

SUPPLEMENTAL MATERIALS

for

(E)-N'-Arylidene-2-(4-oxoquinazolin-4(3H)-yl)acetohydrazides: Synthesis and Evaluation of Caspase Activation Activity and Cytotoxicity

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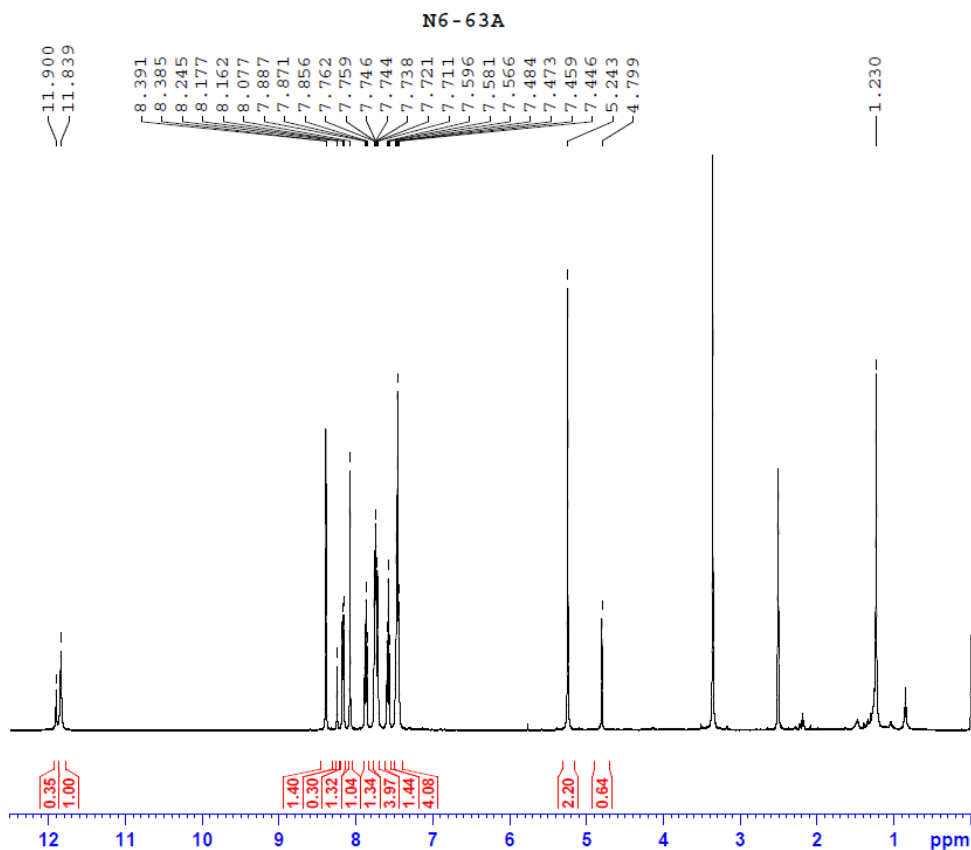
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Keywords: Acetohydrazides, quinazolin-4-one, cytotoxicity, caspase activation.

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ALL ¹H & ¹³C NMR SPECTRA OF THE COMPOUNDS

¹H NMR of compound 5a



Current Data Parameters
 NAME N6-63A
 EXPNO 12
 PROCNO 1

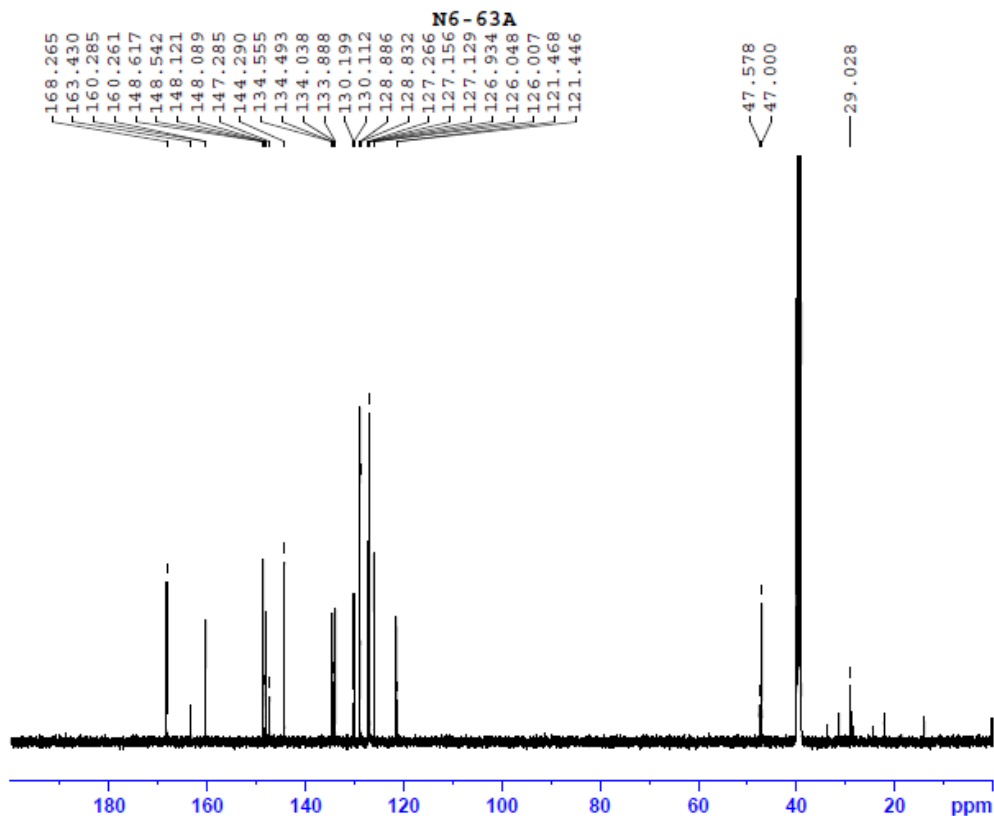
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 Time 9.43
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 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 296.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SF01 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

----- CHANNEL f2 -----
 SF02 500.1320005 MHz
 NUC2 1H
 CPOPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7578474 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹³C NMR of compound 5a



Current Data Parameters
 NAME N6-63A
 EXPNO 12
 PROCNO 1

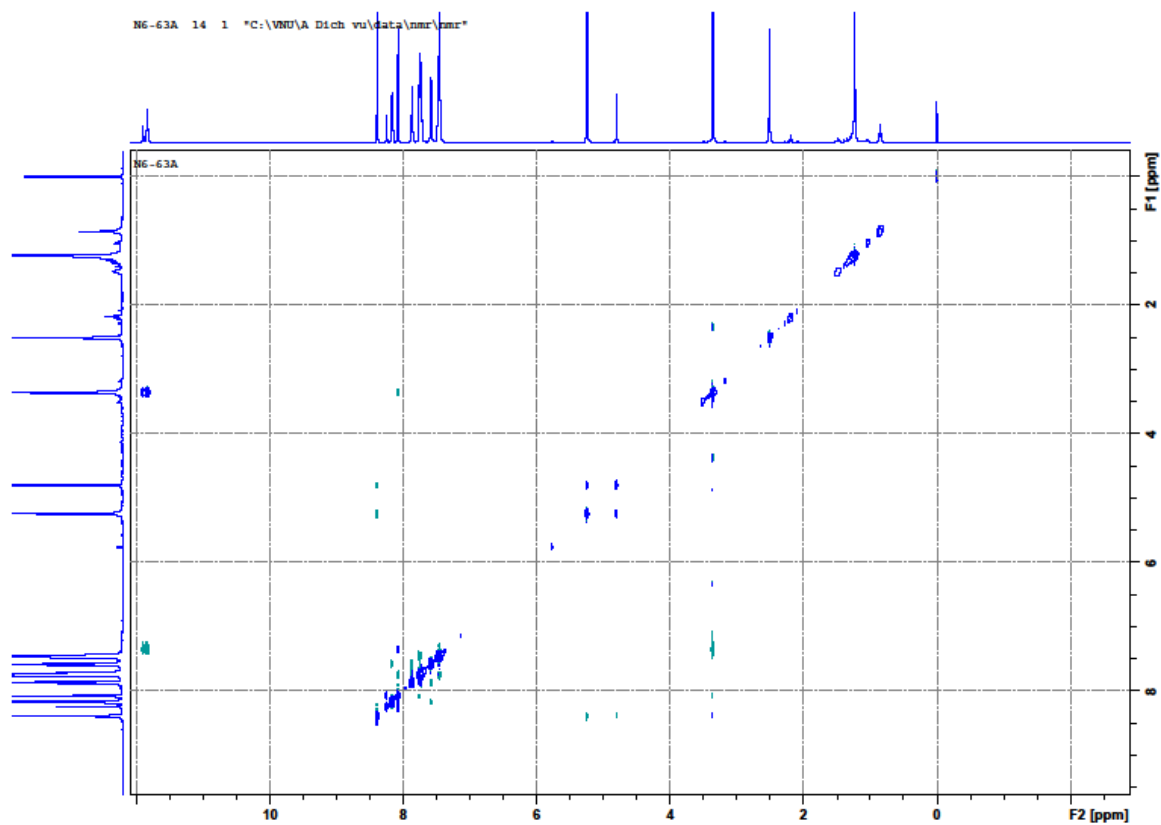
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 Time 9.43
 INSTRUM spect
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 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 296.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SF01 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

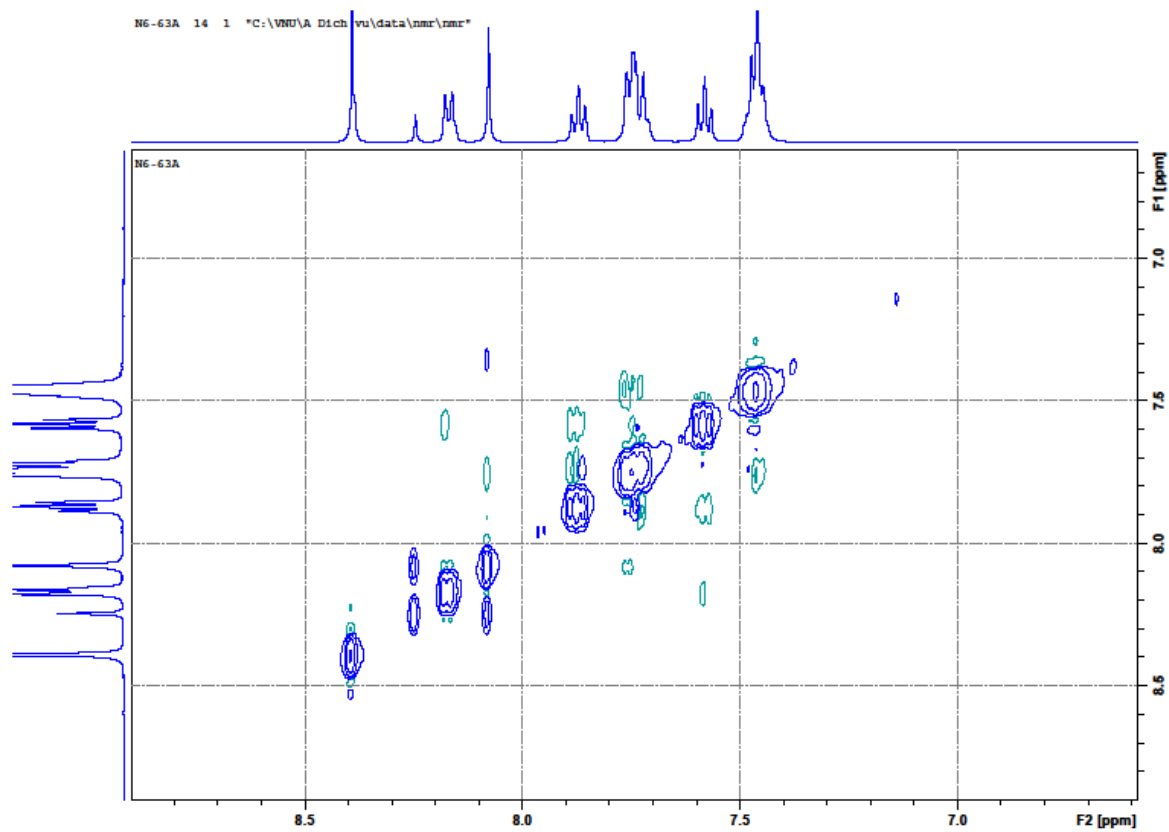
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 SF02 500.1320005 MHz
 NUC2 1H
 CPOPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7578474 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

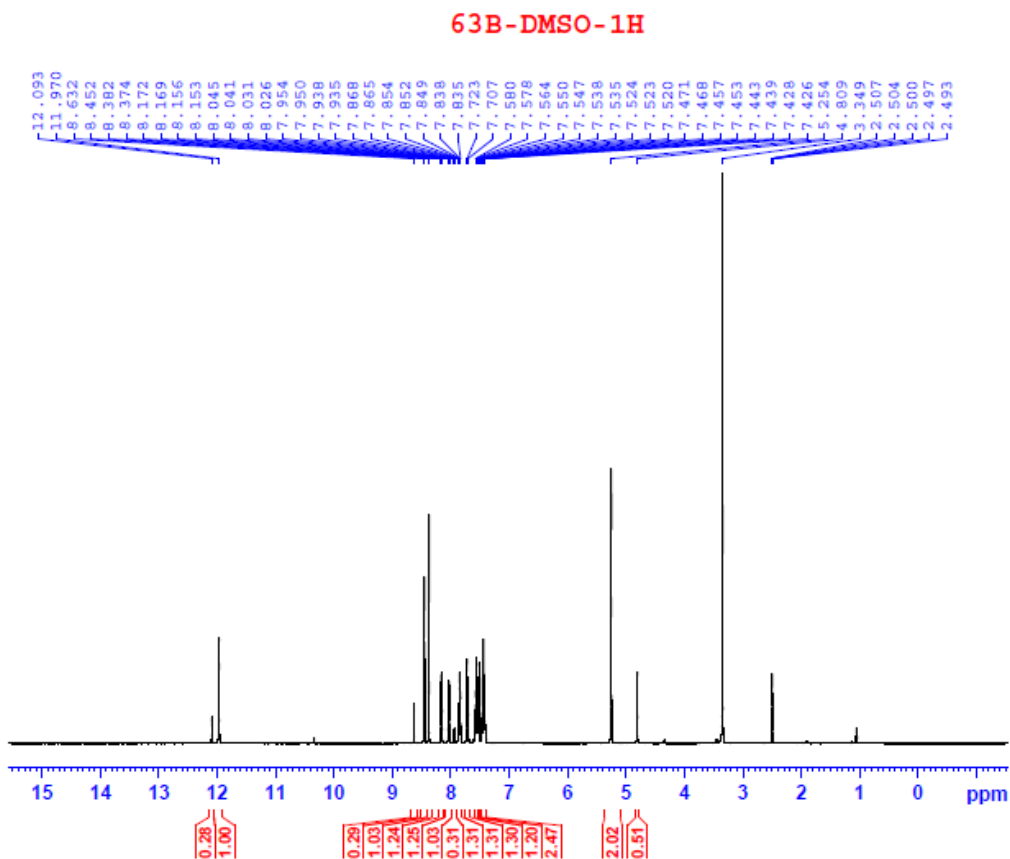
NOESY-1 of compound 5a



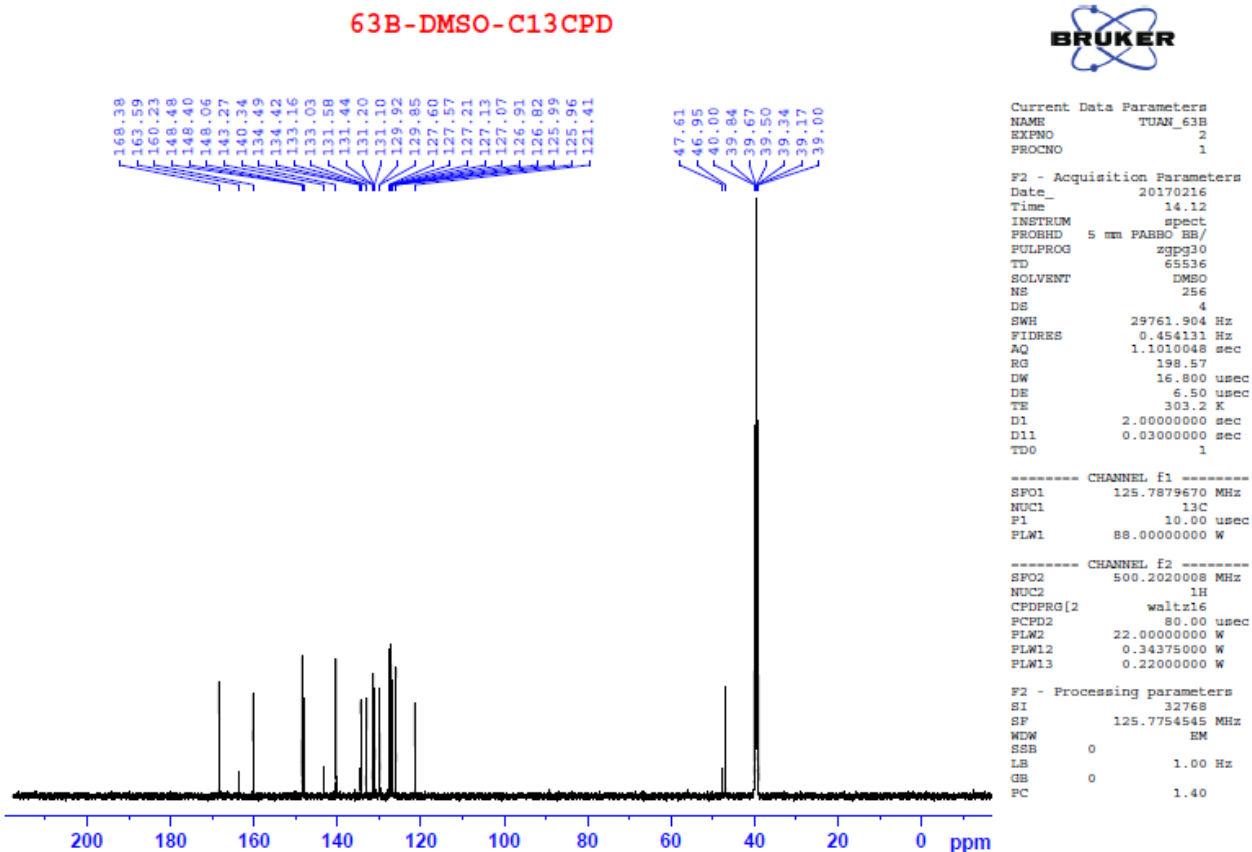
NOESY-2 of compound 5a



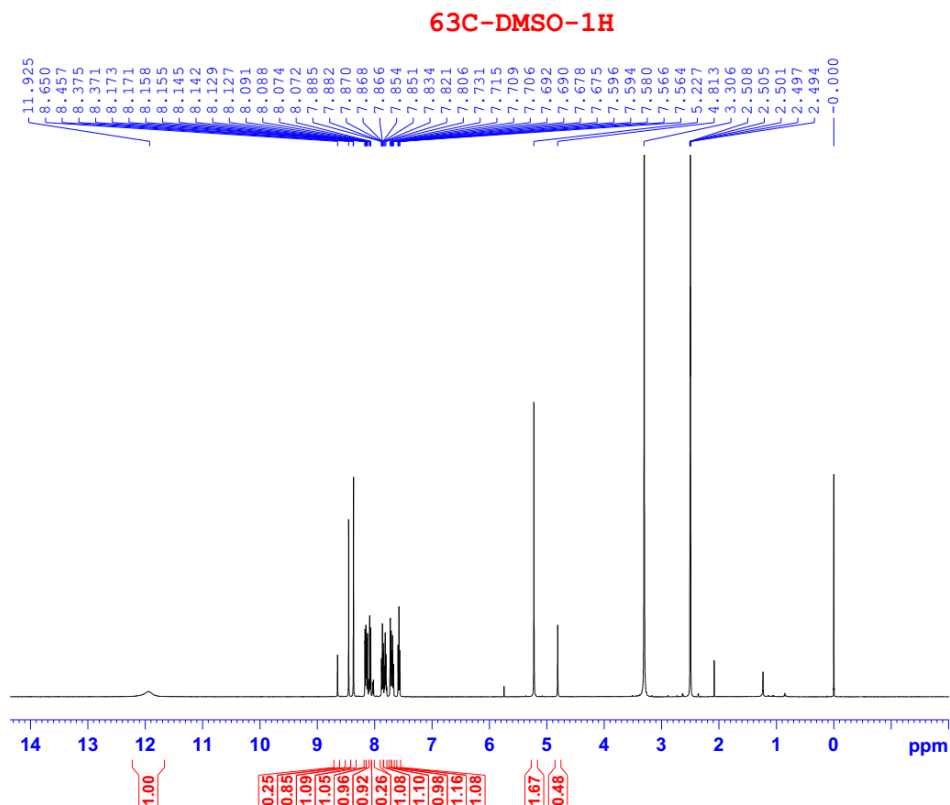
¹H NMR of compound 5b



¹³C NMR of compound 5b



¹H NMR of compound 5c



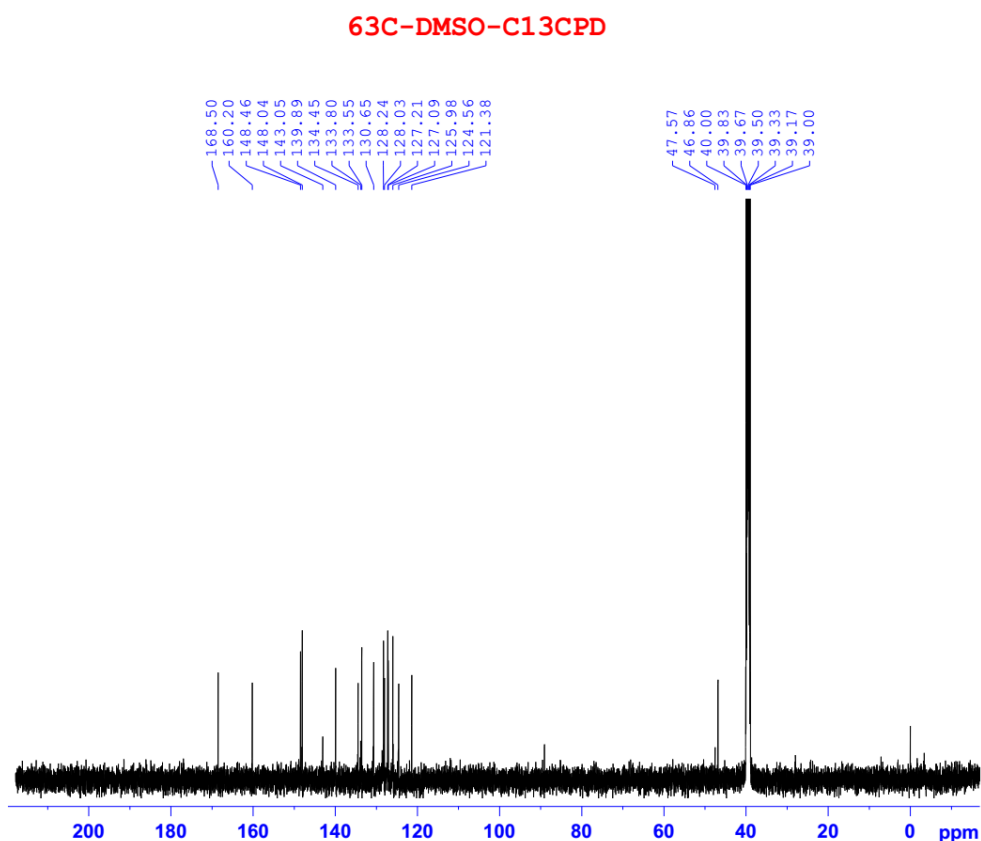
Current Data Parameters
 NAME TUAN_63C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20170321
 Time 16.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 175.34
 DW 50.000 usec
 DE 6.50 usec
 TE 303.2 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 500.2030889 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 22.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.2000046 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5c



Current Data Parameters
 NAME TUAN_63C
 EXPNO 2
 PROCNO 1

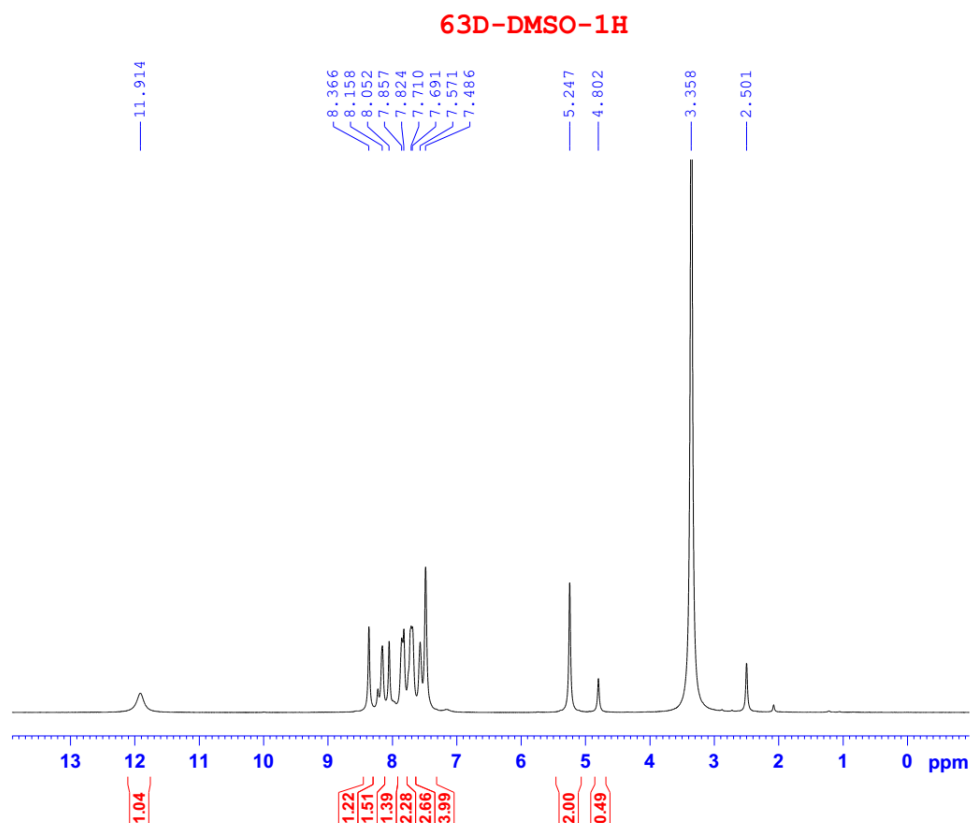
F2 - Acquisition Parameters
 Date 20170322
 Time 2.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 198.57
 DW 16.800 usec
 DE 6.50 usec
 TE 303.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 125.7879670 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 88.00000000 W

===== CHANNEL f2 =====
 SFO2 500.2020008 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 22.00000000 W
 PLW12 0.34375000 W
 PLW13 0.22000000 W

F2 - Processing parameters
 SI 32768
 SF 125.7754570 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR of compound 5d



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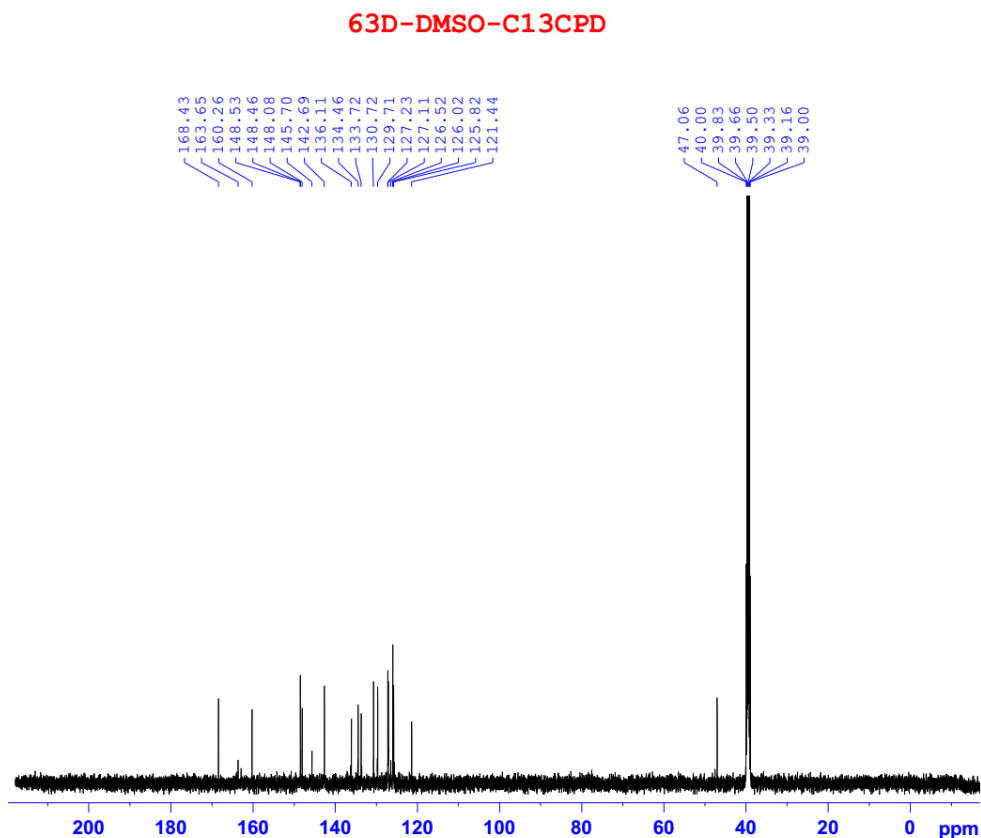
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NAME          TUAN_63D
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20170412
Time_         15.51
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            16
DS            2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            79.36
DW            50.000 usec
DE            6.50 usec
TE            302.7 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          500.2030889 MHz
NUC1           1H
P1            10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI            65536
SF            500.2000083 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
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¹³C NMR of compound 5d



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Current Data Parameters
NAME          TUAN_63D
EXPNO         2
PROCNO        1

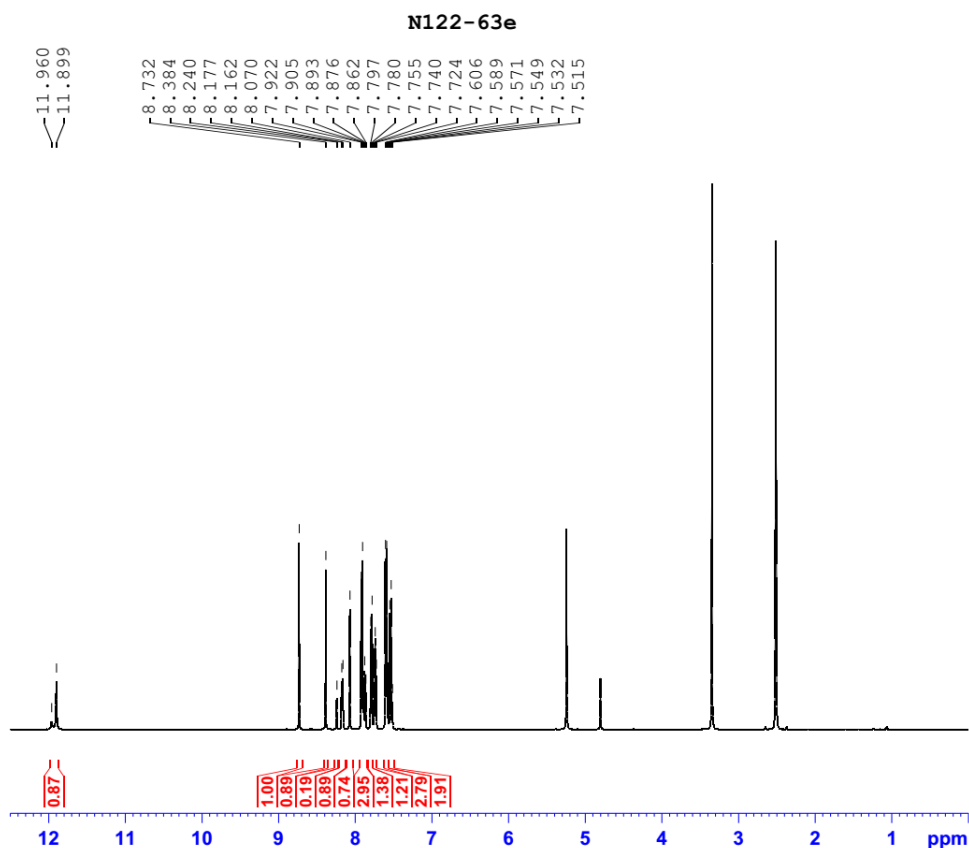
F2 - Acquisition Parameters
Date_         20170414
Time_         10.06
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            128
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG            198.57
DW            16.800 usec
DE            6.50 usec
TE            302.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          125.7879670 MHz
NUC1           13C
P1            10.00 usec
PLW1          88.00000000 W

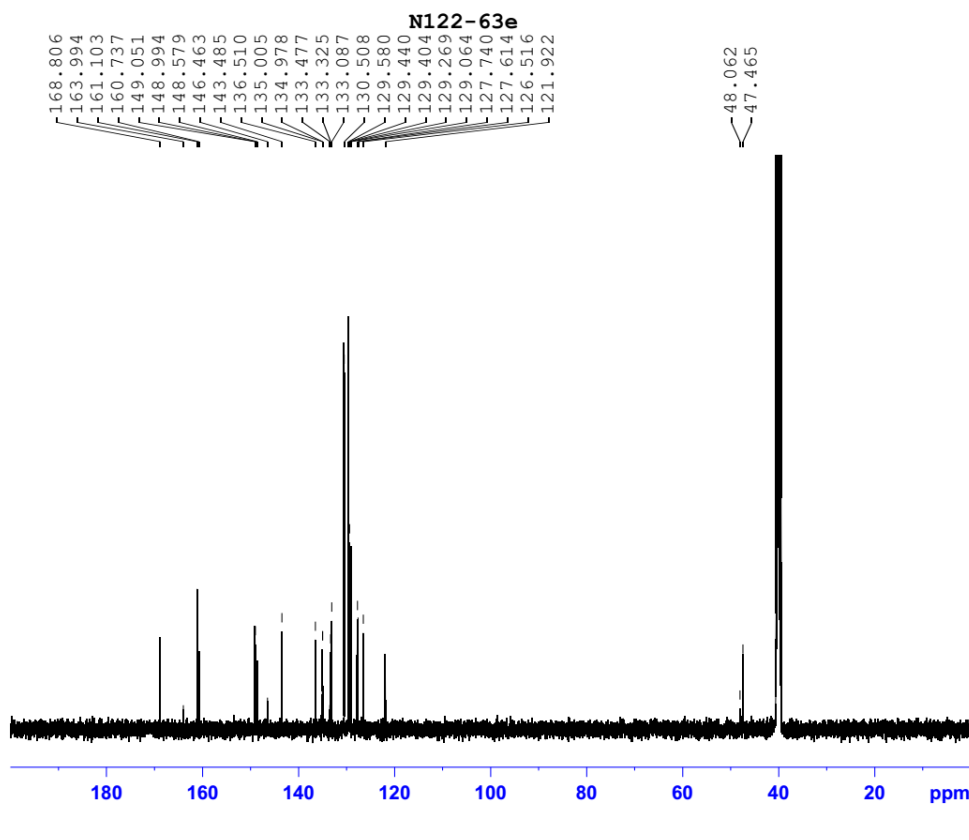
===== CHANNEL f2 =====
SFO2          500.2020008 MHz
NUC2           1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI            32768
SF            125.7754518 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
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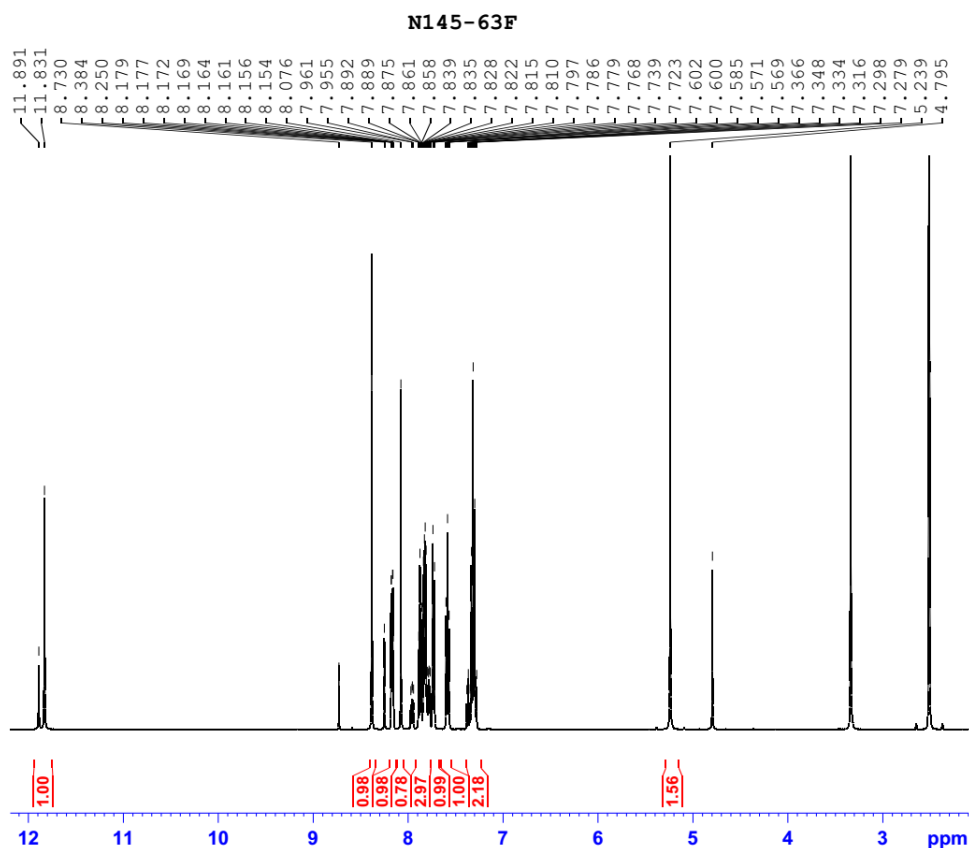
¹H NMR of compound 5e



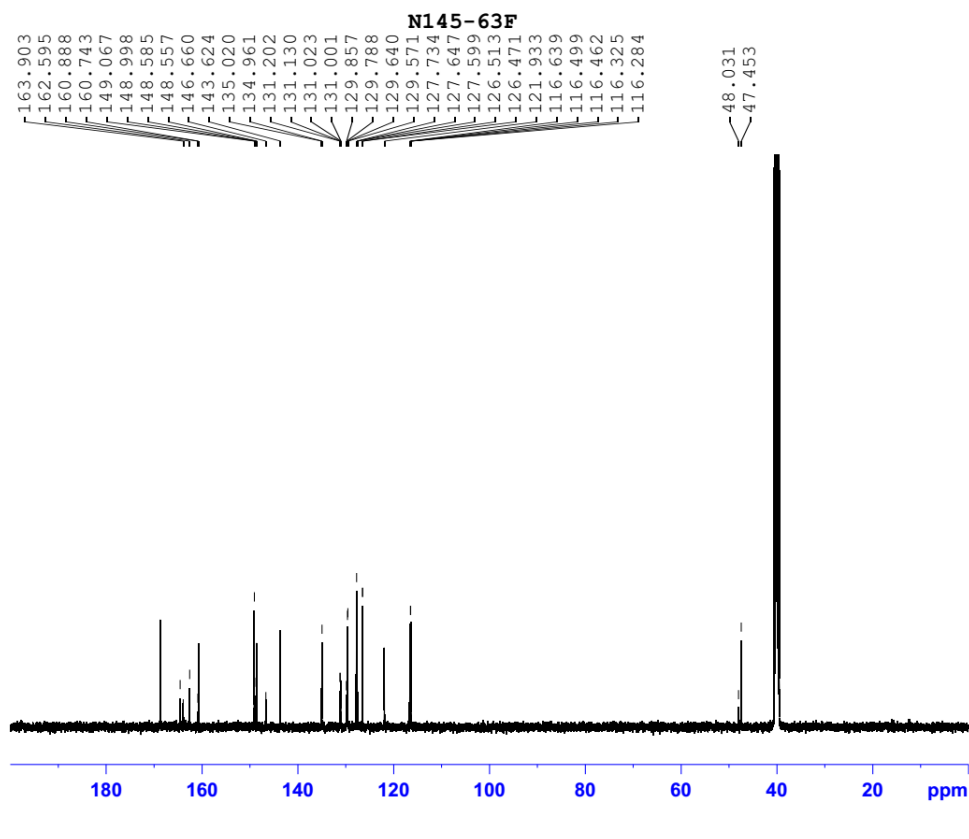
¹³C NMR of compound 5e



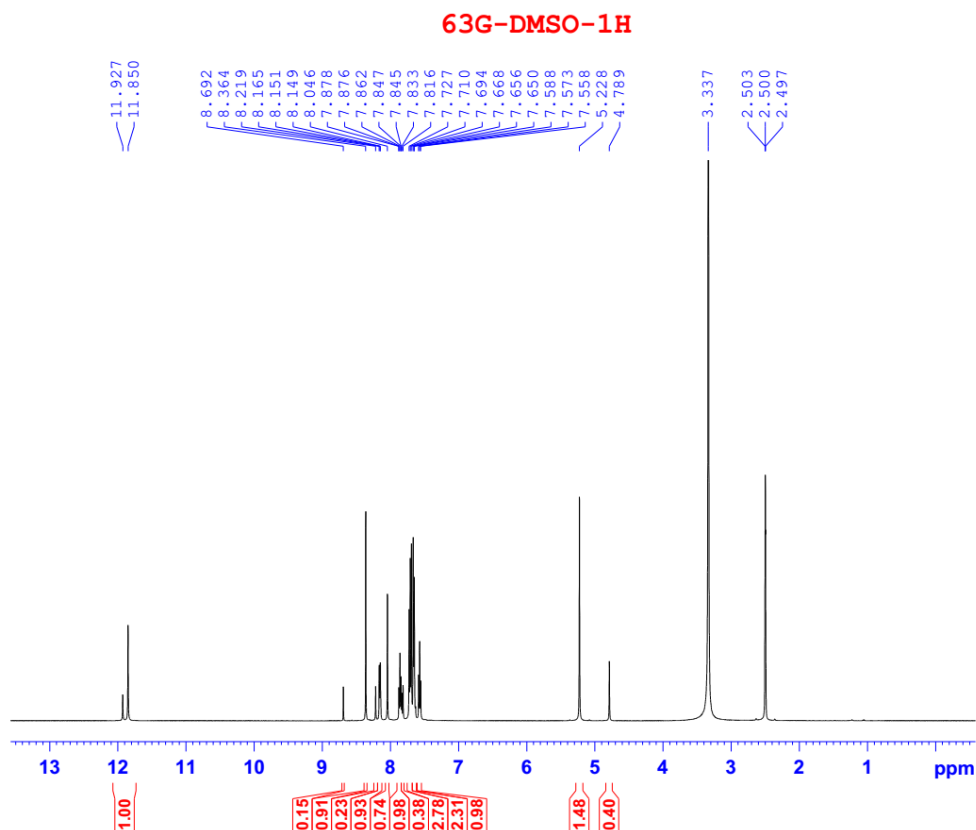
¹H NMR of compound 5f



¹³C NMR of compound 5f



¹H NMR of compound 5g



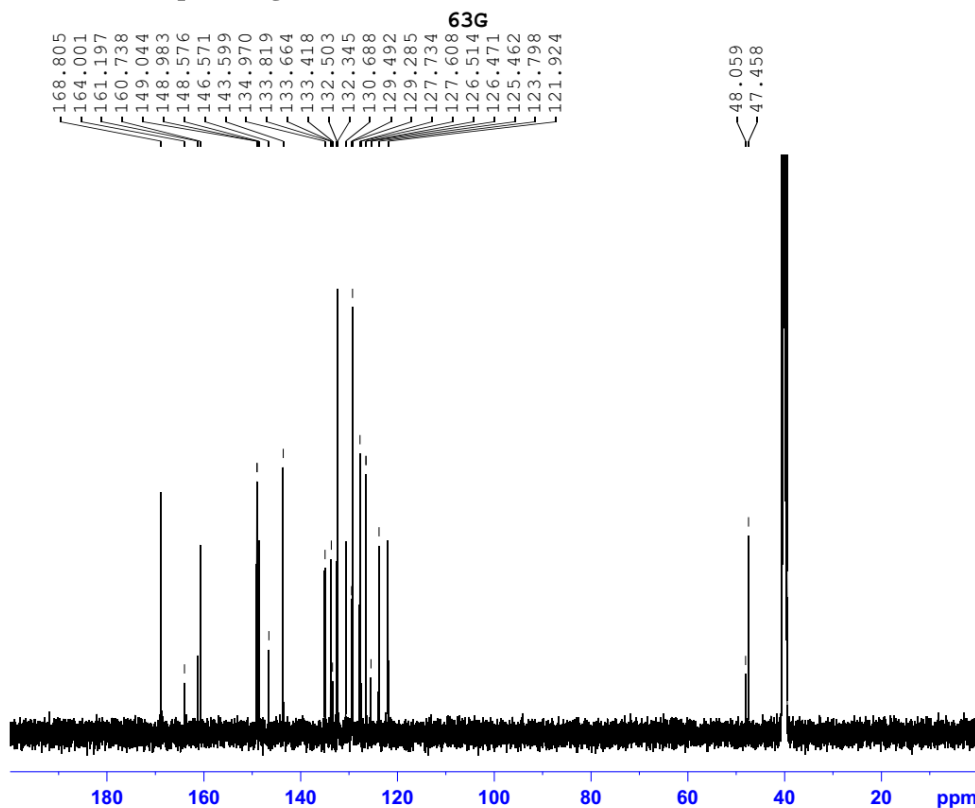
Current Data Parameters
 NAME TUAN_63G
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170308
 Time 15.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 97.76
 DW 50.000 usec
 DE 6.50 usec
 TE 303.1 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 500.2030889 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 22.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.2000063 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5g



Current Data Parameters
 NAME 63G
 EXPNO 41
 PROCNO 1

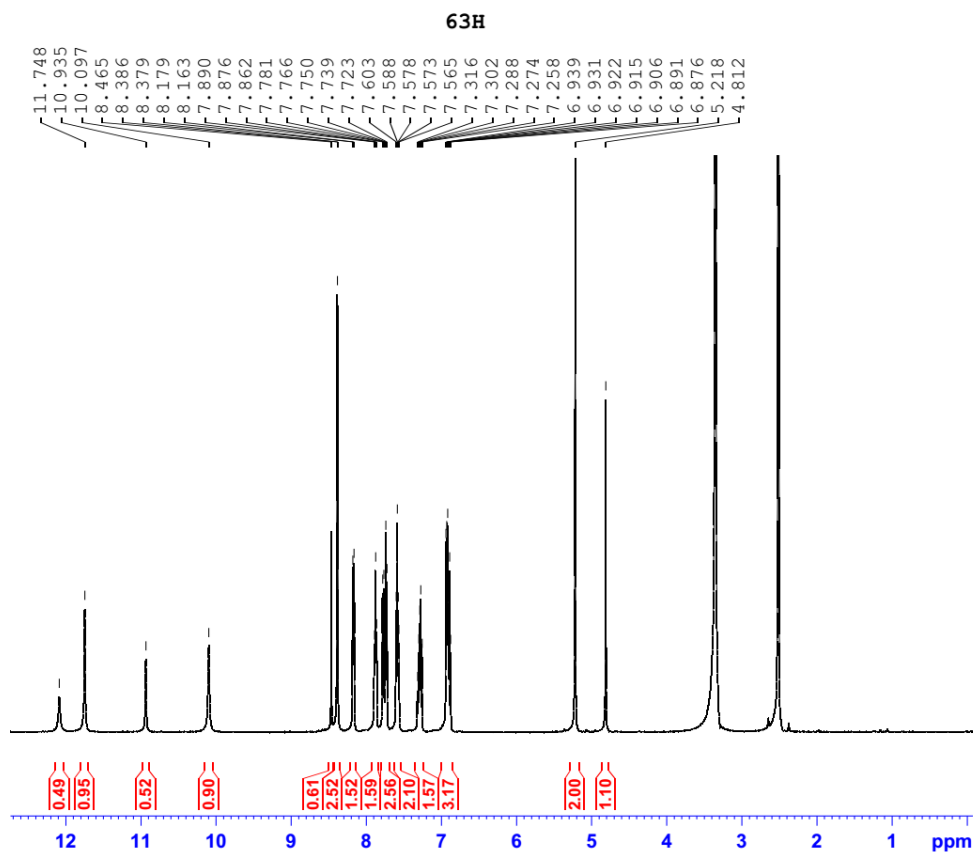
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 Time 0.05
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 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

----- CHANNEL f2 -----
 SFO2 500.1320005 MHz
 NUC2 1H
 CDPORG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR of compound 5h



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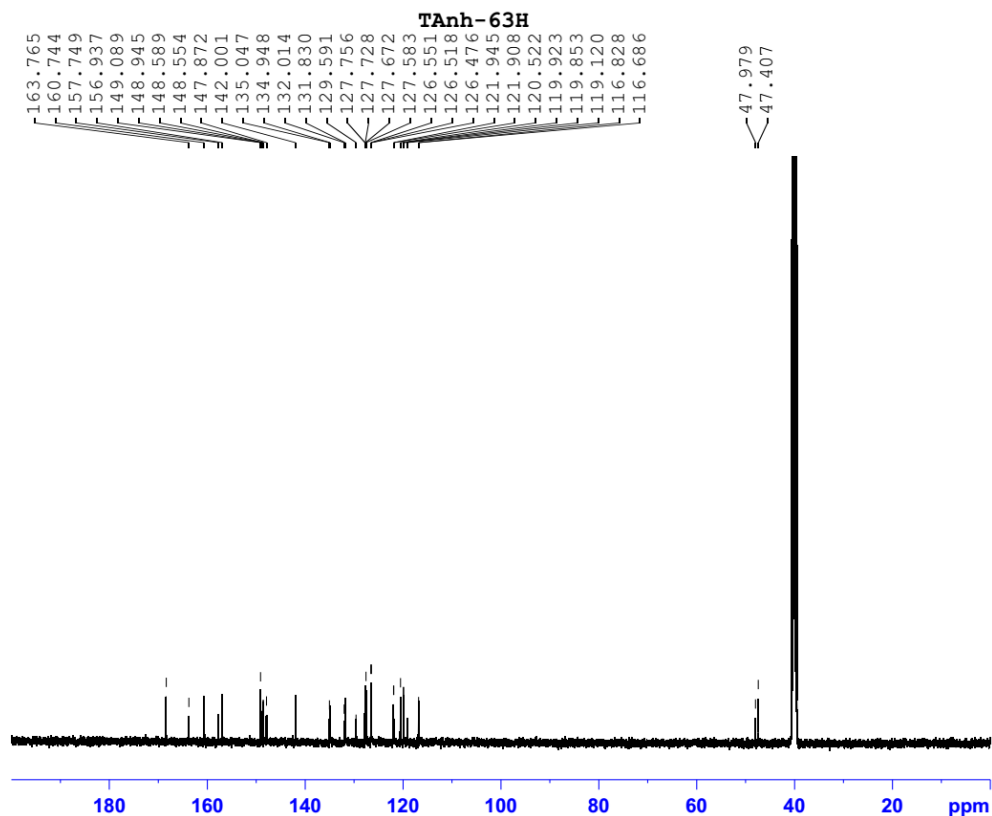
Current Data Parameters
NAME      N220 - 63H
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20170727
Time     15.36
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      10000.000 Hz
FIDRES   0.152588 Hz
AQ       3.2767999 sec
RG       191.38
DW       50.000 usec
DE       6.50 usec
TE       297.6 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    500.1330885 MHz
NUC1    1H
F1      9.80 usec
PLW1    24.00000000 W

F2 - Processing parameters
SI      65536
SF      500.1300000 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
    
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¹³C NMR of compound 5h



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Current Data Parameters
NAME      TAnh-63H
EXPNO    11
PROCNO   1

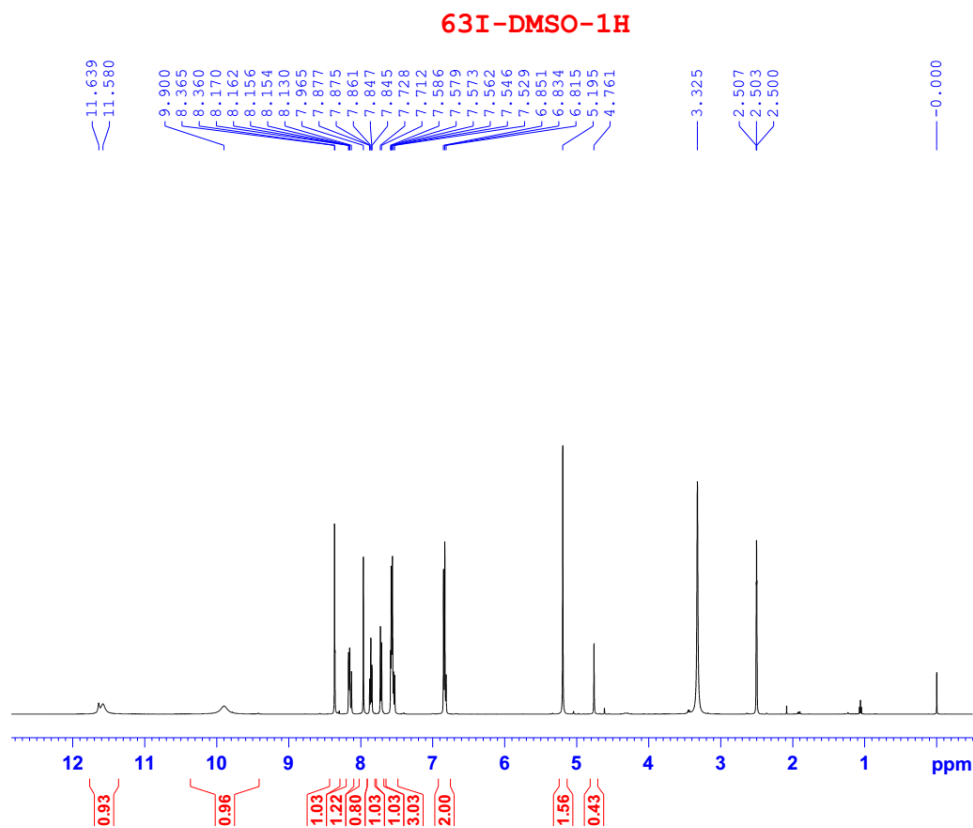
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Date_    20171005
Time     21.50
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       2048
DS       4
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0485760 sec
RG       191.38
DW       16.000 usec
DE       6.50 usec
TE       299.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    125.7703637 MHz
NUC1    13C
P1      9.50 usec
PLW1    90.00000000 W

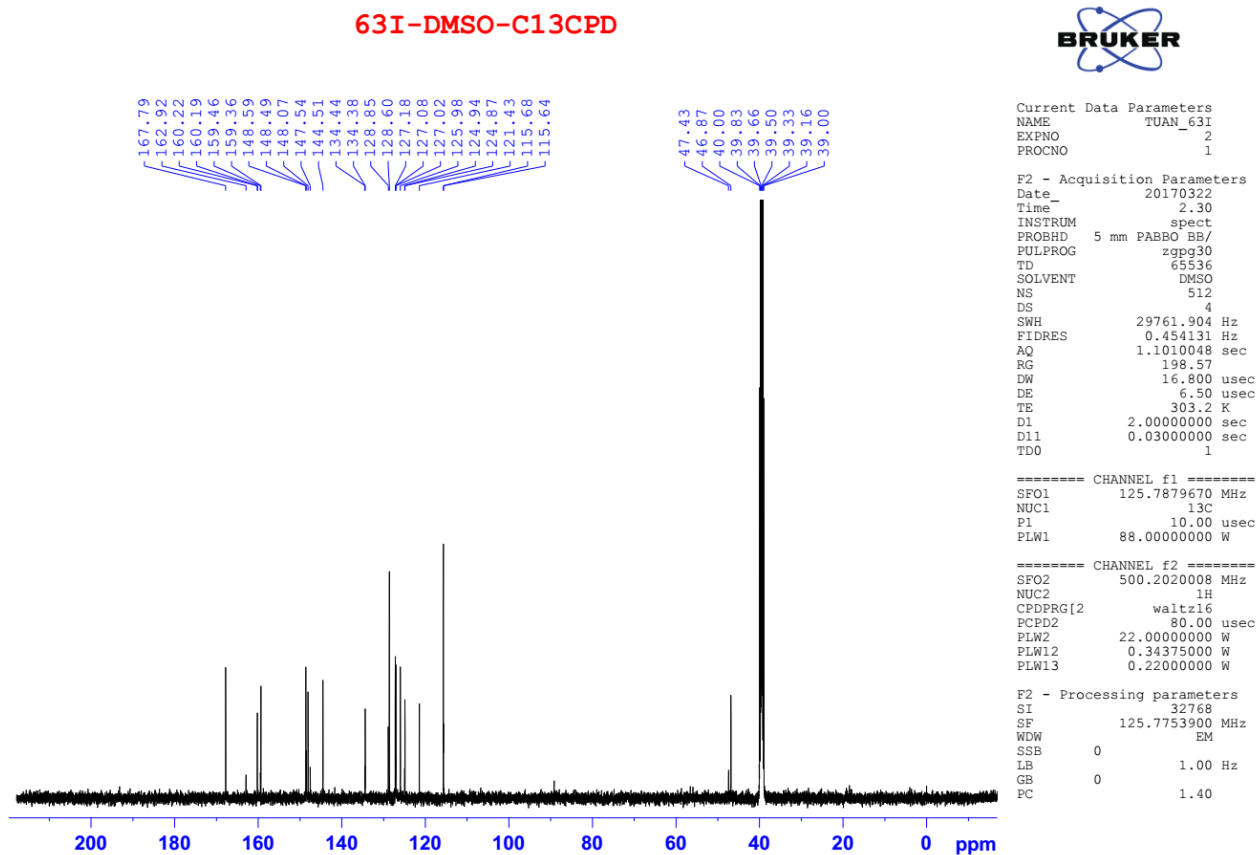
===== CHANNEL f2 =====
SFO2    500.1320005 MHz
NUC2    1H
CPDPRG[2] waltz16
PCPD2   80.00 usec
PLW2    24.00000000 W
PLW12   0.36015001 W
PLW13   0.23050000 W

F2 - Processing parameters
SI      65536
SF      125.7577885 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
    
```

¹H NMR of compound 5i

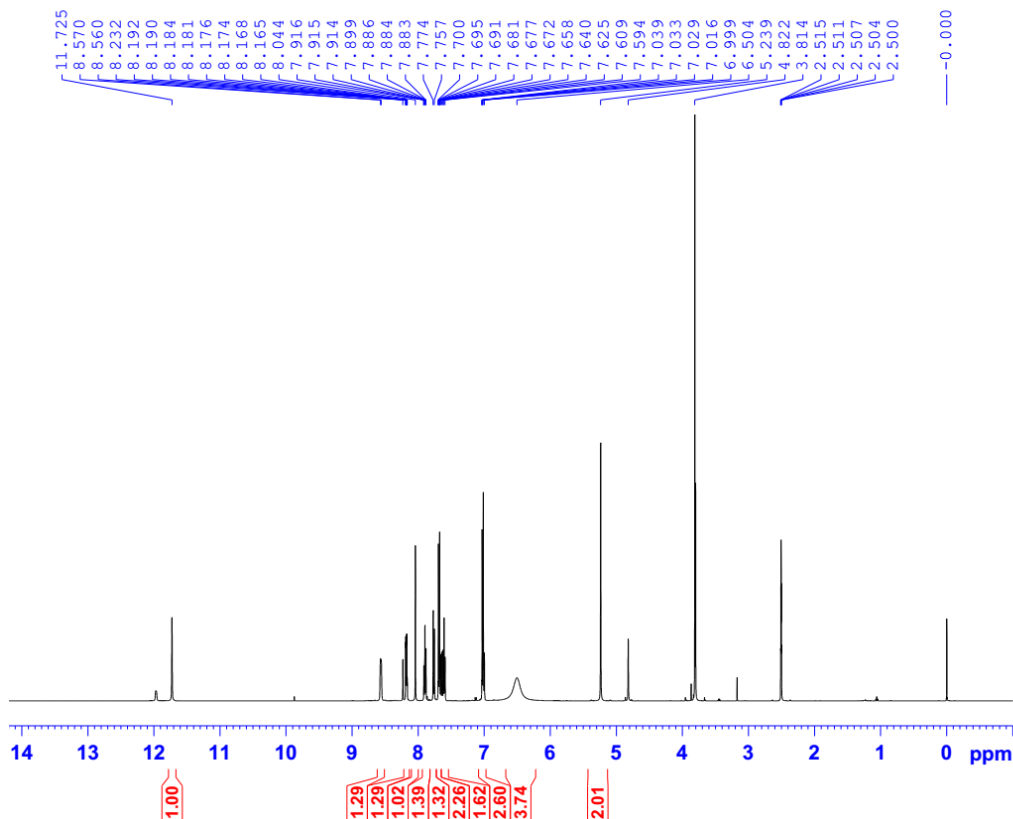


¹³C NMR of compound 5i



¹H NMR of compound 5j

63J-DMSO-1H



Current Data Parameters
 NAME TUAN63J
 EXPNO 1
 PROCNO 1

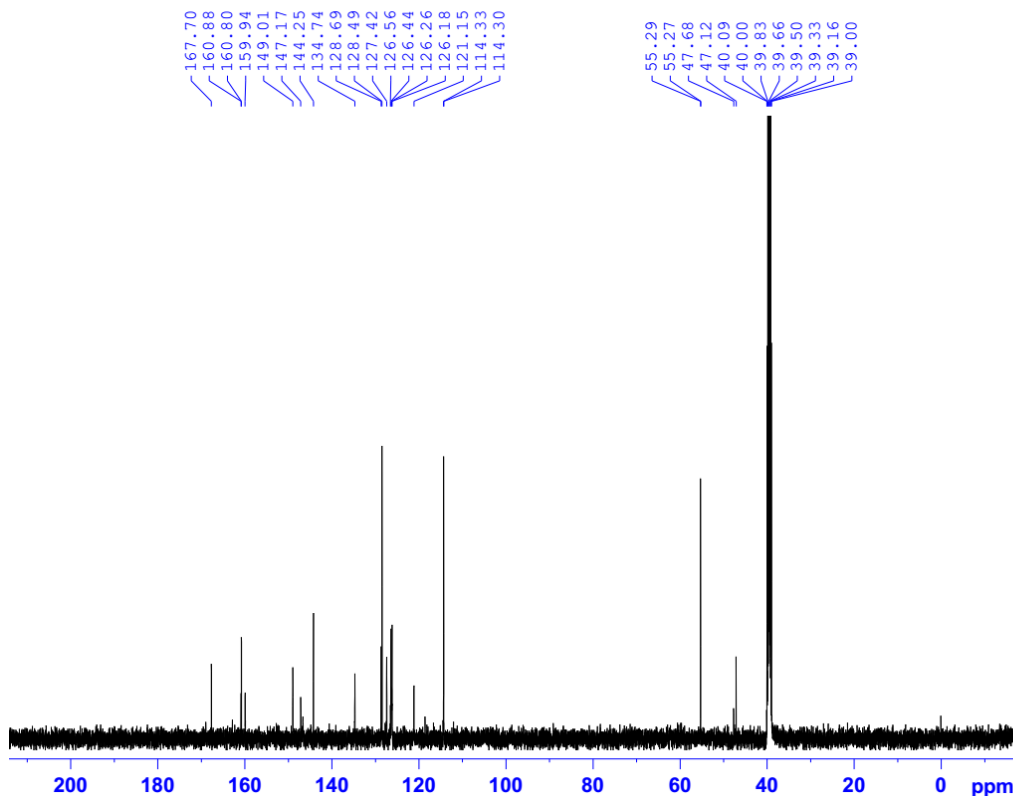
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 Time 11.10
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 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 127.68
 DW 50.000 usec
 DE 6.50 usec
 TE 303.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.2030889 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 22.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.2000013 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5j

63J-DMSO-C13CPD



Current Data Parameters
 NAME TUAN63J
 EXPNO 2
 PROCNO 1

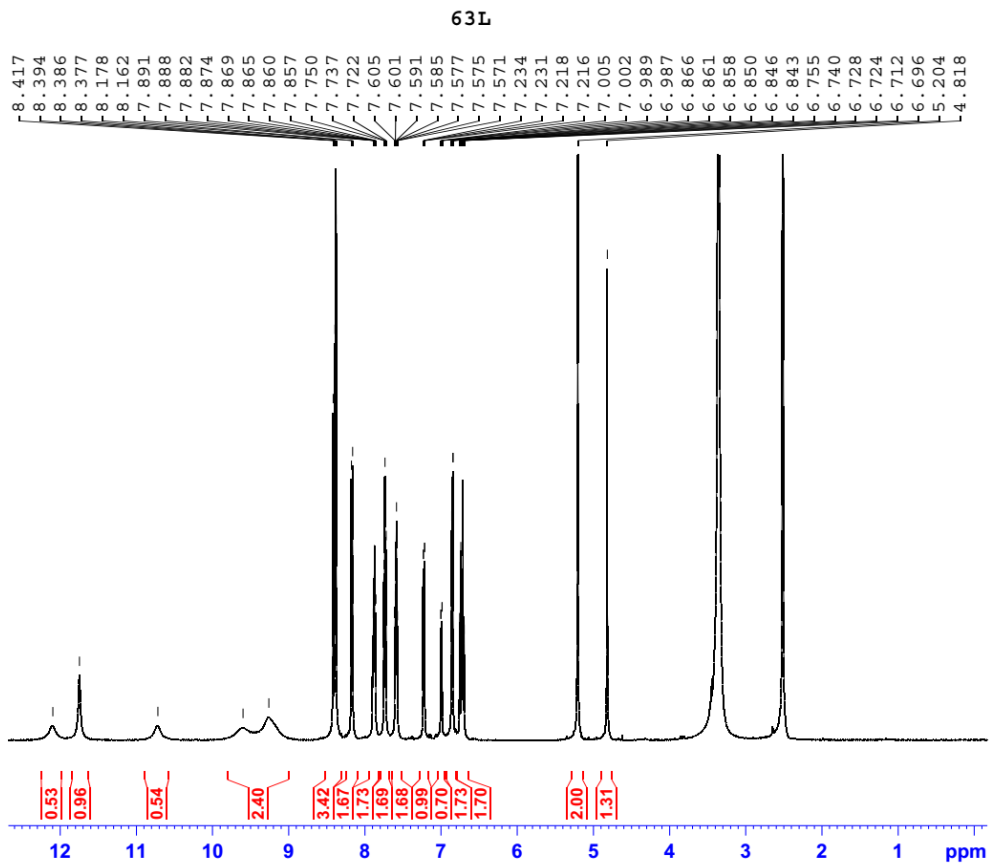
F2 - Acquisition Parameters
 Date_ 20170223
 Time 15.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 256
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 198.57
 DW 16.800 usec
 DE 6.50 usec
 TE 303.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7879670 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 88.00000000 W

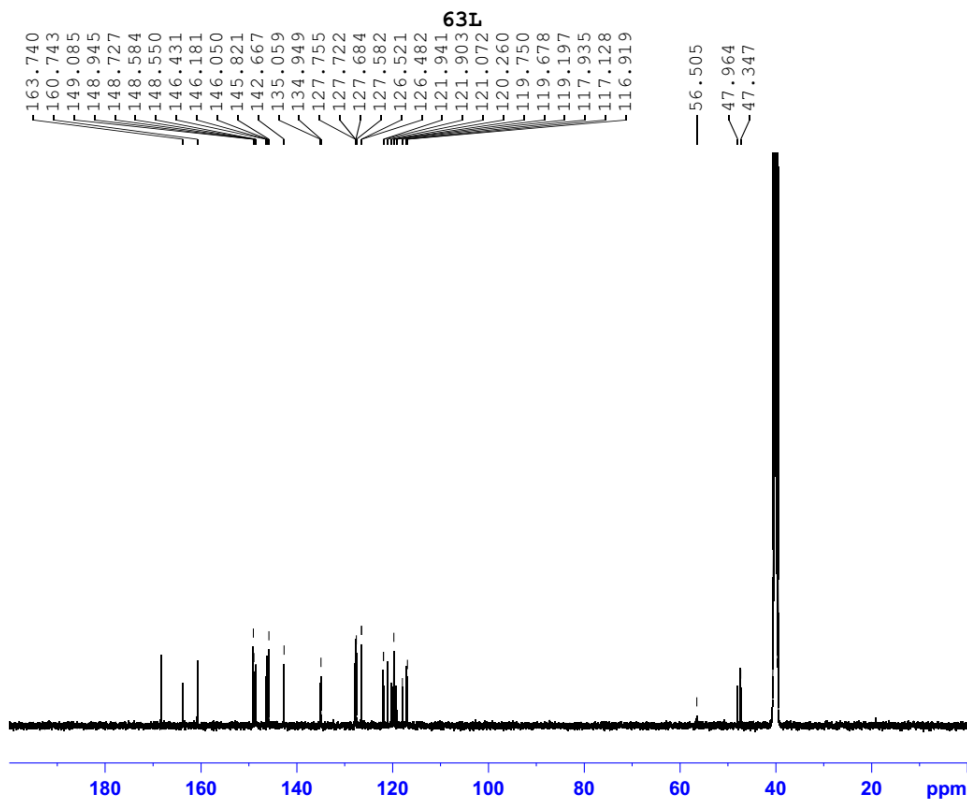
===== CHANNEL f2 =====
 SFO2 500.2020008 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 80.00 usec
 PLW2 22.00000000 W
 PLW12 0.34375000 W
 PLW13 0.22000000 W

F2 - Processing parameters
 SI 32768
 SF 125.7754547 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

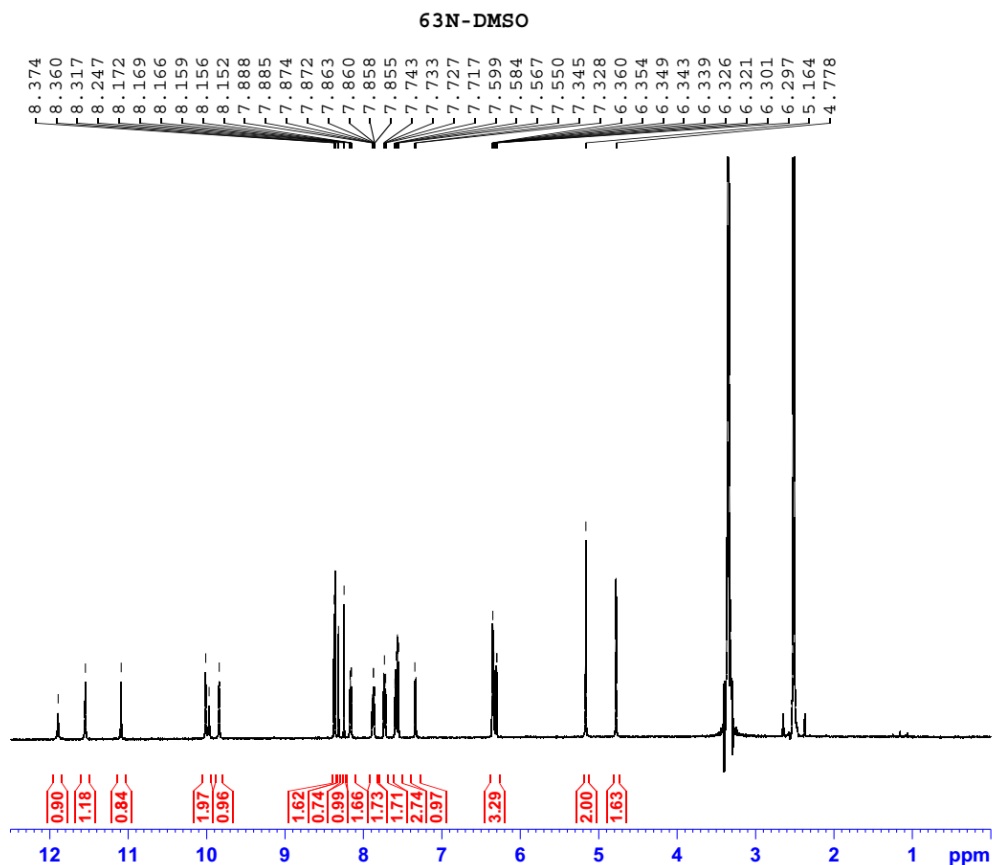
¹H NMR of compound 5k



¹³C NMR of compound 5k



¹H NMR of compound 5l



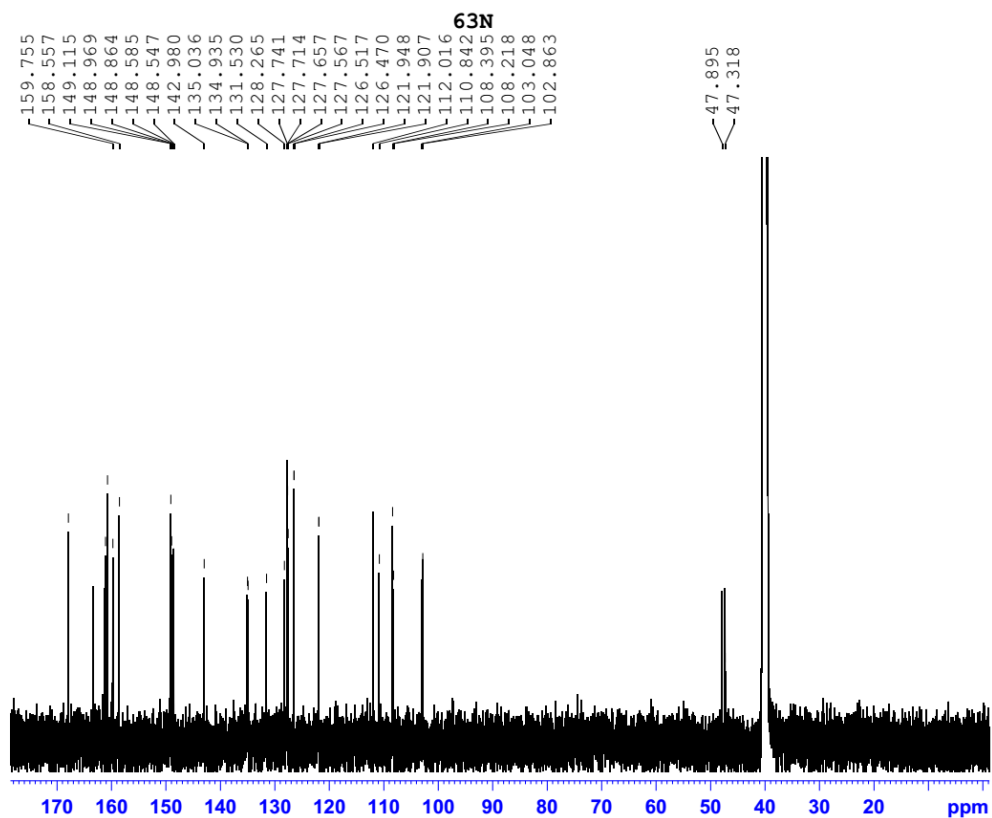
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 NAME 63N-DMSO
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170726
 Time 14.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 191.38
 DW 50.000 usec
 DE 6.50 usec
 TE 297.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1330000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5l



Current Data Parameters
 NAME 63N-DMSO
 EXPNO 20
 PROCNO 1

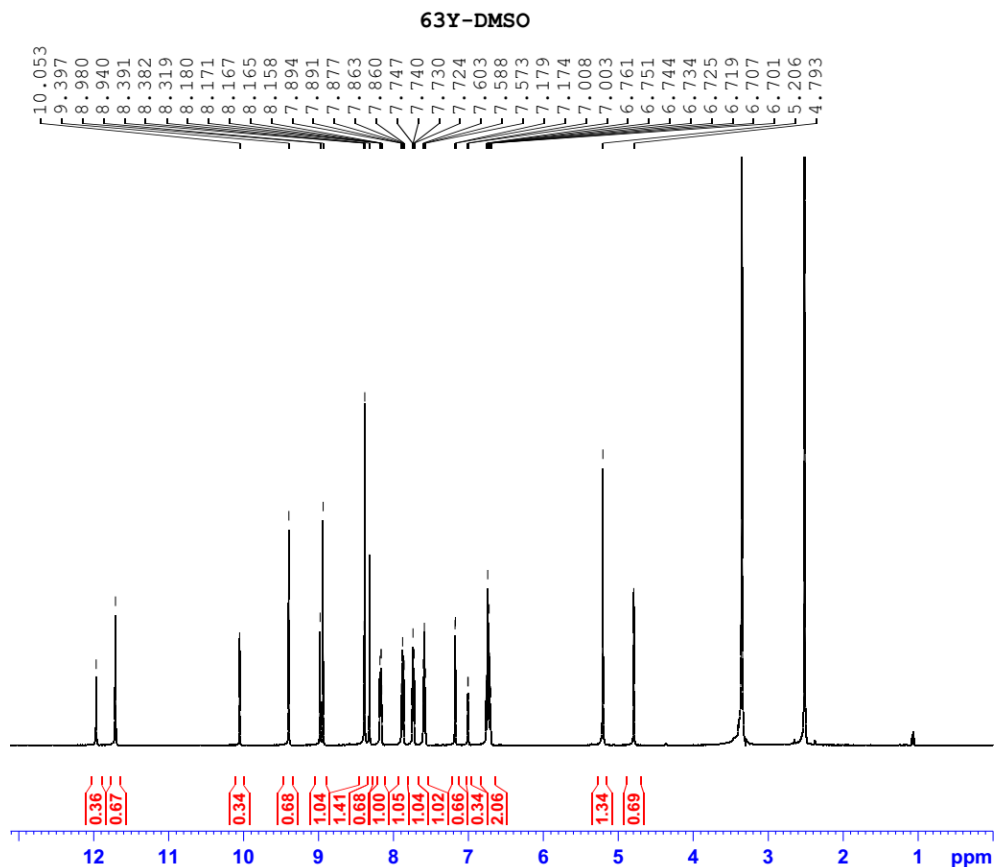
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 Date_ 20170728
 Time 1.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 8192
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 298.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

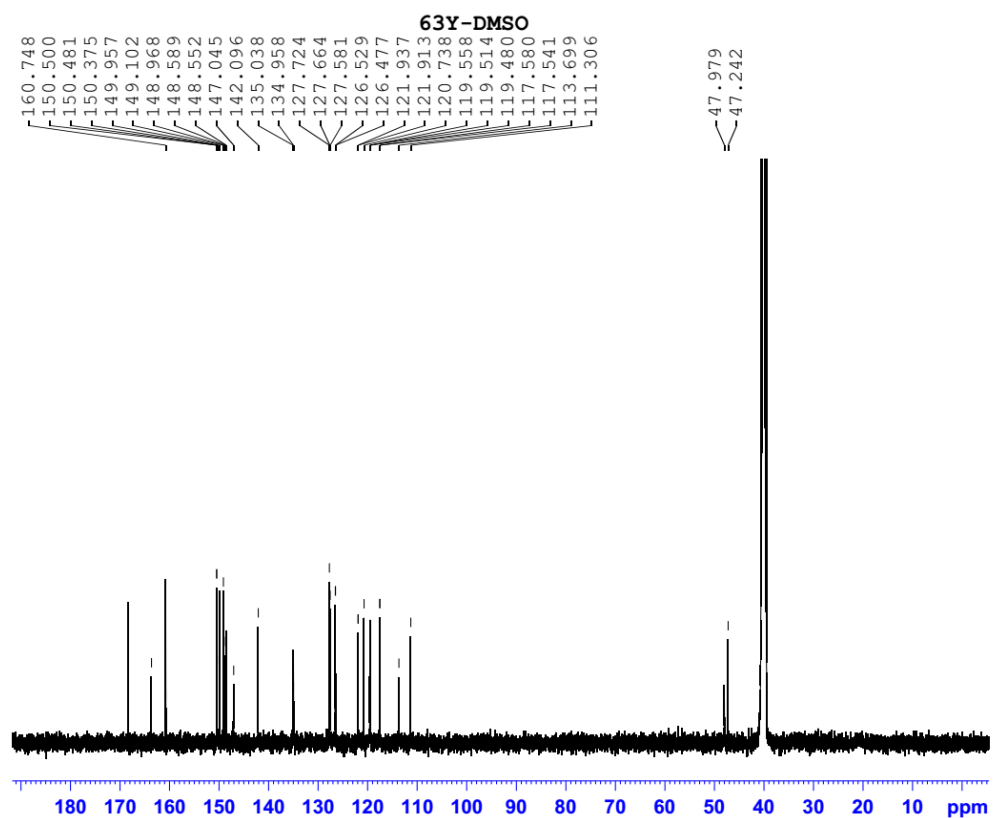
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

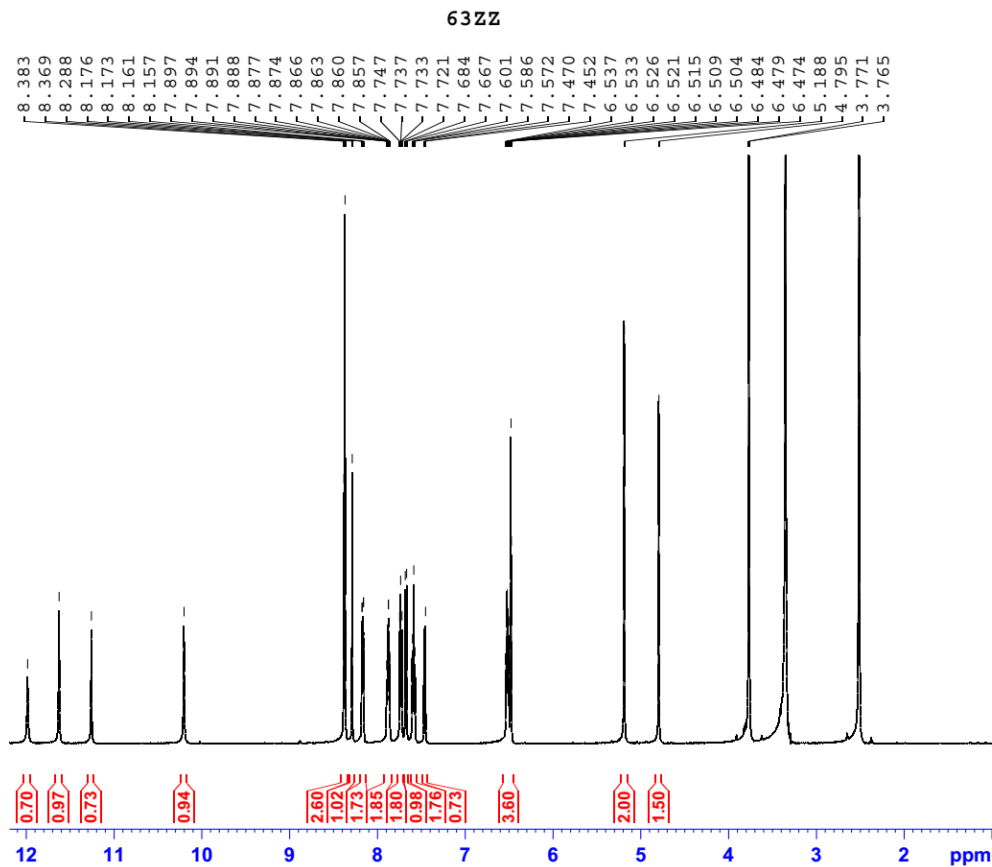
¹H NMR of compound 5m



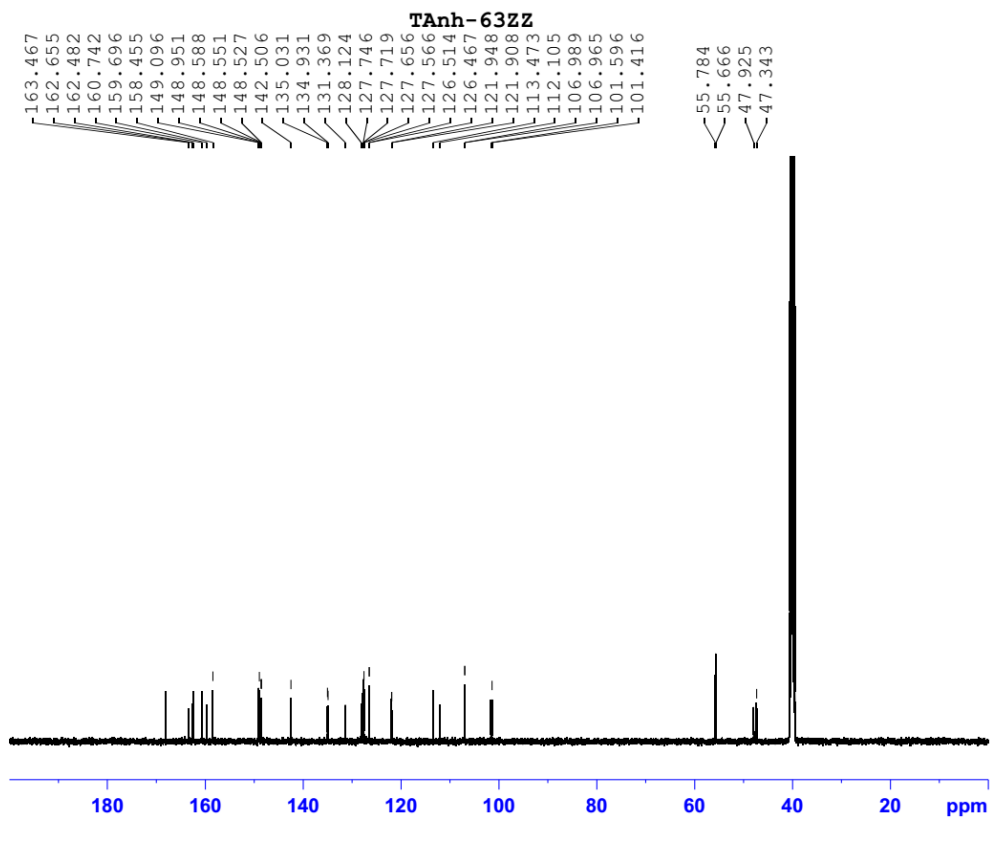
¹³C NMR of compound 5m



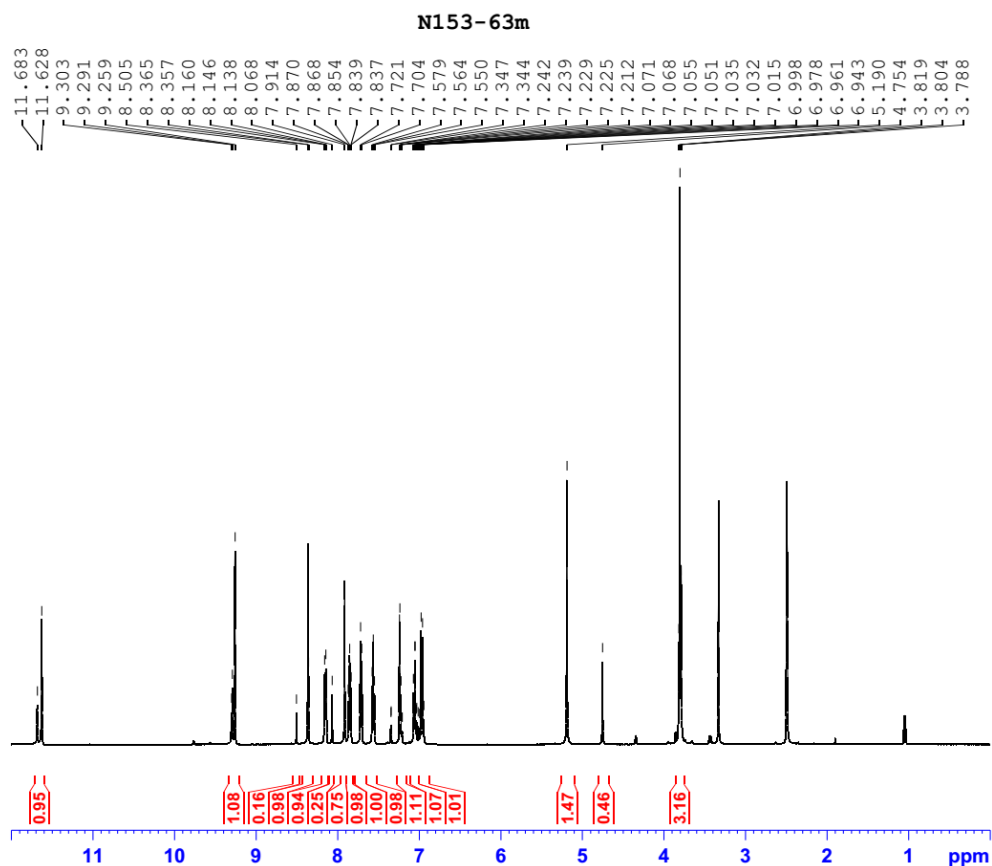
¹H NMR of compound 5n



¹³C NMR of compound 5n



¹H NMR of compound 5o



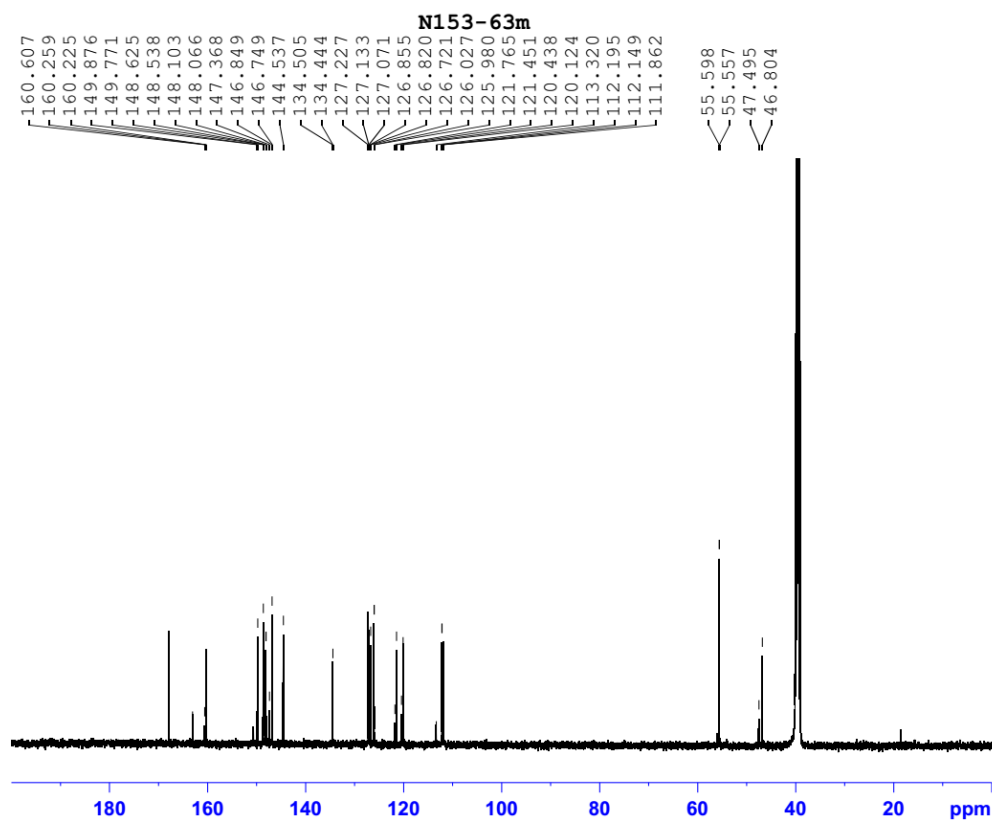
Current Data Parameters
 NAME N153-63m
 EXPNO 30
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170518
 Time_ 0.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 123.67
 DW 50.000 usec
 DE 6.50 usec
 TE 297.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300104 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5o



Current Data Parameters
 NAME N153-63m
 EXPNO 32
 PROCNO 1

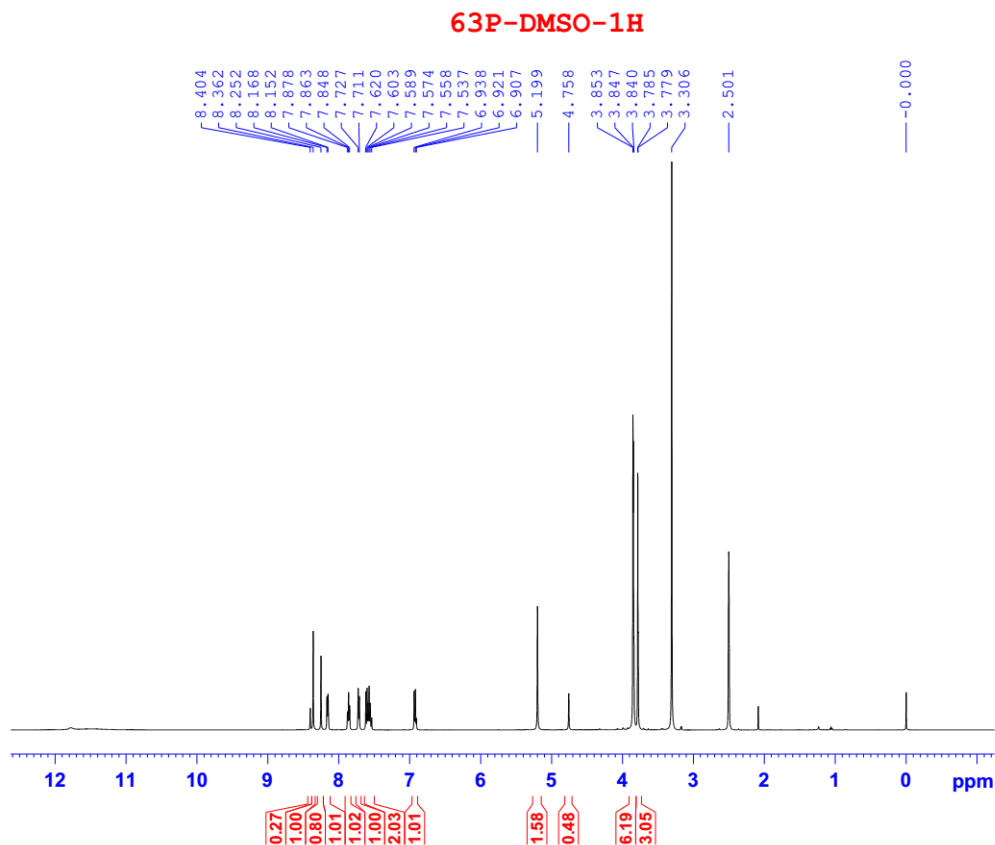
F2 - Acquisition Parameters
 Date_ 20170518
 Time_ 2.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 298.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7578510 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR of compound 5p



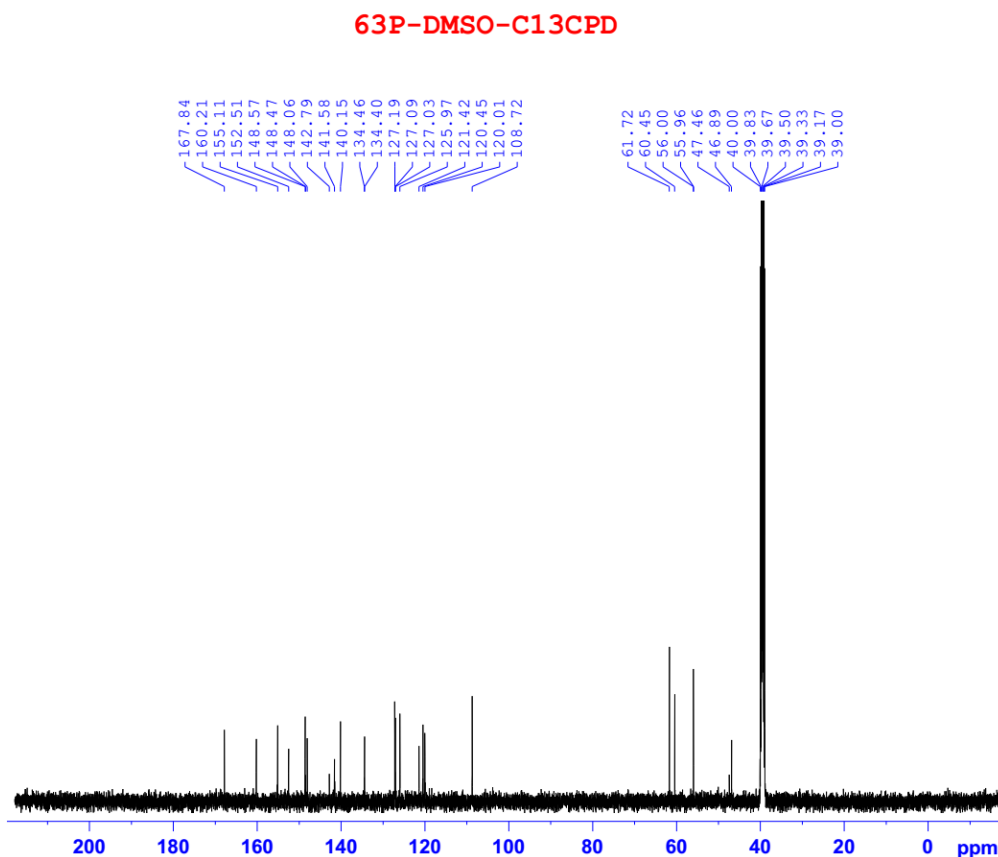
Current Data Parameters
 NAME TUAN_63P
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170321
 Time 16.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 142.98
 DW 50.000 usec
 DE 6.50 usec
 TE 303.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 500.2030889 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 22.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.2000047 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5p



Current Data Parameters
 NAME TUAN_63P
 EXPNO 2
 PROCNO 1

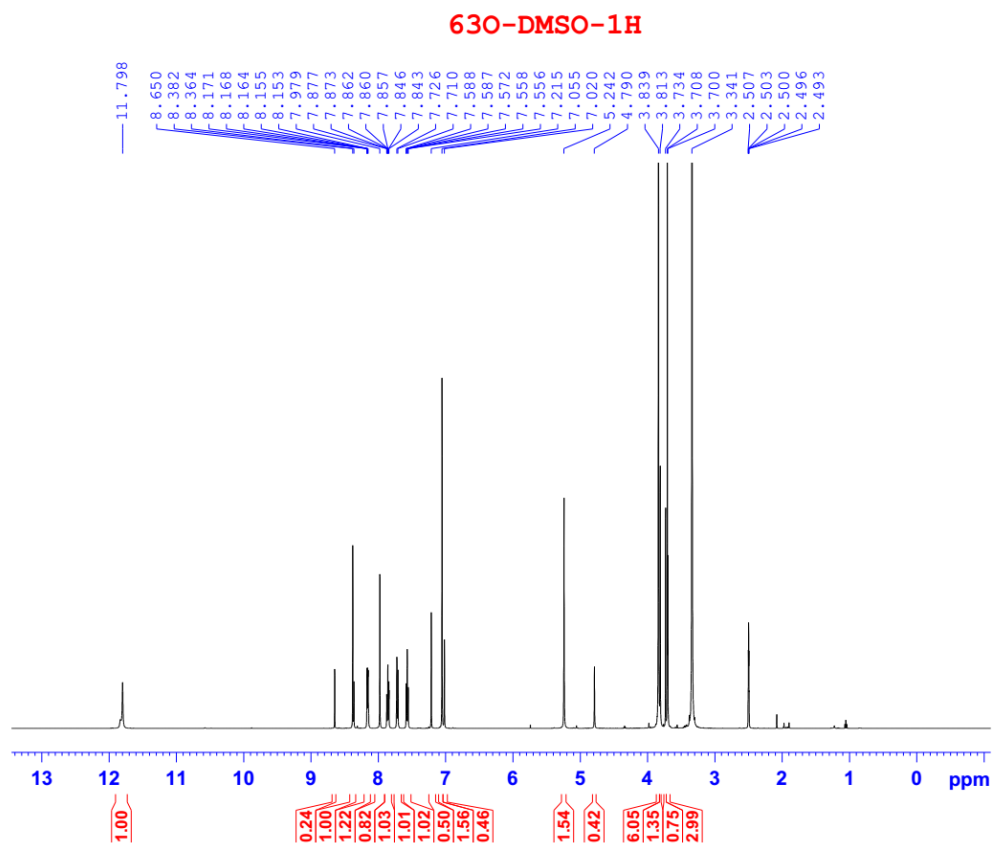
F2 - Acquisition Parameters
 Date_ 20170322
 Time 3.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 198.57
 DW 16.800 usec
 DE 6.50 usec
 TE 303.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 125.7879670 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 88.00000000 W

===== CHANNEL f2 =====
 SF02 500.2020008 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 22.00000000 W
 PLW12 0.34375000 W
 PLW13 0.22000000 W

F2 - Processing parameters
 SI 32768
 SF 125.7754570 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR of compound 5q



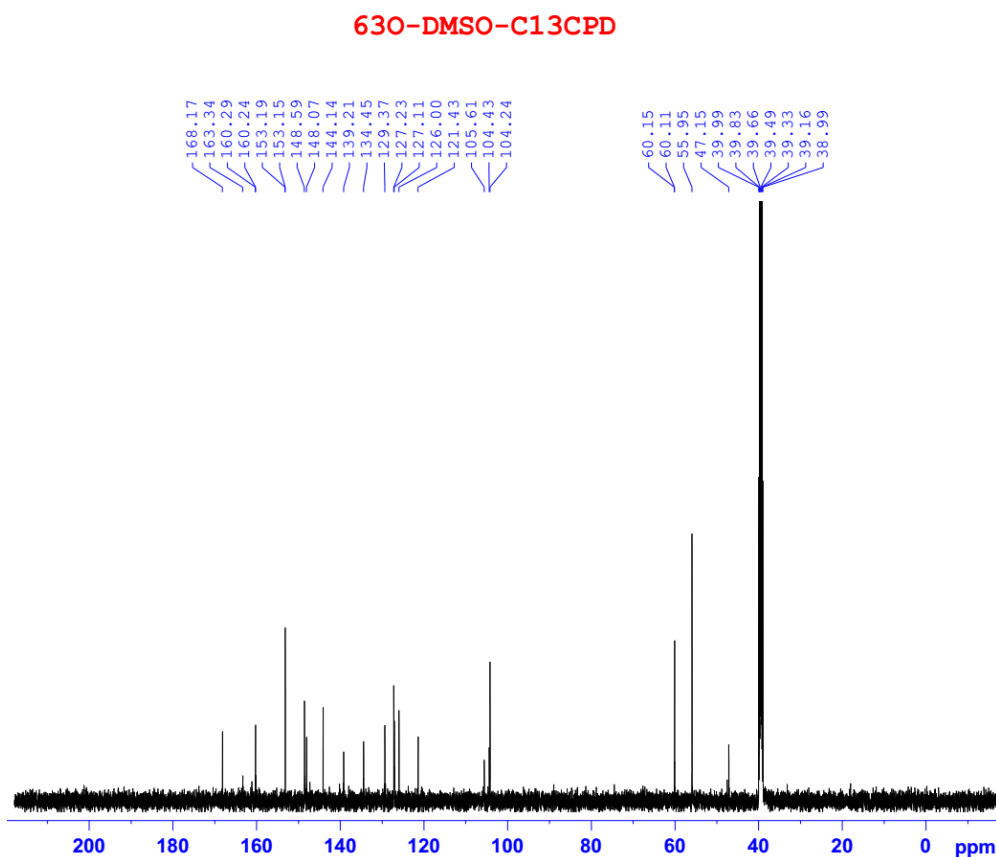
Current Data Parameters
NAME TUAN_630
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170412
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 89.63
DW 50.000 usec
DE 6.50 usec
TE 302.6 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 500.2030889 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 500.2000053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of compound 5q



Current Data Parameters
NAME TUAN_630
EXPNO 2
PROCNO 1

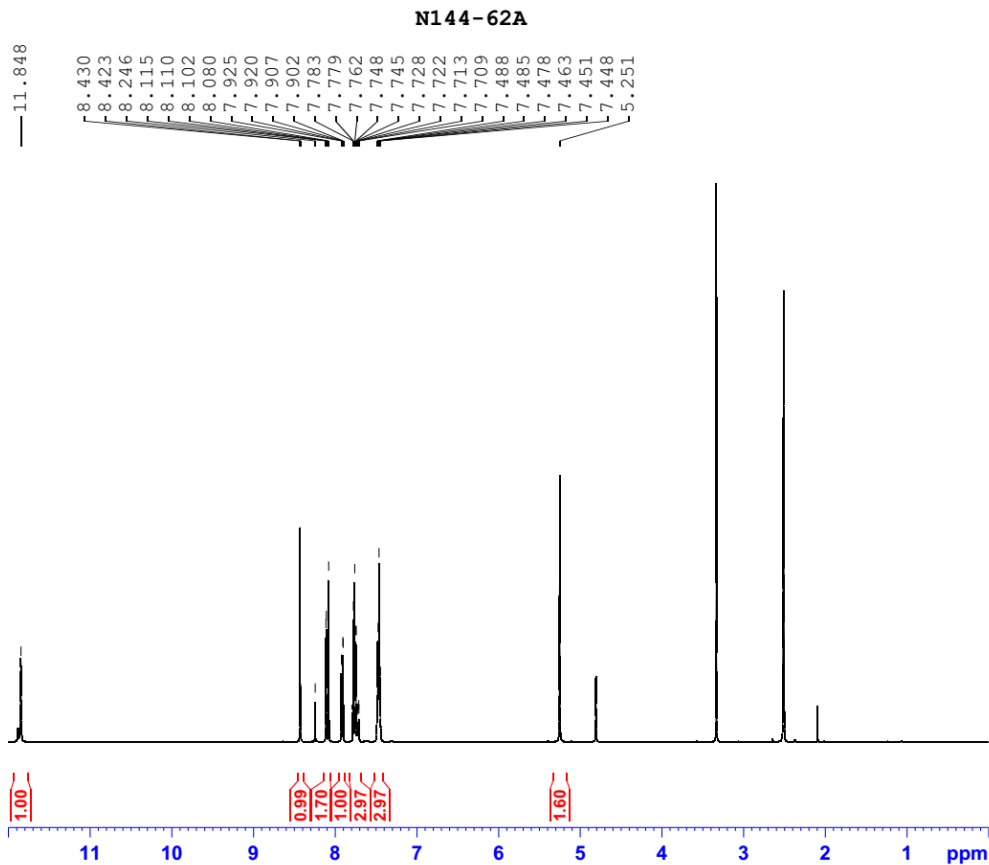
F2 - Acquisition Parameters
Date_ 20170413
Time 17.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 128
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 198.57
DW 16.800 usec
DE 6.50 usec
TE 302.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 125.7879670 MHz
NUC1 13C
P1 10.00 usec
PLW1 88.00000000 W

===== CHANNEL f2 =====
SF02 500.2020008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 22.00000000 W
PLW12 0.34375000 W
PLW13 0.22000000 W

F2 - Processing parameters
SI 32768
SF 125.7754525 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of compound 5r



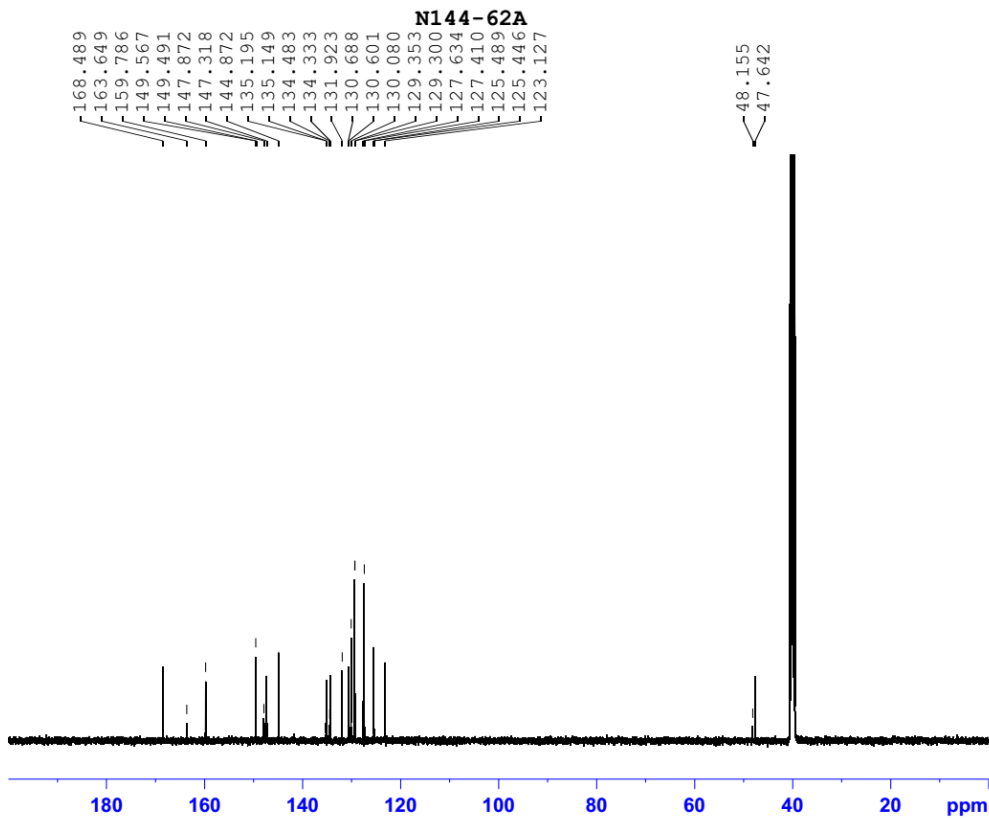
Current Data Parameters
 NAME N144-62A
 EXPNO 50
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170509
 Time 23.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 191.38
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5r



Current Data Parameters
 NAME N144-62A
 EXPNO 52
 PROCNO 1

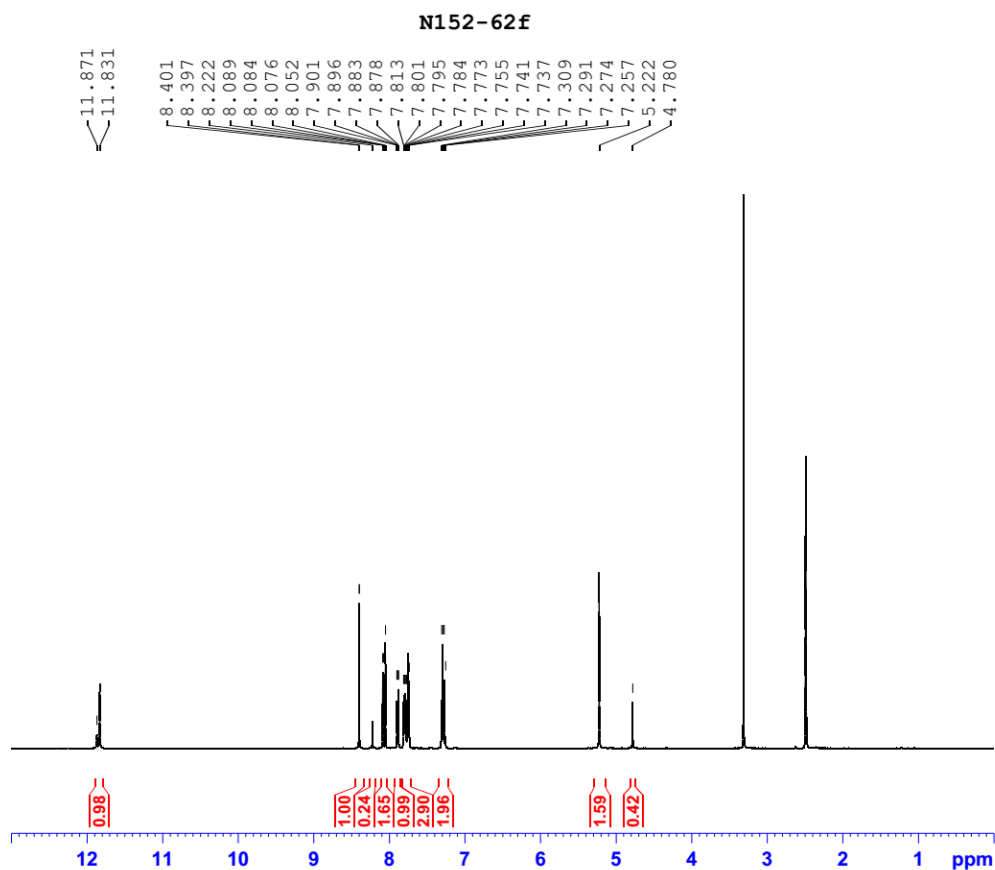
F2 - Acquisition Parameters
 Date_ 20170510
 Time 1.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR of compound 5s



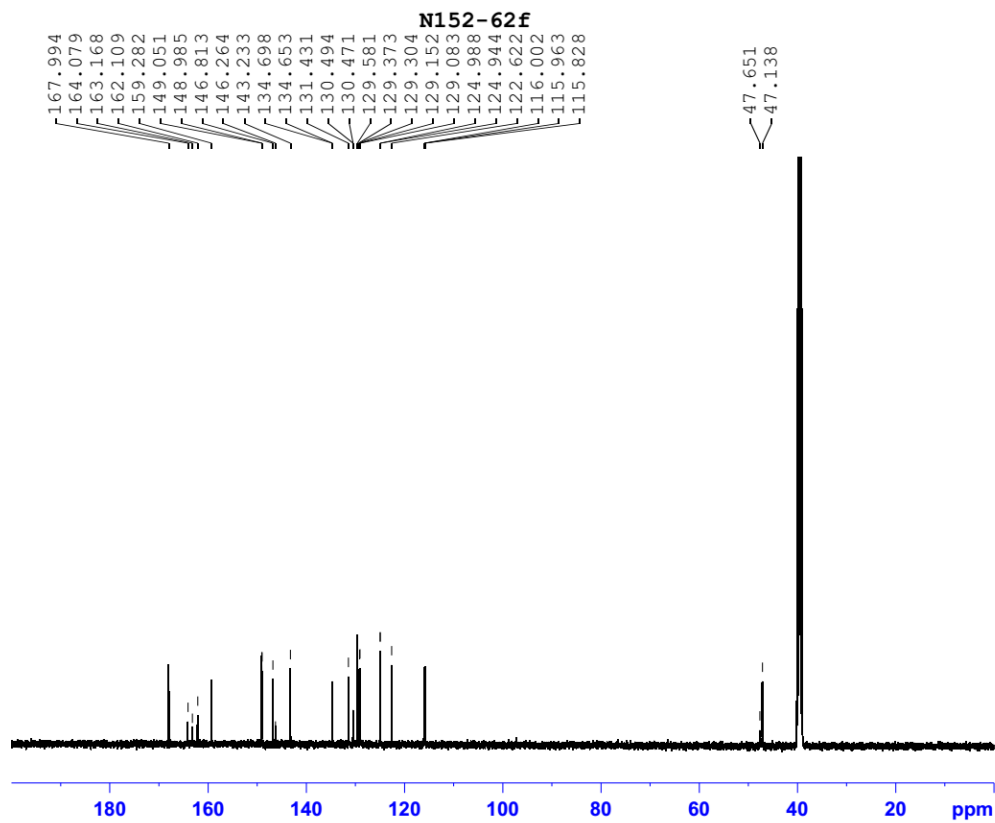
Current Data Parameters
 NAME N152-62f
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170519
 Time 2.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 191.38
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.0000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300110 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5s



Current Data Parameters
 NAME N152-62f
 EXPNO 11
 PROCNO 1

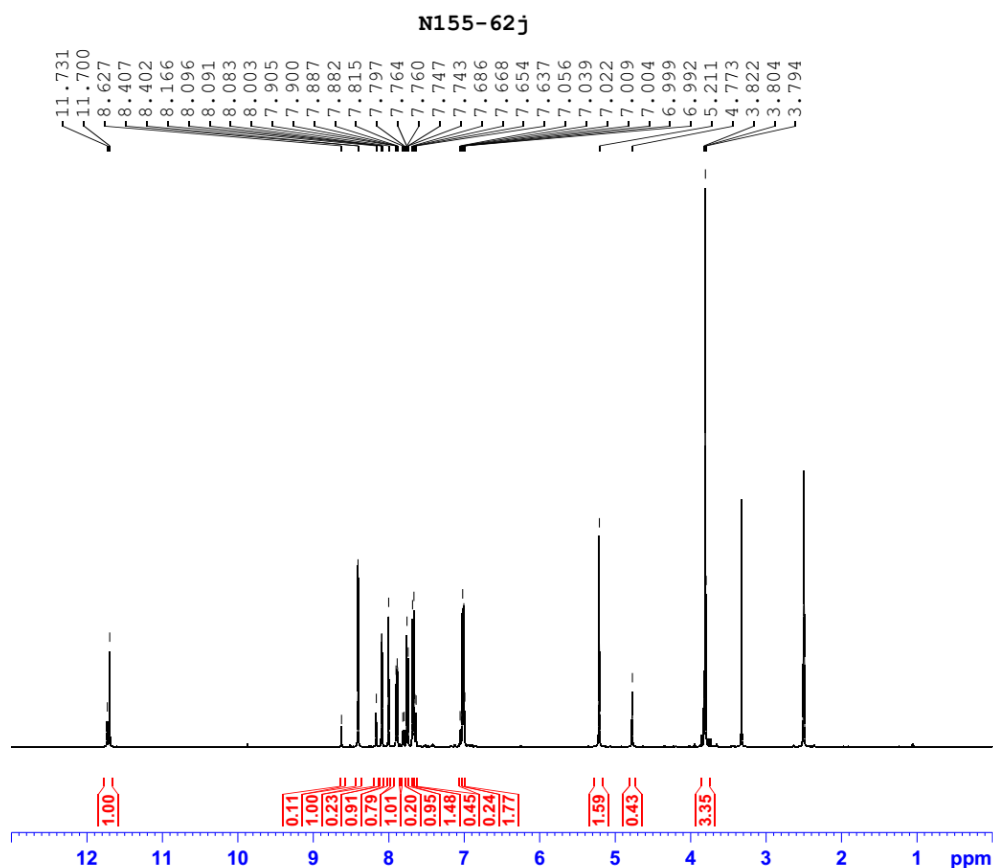
F2 - Acquisition Parameters
 Date_ 20170519
 Time 3.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.0000000 W

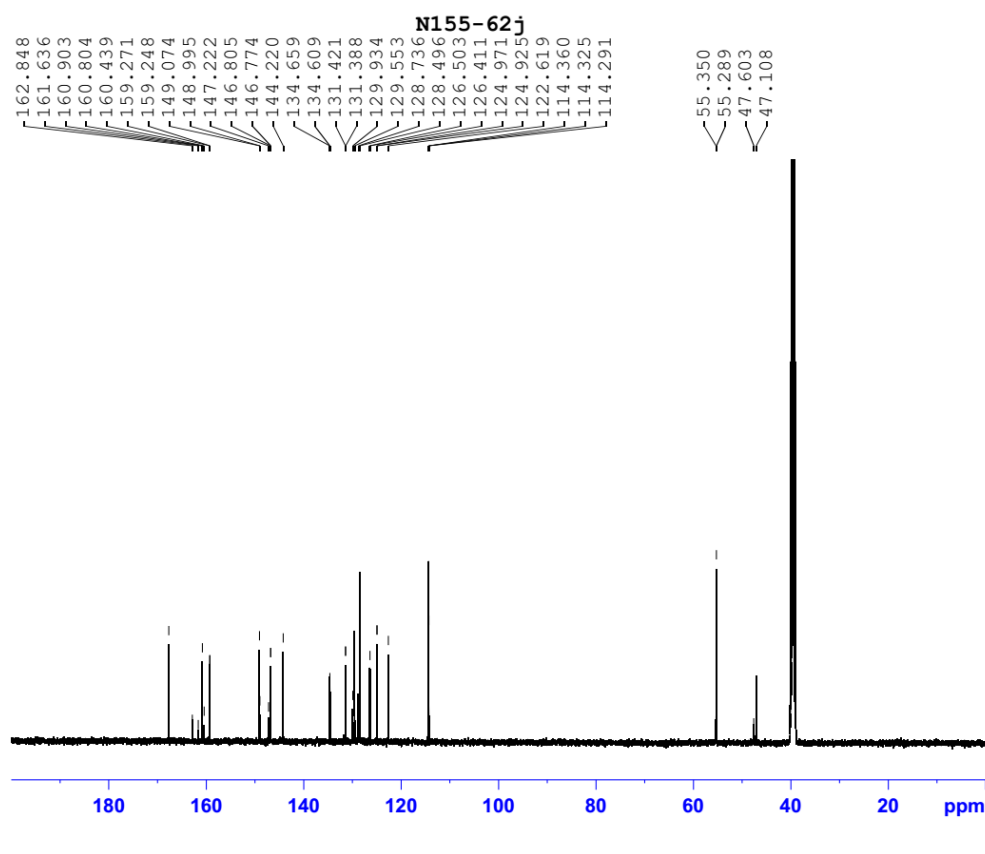
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.0000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7578510 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

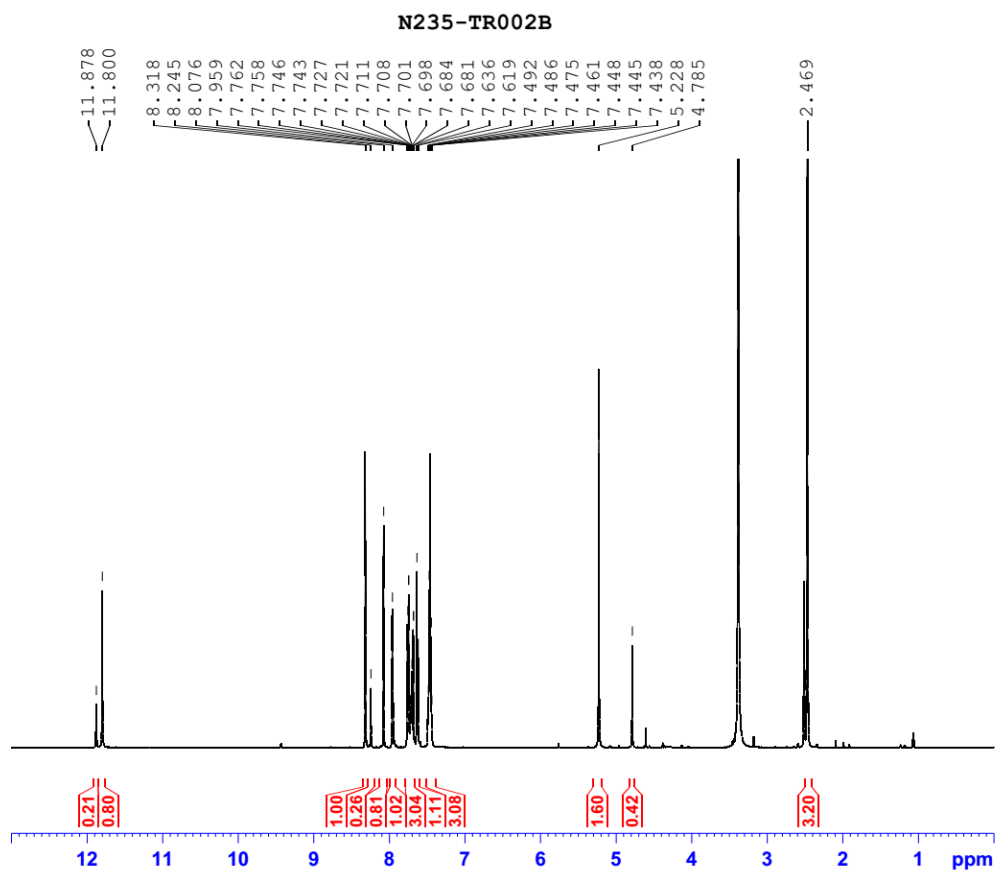
¹H NMR of compound 5t



¹³C NMR of compound 5t



¹H NMR of compound 5u



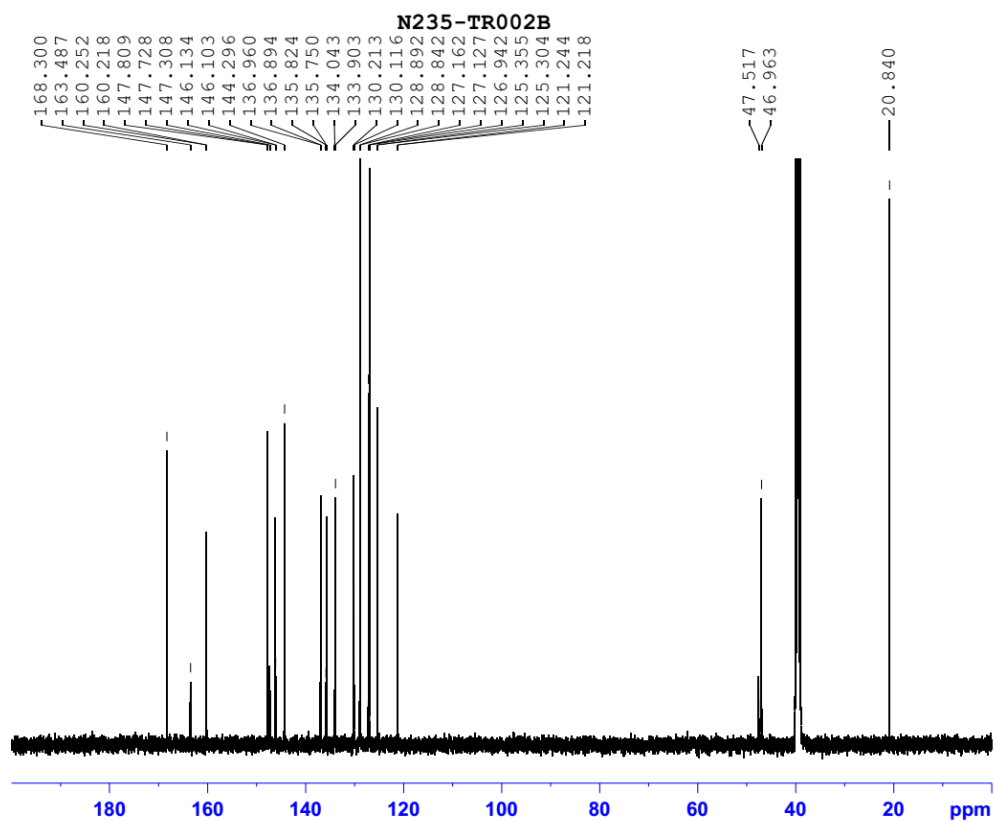
Current Data Parameters
 NAME N235-TR002B
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161102
 Time 16.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 87.53
 DW 50.000 usec
 DE 6.50 usec
 TE 298.6 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.0000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5u



Current Data Parameters
 NAME N235-TR002B
 EXPNO 21
 PROCNO 1

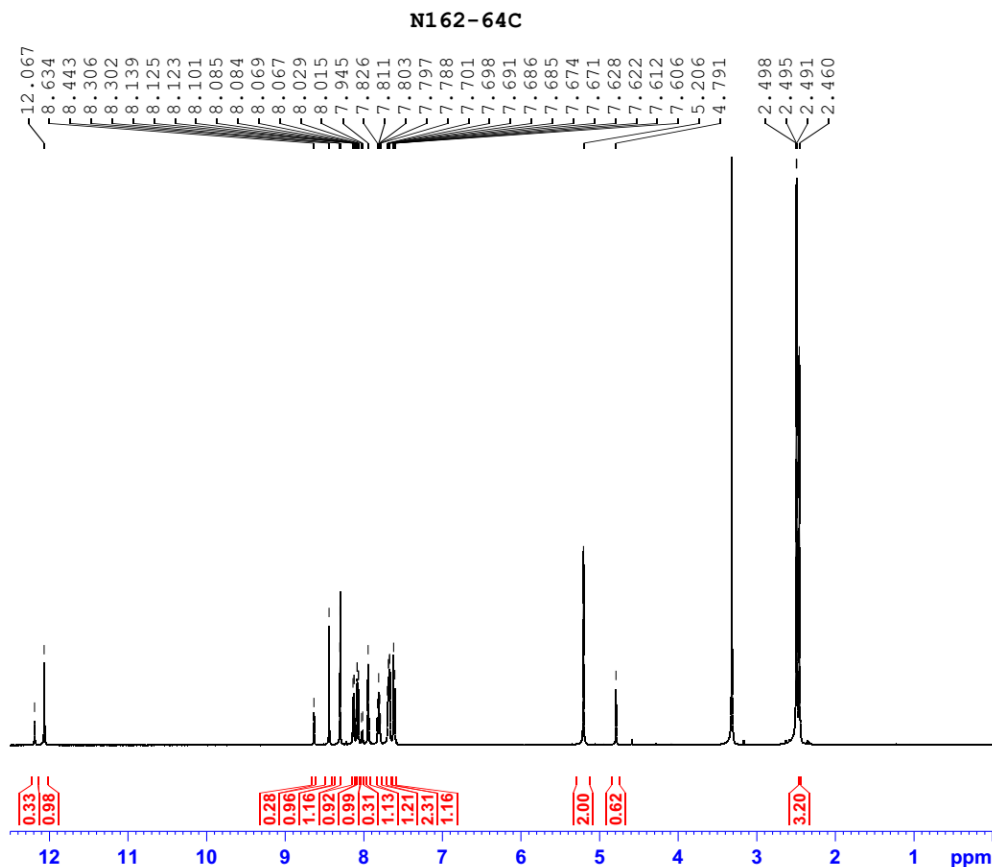
F2 - Acquisition Parameters
 Date_ 20161102
 Time 18.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.8 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.0000000 W

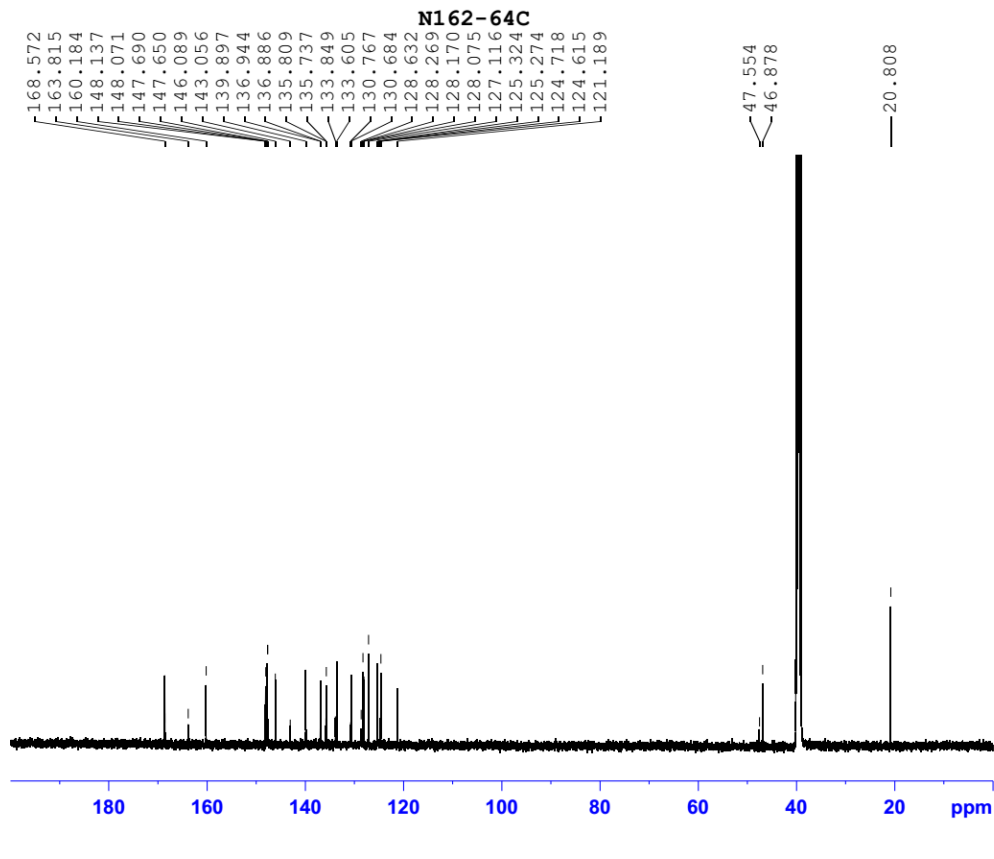
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.0000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7578459 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

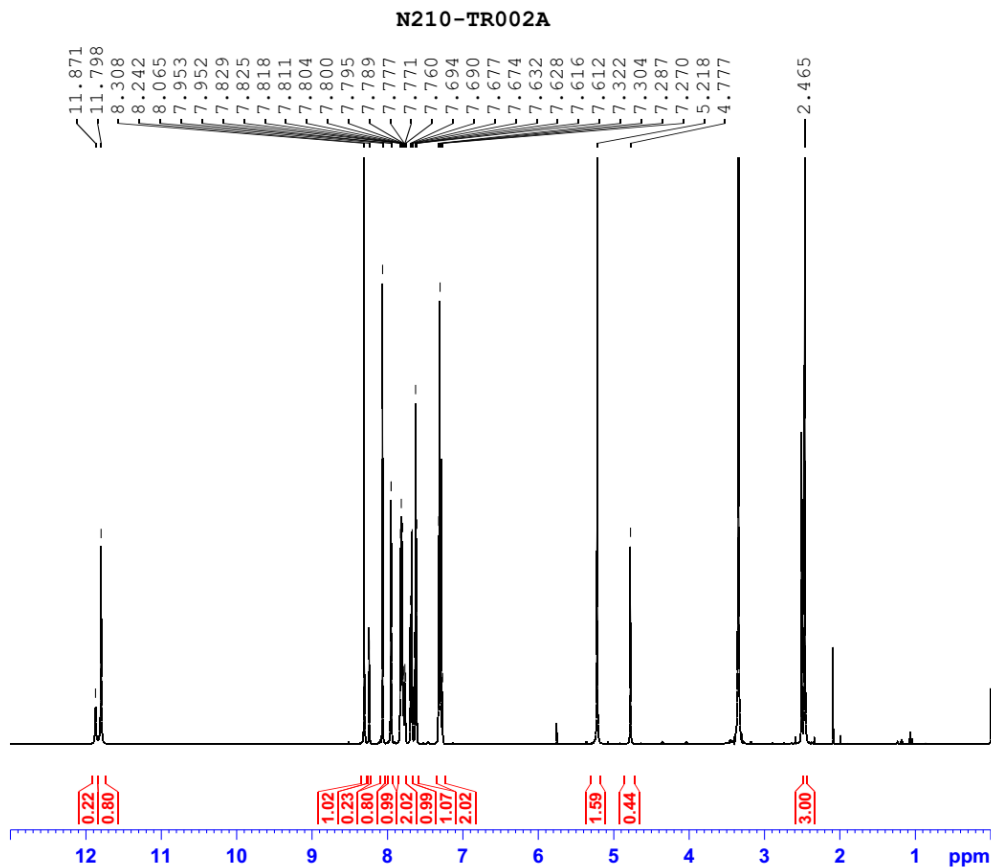
¹H NMR of compound 5v



¹³C NMR of compound 5v



¹H NMR of compound 5w



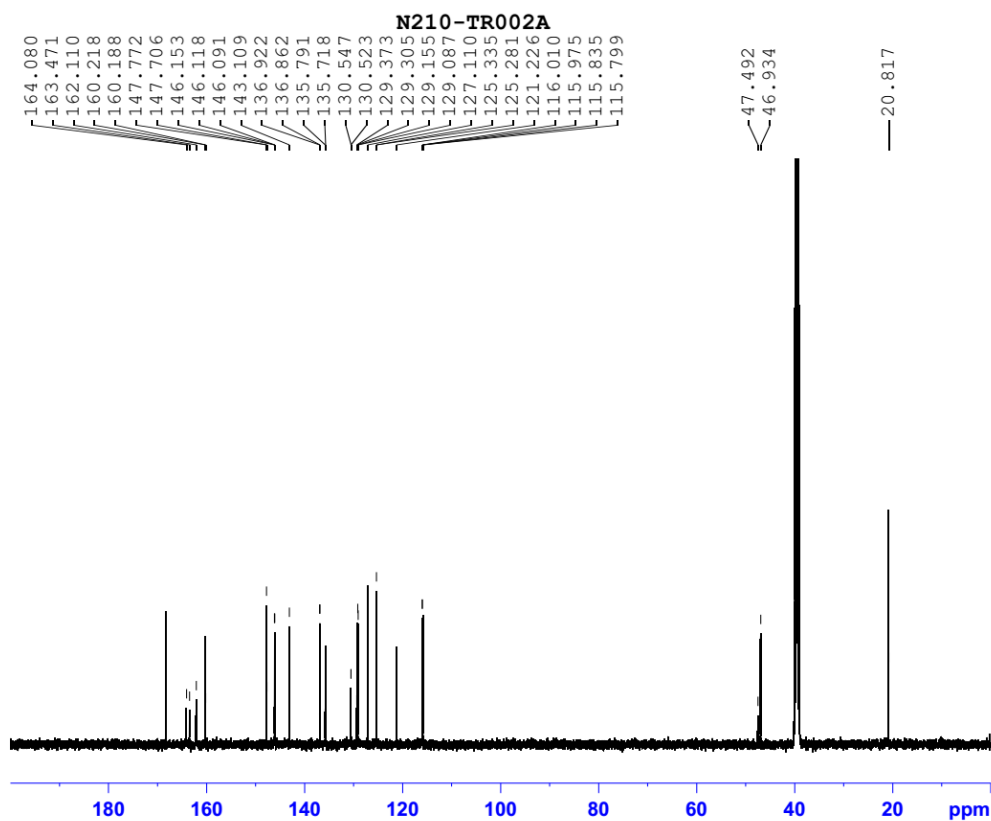
Current Data Parameters
 NAME N210-TR002A
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160928
 Time 8.26
 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 123.67
 DW 50.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 9.50 usec
 PLW1 24.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300024 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 5w



Current Data Parameters
 NAME N210-TR002A
 EXPNO 11
 PROCNO 1

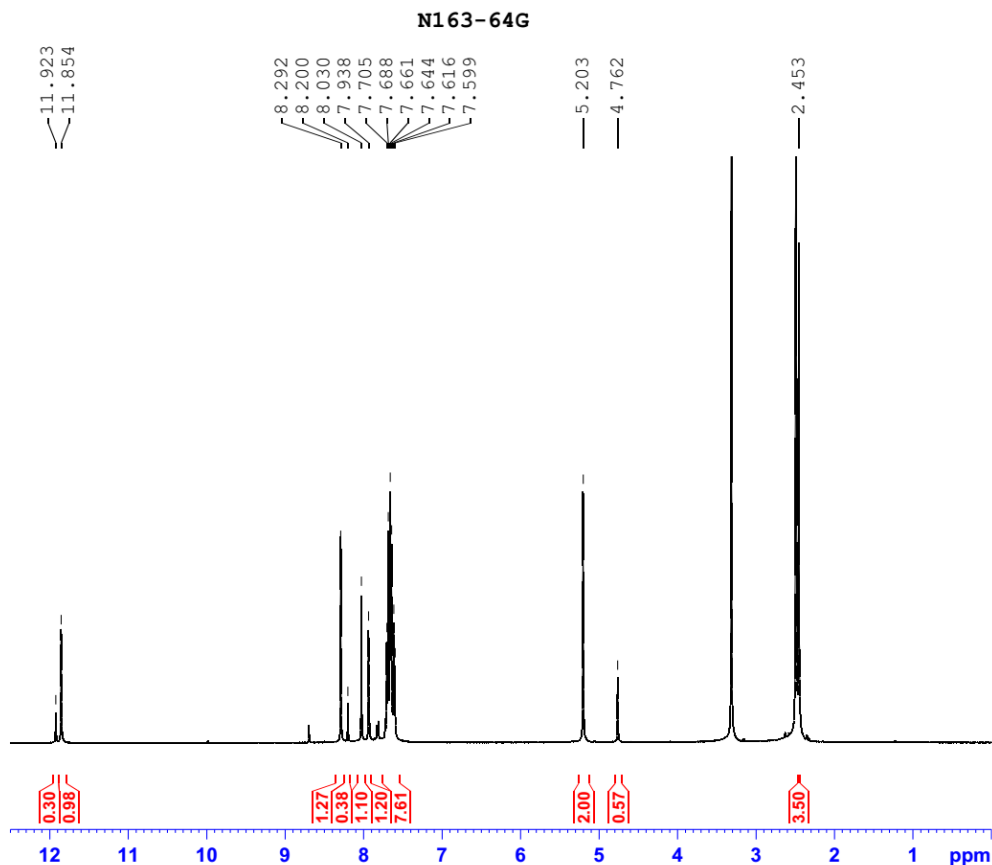
F2 - Acquisition Parameters
 Date_ 20160928
 Time 14.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1114
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

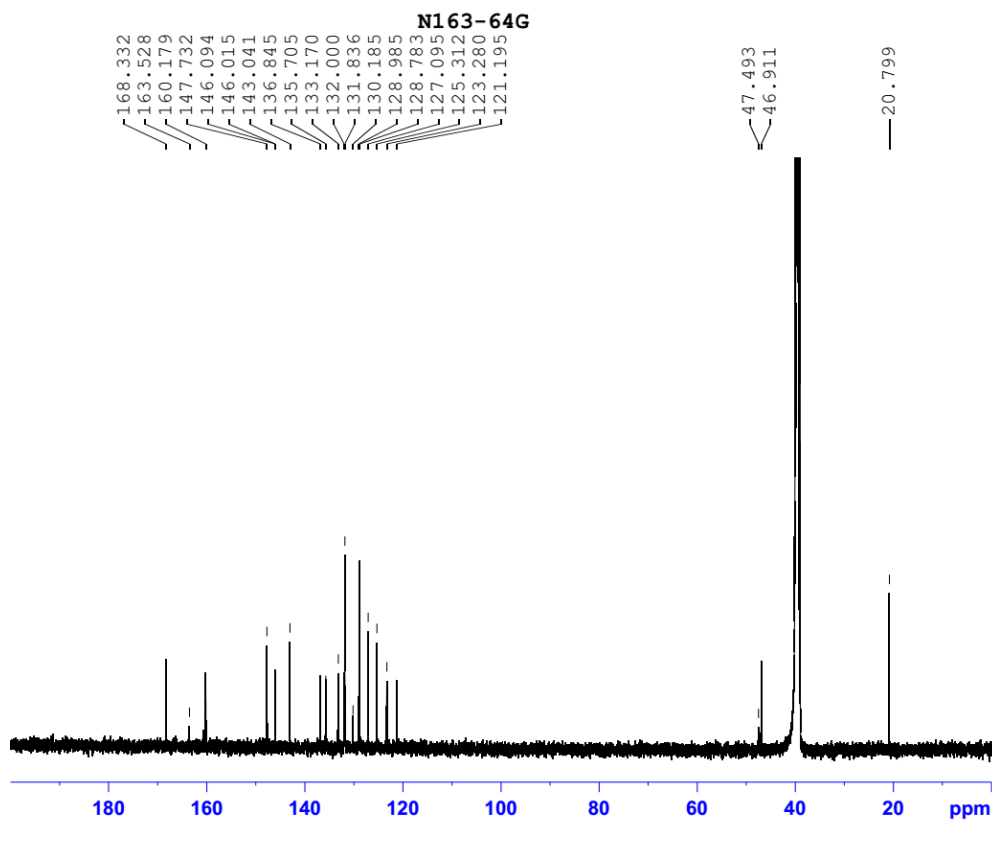
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.35284001 W
 PLW13 0.22582000 W

F2 - Processing parameters
 SI 65536
 SF 125.7578485 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

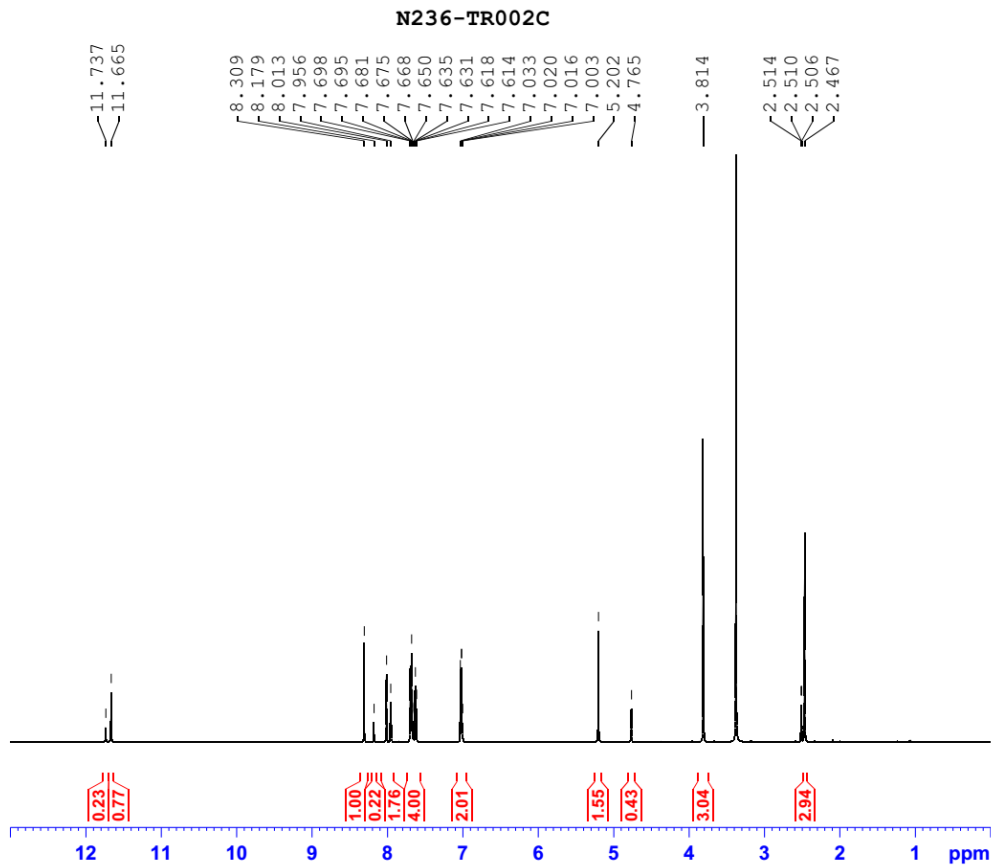
¹H NMR of compound 5y



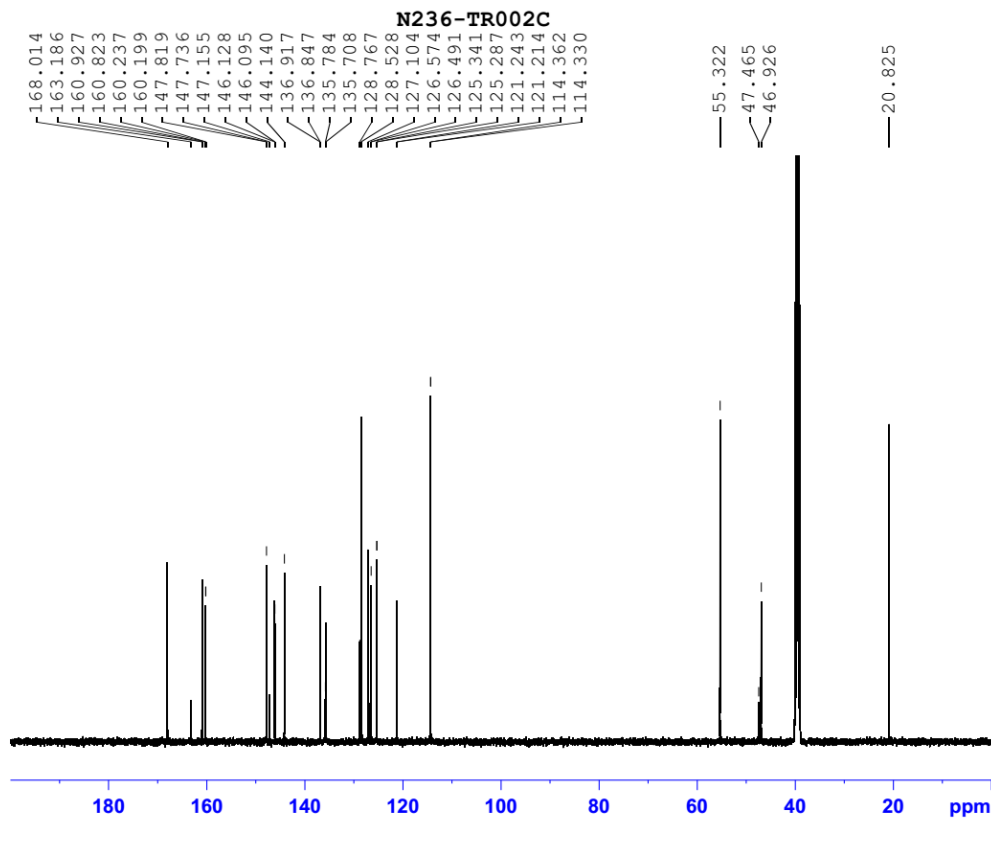
¹³C NMR of compound 5y



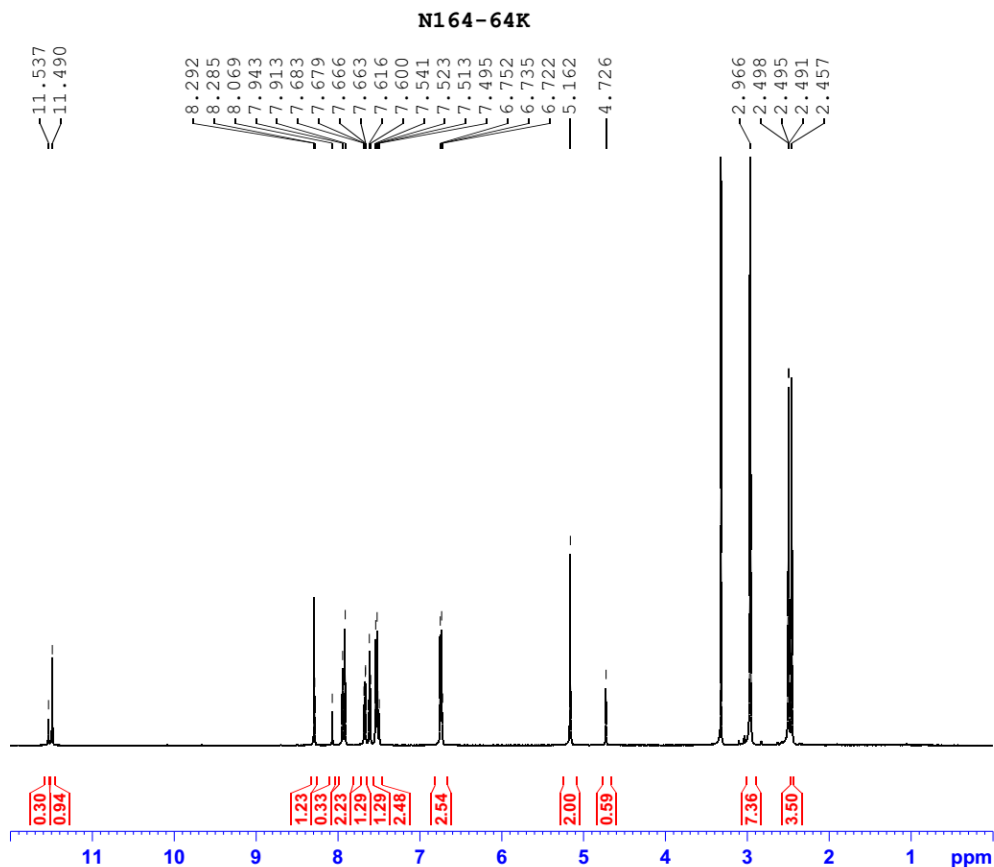
¹H NMR of compound 5x



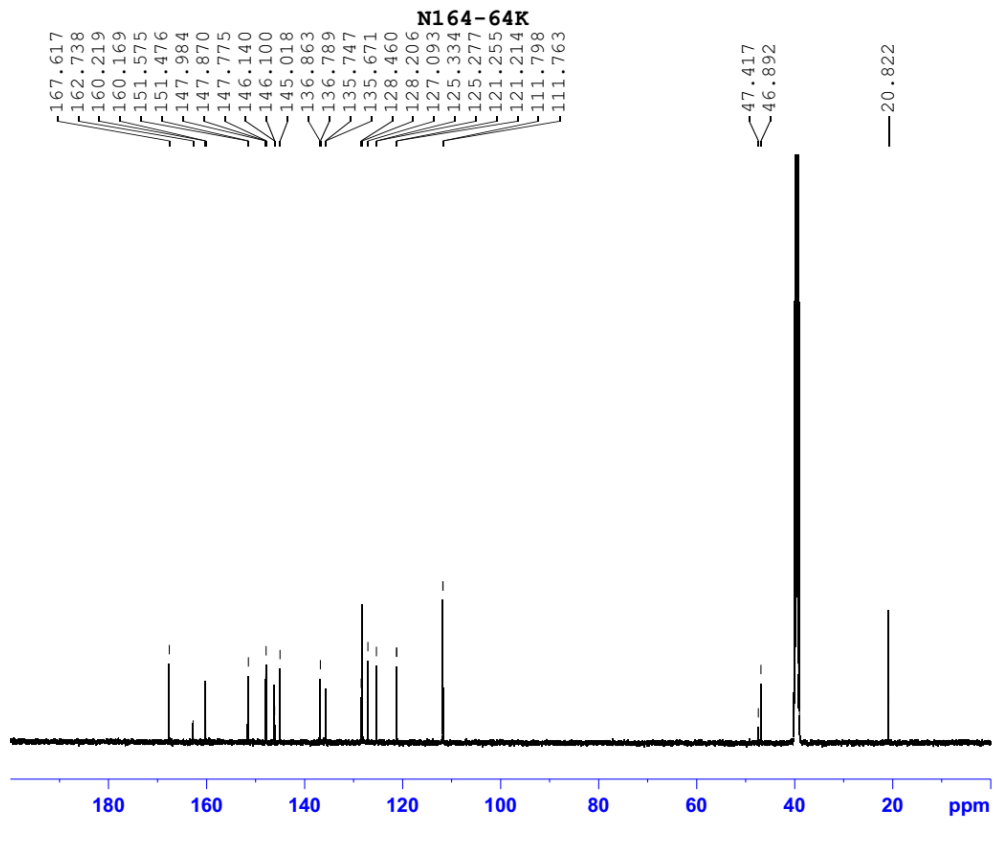
¹³C NMR of compound 5x



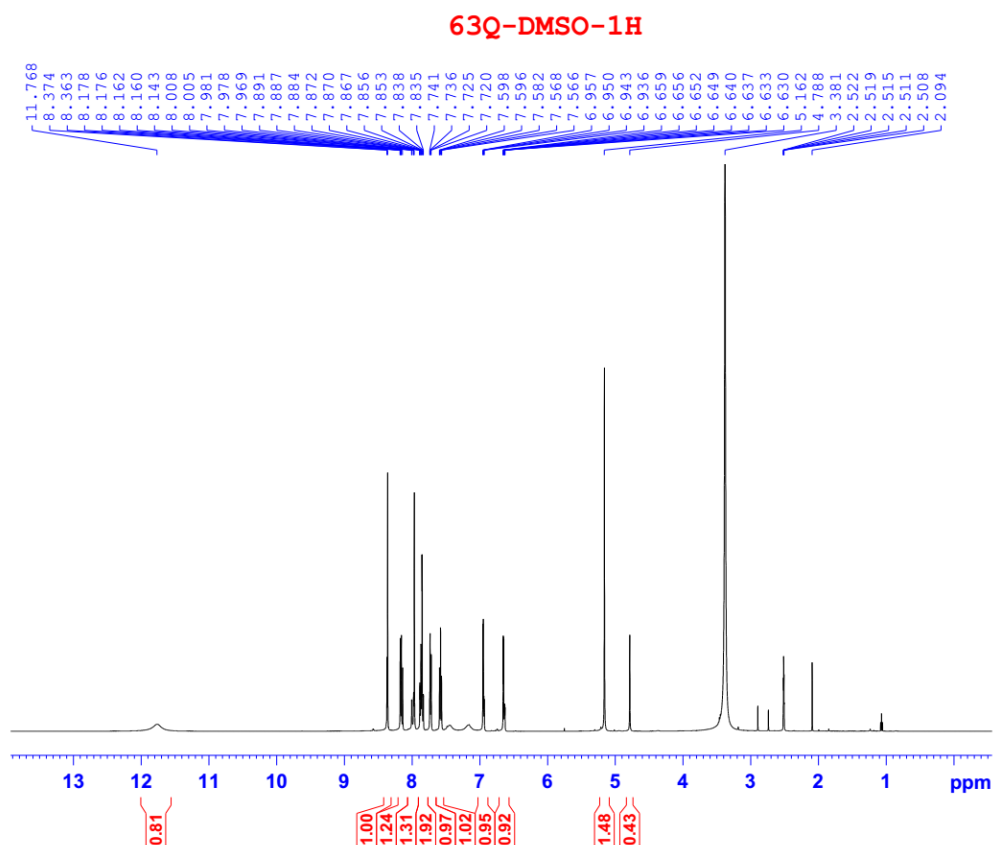
¹H NMR of compound 5z



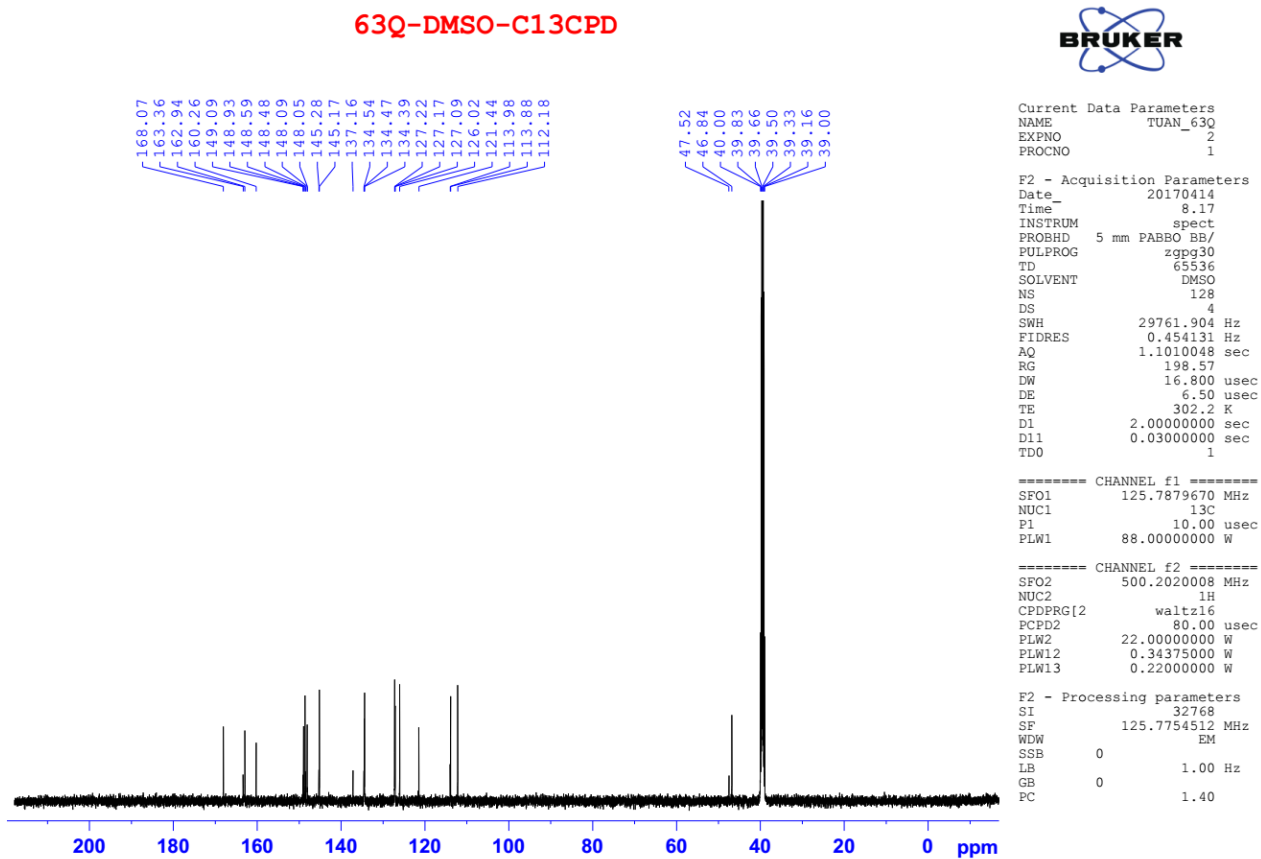
¹³C NMR of compound 5z



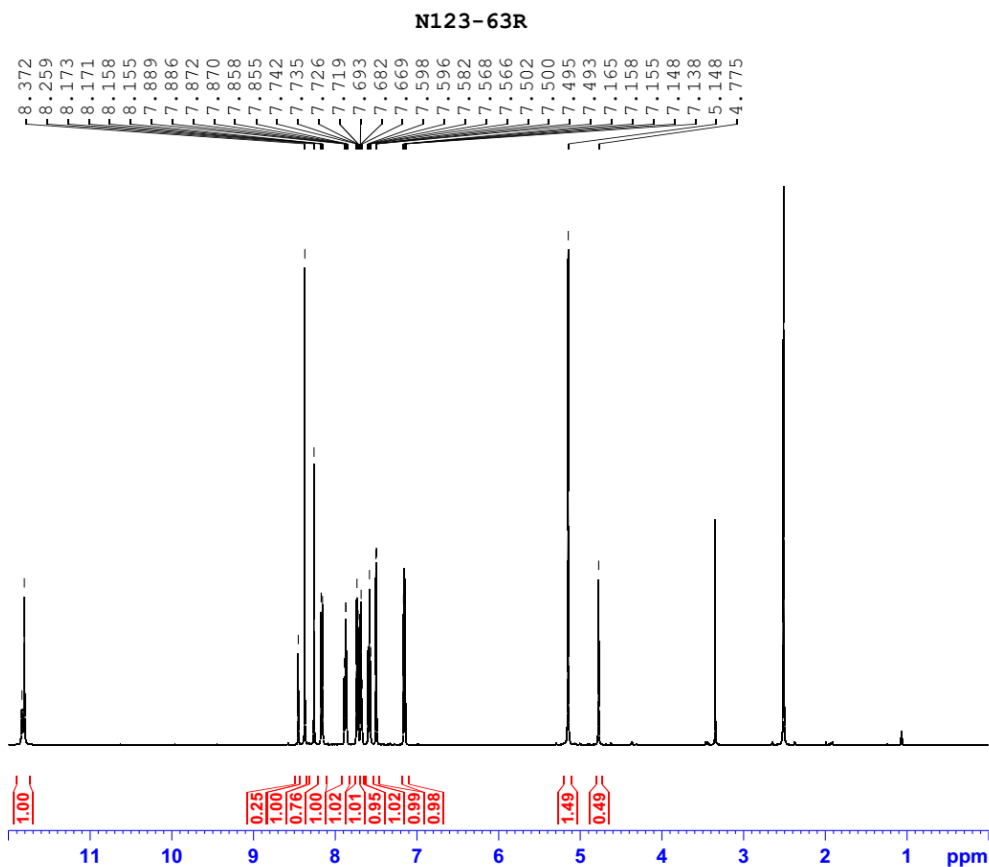
¹H NMR of compound 6a



¹³C NMR of compound 6a



¹H NMR of compound 6b



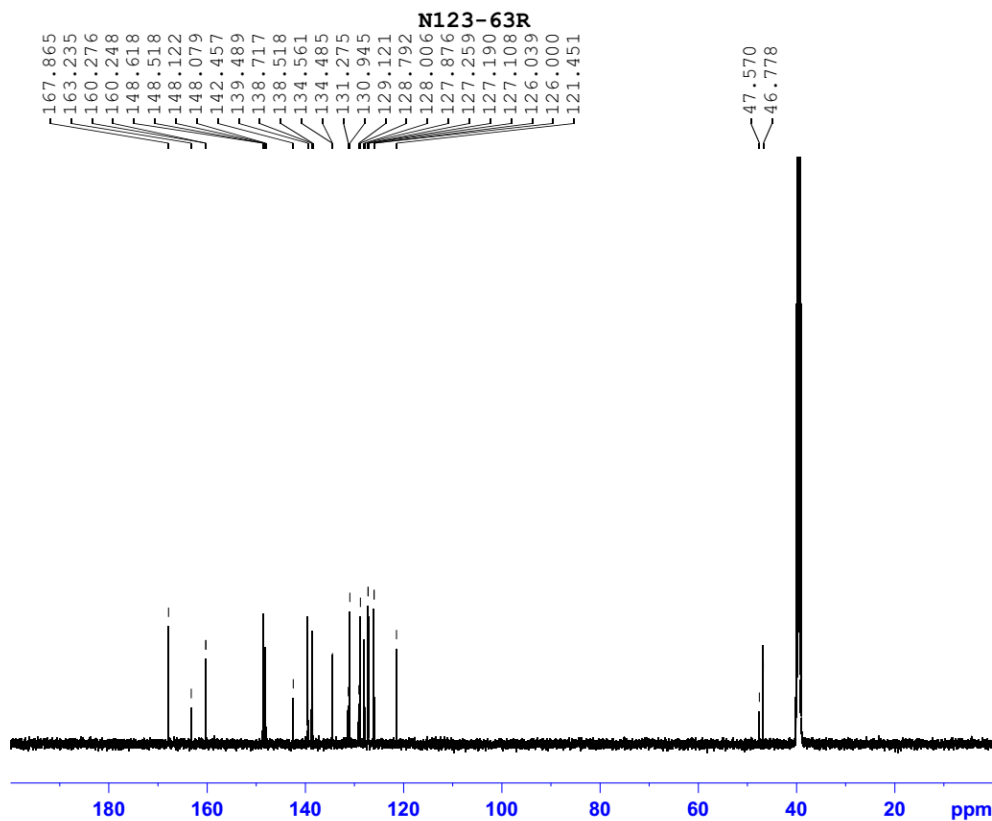
Current Data Parameters
 NAME N123-63R
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170425
 Time 17.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 191.38
 DW 50.000 usec
 DE 6.50 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 6b



Current Data Parameters
 NAME N123-63R
 EXPNO 22
 PROCNO 1

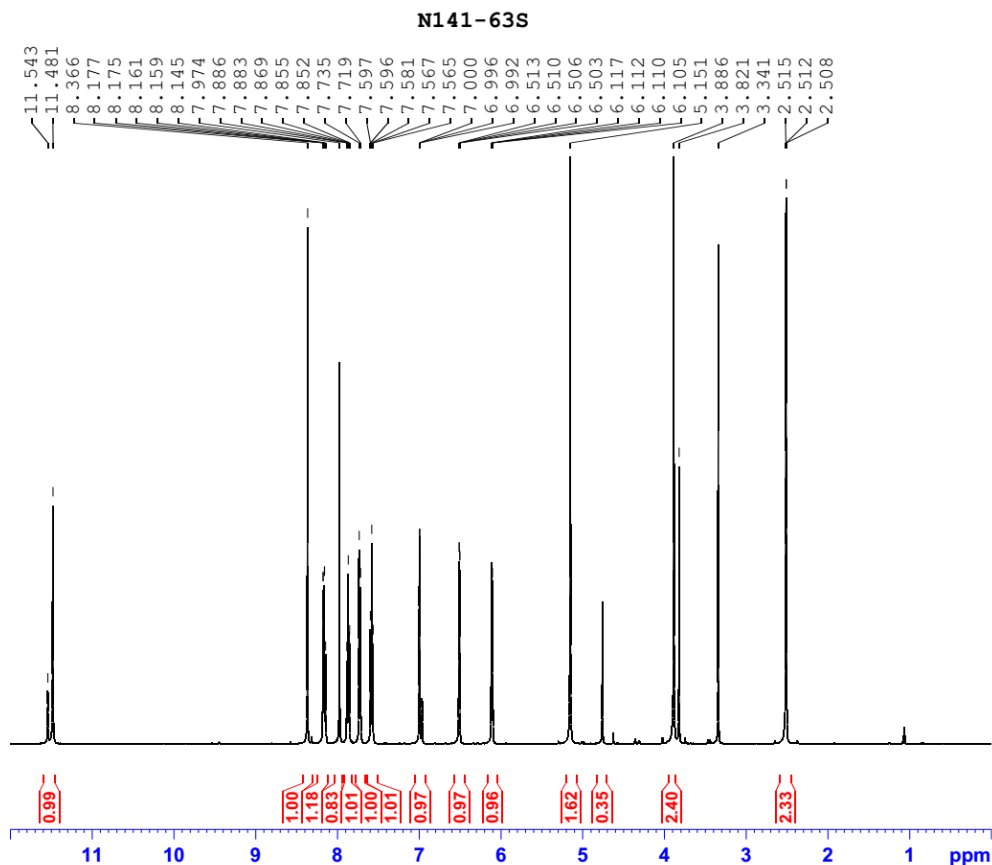
F2 - Acquisition Parameters
 Date_ 20170425
 Time 18.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 FULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 296.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

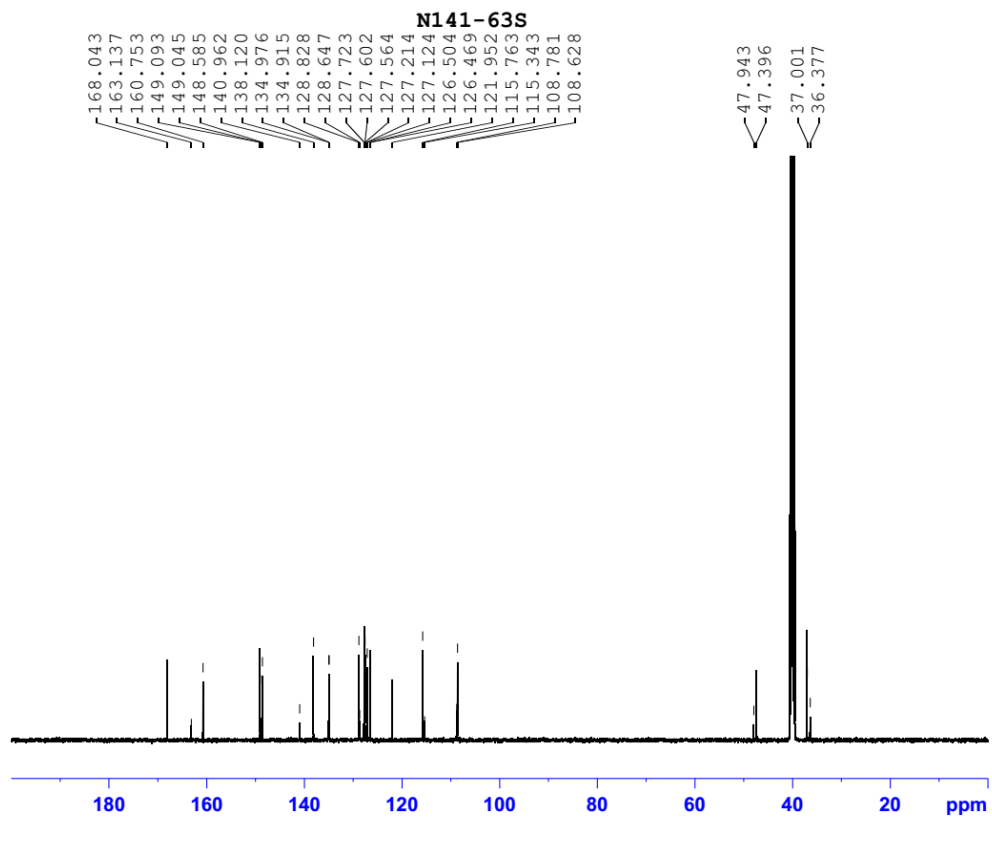
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7578471 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

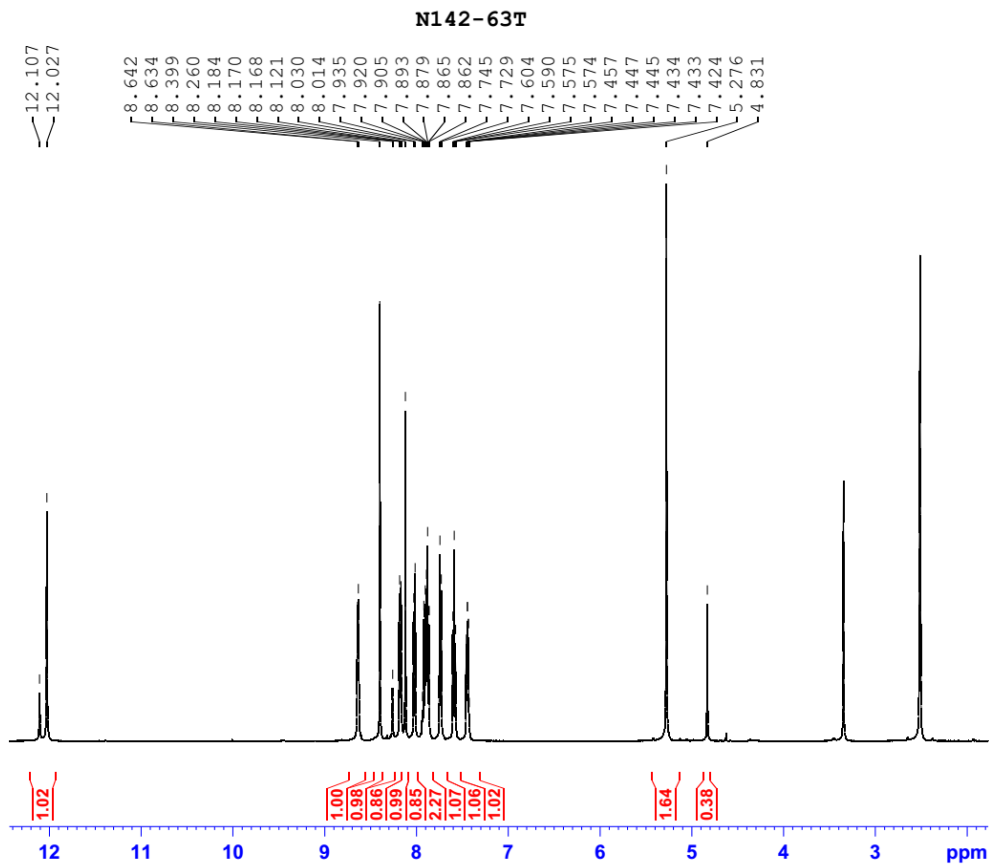
¹H NMR of compound 6c



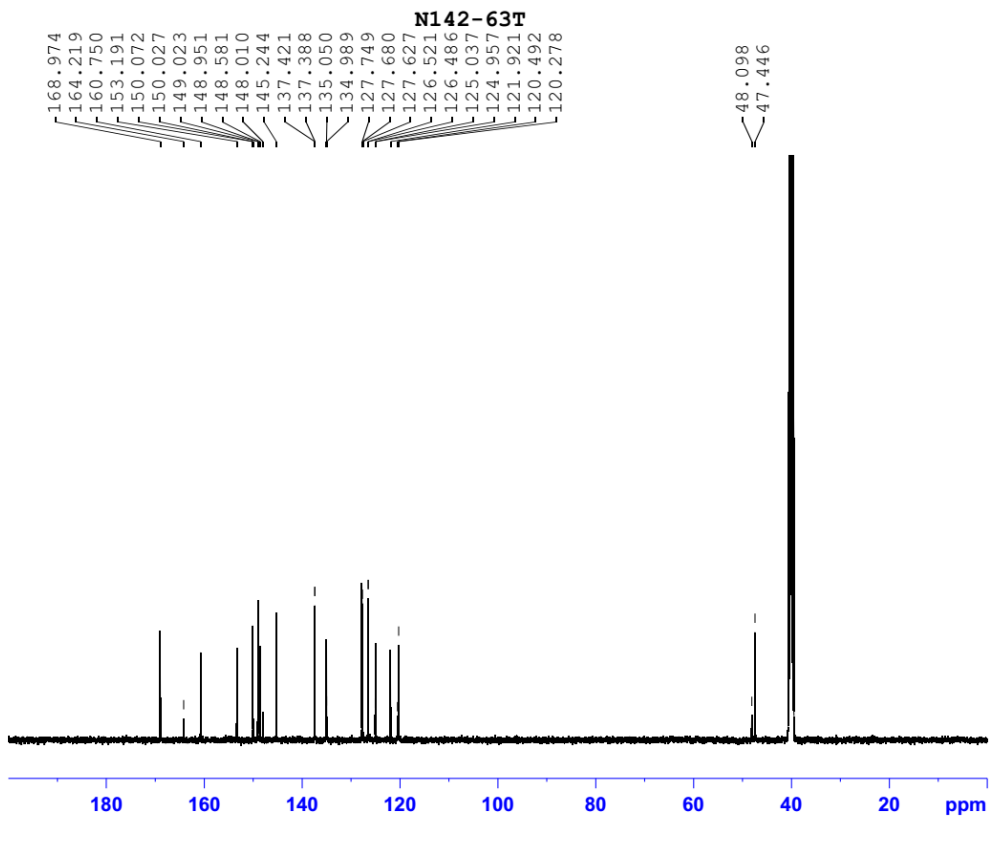
¹³C NMR of compound 6c



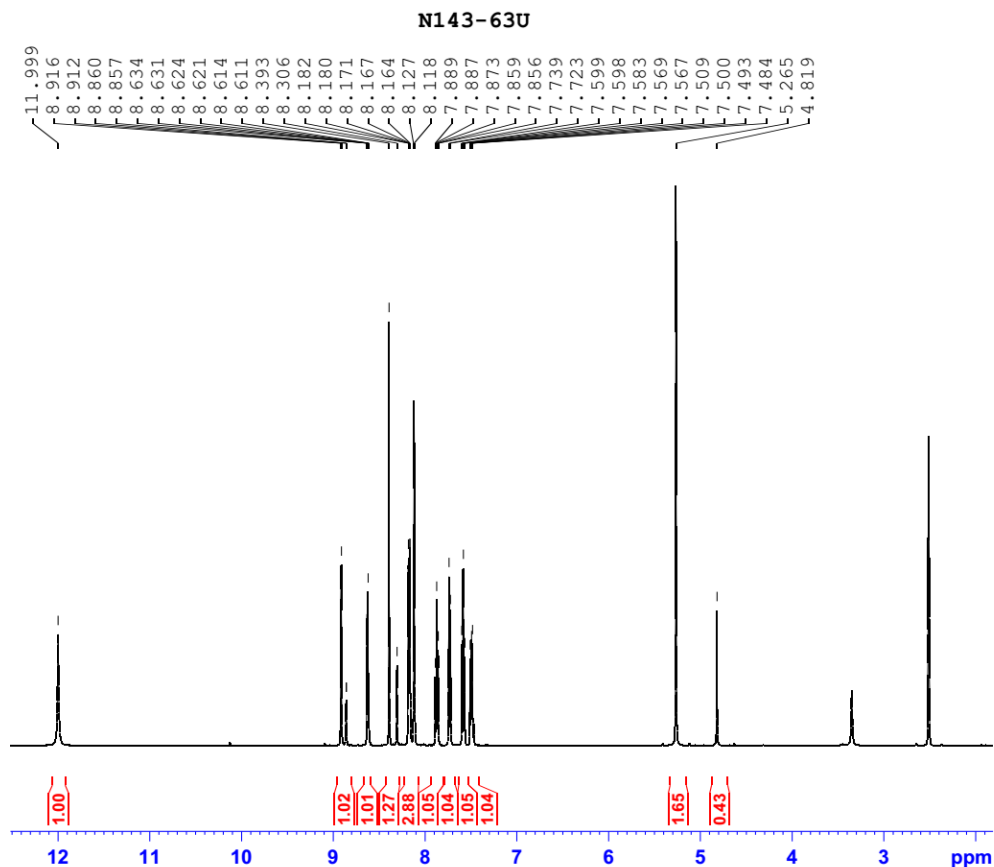
¹H NMR of compound 6d



¹³C NMR of compound 6d



¹H NMR of compound 6e



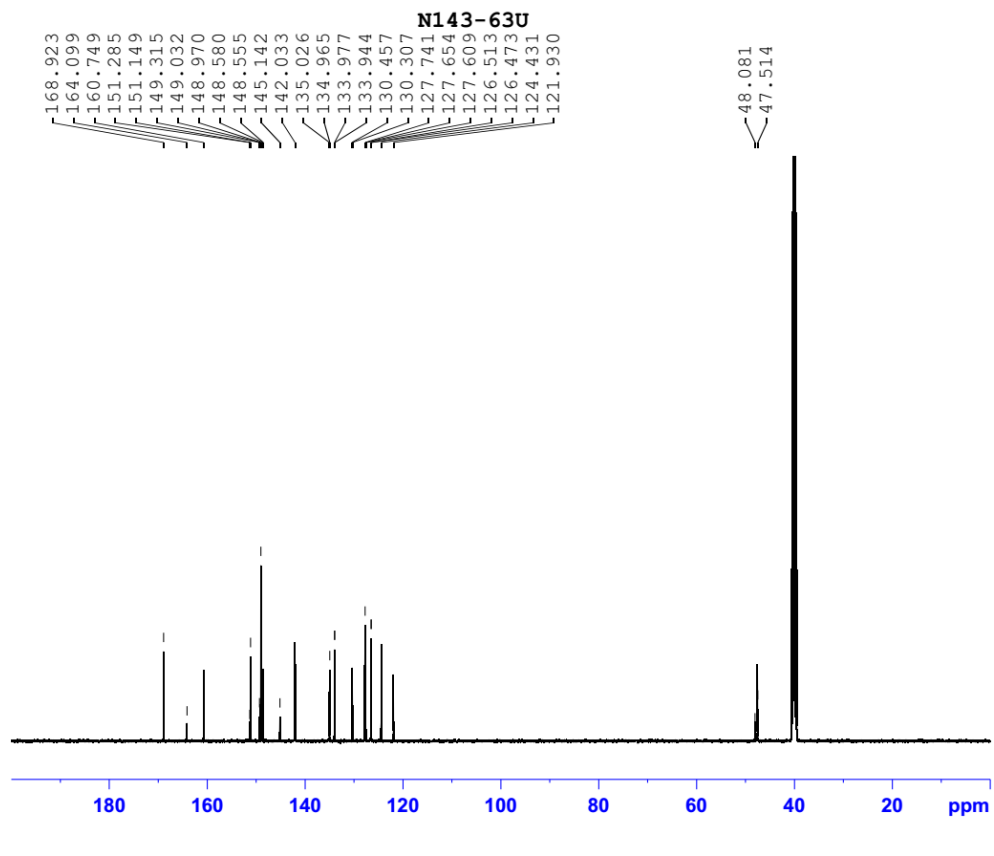
Current Data Parameters
 NAME N143-63U
 EXPNO 40
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170509
 Time_ 21.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 123.67
 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 9.80 usec
 PLW1 24.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 6e



Current Data Parameters
 NAME N143-63U
 EXPNO 42
 PROCNO 1

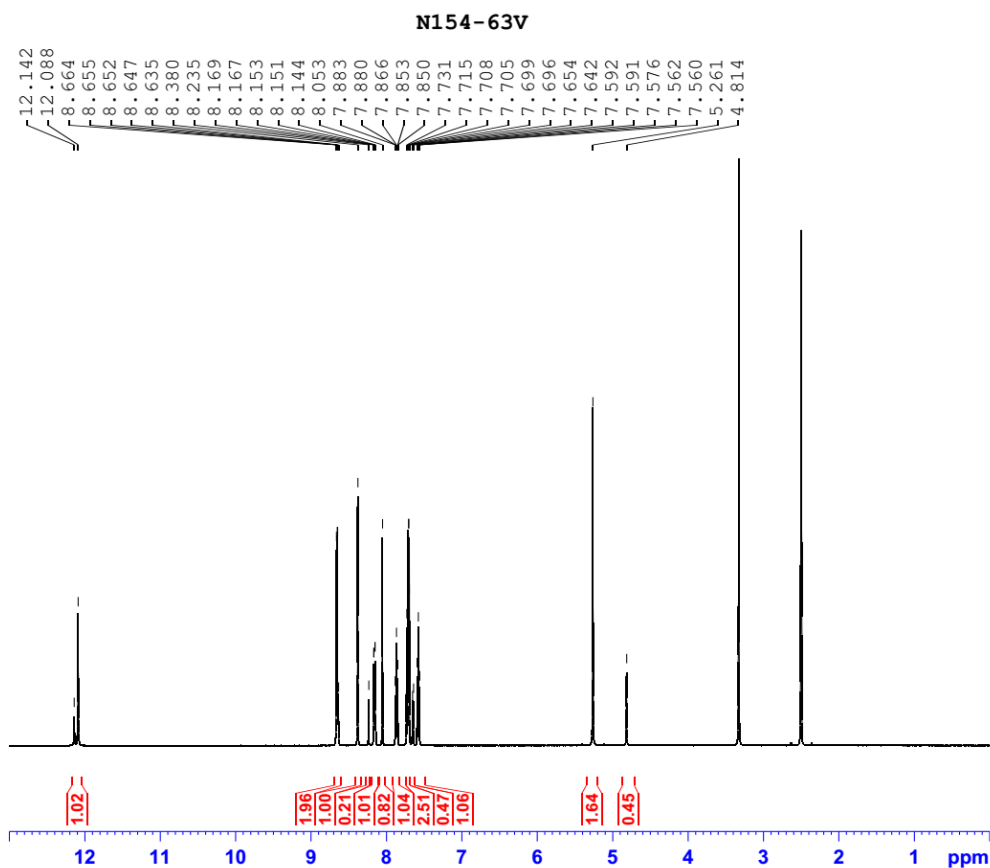
F2 - Acquisition Parameters
 Date_ 20170509
 Time_ 23.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

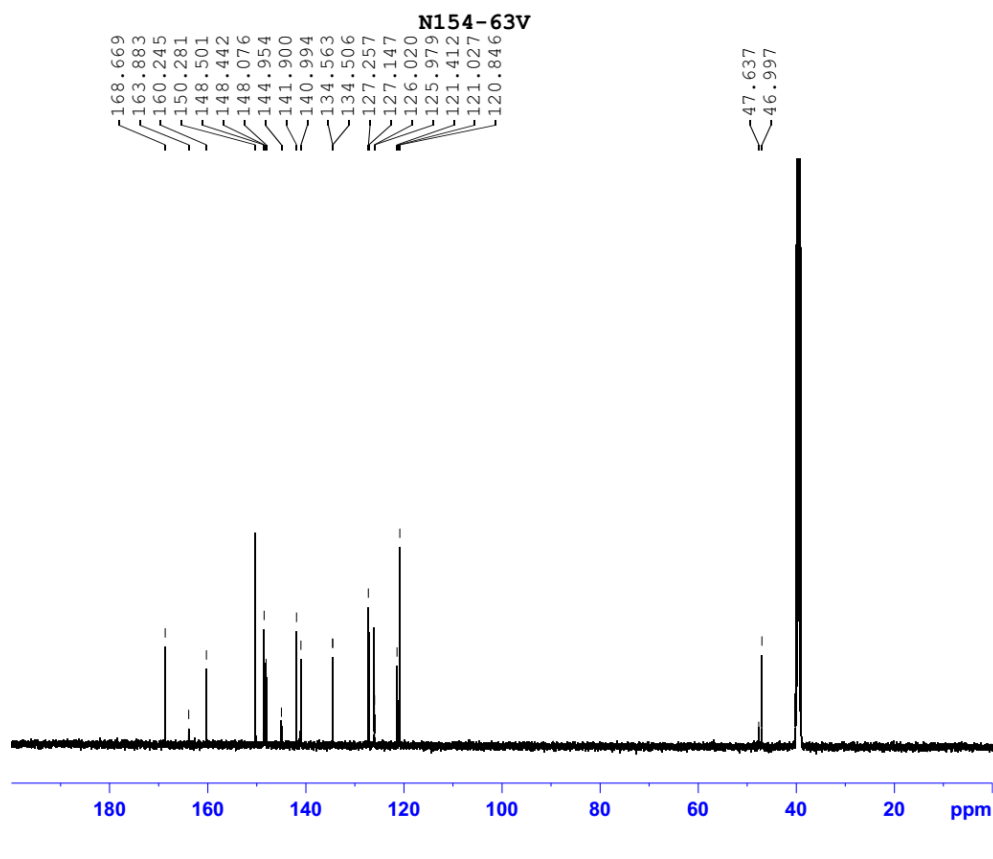
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

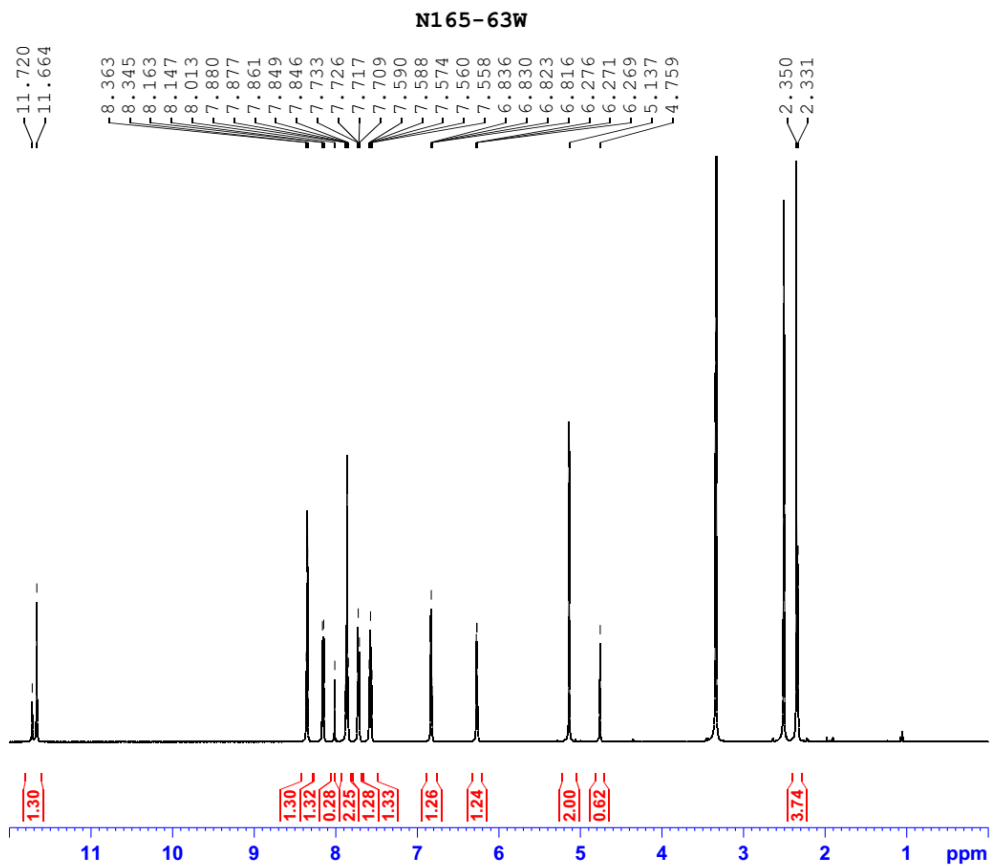
¹H NMR of compound 6f



¹³C NMR of compound 6f



¹H NMR of compound 6g



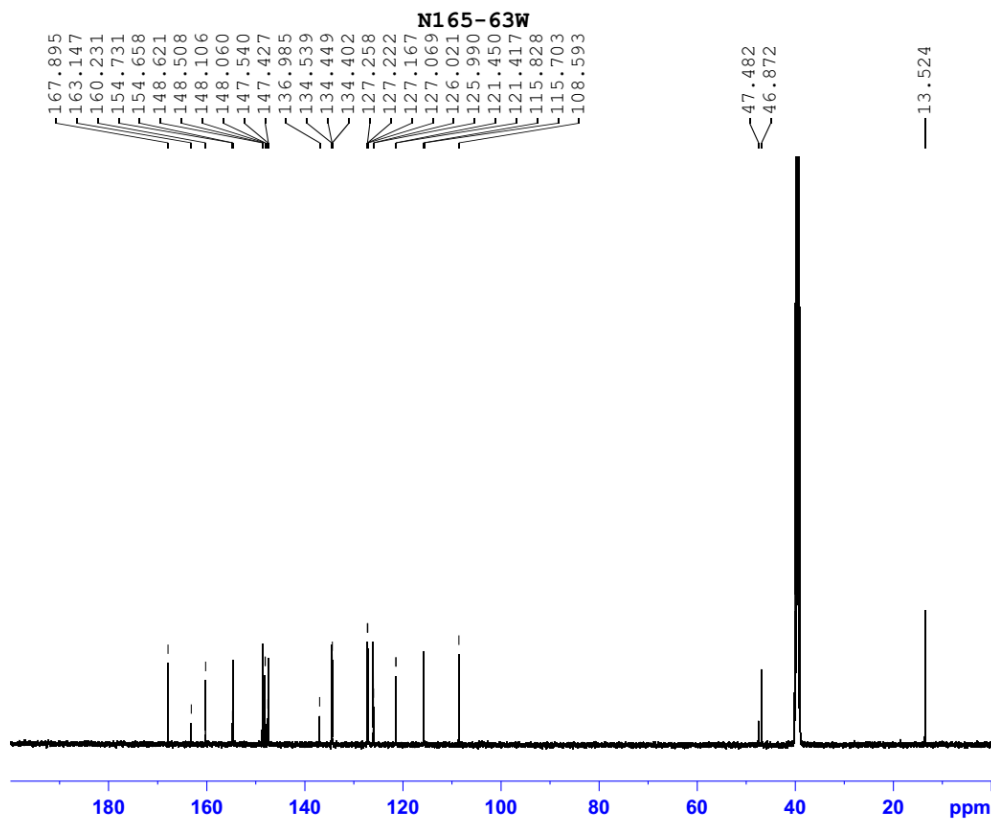
Current Data Parameters
 NAME N165-63W
 EXPNO 50
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170527
 Time_ 7.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 152.54
 DW 50.000 usec
 DE 6.50 usec
 TE 297.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1330040 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR of compound 6g



Current Data Parameters
 NAME N165-63W
 EXPNO 52
 PROCNO 1

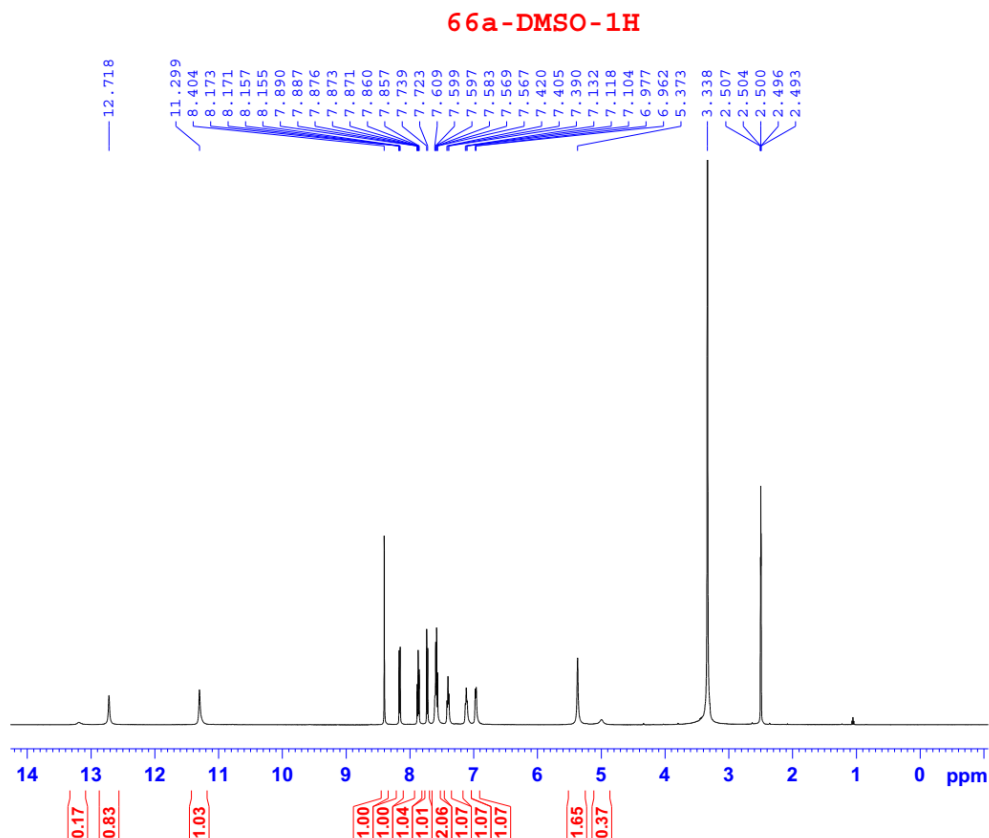
F2 - Acquisition Parameters
 Date_ 20170527
 Time_ 10.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 298.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7578498 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR of compound 7a



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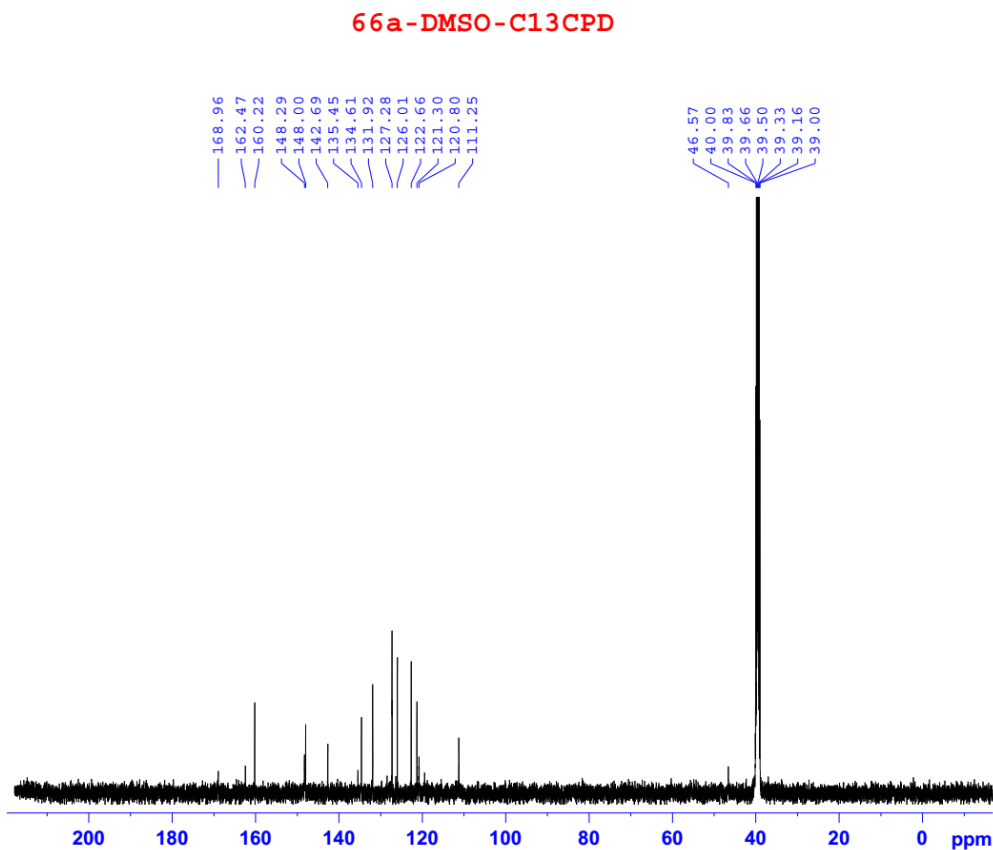
Current Data Parameters
NAME          66a
EXPNO        1
PROCNO       1

F2 - Acquisition Parameters
Date_        20170308
Time         16.02
INSTRUM      spect
PROBHD       5 mm PABBO BB/
PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS           16
DS           2
SWH          10000.000 Hz
FIDRES       0.152588 Hz
AQ           3.2767999 sec
RG           97.76
DW           50.000 usec
DE           6.50 usec
TE           303.1 K
D1           1.00000000 sec
D11          1
D10          1

===== CHANNEL f1 =====
SFO1         500.2030889 MHz
NUC1         1H
P1           10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI           65536
SF           500.2000068 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```

¹³C NMR of compound 7a



```

Current Data Parameters
NAME          66a
EXPNO        2
PROCNO       1

F2 - Acquisition Parameters
Date_        20170308
Time         18.10
INSTRUM      spect
PROBHD       5 mm PABBO BB/
PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS           256
DS           4
SWH          29761.904 Hz
FIDRES       0.454131 Hz
AQ           1.1010048 sec
RG           198.57
DW           16.800 usec
DE           6.50 usec
TE           303.2 K
D1           2.00000000 sec
D11          0.03000000 sec
D10          1

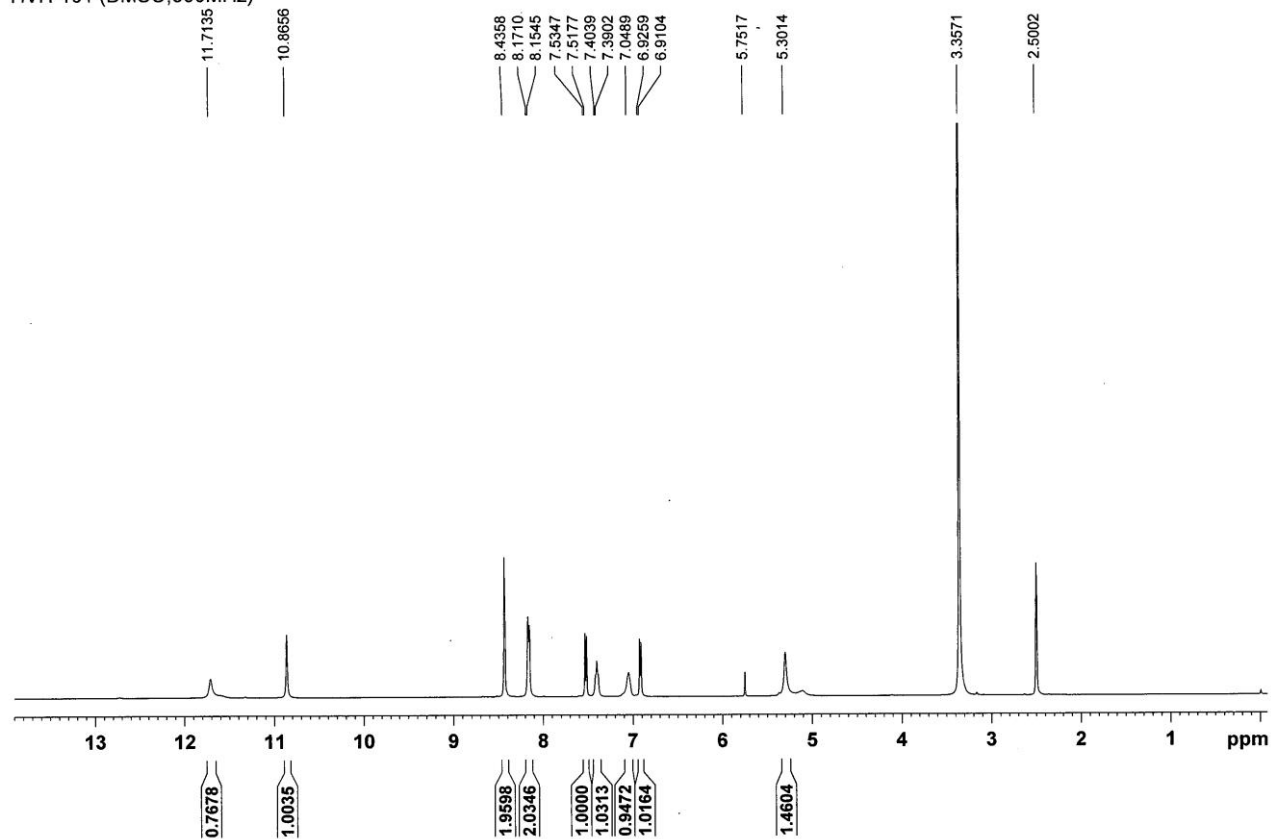
===== CHANNEL f1 =====
SFO1         125.7879670 MHz
NUC1         13C
P1           10.00 usec
PLW1         88.00000000 W

===== CHANNEL f2 =====
SFO2         500.2020008 MHz
NUC2         1H
CPDPRG[2]    waltz16
PCPD2        80.00 usec
PLW2         22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI           32768
SF           125.7754545 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
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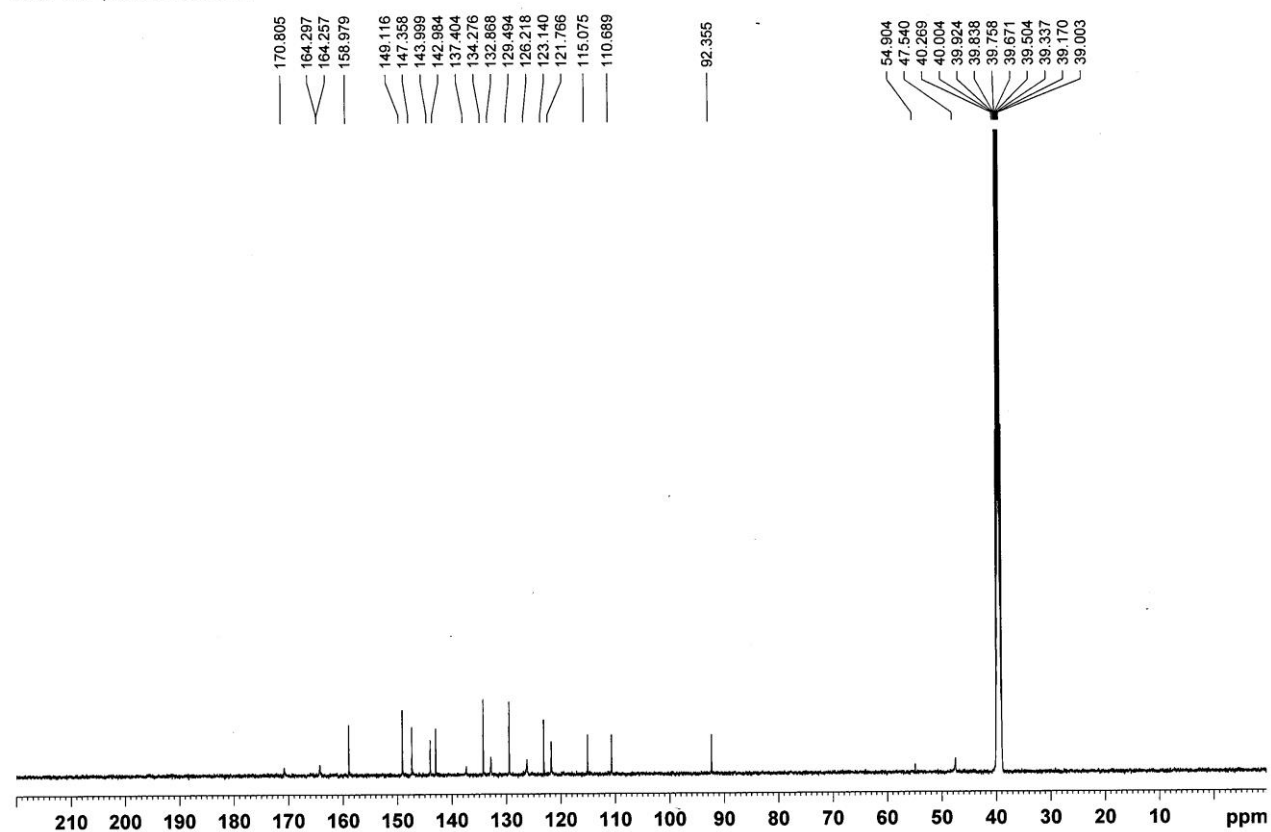
¹H NMR of compound 7b

HVH-101 (DMSO,500MHz)



¹³C NMR of compound 7b

HVH-101 (DMSO,500MHz)



Caption for the Graphical Abstract

A series of (E)-N'-arylidene-2-(4-oxoquinazolin-4(3H)-yl)acetohydrazides with significant cytotoxicity against three human cancer cell lines. Compound 5t displayed cytotoxicity up to 5-fold more potent than 5-FU, meanwhile compound 7b activated caspases activity by almost 200% in comparison to that of PAC-1.