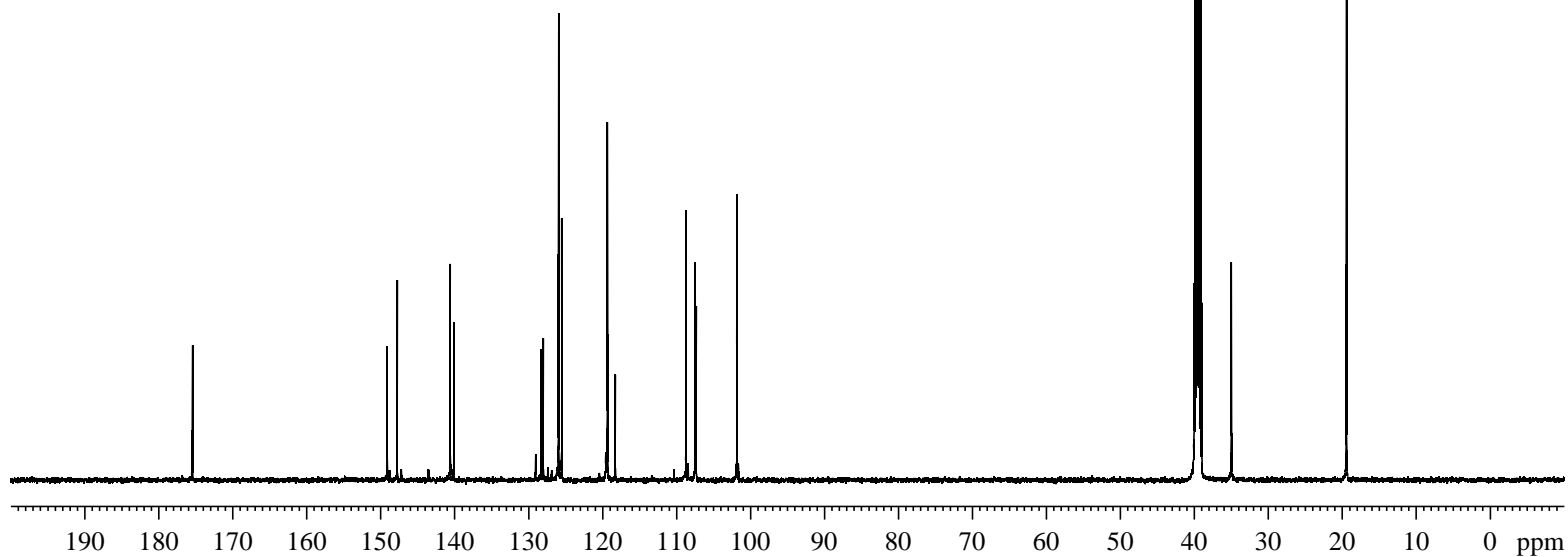
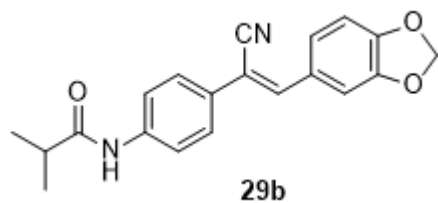
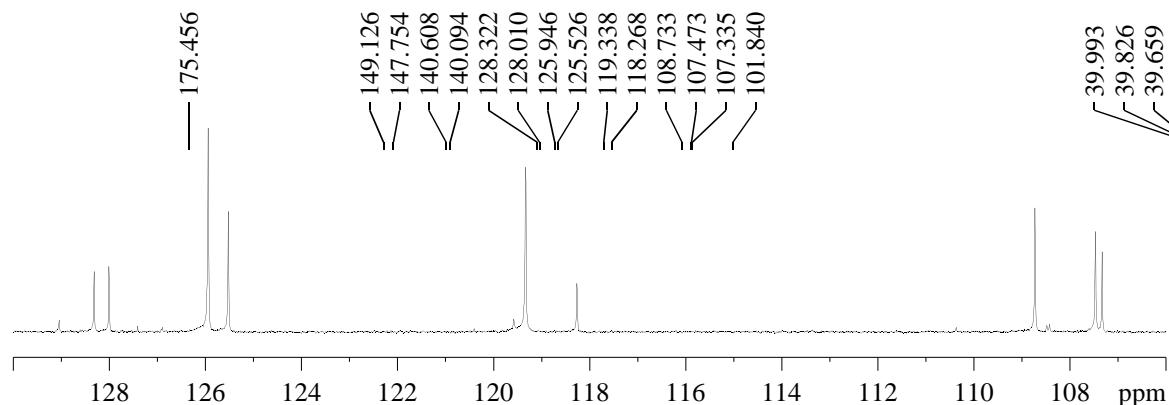
NAME MCX-70
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190221
Time 18.44 h
INSTRUM spect
PROBHD Z116098_0436 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 111.98
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P1 8.00 usec
PLW1 15.00300026 W

F2 - Processing parameters

SI 65536
SF 400.1500008 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



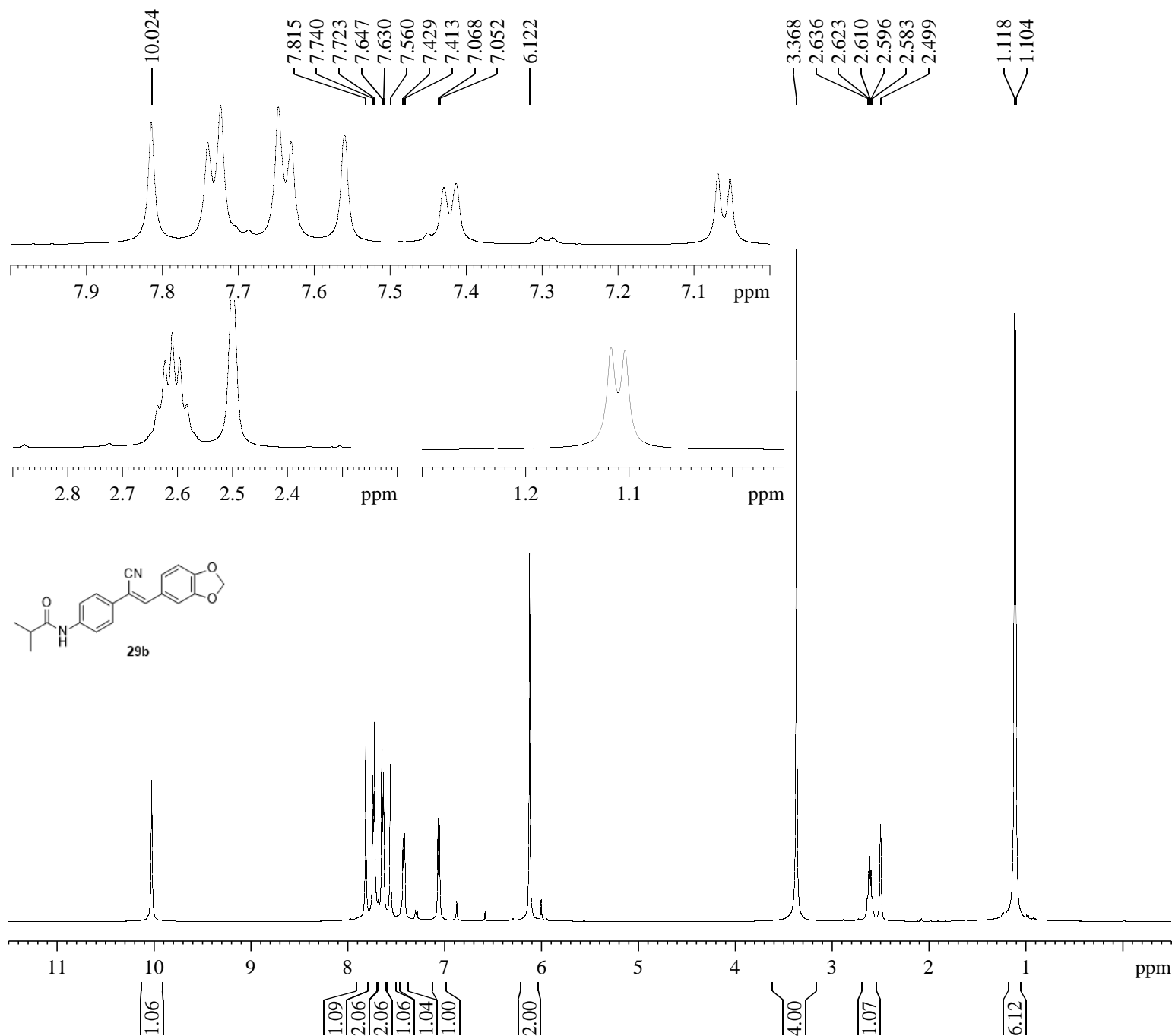
Current Data Parameters
 NAME NMR16090172-LSS-35-C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160930
 Time 12.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 34722.223 Hz
 FIDRES 0.529819 Hz
 AQ 0.9437184 sec
 RG 198.55
 DW 14.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.12 usec
 PLW1 125.88999939 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.41303000 W
 PLW13 0.26434001 W

F2 - Processing parameters
 SI 32768
 SF 125.7578495 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



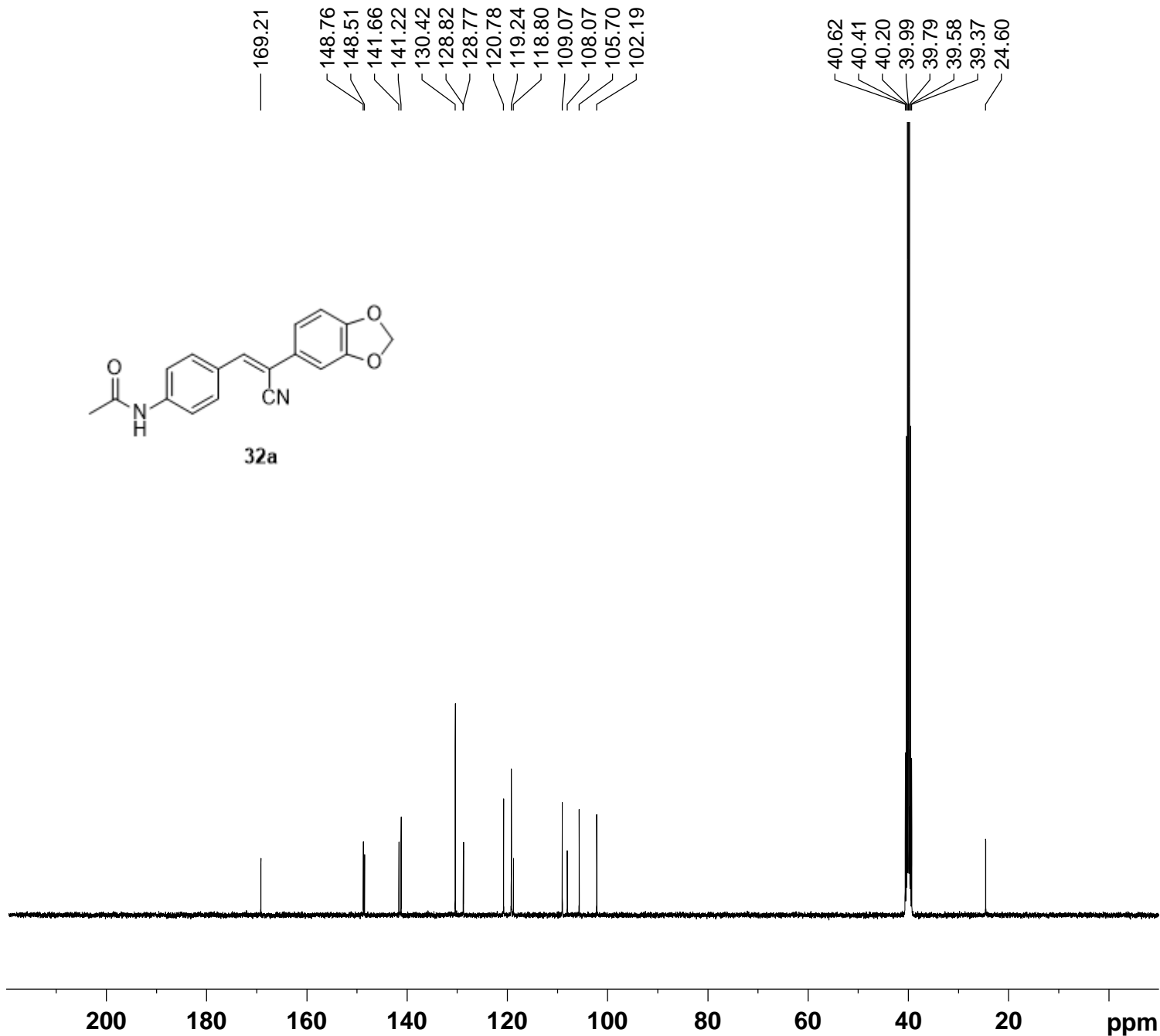
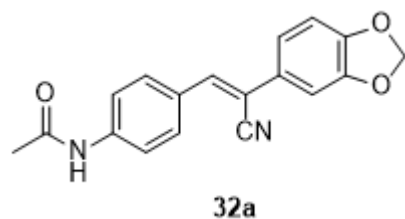
Current Data Parameters
 NAME NMR16090160-LSS-35
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160928
 Time 13.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 128
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 62.41
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.51 usec
 PLW1 19.95299911 W

F2 - Processing parameters
 SI 65536
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

MCX

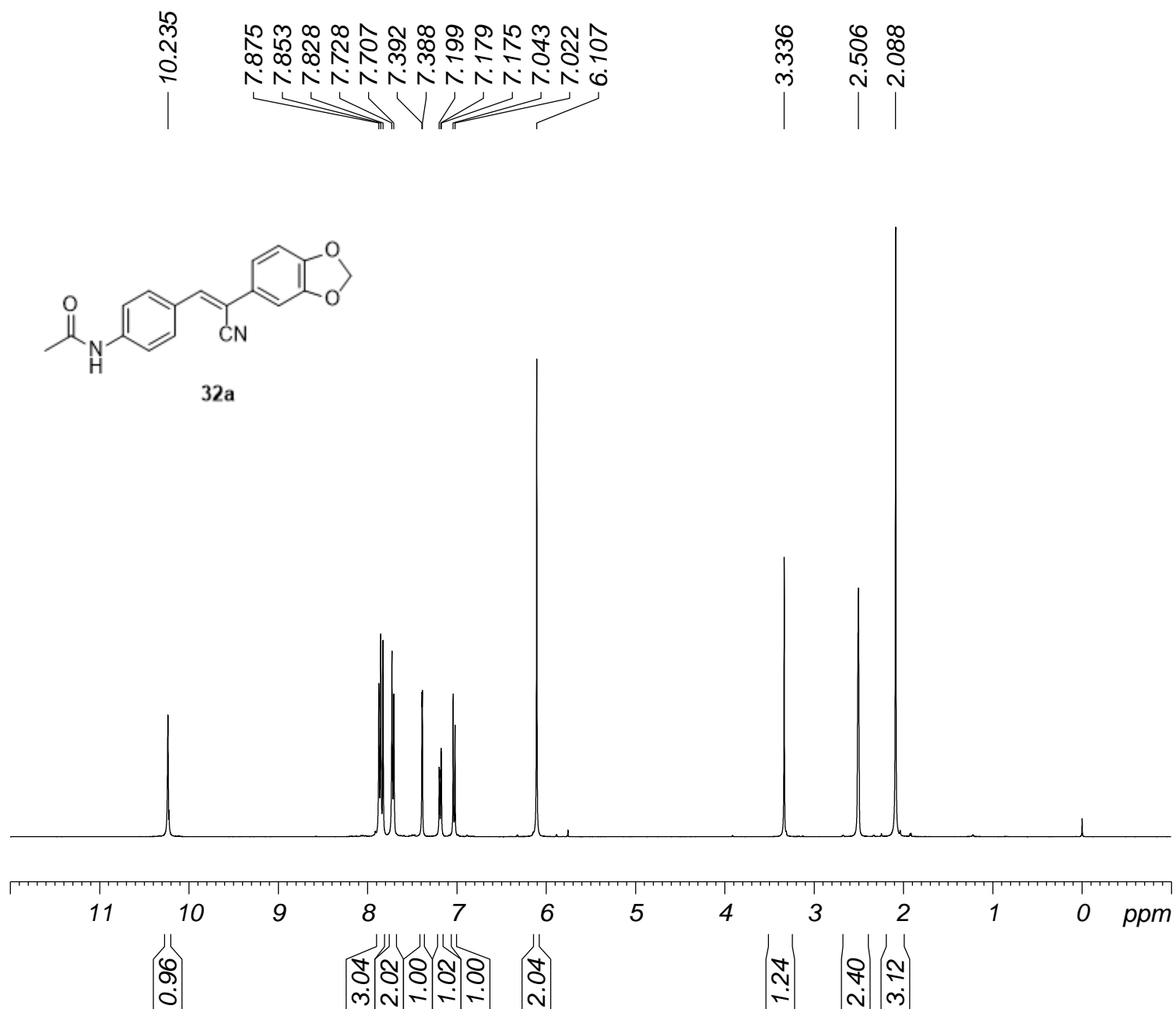


Current Data Parameters
NAME MCX-71
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190225
Time 13.51 h
INSTRUM spect
PROBHD Z116098_0436 (zpgpg30)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.03199768 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.00300026 W
PLW12 0.20275000 W
PLW13 0.10182000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

MCX



Current Data Parameters

NAME MCX-71
EXPNO 1
PROCNO 1

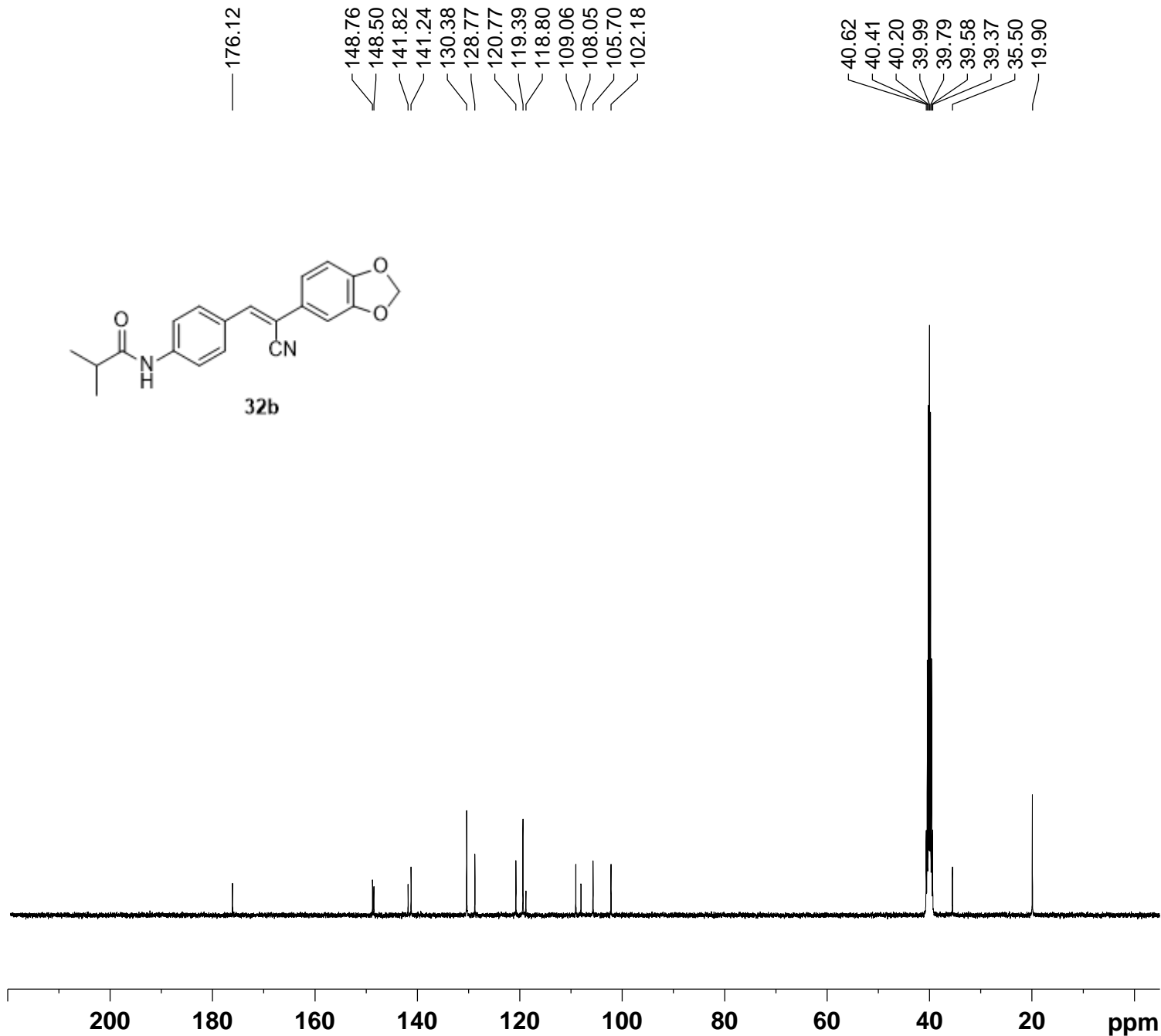
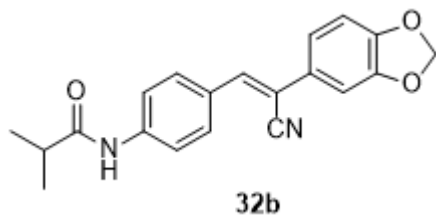
F2 - Acquisition Parameters

Date_ 20190221
Time 18.33 h
INSTRUM spect
PROBHD Z116098_0436 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 111.98
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P1 8.00 usec
PLW1 15.00300026 W

F2 - Processing parameters

SI 65536
SF 400.1500006 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

MCX

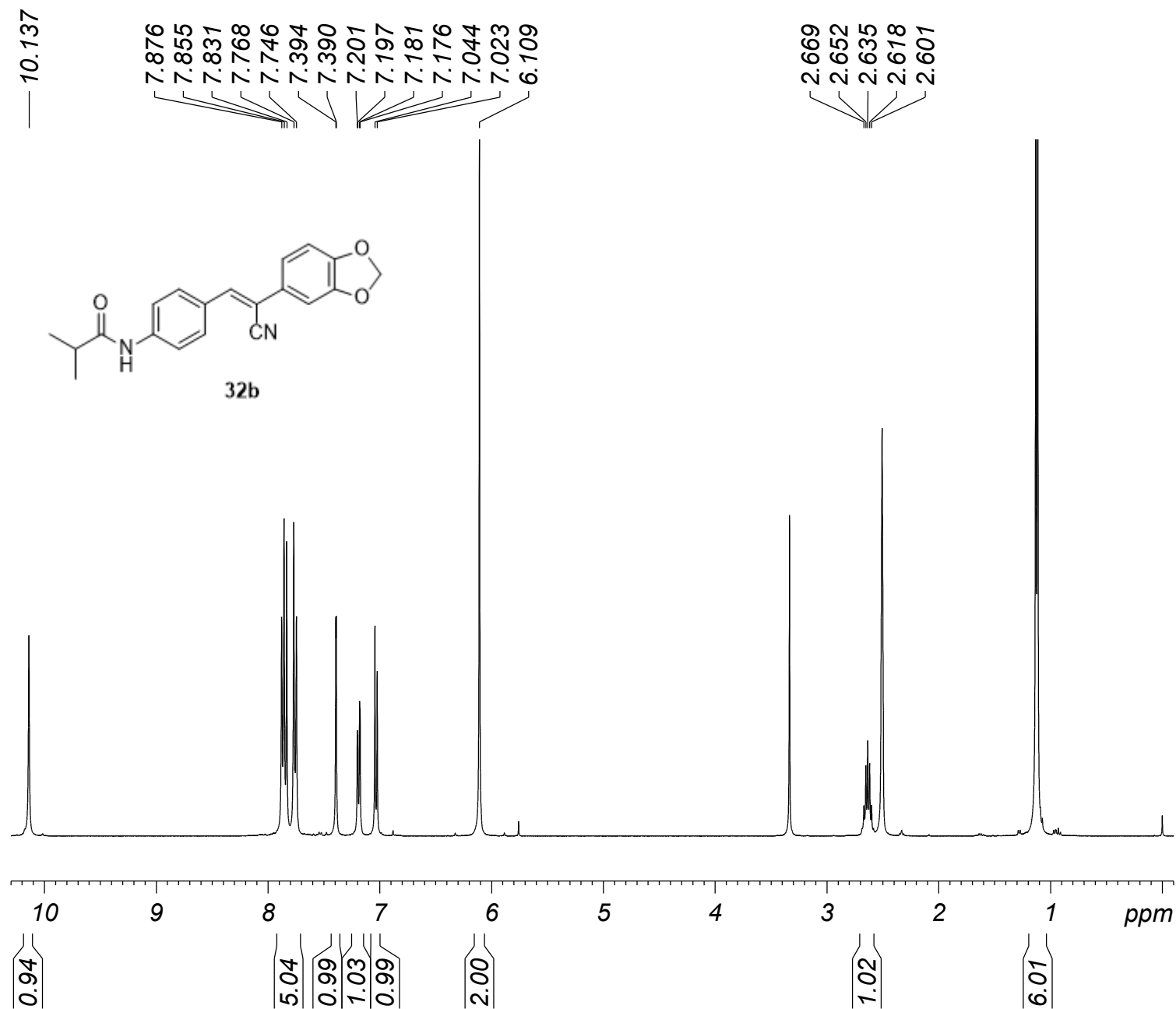


Current Data Parameters
NAME MCX-67-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190111
Time 16.35 h
INSTRUM spect
PROBHD Z116098_0436 (zpgp30)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 835
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.03199768 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.00300026 W
PLW12 0.15003000 W
PLW13 0.07534400 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

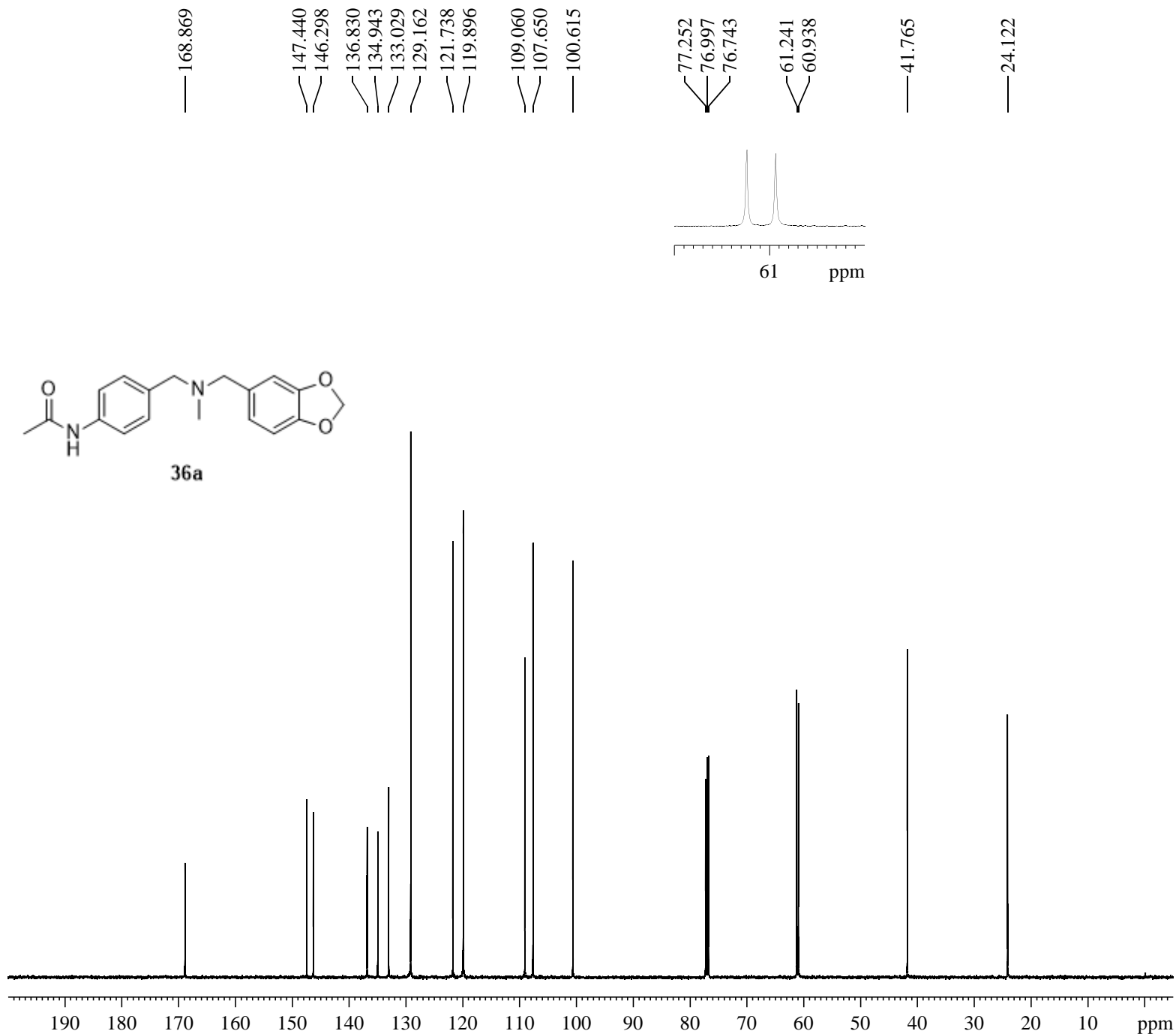
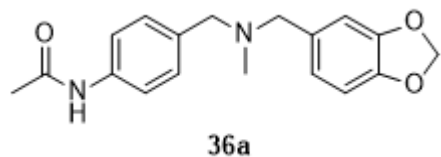
MCX



Current Data Parameters
 NAME MCX-67-H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190221
 Time_ 18.48 h
 INSTRUM spect
 PROBHD Z116098_0436 (zg30)
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 98.25
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1524709 MHz
 NUC1 1H
 P1 8.00 usec
 PLW1 15.00300026 W

F2 - Processing parameters
 SI 65536
 SF 400.1500005 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



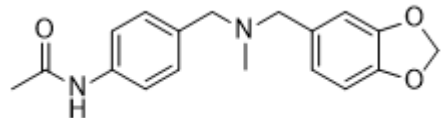
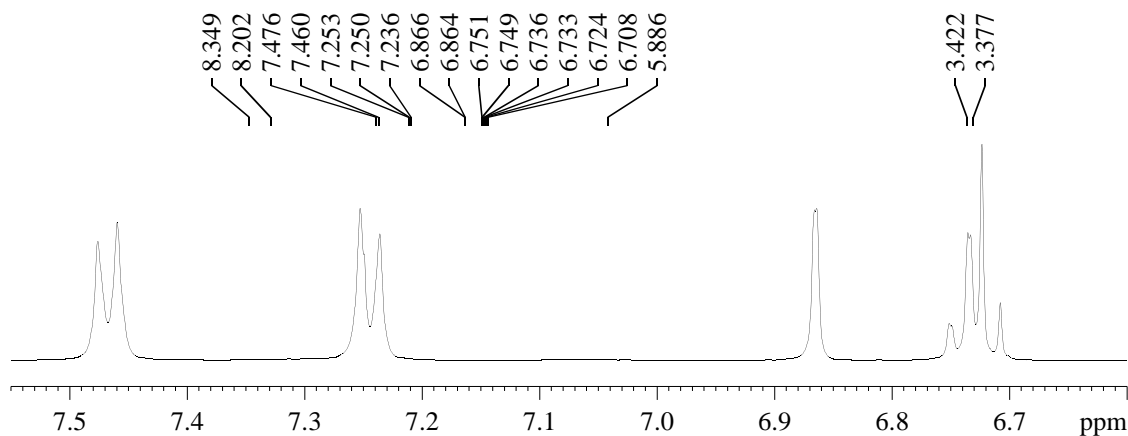
Current Data Parameters
 NAME 150033-LSS-3
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150612
 Time 7.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 34722.223 Hz
 FIDRES 0.529819 Hz
 AQ 0.9437184 sec
 RG 198.55
 DW 14.400 usec
 DE 6.50 usec
 TE 303.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

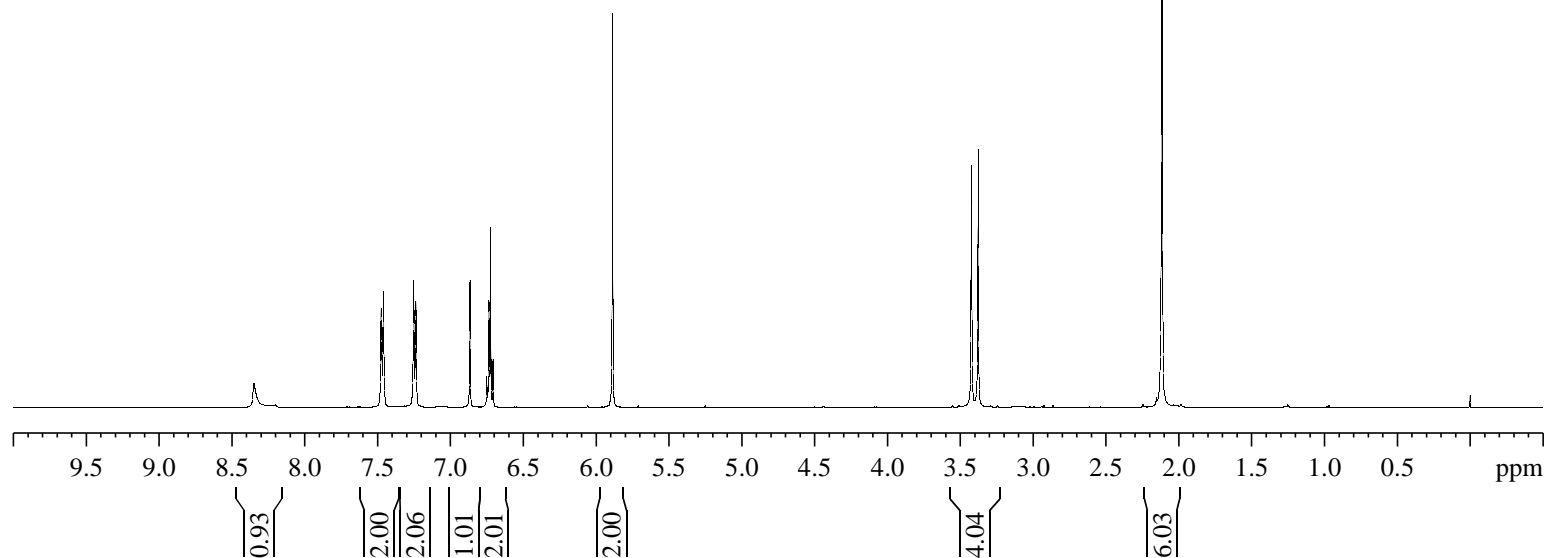
===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.99 usec
 PLW1 125.88999939 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 19.95299911 W
 PLW12 0.39528000 W
 PLW13 0.25297999 W

F2 - Processing parameters
 SI 32768
 SF 125.7578151 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



36a



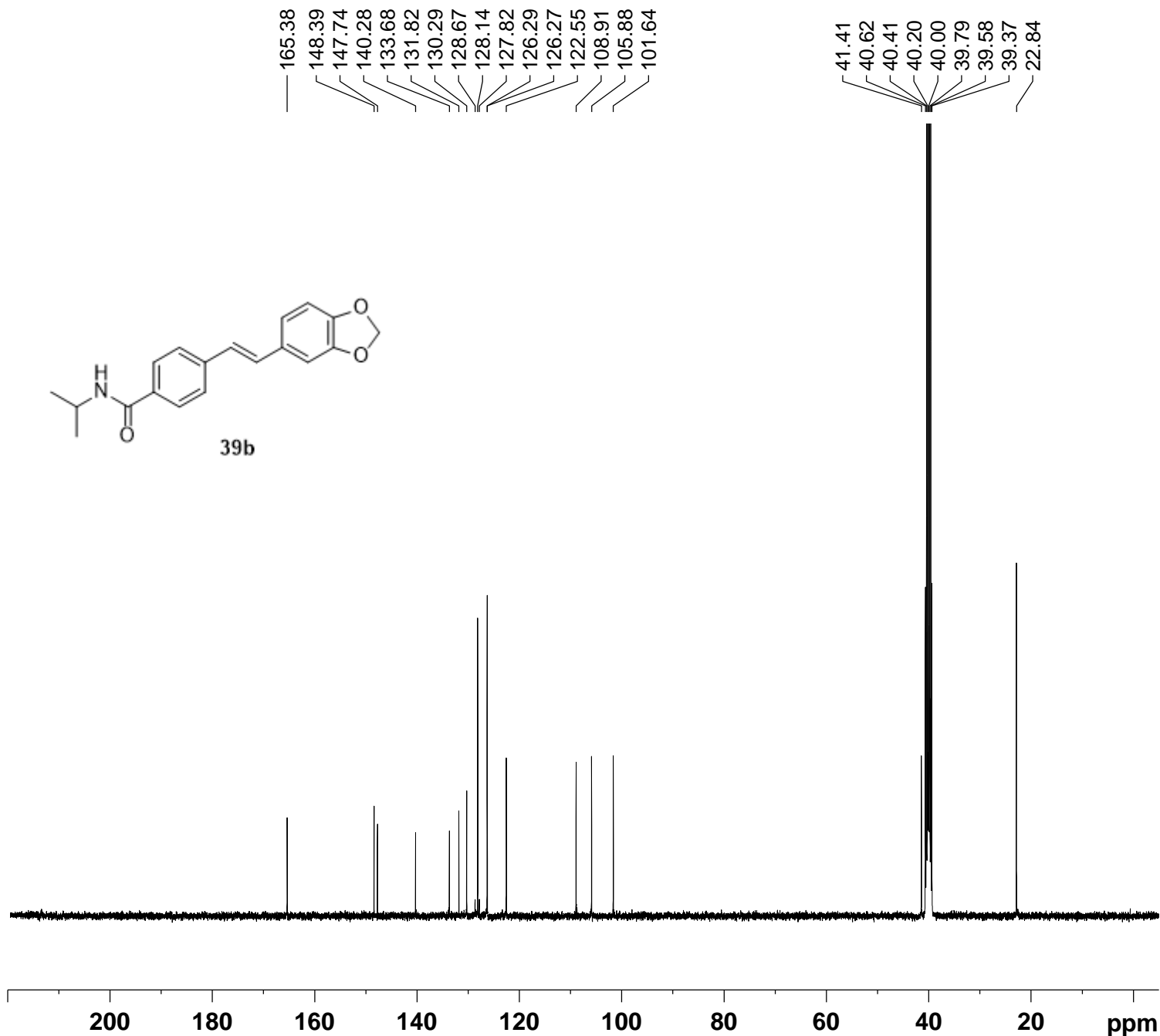
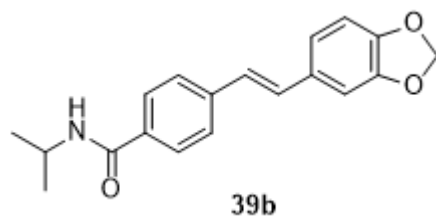
Current Data Parameters
 NAME 150033-LSS-3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150610
 Time 11.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 20.1
 DW 50.000 usec
 DE 6.50 usec
 TE 303.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.26 usec
 PLW1 19.95299911 W

F2 - Processing parameters
 SI 65536
 SF 500.1300170 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

FBZ

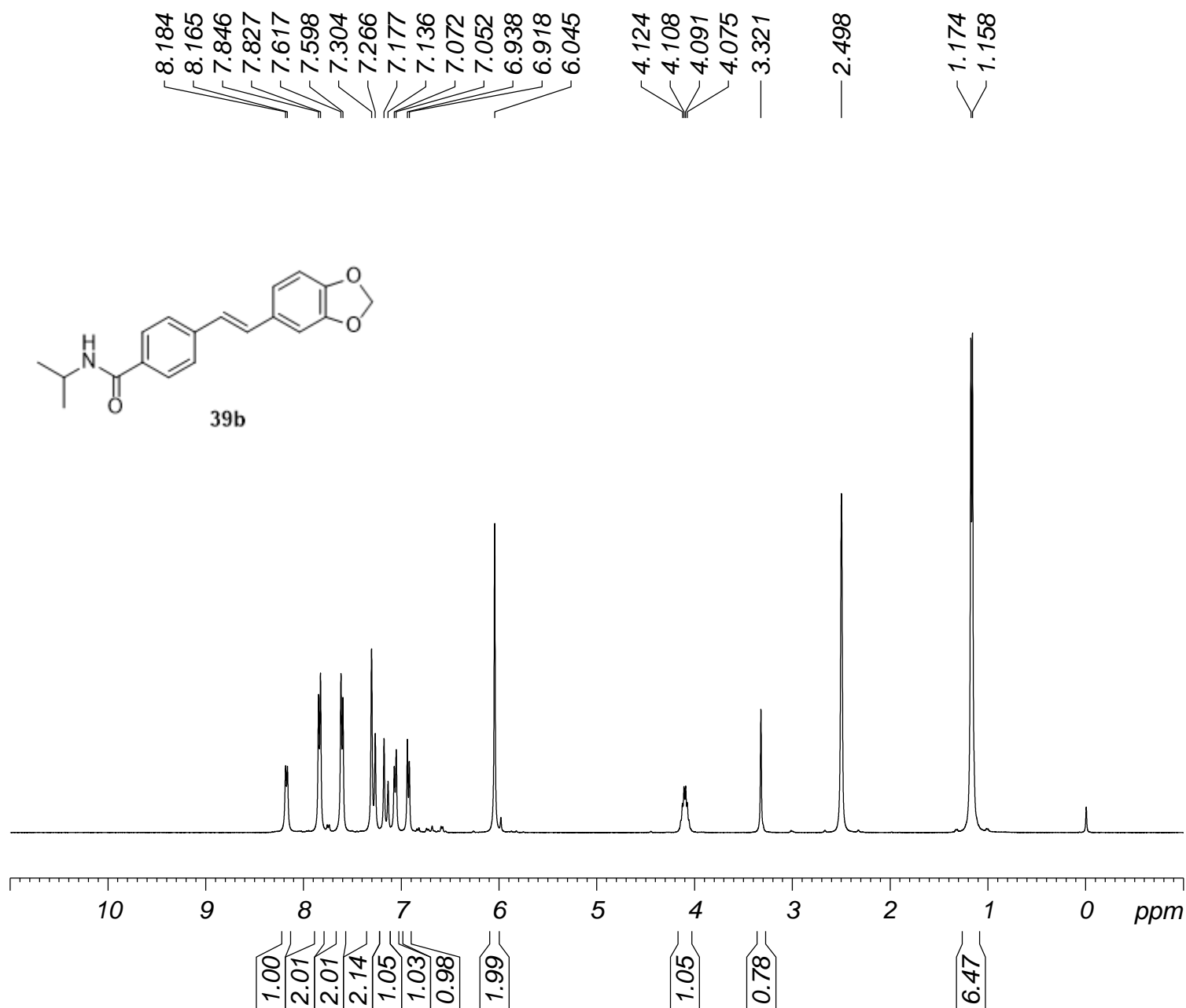


Current Data Parameters
NAME MCX-1-1201-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171201
Time 23.17 h
INSTRUM spect
PROBHD Z116098_0436 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2200
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.03199768 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.00300026 W
PLW12 0.22284999 W
PLW13 0.11191000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

FBZ



Current Data Parameters

NAME MCX-1-1201
EXPNO 1
PROCNO 1

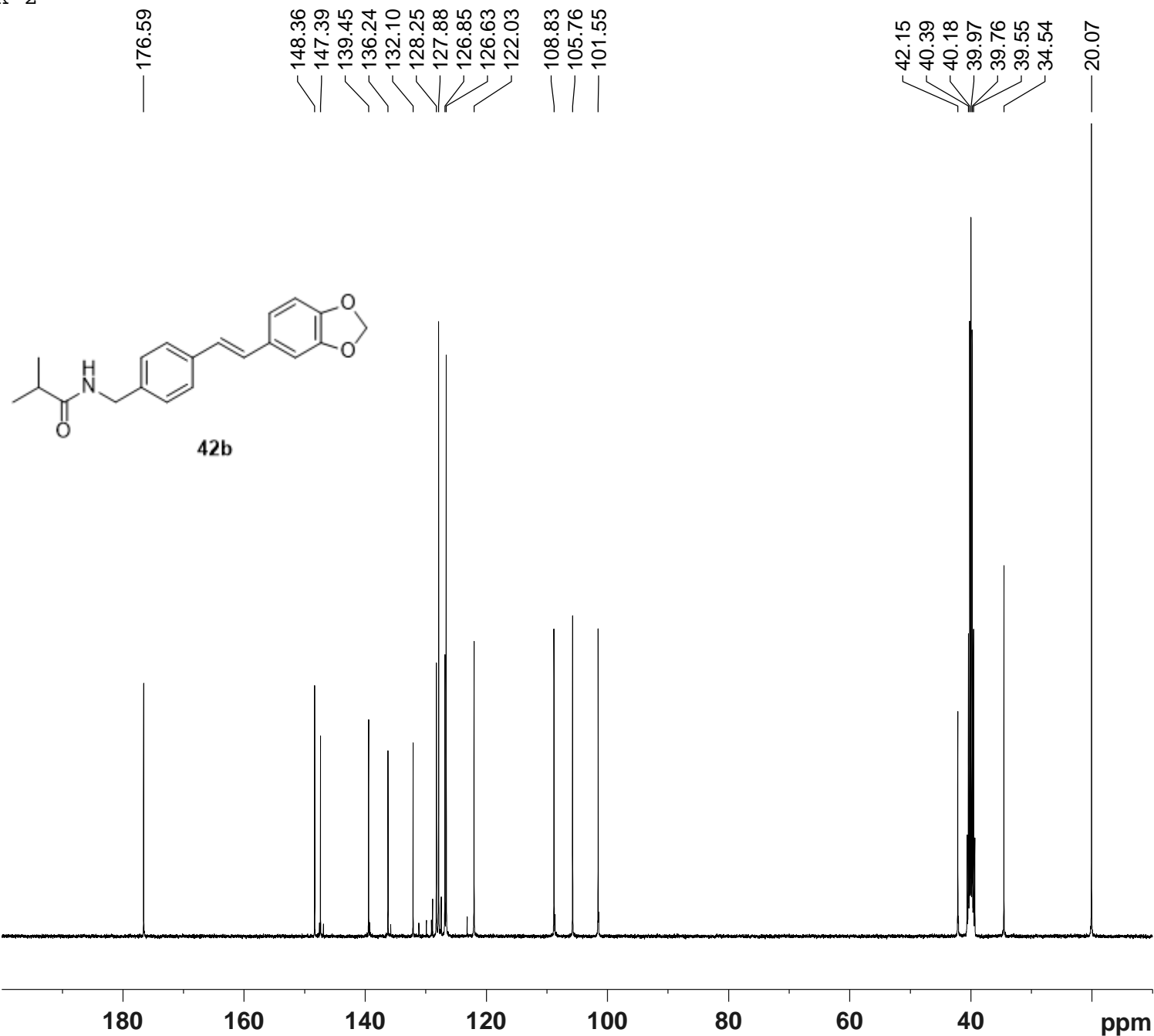
F2 - Acquisition Parameters

Date_ 20171201
Time 11.12 h
INSTRUM spect
PROBHD Z116098_0436 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 98.25
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P1 9.75 usec
PLW1 15.00300026 W

F2 - Processing parameters

SI 65536
SF 400.1500033 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

MCX-2



Current Data Parameters

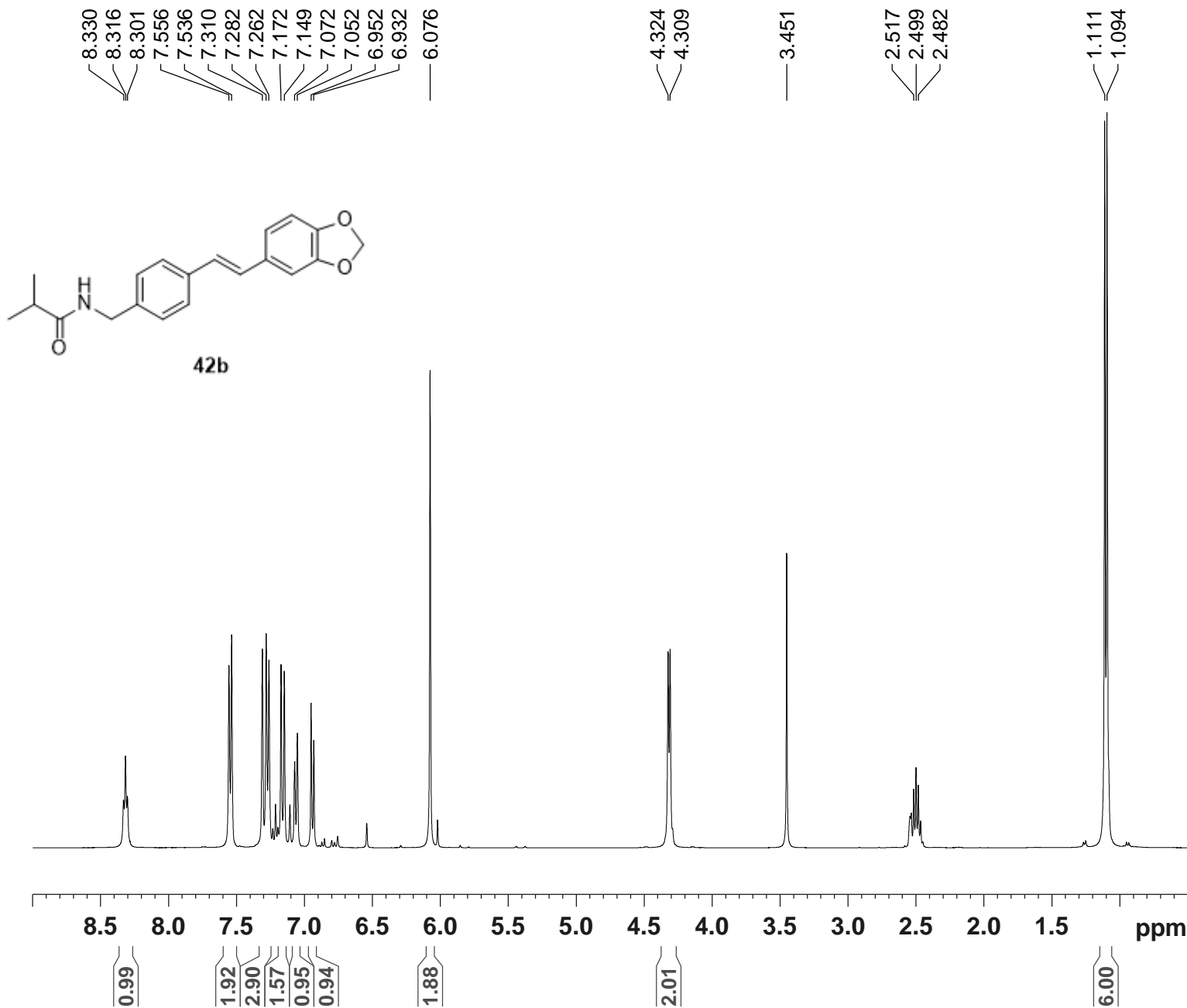
NAME MCX-2-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20161215
Time 11.08 h
INSTRUM spect
PROBHD Z116098_0436 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P1 10.00 usec
PLW1 68.03199768 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.00300026 W
PLW12 0.22284999 W
PLW13 0.11191000 W

F2 - Processing parameters

SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters

NAME MCX-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

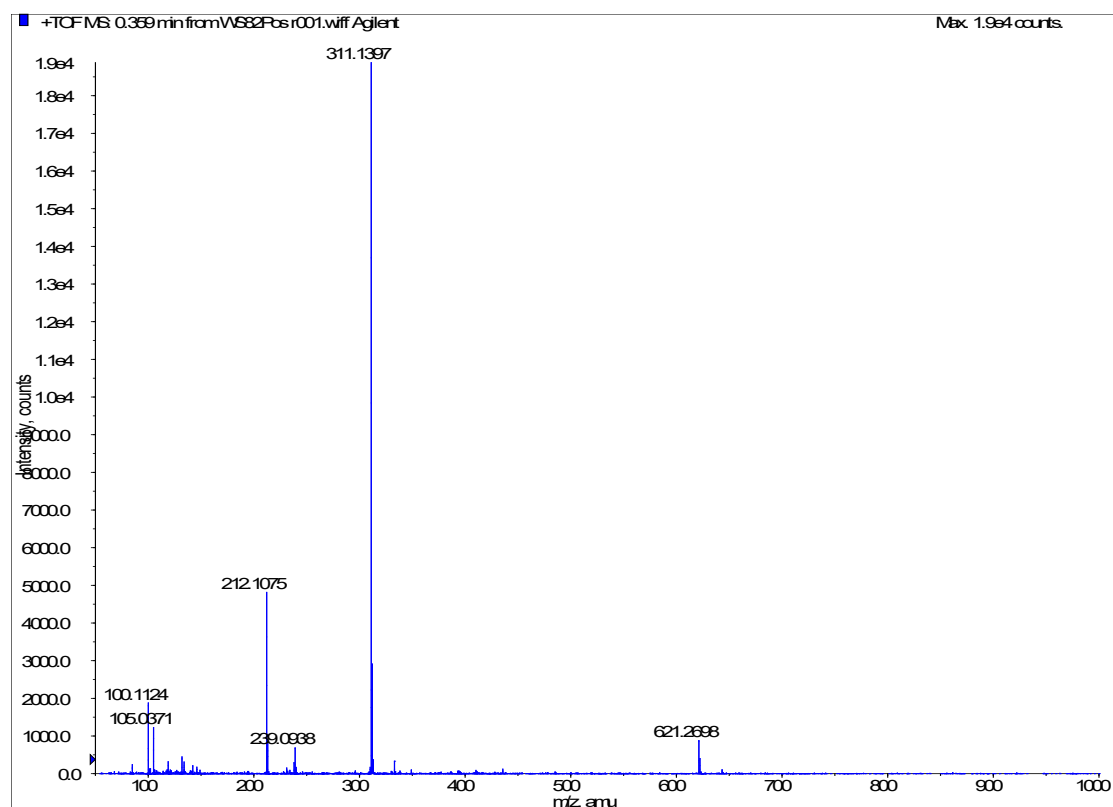
Date_ 20161214
Time 13.13 h
INSTRUM spect
PROBHD Z116098_0436 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 13.82
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P1 9.75 usec
PLW1 15.00300026 W

F2 - Processing parameters

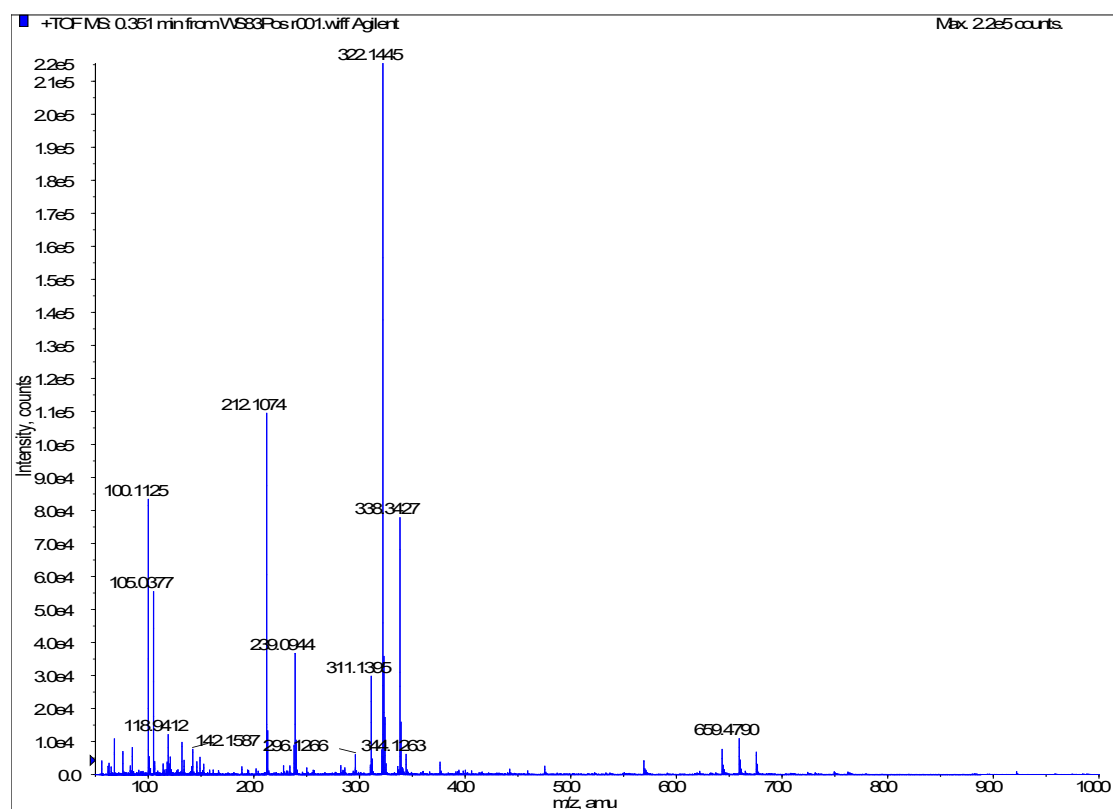
SI 65536
SF 400.1499852 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

HRMS for the representative compounds.

8c



8d



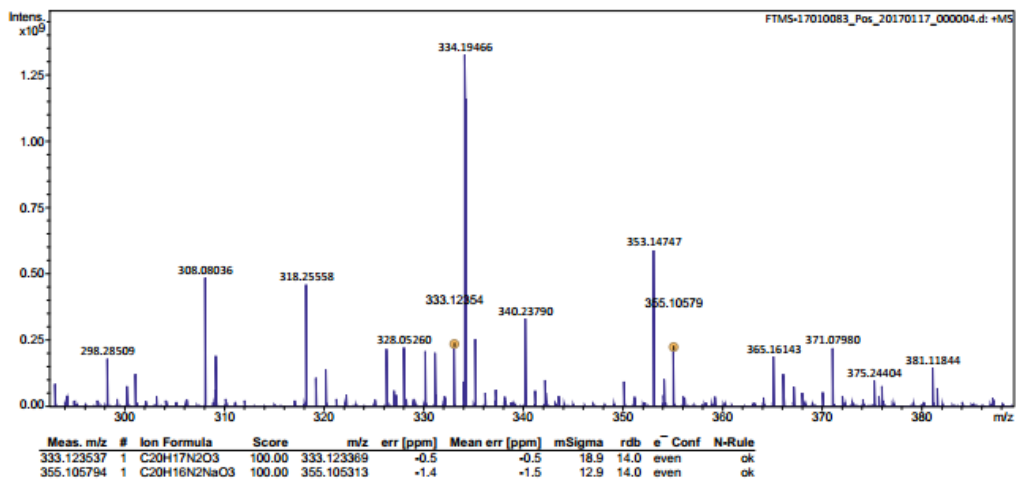
8e

Peking University Mass Spectrometry Sample Analysis Report

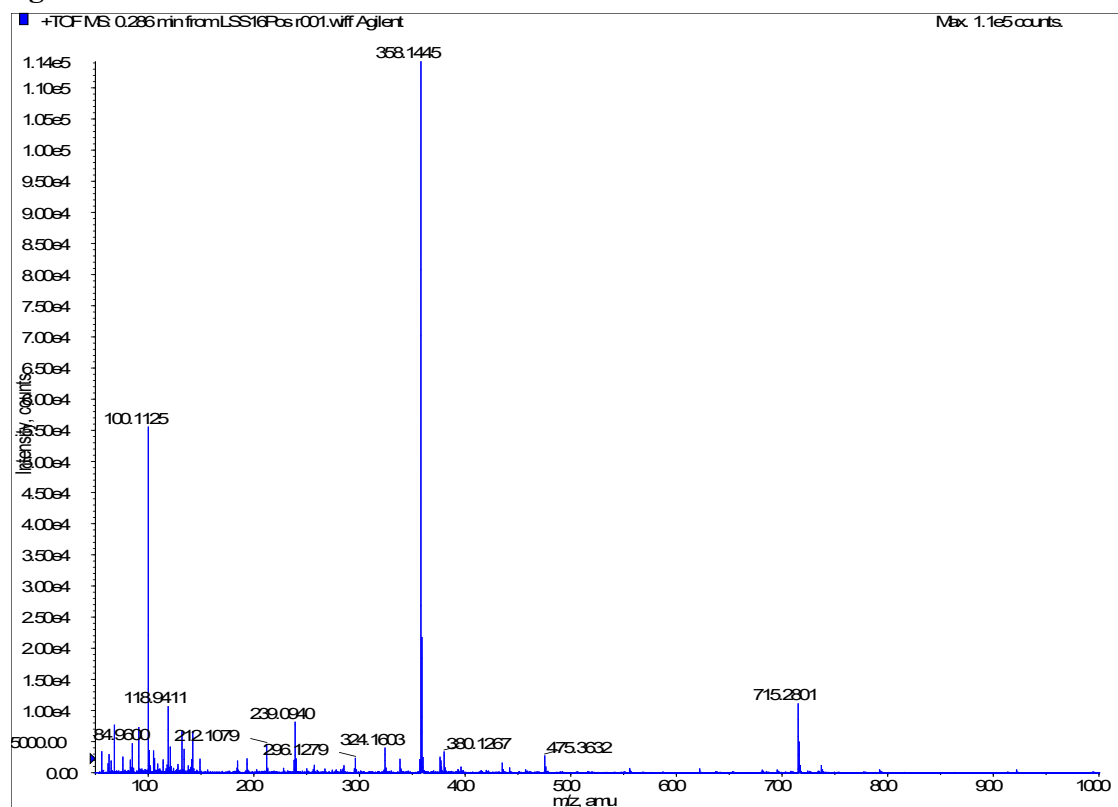
Analysis Info

Analysis Name FTMS-17010083_Pos_20170117_000004.d
Sample LSS-50
Comment

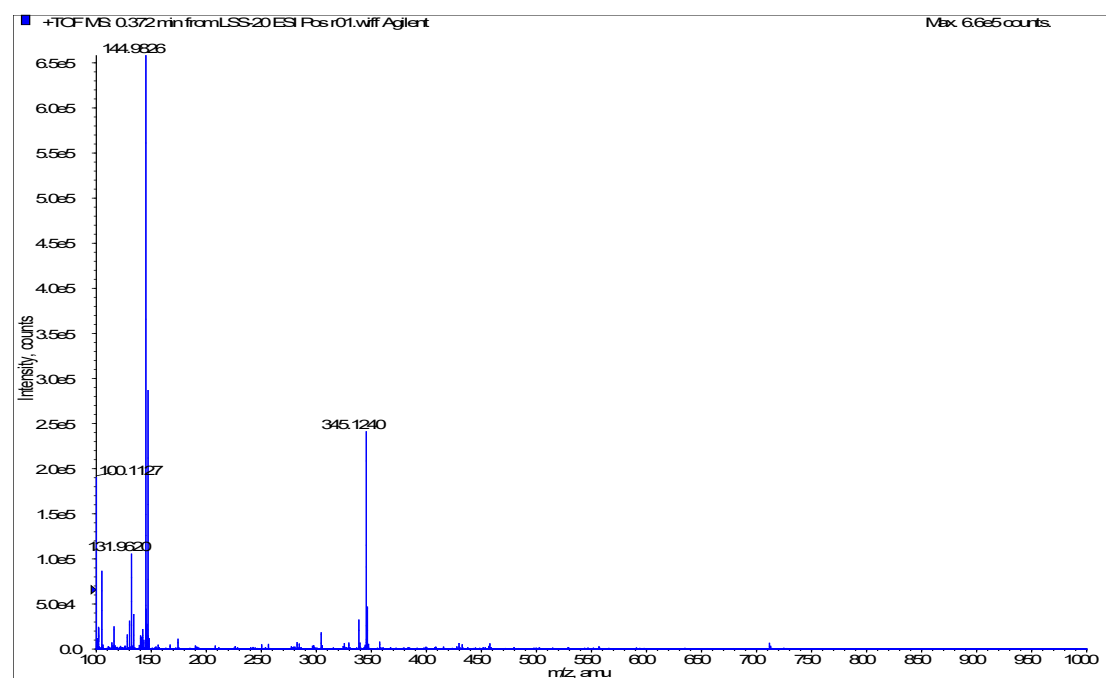
Acquisition Date 1/17/2017 3:18:35 PM
Instrument Bruker Solarix XR FTMS
Operator Peking University



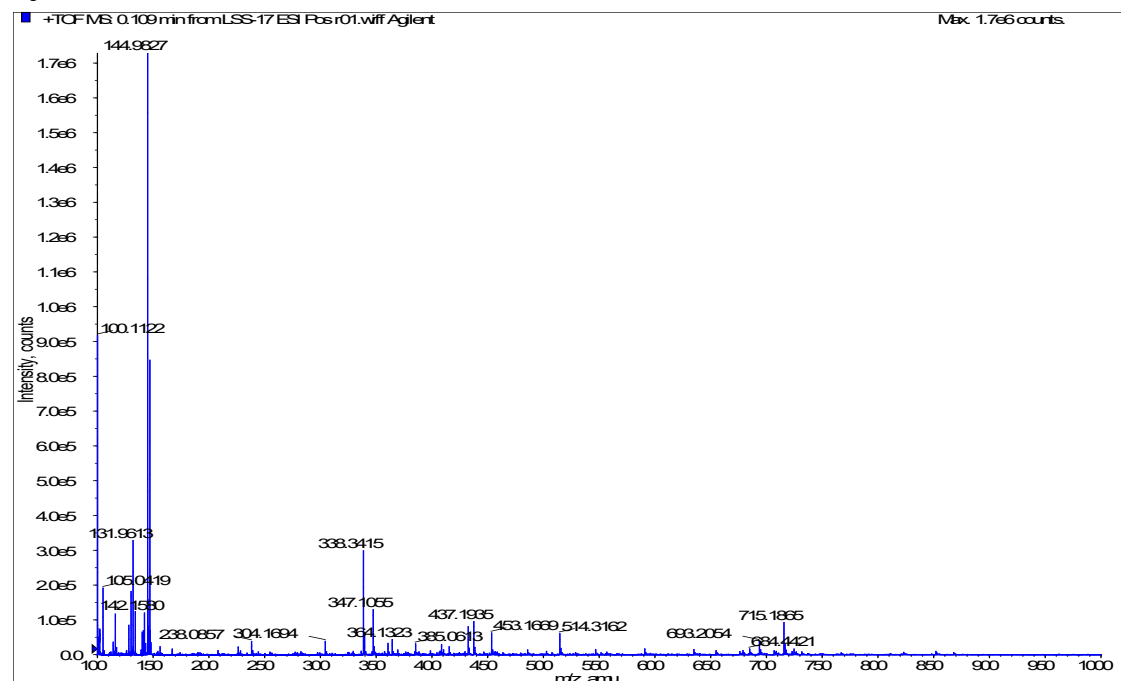
8g



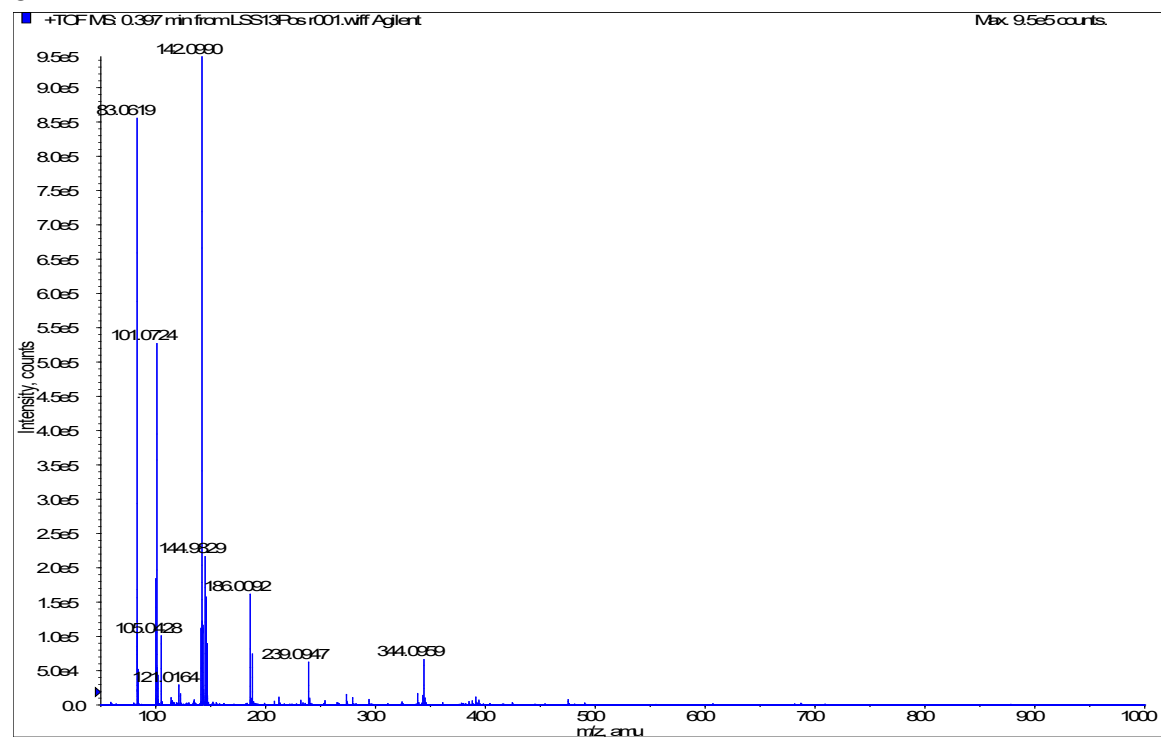
8h



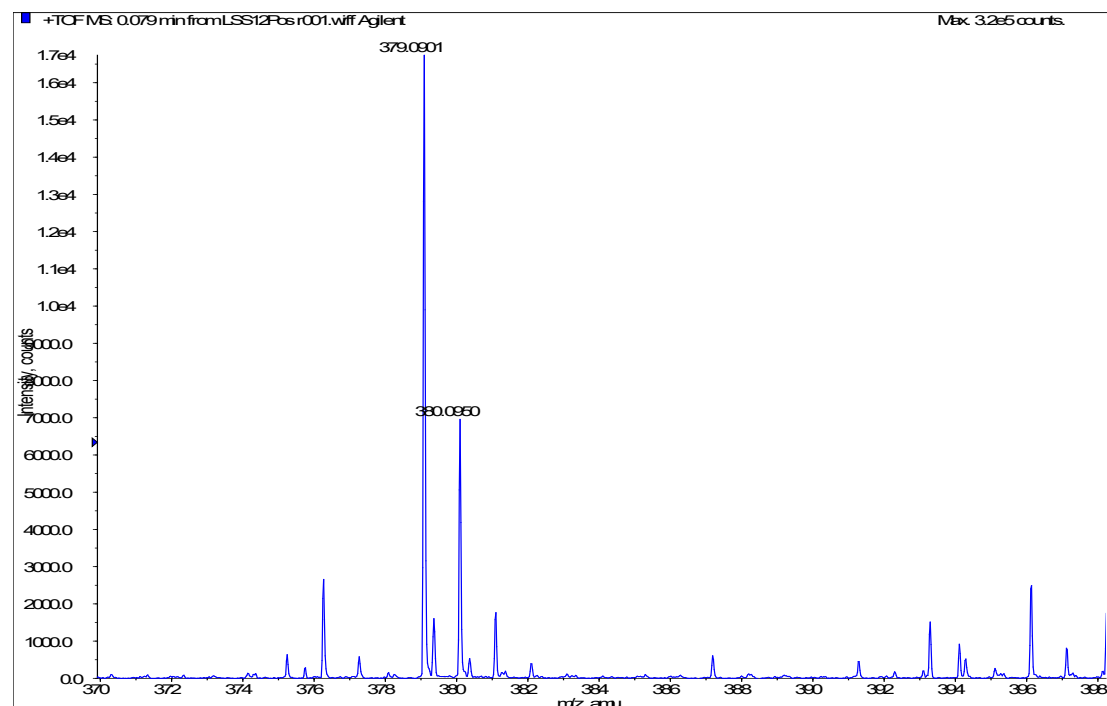
8j



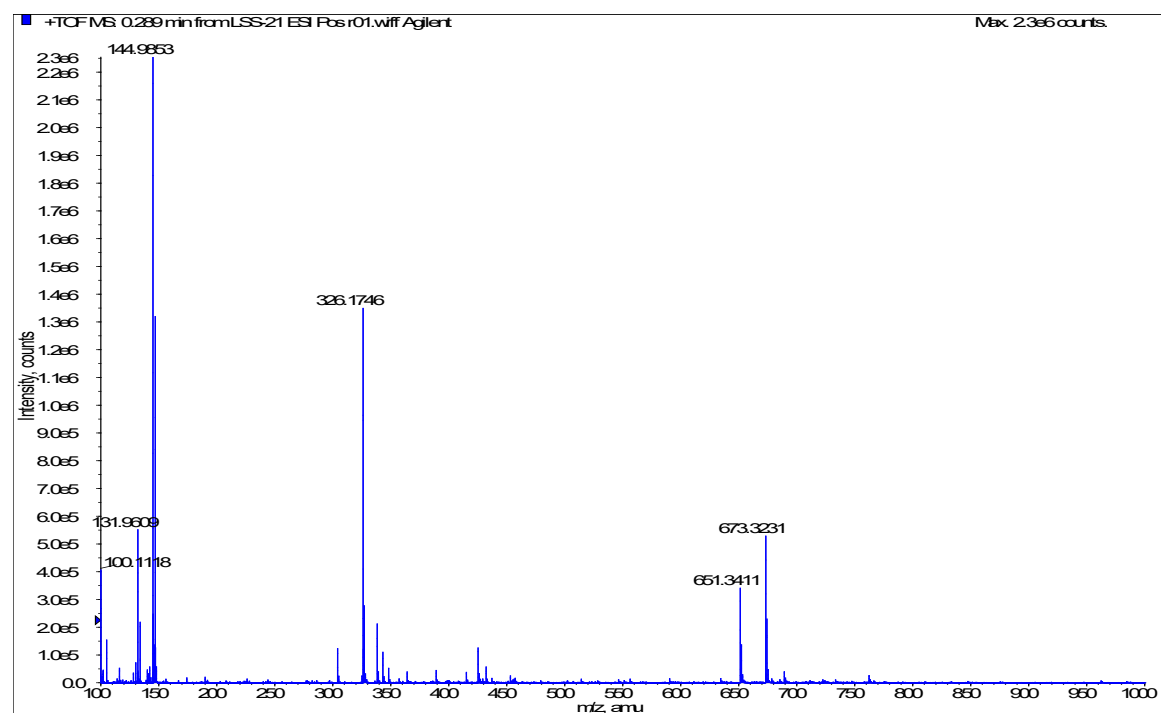
8k



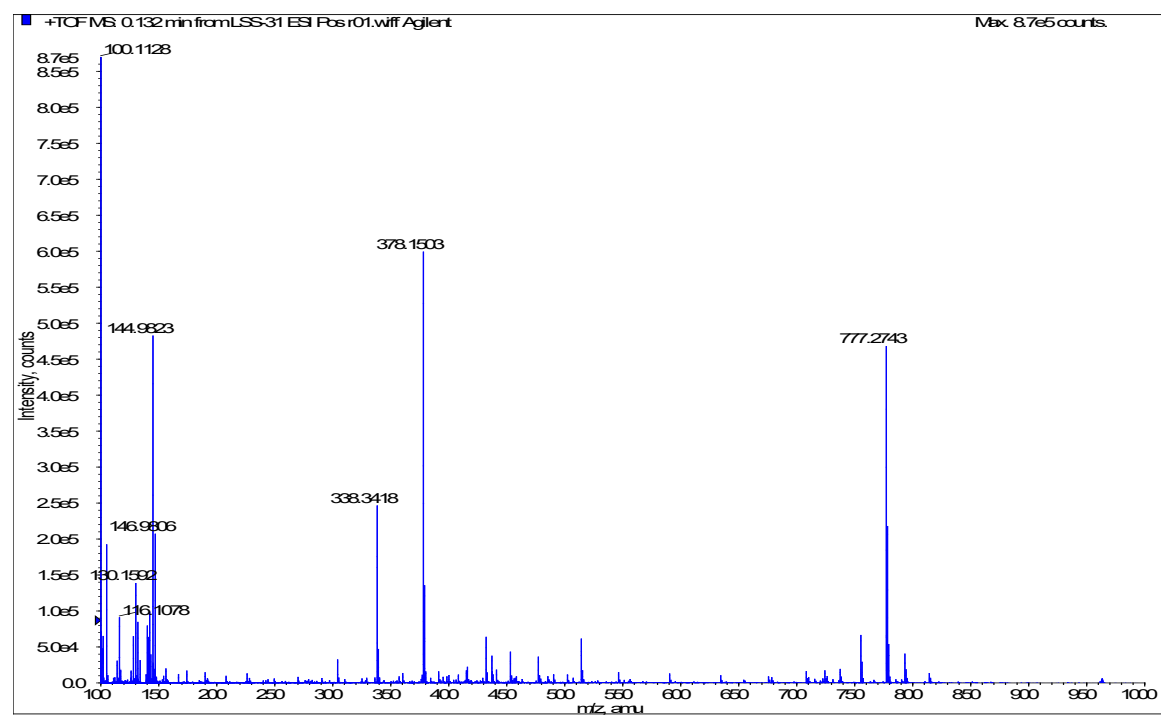
8l



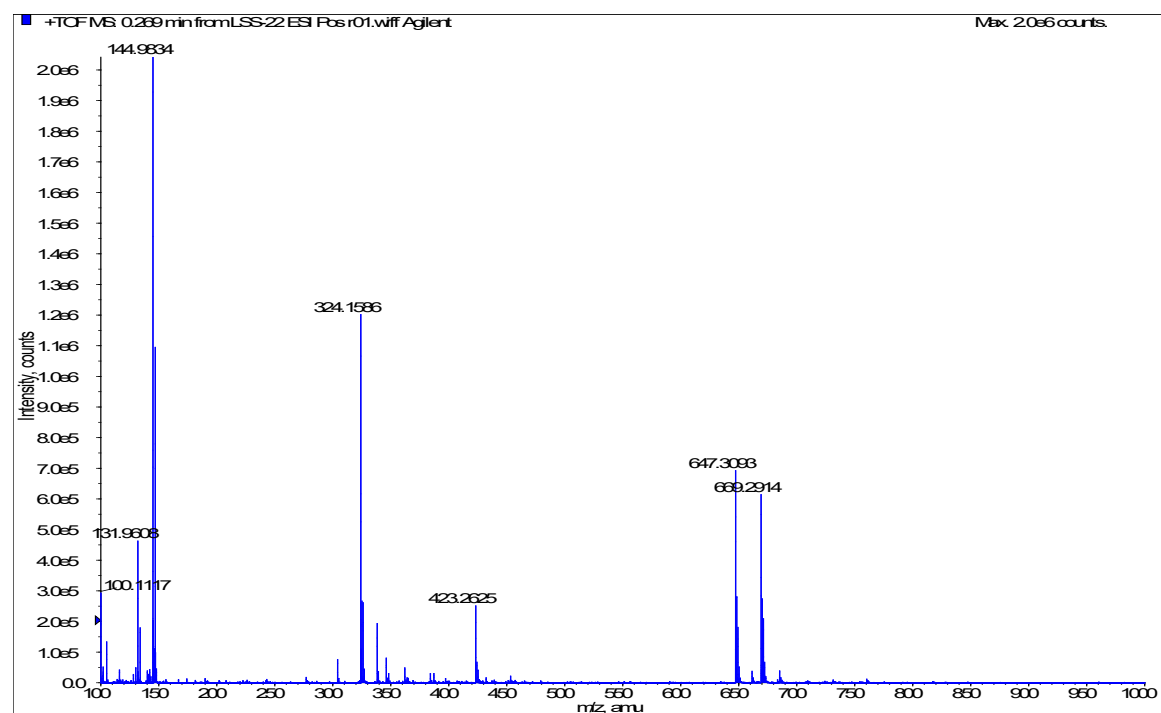
9b



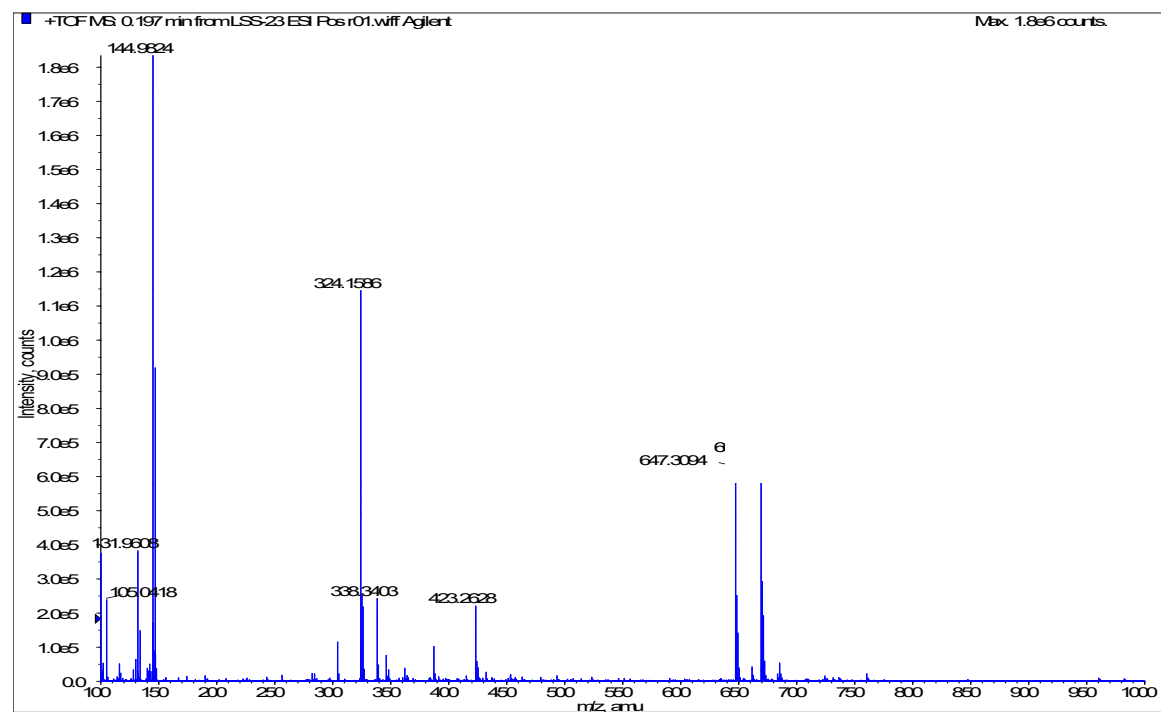
12f



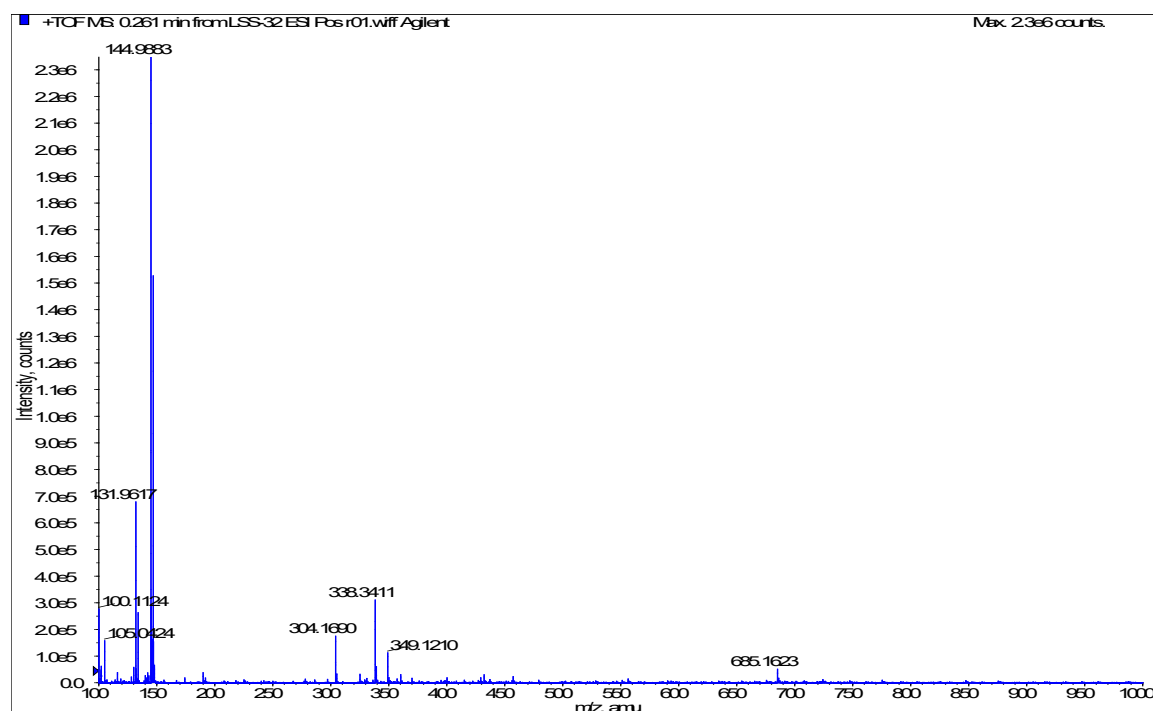
18b



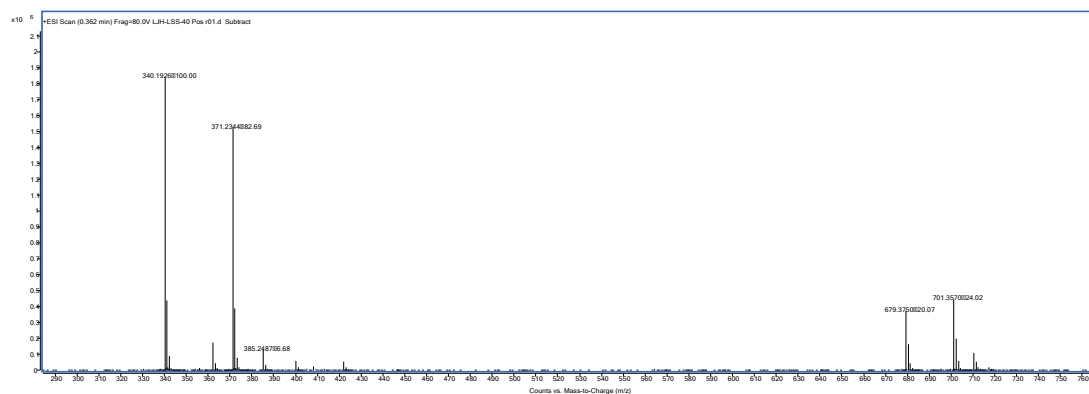
23b



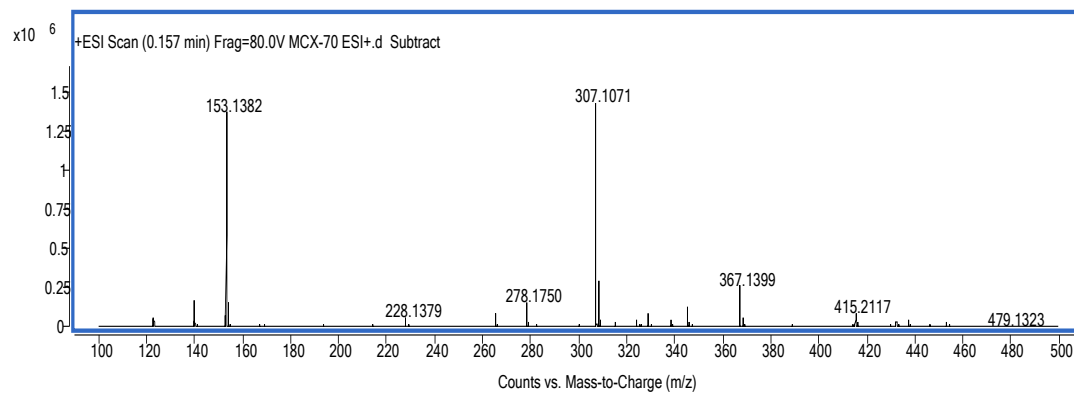
23i



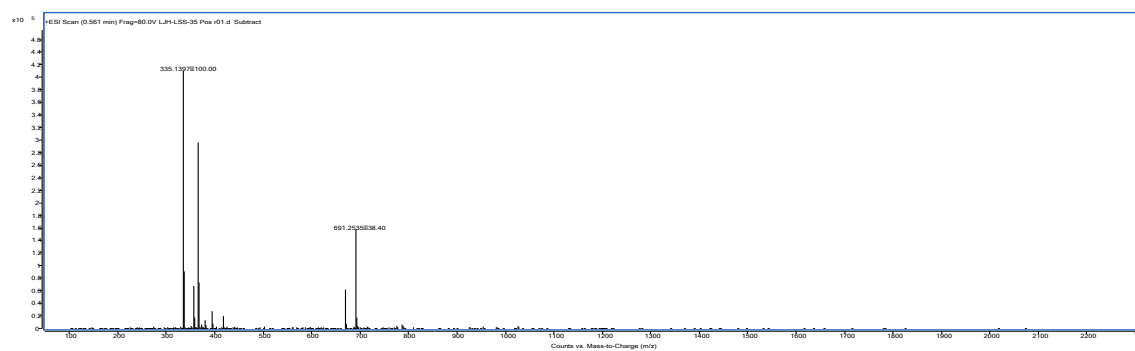
24b



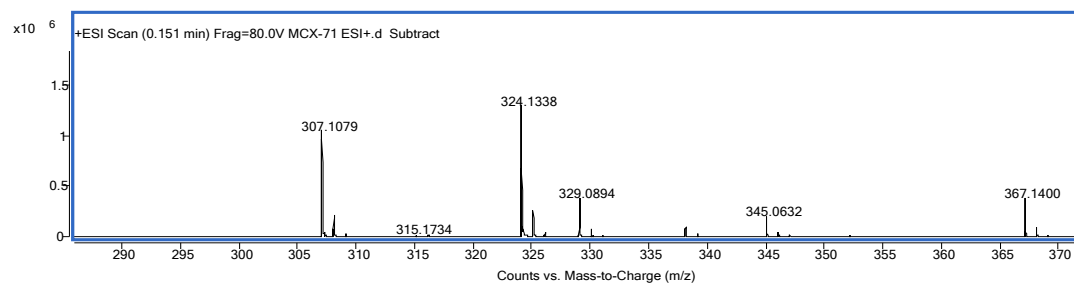
29a



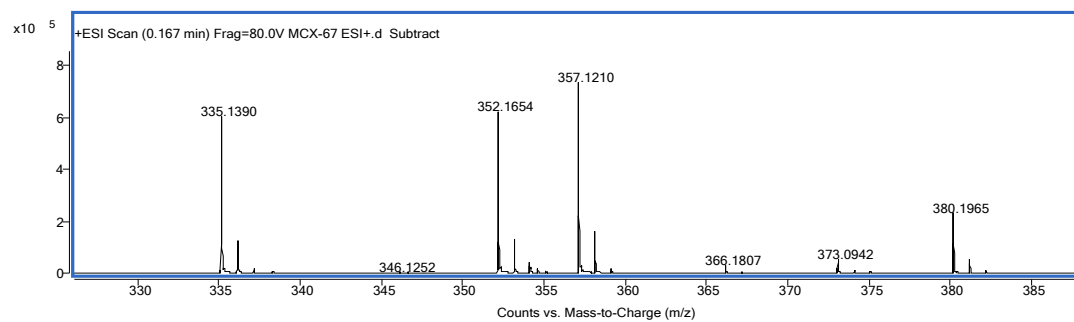
29b



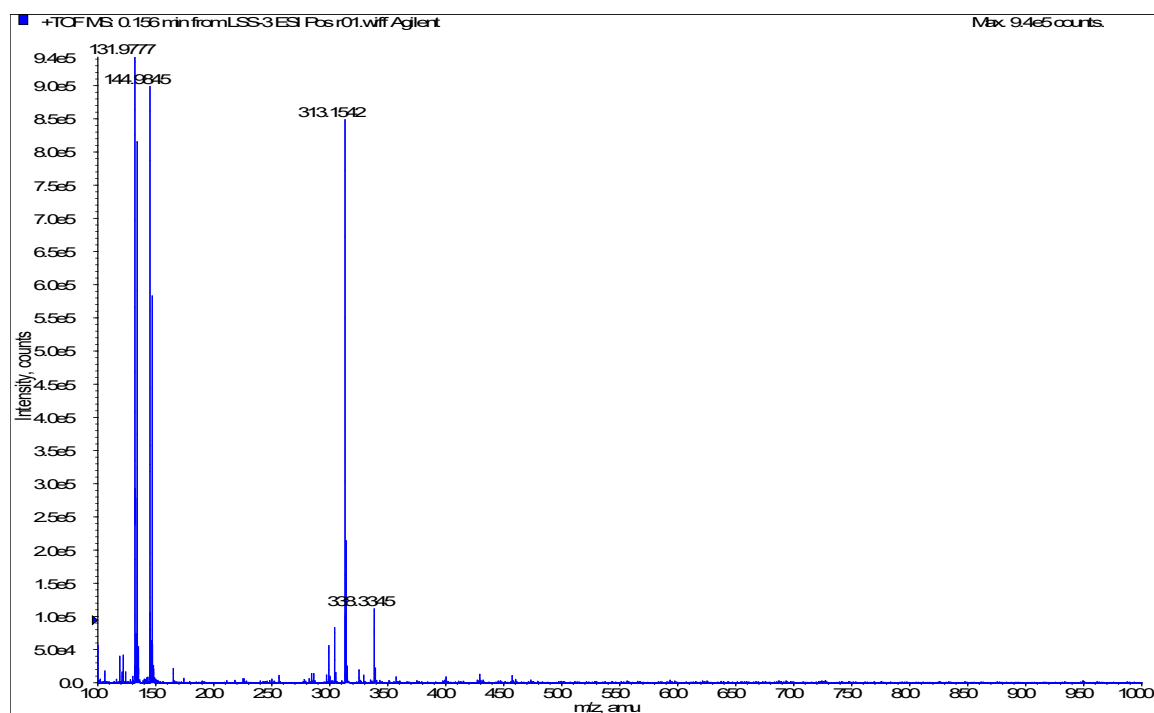
32a



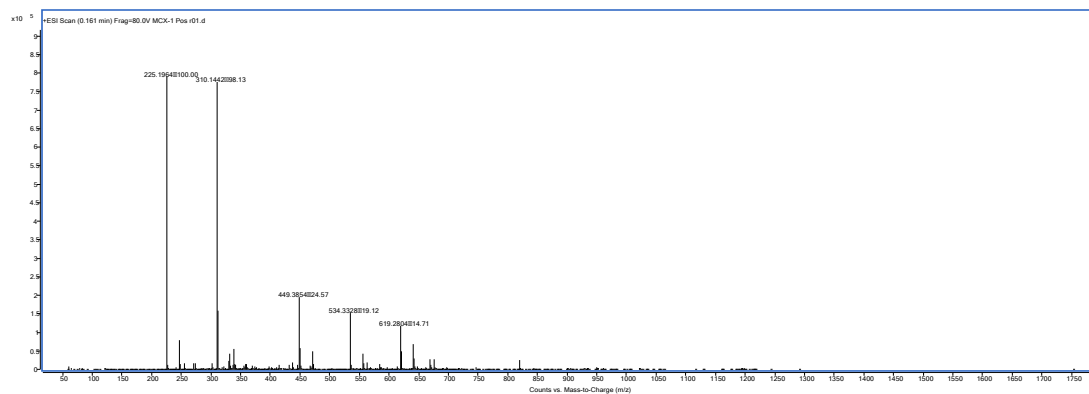
32b



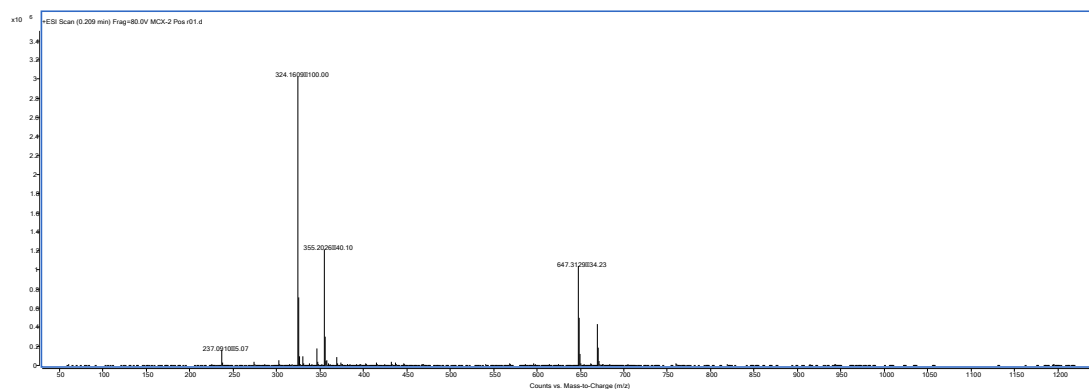
36a



39b



42b



Pharmacokinetic experimental conditions of compound **32b**.

LC-MS method: It was performed on a Thermo Scientific Q Exactive HF-X instrument, the column was an ACQUITY UPLC BEH C18 Column, 130 Å, 1.7 µm, 2.1 mm×100 mm, and the pre-column was an ACQUITY UPLC BEH C18 VanGuard Pre- column, 130Å, 1.7 µm, 2.1 mm×5 mm, and the liquid-phase was based on gradient elution with acetonitrile and 0.1% aqueous formic acid, and the mass spectrometry was performed in positive ion mode. The drug concentration in plasma samples was quantified by internal standard method and the pharmacokinetic parameters were calculated by phoenix winnonlin.

Mass spectrometry conditions: **32b** mass spectrometry acquisition mode is positive ion mode, the molecular weight of the precursor ion is $[M+H]^+$: 335.1384, the molecular weight of the daughter ion is: 265.0969.

Column Details:	ACQUITY UPLC BEH C18 Column (1.7 µm, 2.1 mm×100 mm)
Column Temperature:	30°C
Flow Rate:	0.3 mL/min
Injection volum:	3 µL

Solvent A: 0.1% formic acid in water; Solvent B: acetonitrile.

Time	Solvent A	Solvent B
0	60	40
2	60	40
3	2	98
10	2	98
11	60	40
13	60	40

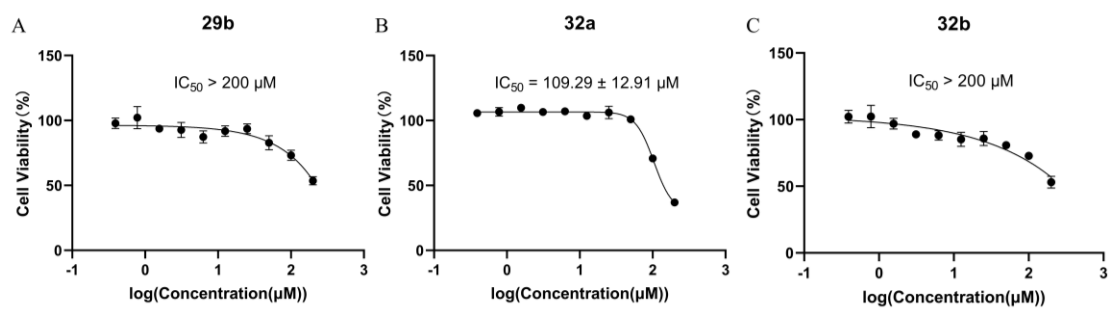


Figure S1. Results of dose-toxicity experiment for compounds **29b**, **32a**, and **32b**.