

SUPPLEMENTAL MATERIALS

for

Design, Synthesis and Evaluation of Novel *N'*-substituted-1-(4-chlorobenzyl)-1*H*-indol-3-carbohydrazides as Antitumor Agents

Le Cong Huan,^{a,d} Duong Tien Anh,^a Pham-The Hai,^a Lai Duc Anh,^a Eun Jae Park,^b A Young Ji,^b Jong Soon Kang,^c Do Thi Mai Dung,^a Dao Thi Kim Oanh,^a Truong Thanh Tung,^{e,f} Dinh Thi Thanh Hai,^{*,a} Sang-Bae Han,^{*,b} Nguyen-Hai Nam^{*,a}

^aHanoi University of Pharmacy, 13-15 Le Thanh Tong, Hanoi, Vietnam

^bCollege of Pharmacy, Chungbuk National University, 194-31, Osongsaengmyung-1, Heungdeok, Cheongju, Chungbuk, 28160, Republic of Korea

^cBio-Evaluation Center, Korea Research Institute of Bioscience and Biotechnology, Cheongju, Chungbuk, Republic of Korea

^dThai Binh University of Medicine and Pharmacy, Thai Binh City, Vietnam

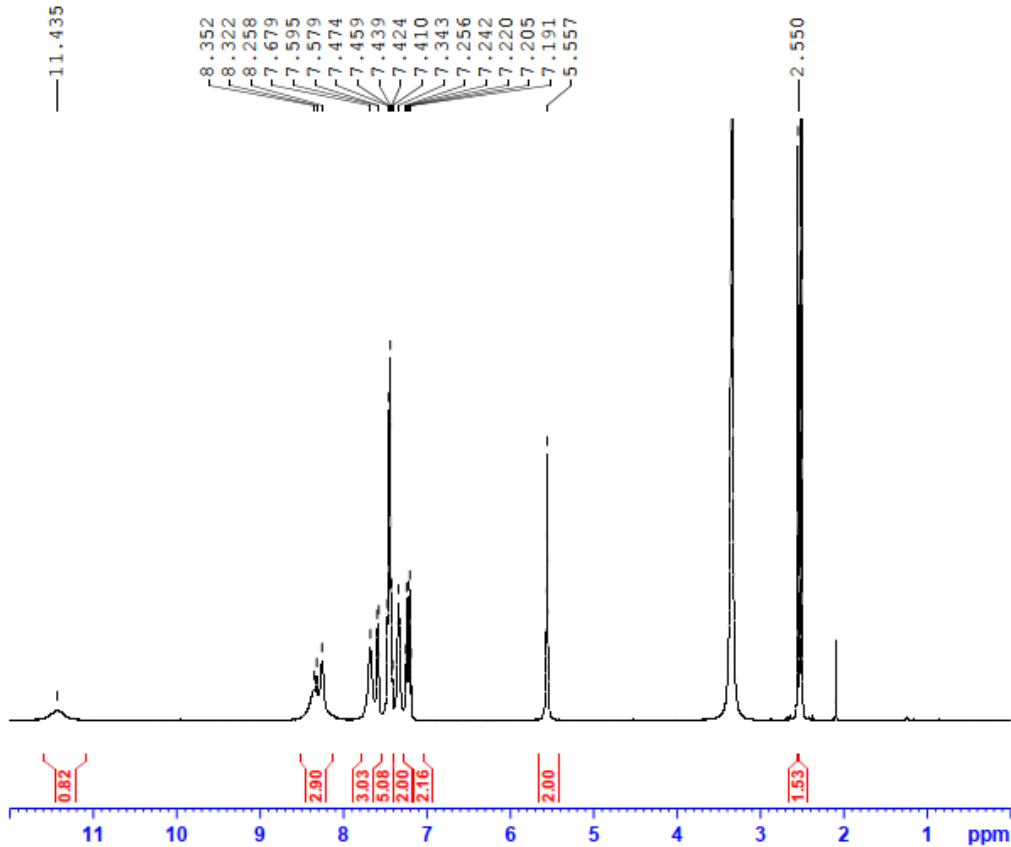
^eFaculty of Pharmacy, PHENIKAA University, Hanoi, 12116, Vietnam

^fPHENIKAA Institute for Advanced Study (PIAS), PHENIKAA University, Hanoi, 12116, Vietnam

Keywords: Acylhydrazones, acetohydrazides, cytotoxicity, caspase activation.

***Corresponding authors:** Tel.: +84-4-39330531; Fax: +84-4-39332332; Emails: shan@cbnu.ac.kr (S.B. Han); namnh@hup.edu.vn (N.H. Nam).

ALL ¹H & ¹³C NMR SPECTRA OF THE COMPOUNDS



¹H-NMR of compound 4a



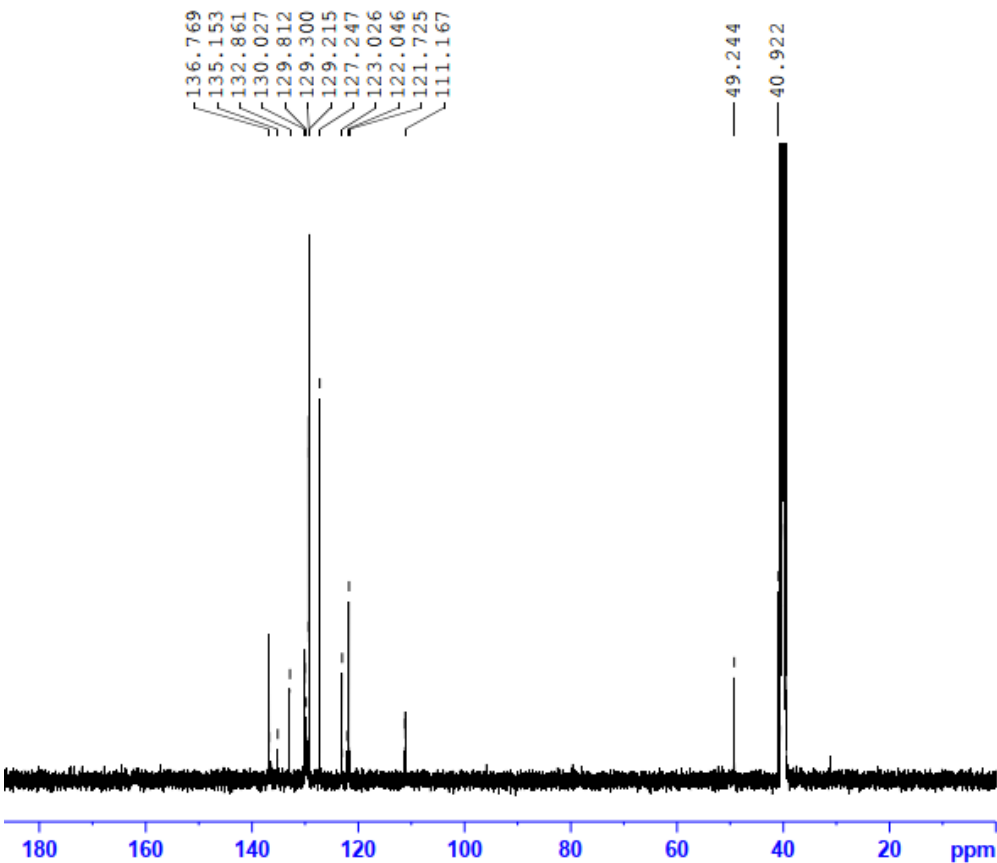
```

Current Data Parameters
NAME      TAnh-105A-2
EXPNO    10
PROCNO   1

FC - Acquisition Parameters
Date_    20191010
Time     13.27
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       3.278799 sec
RG       152.54
DM       50.000 usec
DE       6.50 usec
TE       298.9 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
SF01    500.1320885 MHz
NUC1     1H
P1       9.80 usec
PLW1    24.00000000 W

FC - 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 4a



```

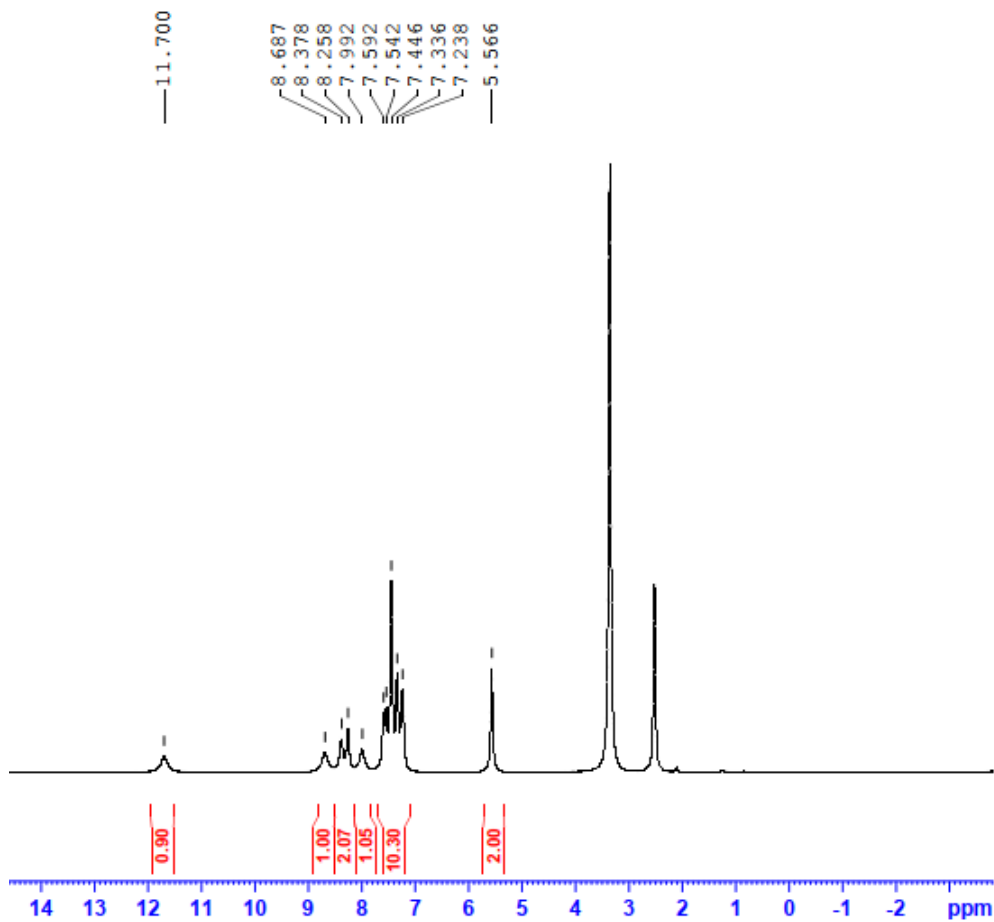
Current Data Parameters
NAME      TAnh-105A-2
EXPNO    11
PROCNO   1

FC - Acquisition Parameters
Date_    20191011
Time     10.54
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       1.0485960 sec
RG       191.38
DM       16.000 usec
DE       6.50 usec
TE       299.7 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
SF01    125.7702627 MHz
NUC1     13C
P1       9.50 usec
PLW1    90.00000000 W

===== CHANNEL f2 =====
SF02    500.1320005 MHz
NUC2     1H
CPDPRG12 waltz16
PCPD2    80.00 usec
PLW2    24.00000000 W
PLW12   0.36015001 W
PLW13   0.23050000 W

FC - Processing parameters
SI       65536
SF       125.7877885 MHz
WDW      EM
SSB      0
TR       1.00 Hz
  
```



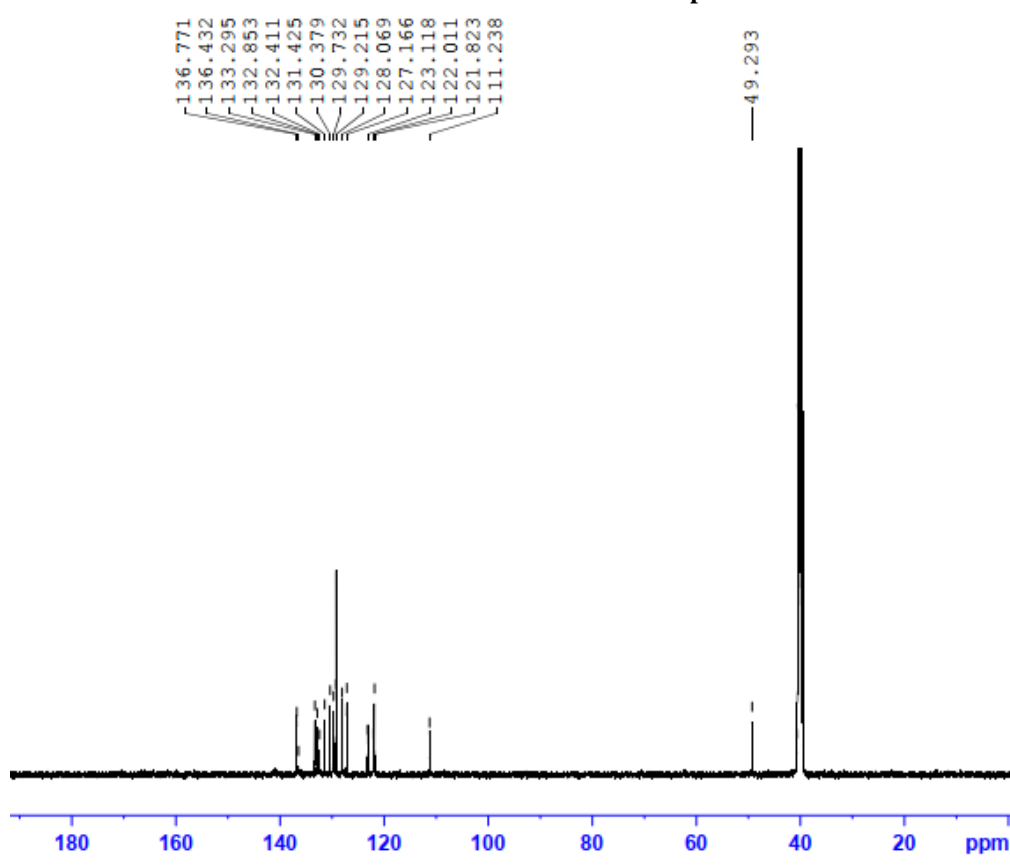
Current Data Parameters
 NAME TAnh-105B
 EXPNO 10
 PROCNO 1

FC - Acquisition Parameters
 Date_ 20191015
 Time 16.56
 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 138.87
 DW 50.000 usec
 DE 6.50 usec
 TE 298.7 K
 D1 1.00000000 sec
 TDO 1

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

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

¹H-NMR of compound 4b



Current Data Parameters
 NAME TAnh-105B
 EXPNO 11
 PROCNO 1

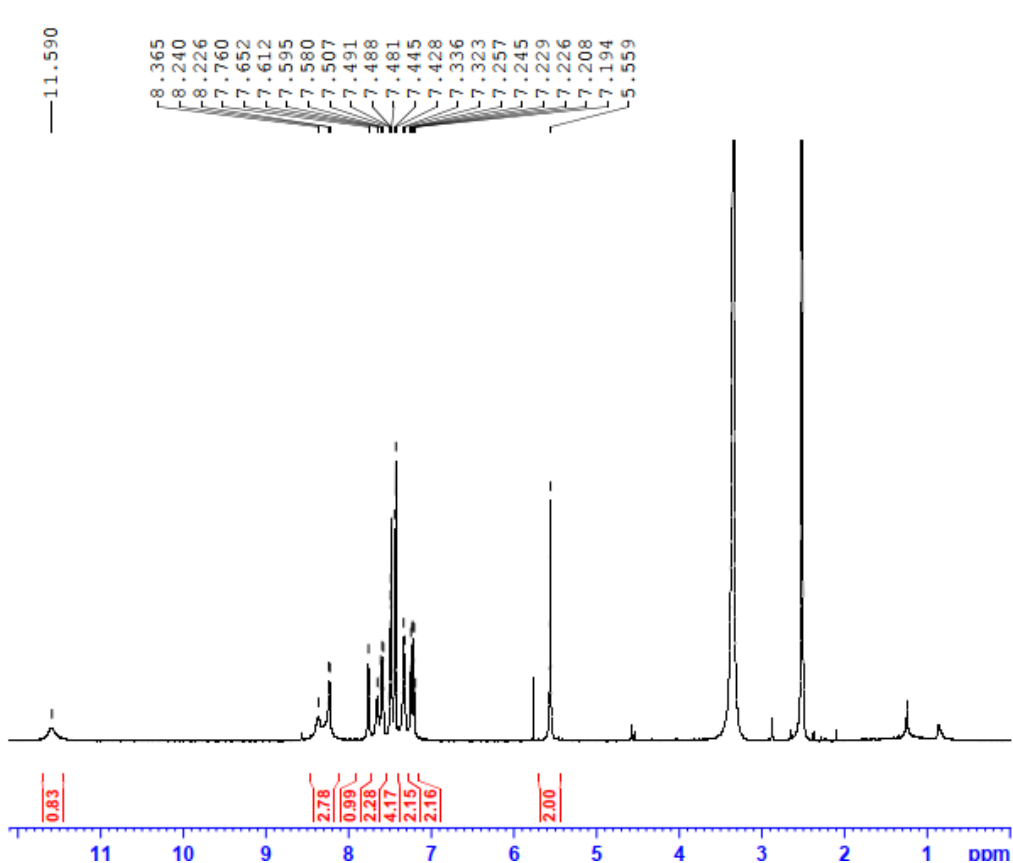
FC - Acquisition Parameters
 Date_ 20191015
 Time 20.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476827 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 129.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLM2 24.00000000 W
 PLM12 0.26015001 W
 PLM13 0.23050000 W

FC - Processing parameters
 SI 65536
 SF 129.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz

¹³C-NMR of compound 4b



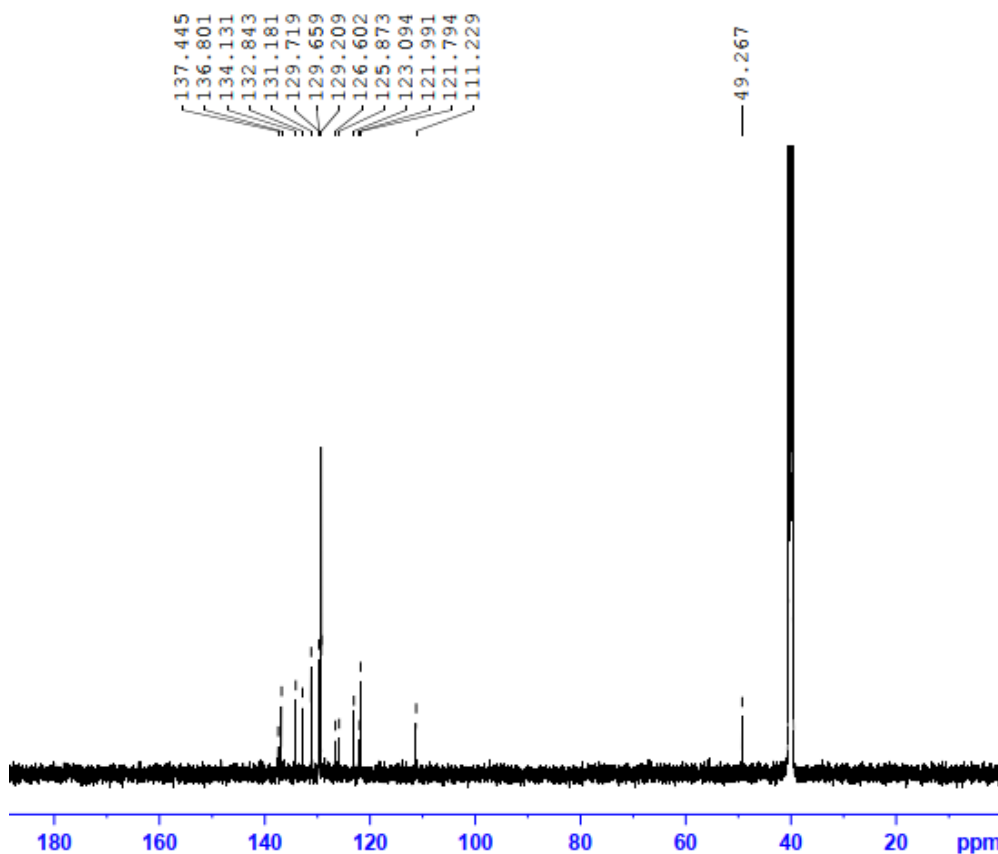
Current Data Parameters
NAME TAnh-105C
EXPNO 10
PROCNO 1

FC - Acquisition Parameters
Date_ 20191125
Time 0.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.162888 Hz
AQ 3.27679999 sec
RG 191.38
DN 50.000 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TDO 1

===== CHANNEL #1 =====
SF01 500.1330888 MHz
NUC1 1H
P1 9.80 usec
PLW1 24.00000000 W

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

¹H-NMR of compound 4c



Current Data Parameters
NAME TAnh-105C
EXPNO 11
PROCNO 1

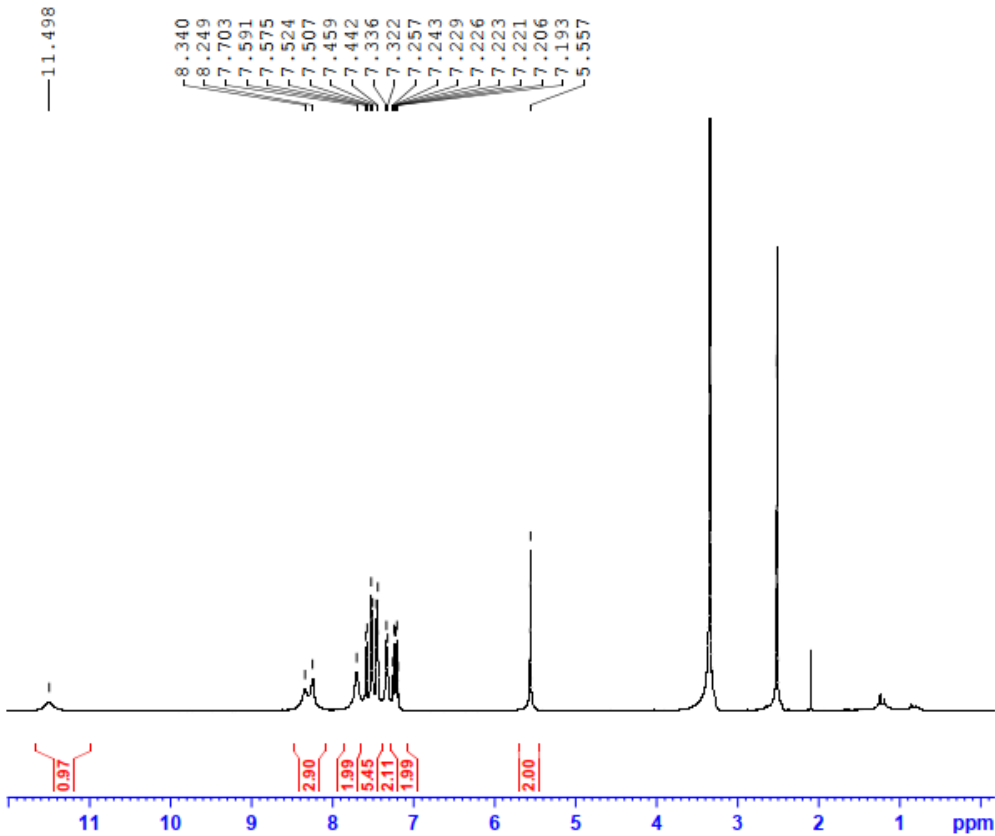
FC - Acquisition Parameters
Date_ 20191125
Time 4.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.04885760 sec
RG 191.38
DN 16.000 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL #1 =====
SF01 125.7703627 MHz
NUC1 13C
P1 9.50 usec
PLW1 90.00000000 W

===== CHANNEL #2 =====
SF02 500.1320005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 80.00 usec
PLW2 24.00000000 W
PLW12 0.26015001 W
PLW13 0.23050000 W

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

¹³C-NMR of compound 4c



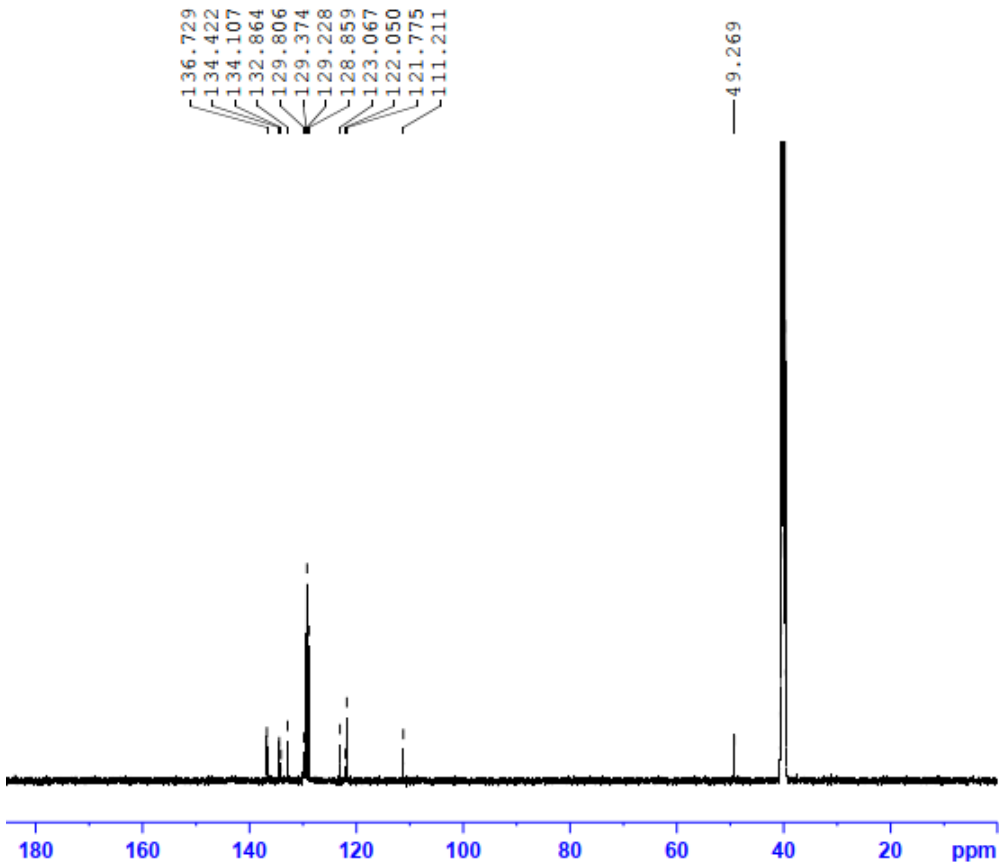
Current Data Parameters
 NAME TANh-105D
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191018
 Time_ 20.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152388 Hz
 AQ 3.2767999 sec
 RG 191.38
 DW 30.000 usec
 DE 6.50 usec
 TE 299.1 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL #1 =====
 SFO1 500.1320885 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

¹H-NMR of compound 4d



Current Data Parameters
 NAME TANh-105D
 EXPNO 21
 PROCNO 1

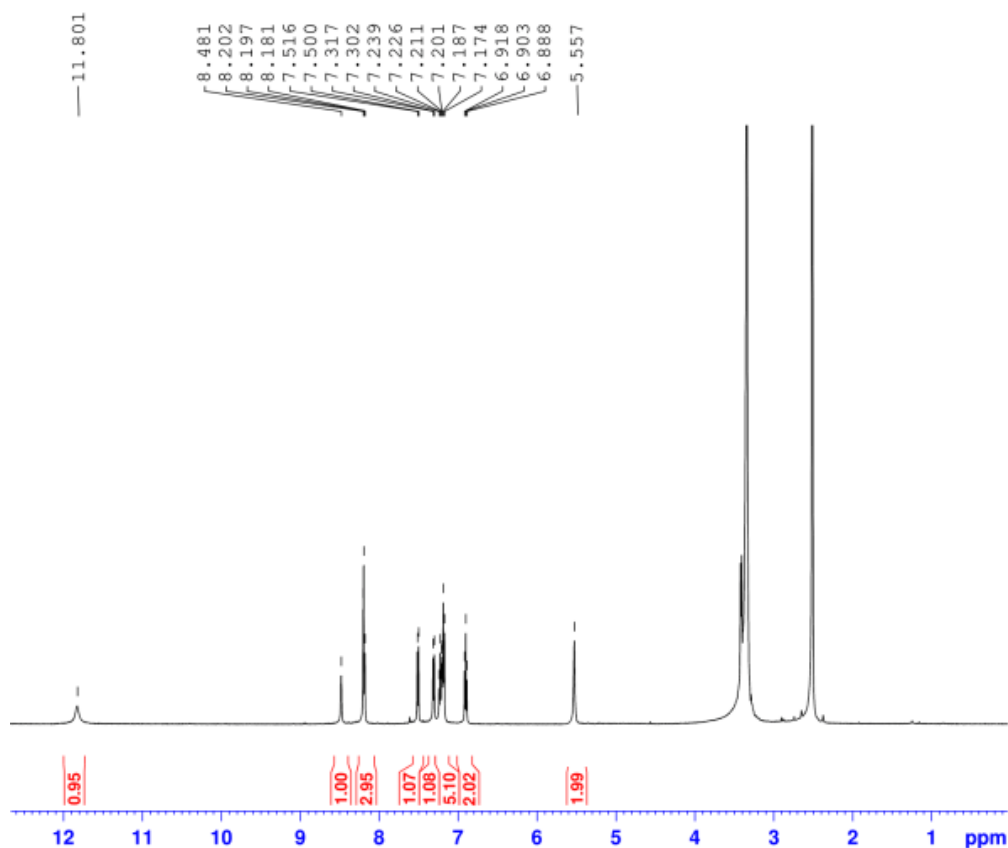
F2 - Acquisition Parameters
 Date_ 20191016
 Time_ 0.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 31260.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL #1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

===== CHANNEL #2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW3 0.26019001 W
 PLW4 0.29050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7577888 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz

¹³C-NMR of compound 4d



¹H-NMR of compound 4e



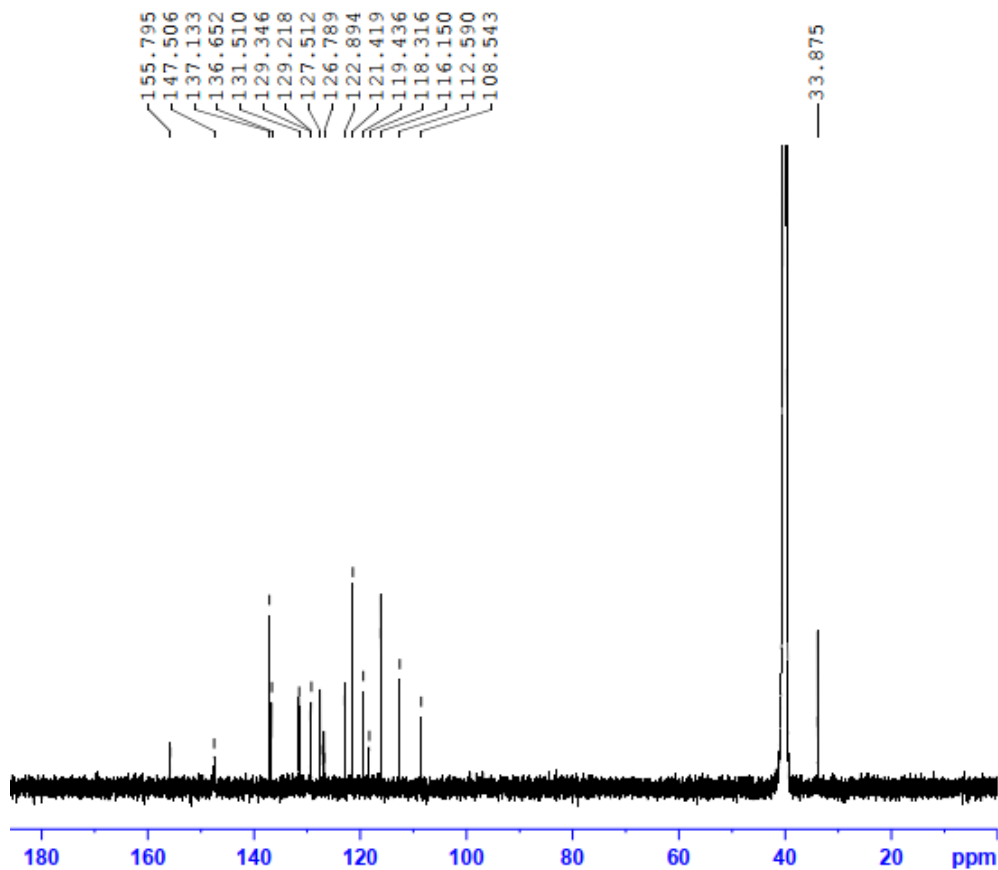
```

Current Data Parameters
NAME      Tanh-105E
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20191116
Time     15.05
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       298.8 K
D1       1.00000000 sec
TD0      1

----- CHANNEL f1 -----
SF01    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 4e



```

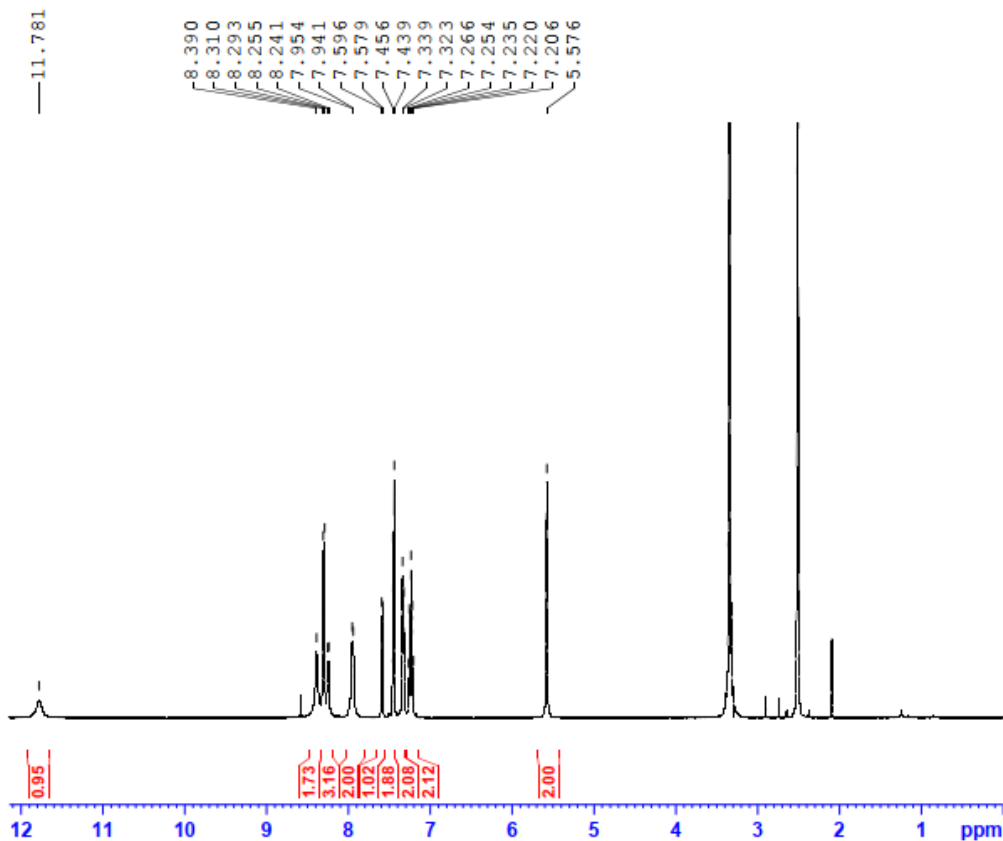
Current Data Parameters
NAME      Tanh-105E
EXPNO    11
PROCNO   1

F2 - Acquisition Parameters
Date_    20191116
Time     22.11
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       8192
DS       4
SWH      31250.000 Hz
FIDRES   0.476827 Hz
AQ       1.0488760 sec
RG       191.38
DW       16.000 usec
DE       6.50 usec
TE       299.4 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
SF01    125.7703627 MHz
NUC1     13C
P1       9.50 usec
PLW1    90.00000000 W

===== CHANNEL f2 =====
SF02    500.1320005 MHz
NUC2     1H
CPDPRG12 waltz16
PCPD0    80.00 usec
PLW2    24.00000000 W
PLW12   0.36015001 W
PLW13   0.23060000 W

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



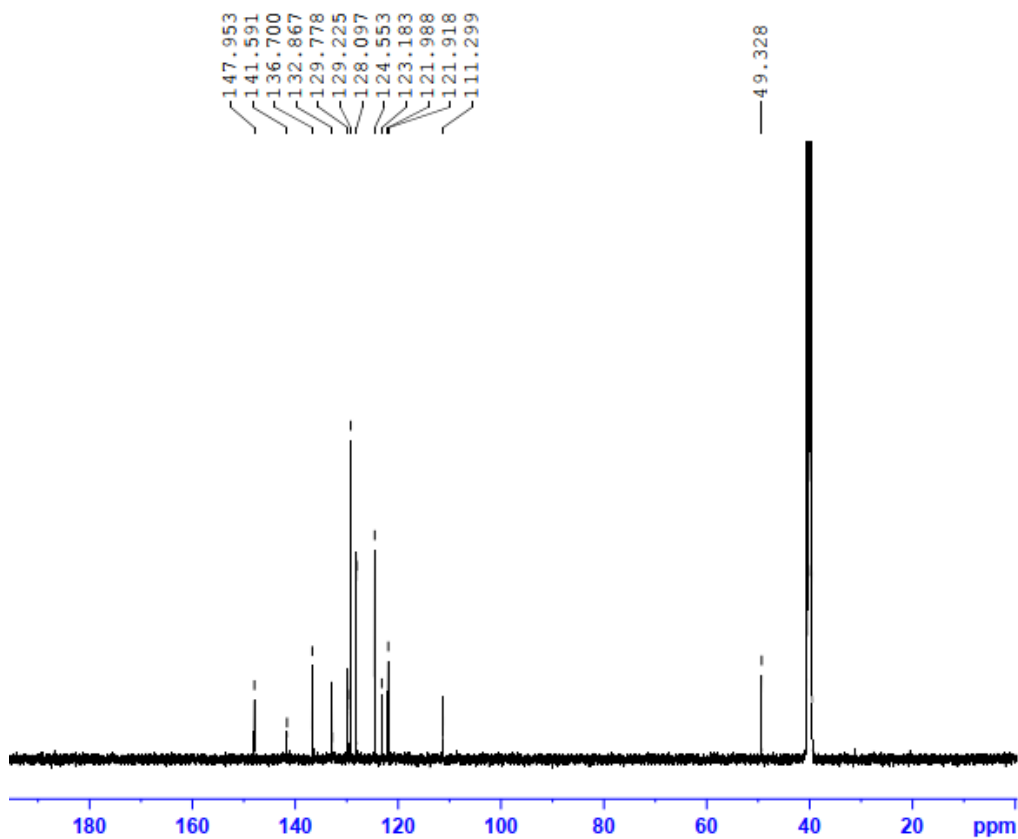
Current Data Parameters
 NAME Tanh-105F
 EXPNO 20
 PROCNO 1

FC - Acquisition Parameters
 Date_ 20191108
 Time 13.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SNH 10000.000 Hz
 FIDRES 0.150588 Hz
 AQ 3.2767999 sec
 RG 191.38
 DW 50.000 use
 DE 6.50 use
 TE 298.6 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 500.1330885 MHz
 NUC1 1H
 P1 9.50 use
 PLW1 24.00000000 W

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

¹H-NMR of compound 4f



Current Data Parameters
 NAME Tanh-105F
 EXPNO 21
 PROCNO 1

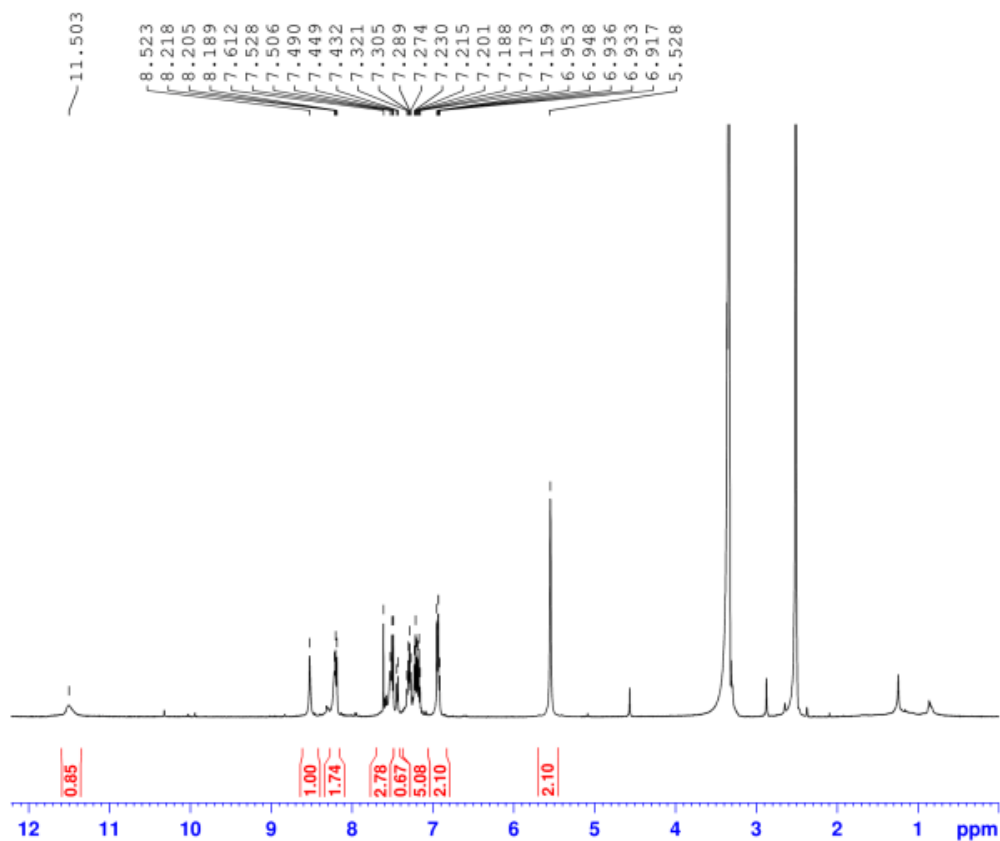
FC - Acquisition Parameters
 Date_ 20191109
 Time 14.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 8192
 DS 4
 SNH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0488760 sec
 RG 191.38
 DW 16.000 use
 DE 6.50 use
 TE 298.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 125.7702637 MHz
 NUC1 13C
 P1 9.50 use
 PLW1 90.00000000 W

===== CHANNEL f2 =====
 SF02 500.1320005 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 80.00 use
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.23050000 W

FC - Processing parameters
 SI 65536
 SF 125.7577685 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz

¹³C-NMR of compound 4f



¹H-NMR of compound 4g



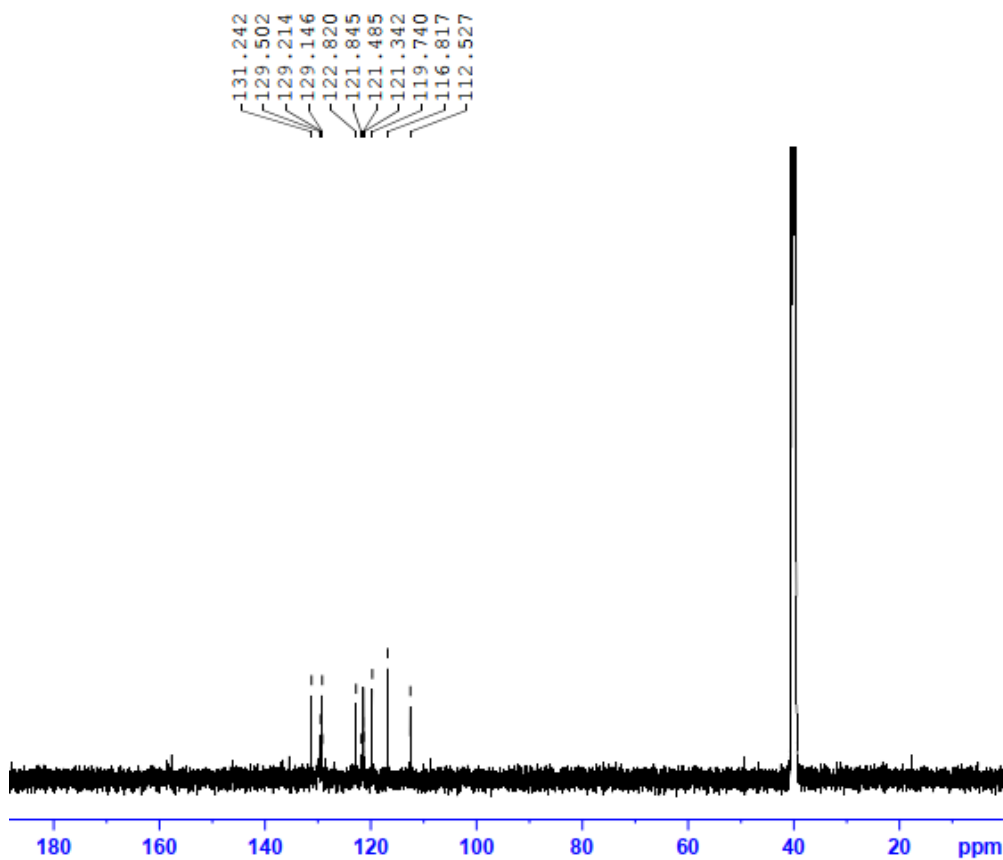
```

Current Data Parameters
NAME      TAnh-105G
EXPNO    30
PROCNO   1

F2 - Acquisition Parameters
Date_    20191117
Time     5.25
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       299.0 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 4g



```

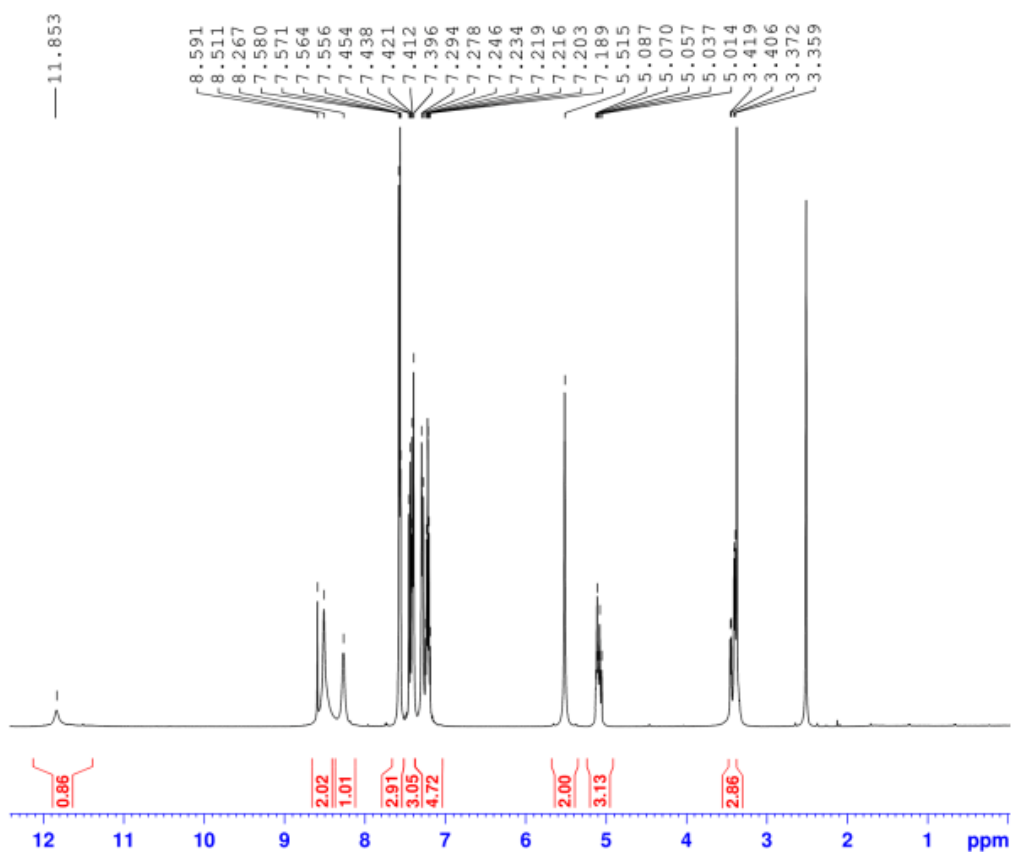
Current Data Parameters
NAME      TAnh-105G
EXPNO    30
PROCNO   1

F2 - Acquisition Parameters
Date_    20191117
Time     12.31
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       299.6 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

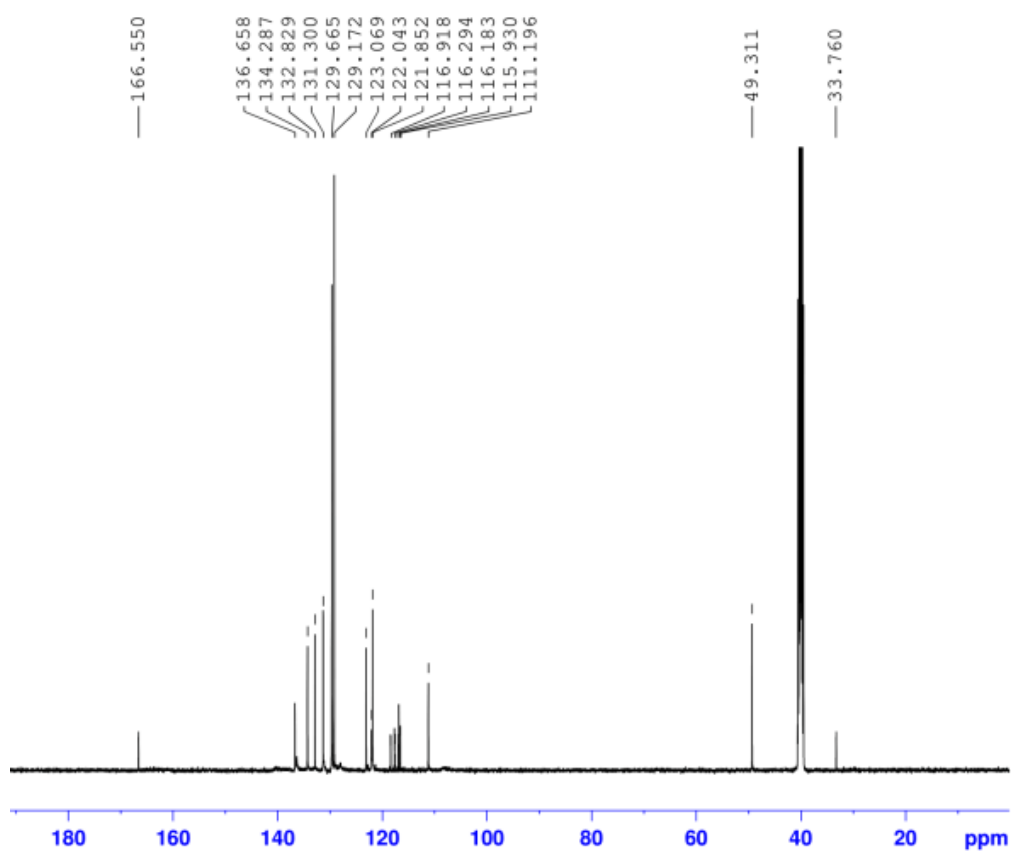
===== CHANNEL f1 =====
SFO1    125.7702637 MHz
NUC1     13C
P1       9.50 usec
PLW1    90.00000000 W

===== CHANNEL f2 =====
SFO2    500.1320005 MHz
NUC2     1H
CPDPRG12 waltz16
PCPD02   80.00 usec
PLW2    24.00000000 W
PLW12   0.26015001 W
PLW13   0.23050000 W

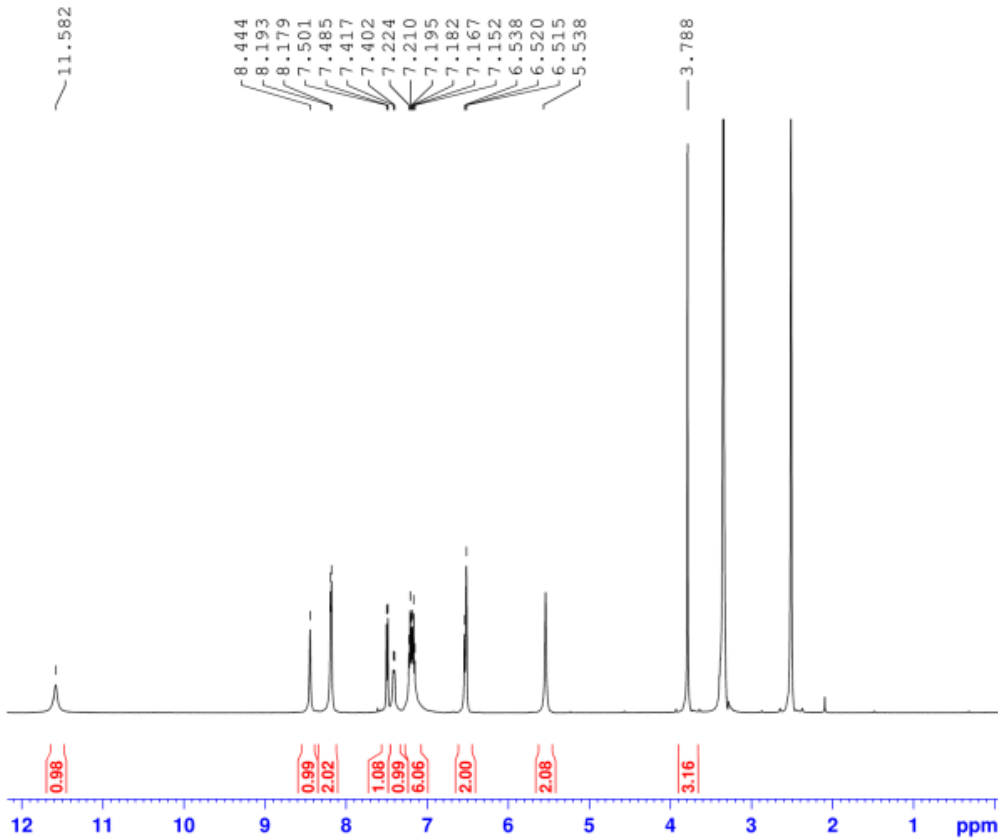
F2 - Processing parameters
SI       65536
SF       125.7577885 MHz
WDW      EM
SSB      0
PC       1.00 usec
  
```

¹H-NMR of compound 4h



¹³C-NMR of compound 4h



```

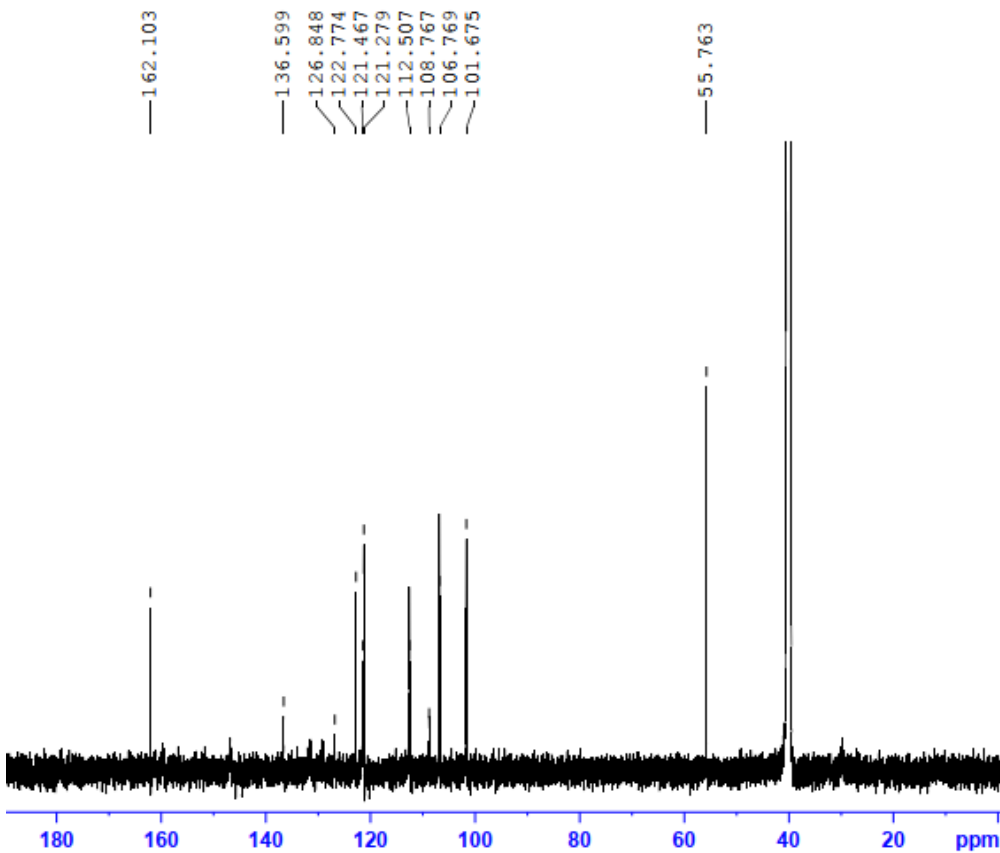
Current Data Parameters
NAME      TANh-105I
EXPNO    20
PROCNO   1

F2 - Acquisition Parameters
Date_    20191029
Time     9.37
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       298.9 K
D1       1.00000000 sec
TD0      1

----- CHANNEL f1 -----
SF01    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
  
```

¹H-NMR of compound 4i



```

Current Data Parameters
NAME      TANh-105I
EXPNO    21
PROCNO   1

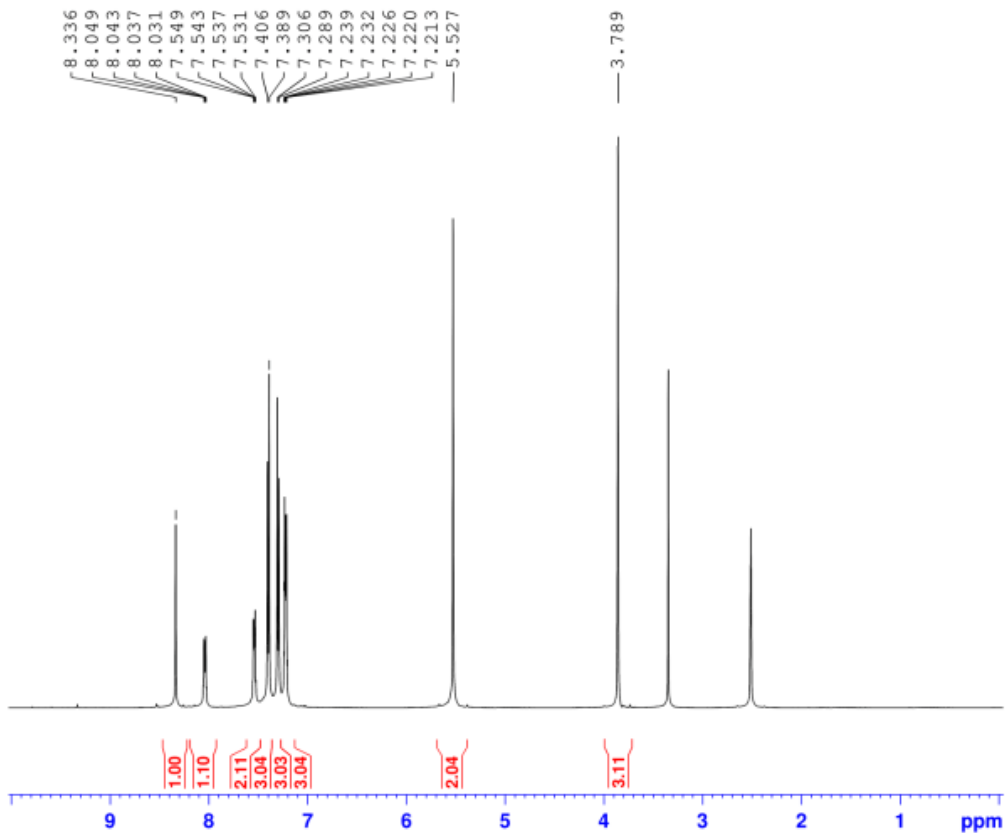
F2 - Acquisition Parameters
Date_    20191029
Time     10.41
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       4096
DS       4
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0488760 sec
RG       191.38
DW       16.000 usec
DE       6.50 usec
TE       299.6 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
CPDPRG12 waltz16
PCPD02   80.00 usec
PLW2    24.00000000 W
PLW12   0.36015001 W
PLW13   0.28050000 W

F2 - Processing parameters
SI       65536
SF       125.7877888 MHz
WDW      EM
SSB      0
LB       1.00 Hz
  
```

¹³C-NMR of compound 4i



¹H-NMR of compound 4j

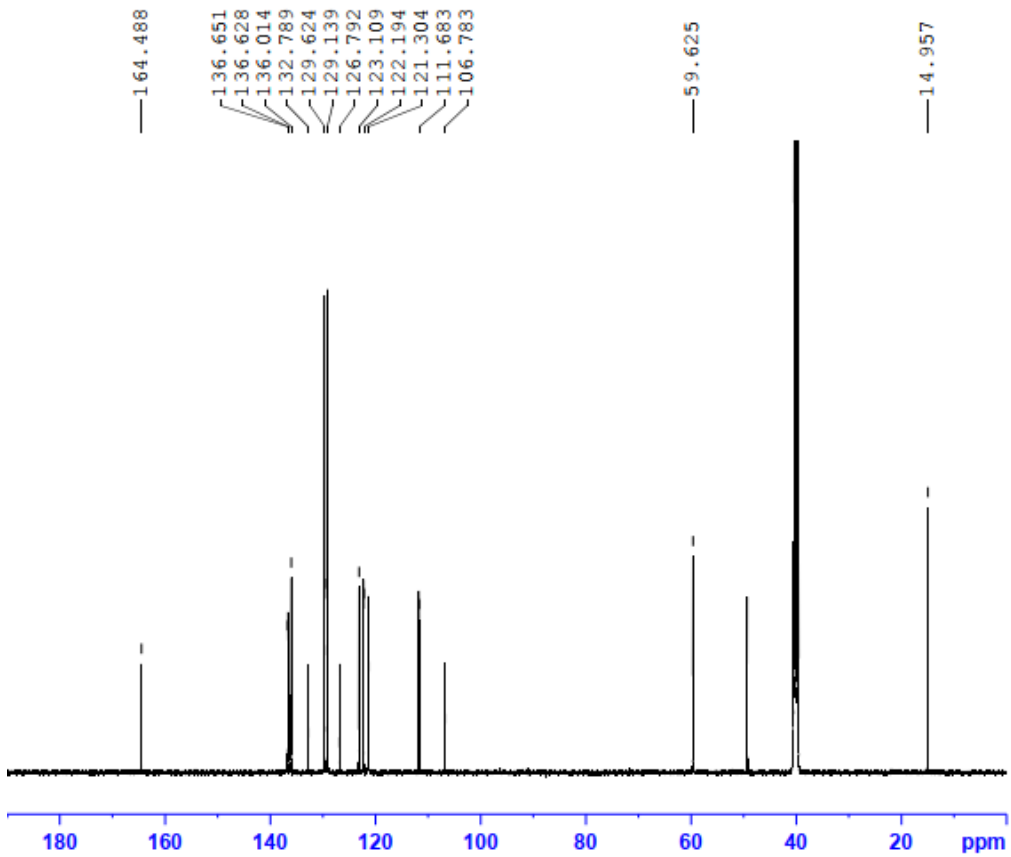


Current Data Parameters
 NAME Tien Anh-105J
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200117
 Time 19.03
 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 108.52
 DW 50.000 usec
 DE 6.50 usec
 TE 298.0 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
 WDN EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



¹³C-NMR of compound 4j



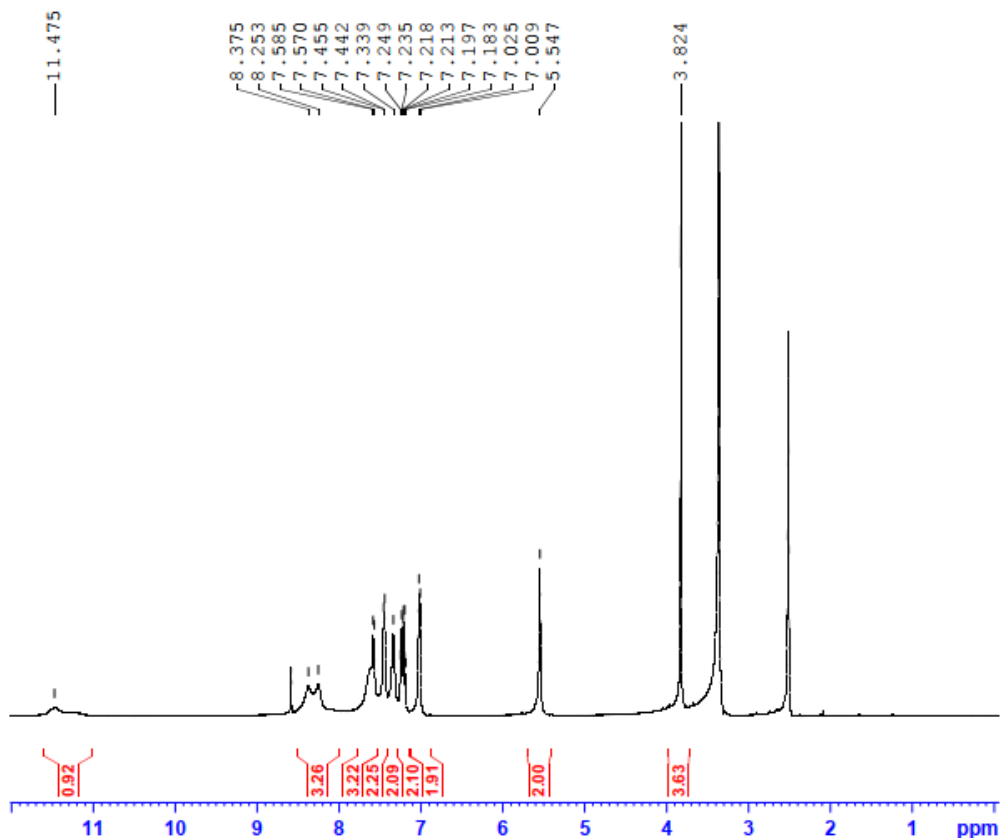
Current Data Parameters
 NAME Tien Anh-105J
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200117
 Time 20.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476827 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.3 K
 D1 2.00000000 sec
 D11 0.02000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7704637 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.22050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7577888 MHz
 WDN EM
 SSB 0
 LB 1.00 Hz



```

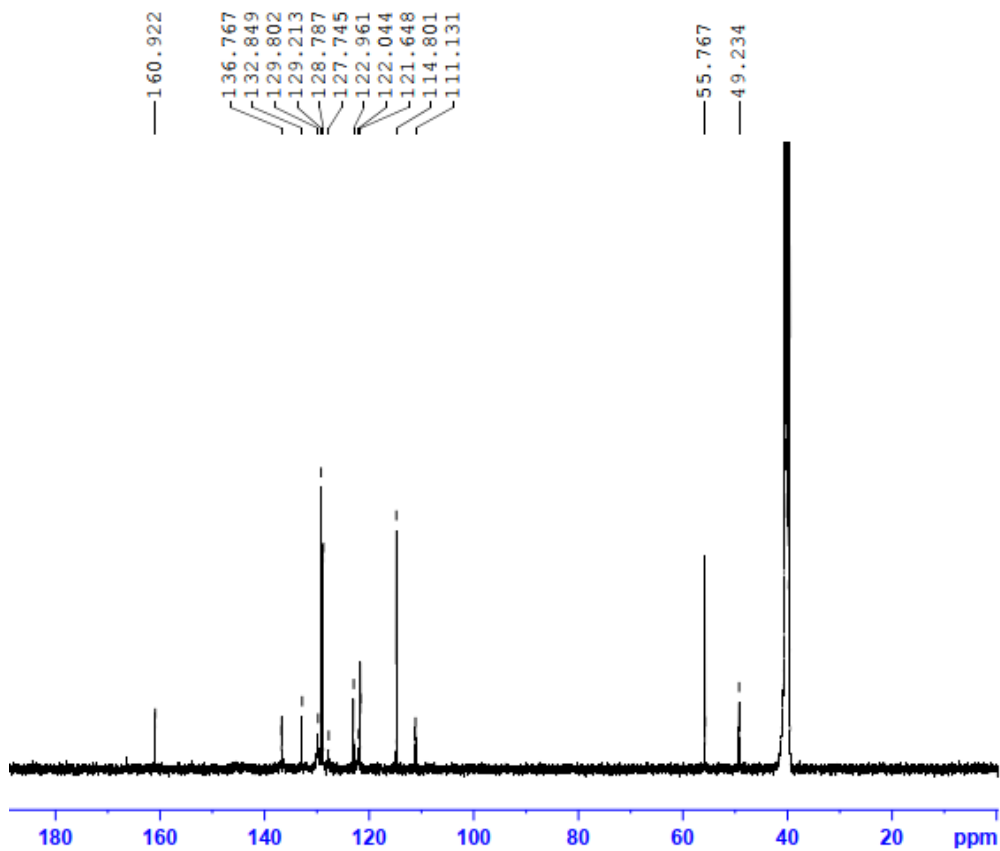
Current Data Parameters
NAME      Tank-105K
EXPNO    20
PROCNO   1

F2 - Acquisition Parameters
Date_    20191125
Time     4.27
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       138.87
DN       80.000 usec
DE       6.50 usec
TE       299.2 K
D1       1.0000000 sec
TDO      1

===== CHANNEL f1 =====
SF01    500.1320885 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      0.20 Hz
GB      0
PC      1.00
  
```

¹H-NMR of compound 4k



```

Current Data Parameters
NAME      Tank-105K
EXPNO    22
PROCNO   1

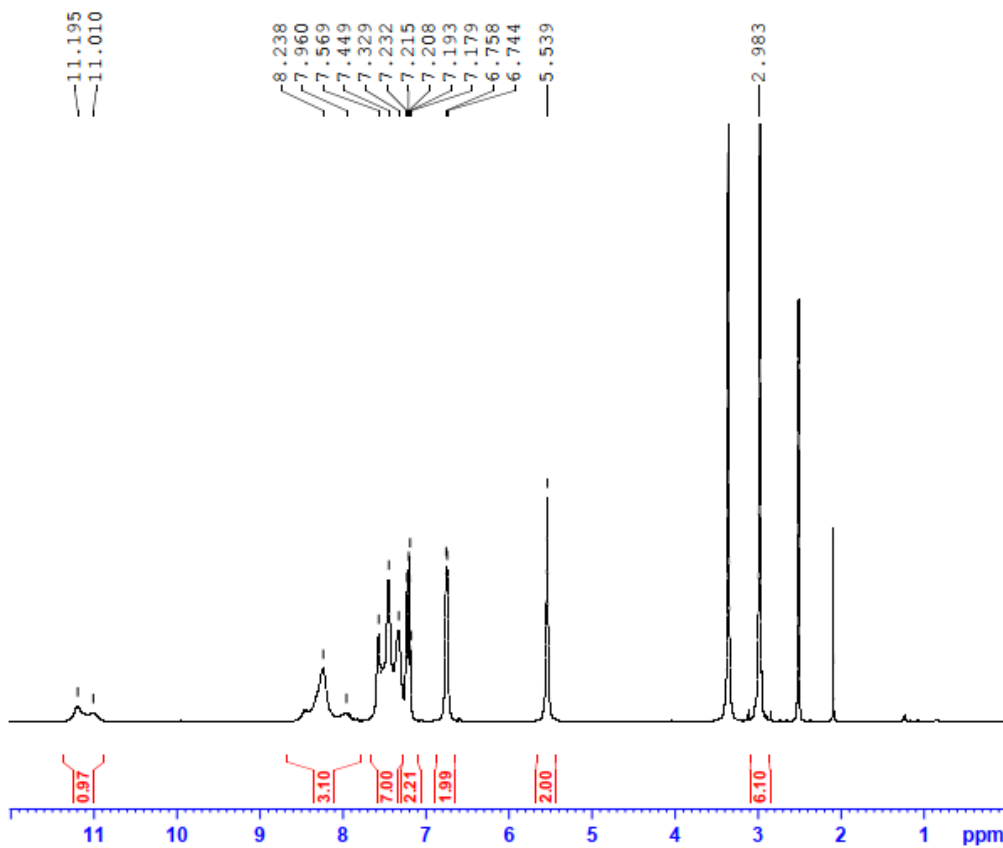
F2 - Acquisition Parameters
Date_    20191125
Time     8.01
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       4096
DS       4
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0488760 sec
RG       191.28
DN       16.000 usec
DE       6.50 usec
TE       299.2 K
D1       2.0000000 sec
D11      0.0300000 sec
TDO      1

===== CHANNEL f1 =====
SF01    125.7702637 MHz
NUC1    13C
P1      9.50 usec
PLW1    90.0000000 W

===== CHANNEL f2 =====
SF02    500.1320008 MHz
NUC2    1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLW2    24.0000000 W
PLW12   0.36018001 W
PLW13   0.23050000 W

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

¹³C-NMR of compound 4k



```

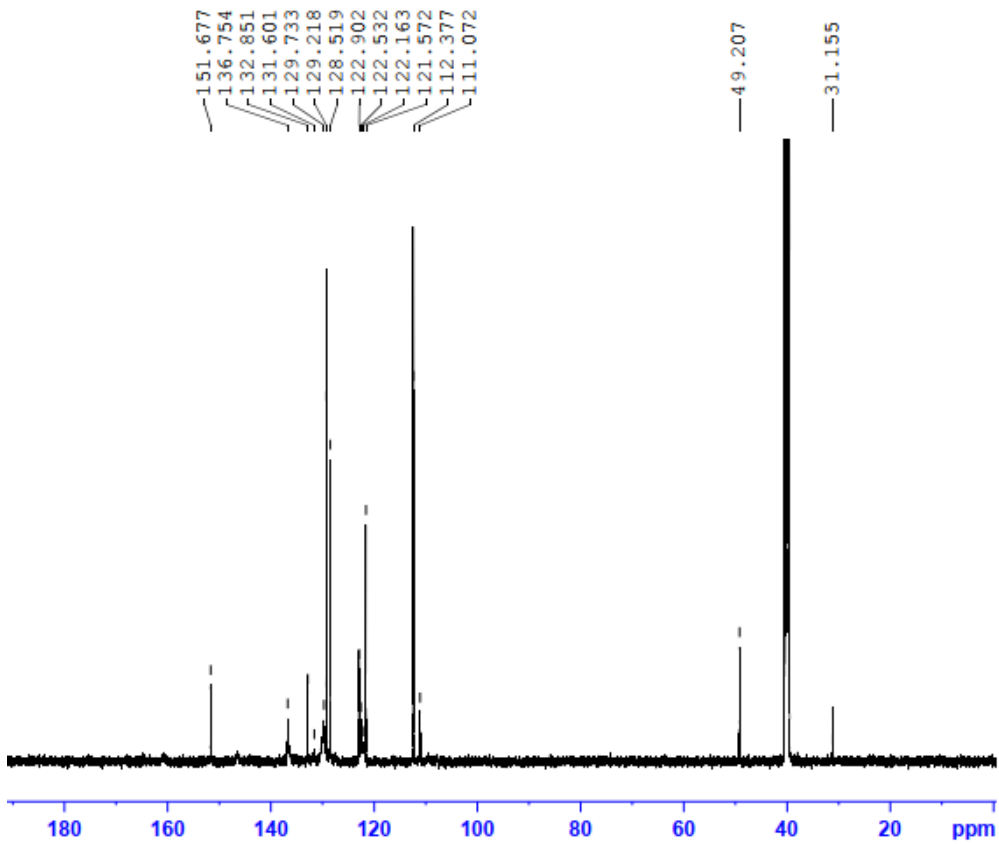
Current Data Parameters
NAME      Tanh-10SL
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20191108
Time     13.48
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      10000.000 Hz
FIDRES   0.152588 Hz
AQ       3.2767999 sec
RG       108.82
DN       50.000 usec
DE       6.50 usec
TE       298.8 K
DL       1.00000000 sec
TDO     1

===== CHANNEL f1 =====
SF01    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      0.20 Hz
GB      0
PC      1.00
  
```

¹H-NMR of compound 4l



```

Current Data Parameters
NAME      Tanh-10SL
EXPNO    11
PROCNO   1

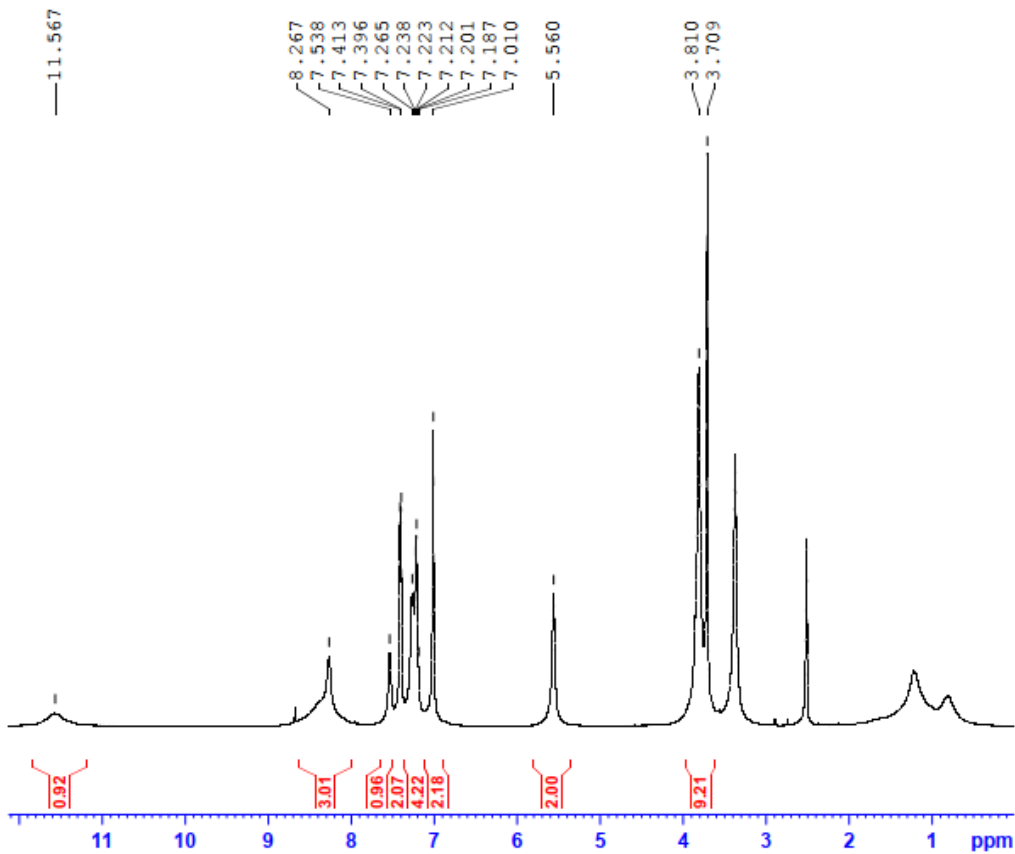
F2 - Acquisition Parameters
Date_    20191109
Time     7.37
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       4096
DS       4
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0488760 sec
RG       191.38
DN       16.000 usec
DE       6.50 usec
TE       299.8 K
DL       2.00000000 sec
D11     0.08000000 sec
TDO     1

===== CHANNEL f1 =====
SF01    125.7709637 MHz
NUC1    13C
P1      9.50 usec
PLW1    90.00000000 W

===== CHANNEL f2 =====
SF02    500.1320005 MHz
NUC2    1H
CPDPRG2  waltz16
PCPD0    80.00 usec
PLW2    24.00000000 W
PLW12   0.36018001 W
PLW13   0.23050000 W

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

¹³C-NMR of compound 4l



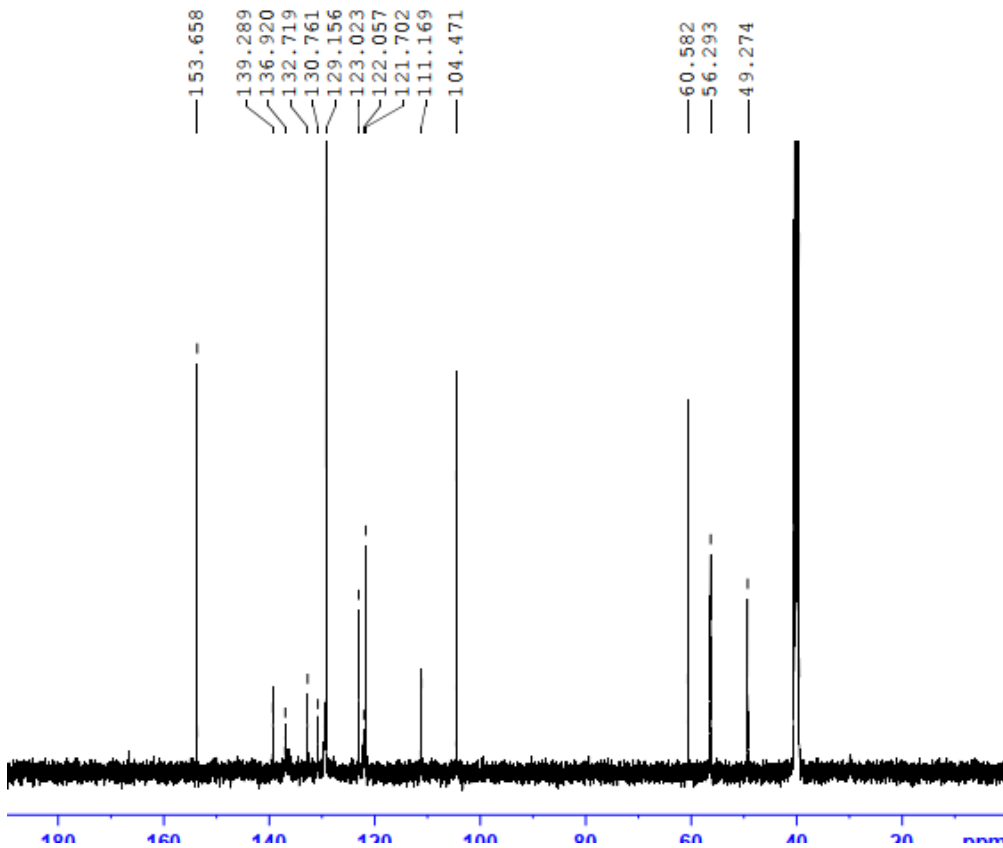
Current Data Parameters
 NAME TANh-105M
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191029
 Time 9.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SMH 10000.000 Hz
 FIDRES 0.182588 Hz
 AQ 3.2767999 sec
 RG 70.26
 DW 50.000 usec
 DE 6.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 500.1320885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1320000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H-NMR of compound 4m



Current Data Parameters
 NAME TANh-105M
 EXPNO 11
 PROCNO 1

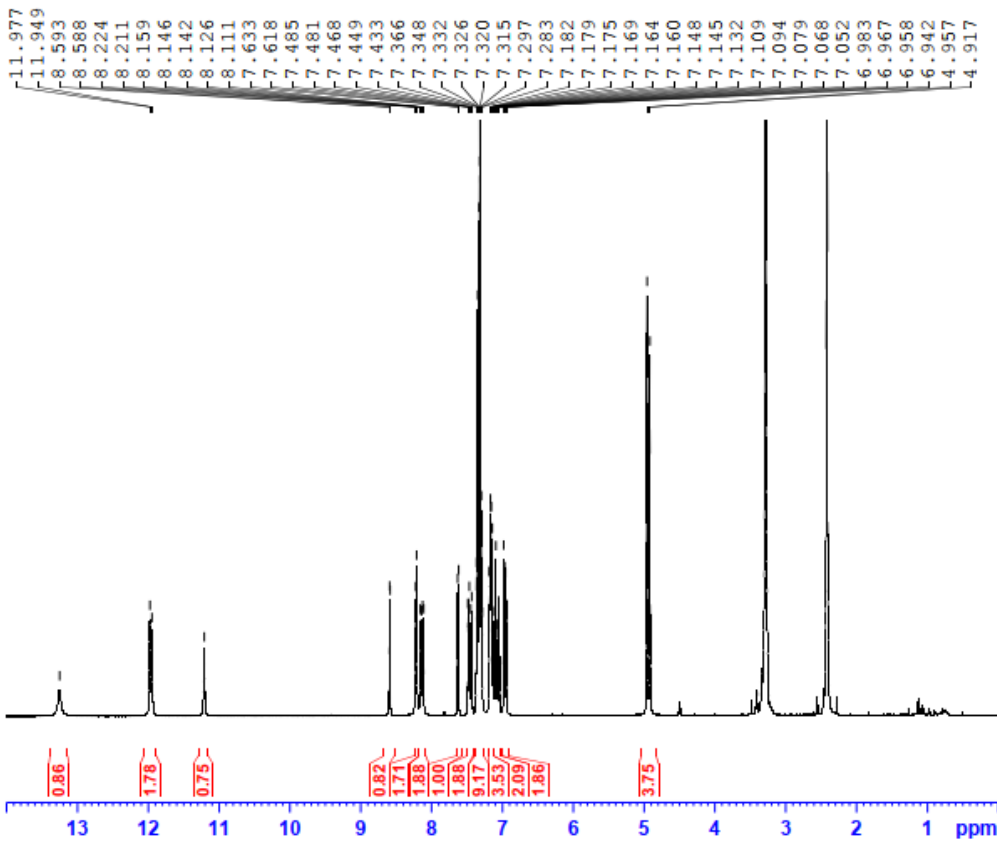
F2 - Acquisition Parameters
 Date_ 20191029
 Time 9.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 4
 SMH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0488780 sec
 RG 191.28
 DW 16.000 usec
 DE 6.50 usec
 TE 299.3 K
 D1 2.00000000 sec
 D11 0.08000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 125.7702627 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

===== CHANNEL f2 =====
 SF02 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.26018001 W
 PLW13 0.23050000 W

F2 - Processing parameters
 SI 65536
 SF 125.7577885 MHz
 WDW em
 SSB 0

¹³C-NMR of compound 4m



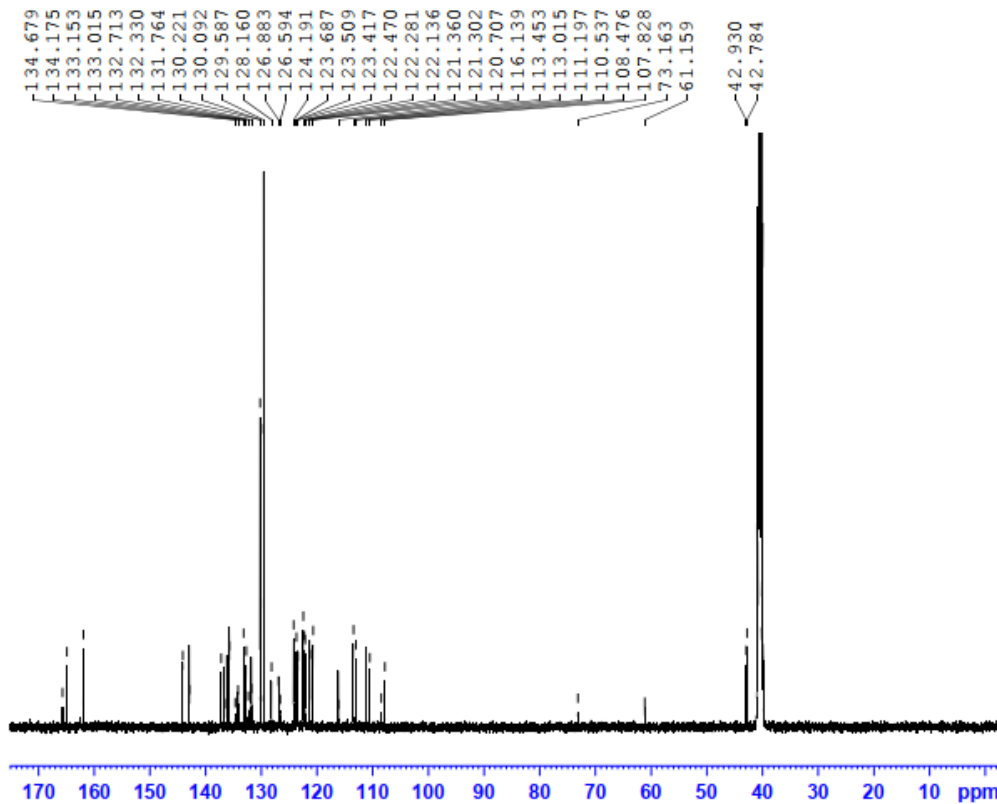
Current Data Parameters
 NAME TAnh-104A
 EXPNO 1
 PROCNO 1

PC - Acquisition Parameters
 Date_ 20191217
 Time 8.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.182388 Hz
 AQ 3.2787999 sec
 RG 87.52
 DW 50.000 usec
 DE 6.50 usec
 TE 298.7 K
 DL 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 500.1300885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.00000000 W

PC - Processing parameters
 SI 65536
 SF 500.1300465 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H-NMR of compound 5a



Current Data Parameters
 NAME TAnh-104A
 EXPNO 1
 PROCNO 1

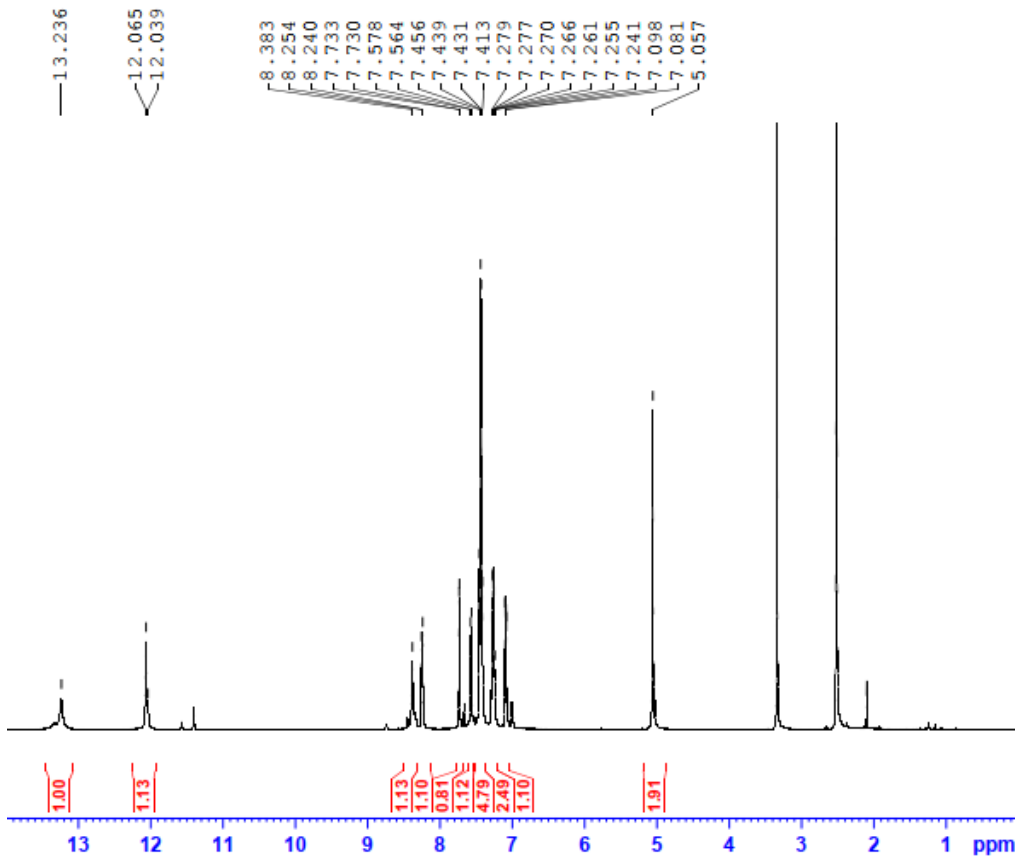
PC - Acquisition Parameters
 Date_ 20191217
 Time 23.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMS
 NS 2048
 DS 4
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.6 K
 DL 2.00000000 sec
 DLI 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 125.7708637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 90.00000000 W

===== CHANNEL f2 =====
 SF02 500.1320005 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36015001 W
 PLW13 0.22080000 W

PC - Processing parameters
 SI 65536
 SF 125.7677885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz

¹³C-NMR of compound 5a



BRUKER

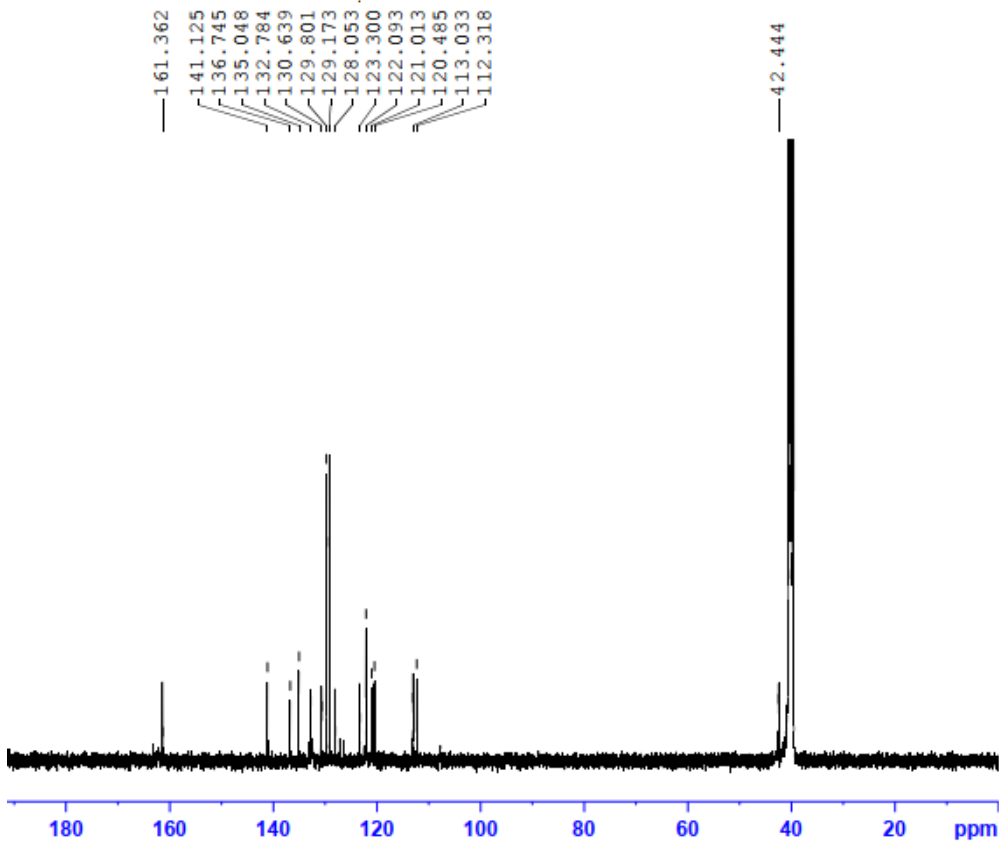
Current Data Parameters
 NAME Tien Anh-104C
 EXPNO 20
 PROCNO 1

PC - Acquisition Parameters
 Date_ 20200117
 Time_ 20.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SSW 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2787999 sec
 RG 191.38
 DW 50.000 usec
 DE 6.50 usec
 TE 298.6 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 500.1320885 MHz
 NUCL 1H
 PL 9.80 usec
 PLW1 24.00000000 W

PC - Processing parameters
 SI 65536
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

¹H-NMR of compound 5c



BRUKER

Current Data Parameters
 NAME Tien Anh-104C
 EXPNO 21
 PROCNO 1

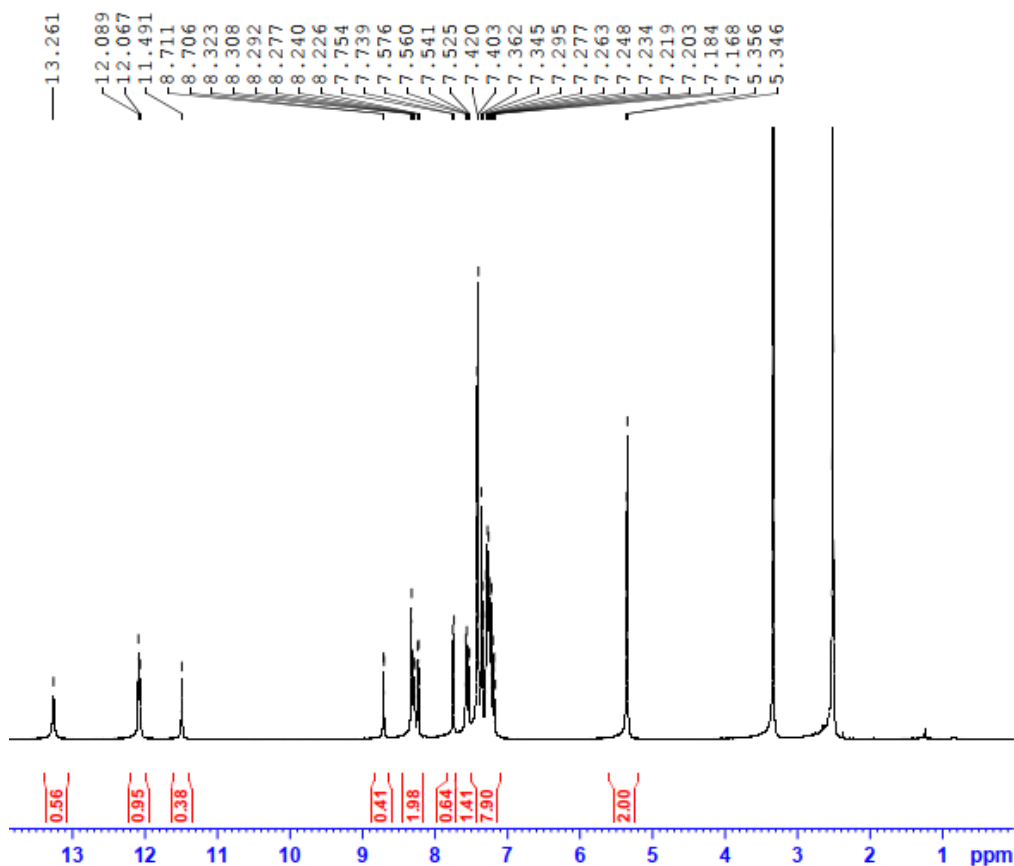
PC - Acquisition Parameters
 Date_ 20200117
 Time_ 22.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SSW 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0488760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 125.7709637 MHz
 NUCL 13C
 PL 9.50 usec
 PLW1 90.00000000 W

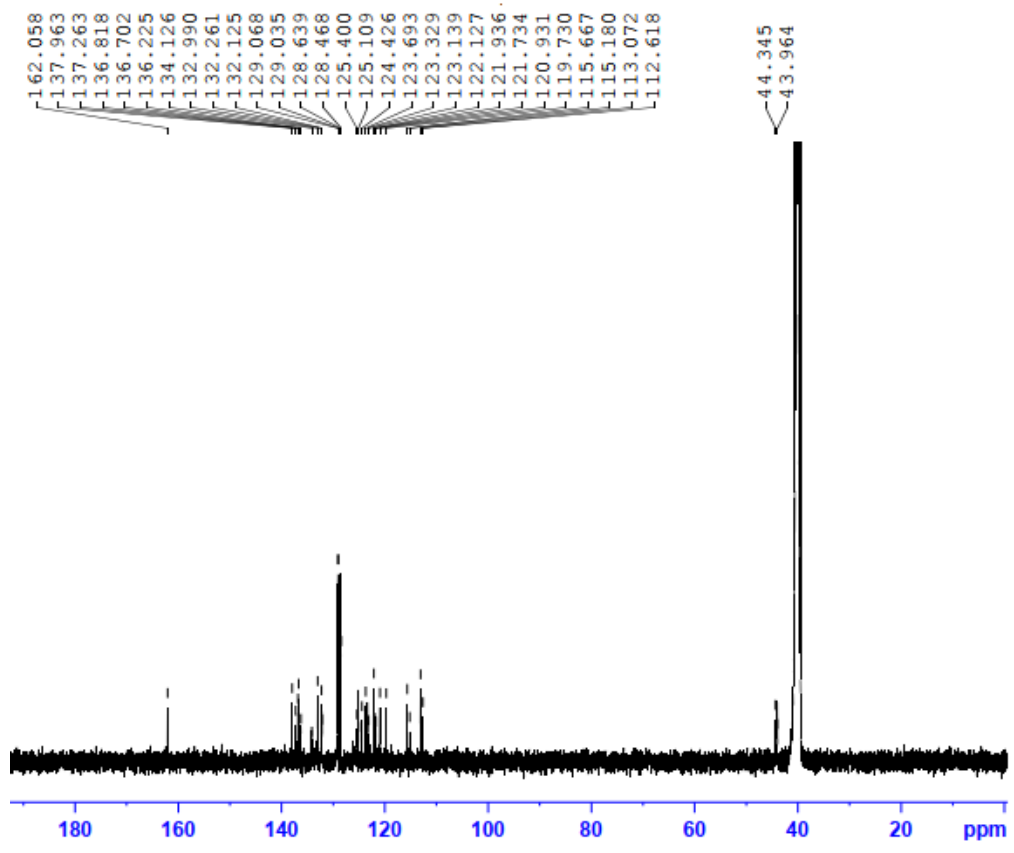
===== CHANNEL f2 =====
 SF02 500.1320005 MHz
 NUCL 1H
 CPDPRG12 waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.36018001 W
 PLW13 0.23050000 W

PC - Processing parameters
 SI 65536
 SF 125.7577888 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz

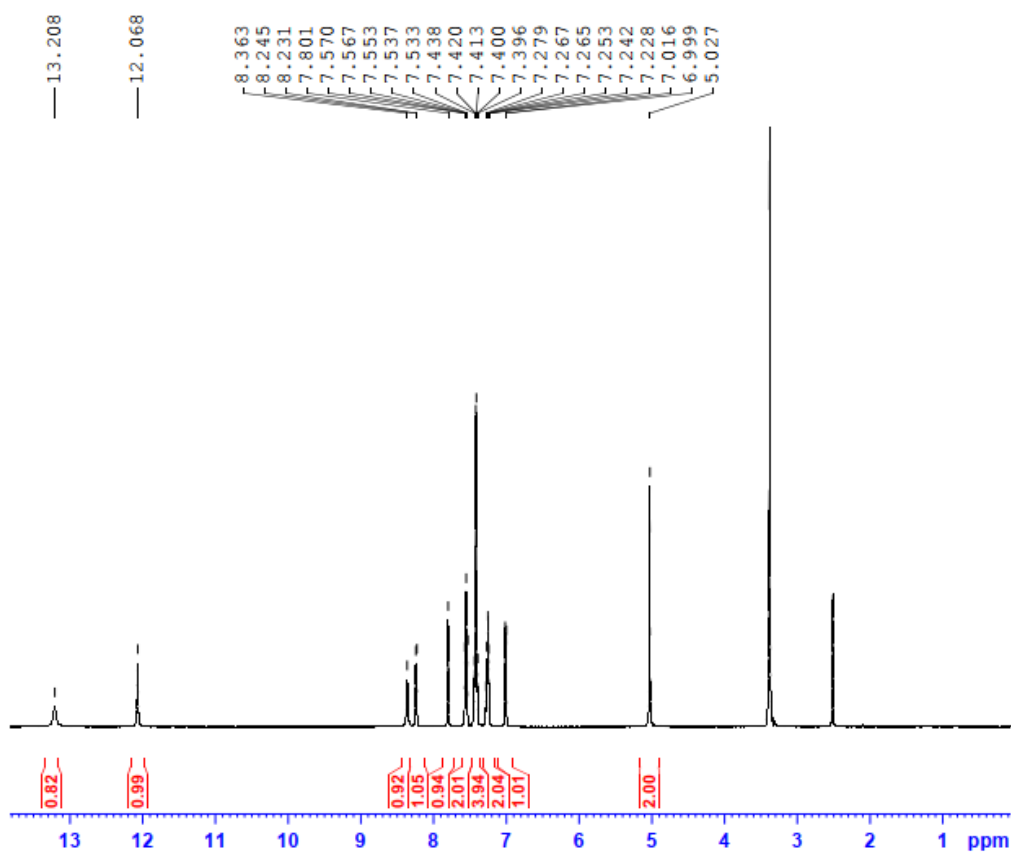
¹³C-NMR of compound 5c



¹H-NMR of compound 5d



¹³C-NMR of compound 5d



¹H-NMR of compound 5e



```

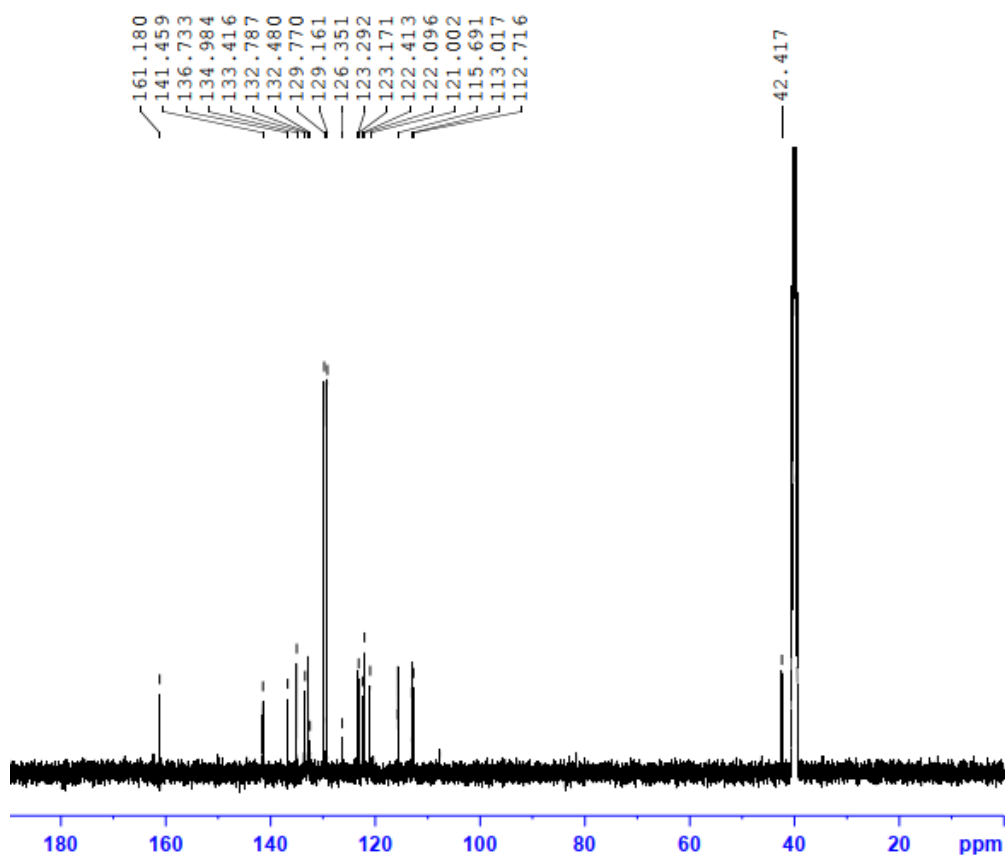
Current Data Parameters
NAME      TAnh-104E-2
EXPNO    20
PROCNO   1

FC - Acquisition Parameters
Date_    20200316
Time     13.47
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       95.24
DN       50.000 usec
DE       6.50 usec
TE       298.5 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
SF01    500.1320885 MHz
NUC1     1H
P1       9.80 usec
PLW1    24.00000000 W

FC - Processing parameters
SI       65536
SF       500.1320000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

```



¹³C-NMR of compound 5e



```

Current Data Parameters
NAME      TAnh-104E-2
EXPNO    21
PROCNO   1

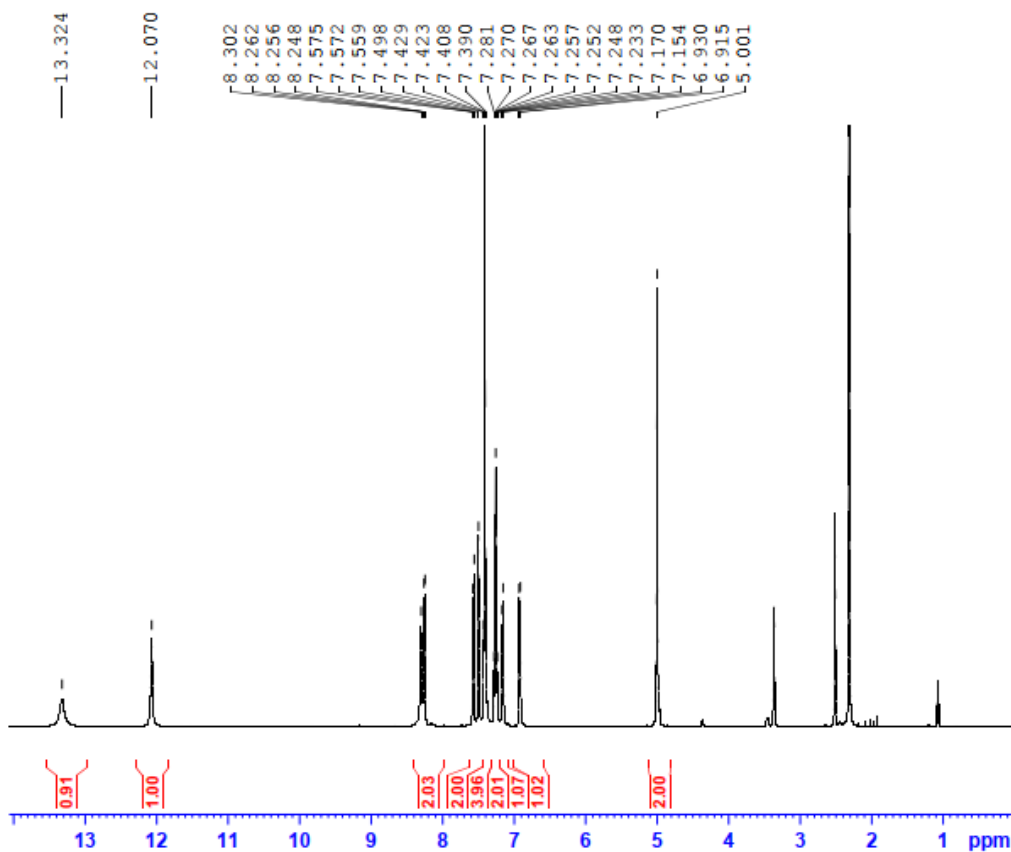
FC - Acquisition Parameters
Date_    20200316
Time     14.21
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       329
DS       4
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0485760 sec
RG       191.28
DN       16.000 usec
DE       6.50 usec
TE       299.2 K
D1       2.00000000 sec
D11     0.03000000 sec
TDO      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
CPDPRG12 waltz16
PCPDPC   80.00 usec
PLW2    24.00000000 W
PLW12   0.36015001 W
PLW13   0.23050000 W

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

```



```

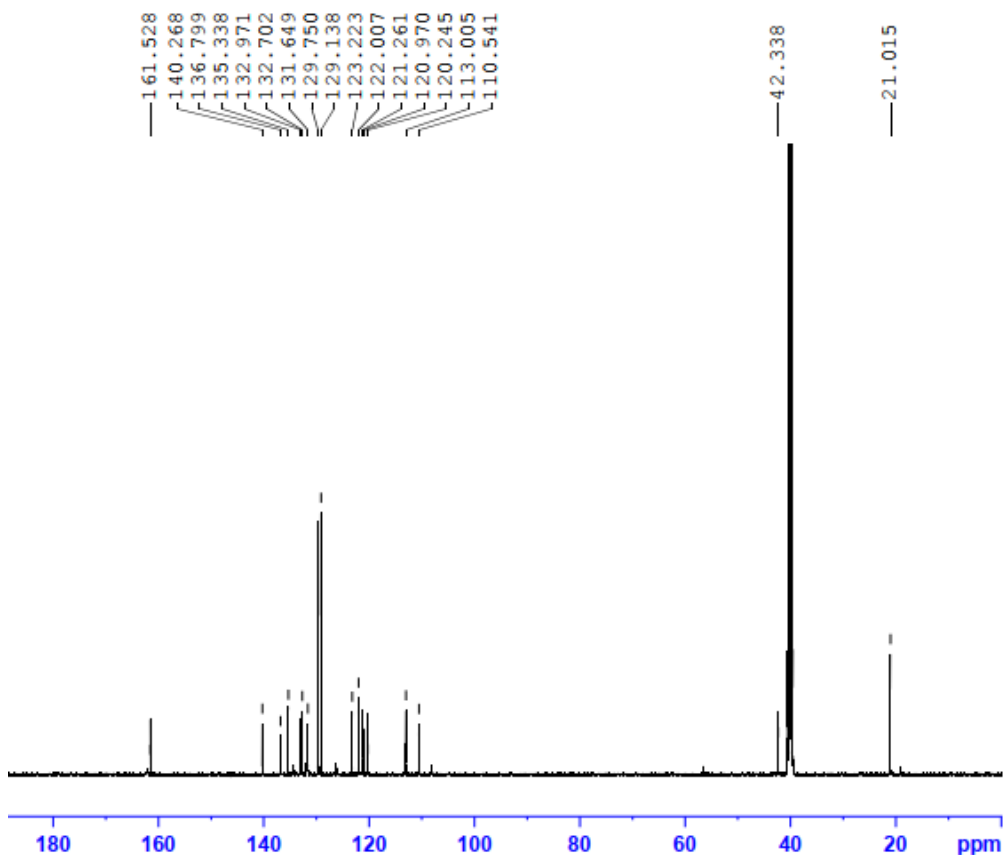
Current Data Parameters
NAME      Tien Anh-104F
EXPNO    50
PROCNO   1

F2 - Acquisition Parameters
Date_    20200118
Time     2.30
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zg30
TD        65536
SOLVENT  DMSO
NS        16
DS         2
SWH       10000.000 Hz
FIDRES    0.182588 Hz
AQ        3.2767999 sec
RG         87.53
DN         50.000 usec
DE         6.50 usec
TE        298.7 K
D1        1.00000000 sec
TDO       1

===== CHANNEL f1 =====
SFO1     500.1320885 MHz
NUC1      1H
P1        9.80 usec
PLW1     24.00000000 W

F2 - Processing parameters
SI        65536
SF        500.1320000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

¹H-NMR of compound 5f



```

Current Data Parameters
NAME      Tien Anh-104F
EXPNO    51
PROCNO   1

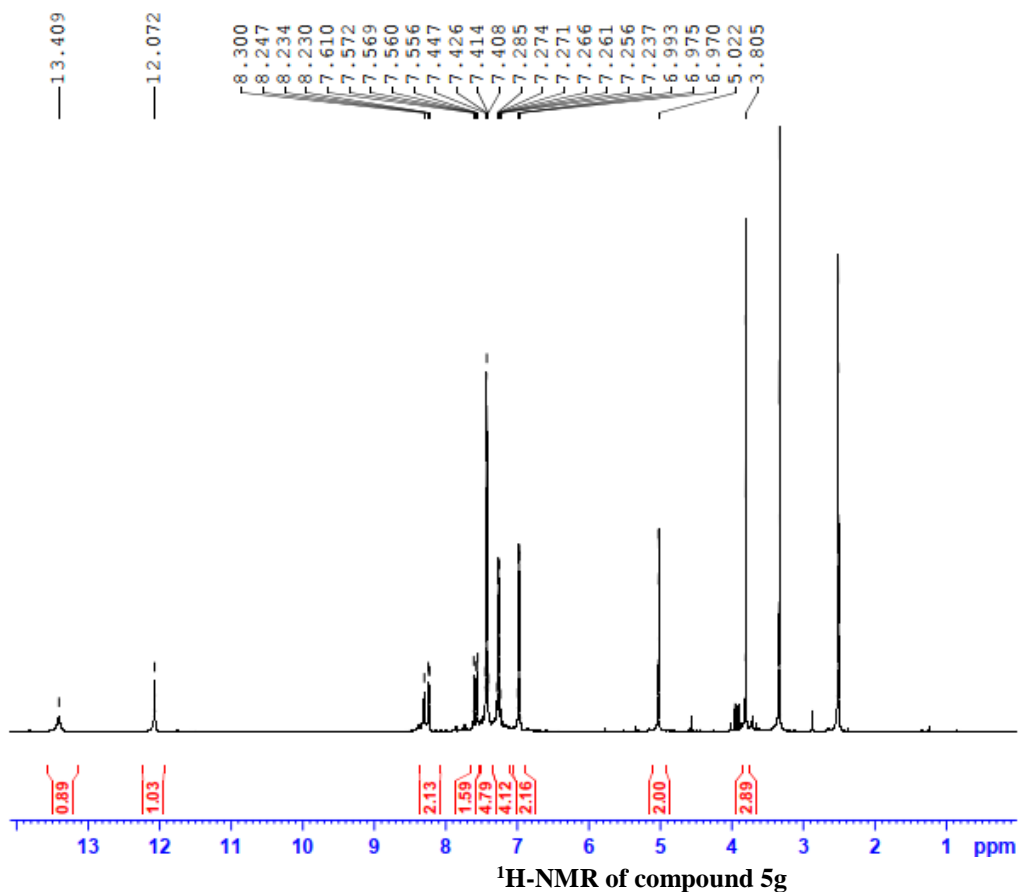
F2 - Acquisition Parameters
Date_    20200118
Time     3.24
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg30
TD        65536
SOLVENT  DMSO
NS        1024
DS         4
SWH       31250.000 Hz
FIDRES    0.476837 Hz
AQ        1.0488760 sec
RG        191.38
DN         16.000 usec
DE         6.50 usec
TE        299.3 K
D1        2.00000000 sec
D11       0.03000000 sec
TDO       1

===== CHANNEL f1 =====
SFO1     125.7703637 MHz
NUC1      13C
P1        9.80 usec
PLW1     90.00000000 W

===== CHANNEL f2 =====
SFO2     500.1320005 MHz
NUC1      1H
CPDPRG12 waltz16
PCPD2    80.00 usec
PLW2     24.00000000 W
PLW12    0.26015001 W
PLW13    0.23050000 W

F2 - Processing parameters
SI        65536
SF        125.7577888 MHz
WDW       EM
SSB       0
LB        1.00 Hz
  
```

¹³C-NMR of compound 5f

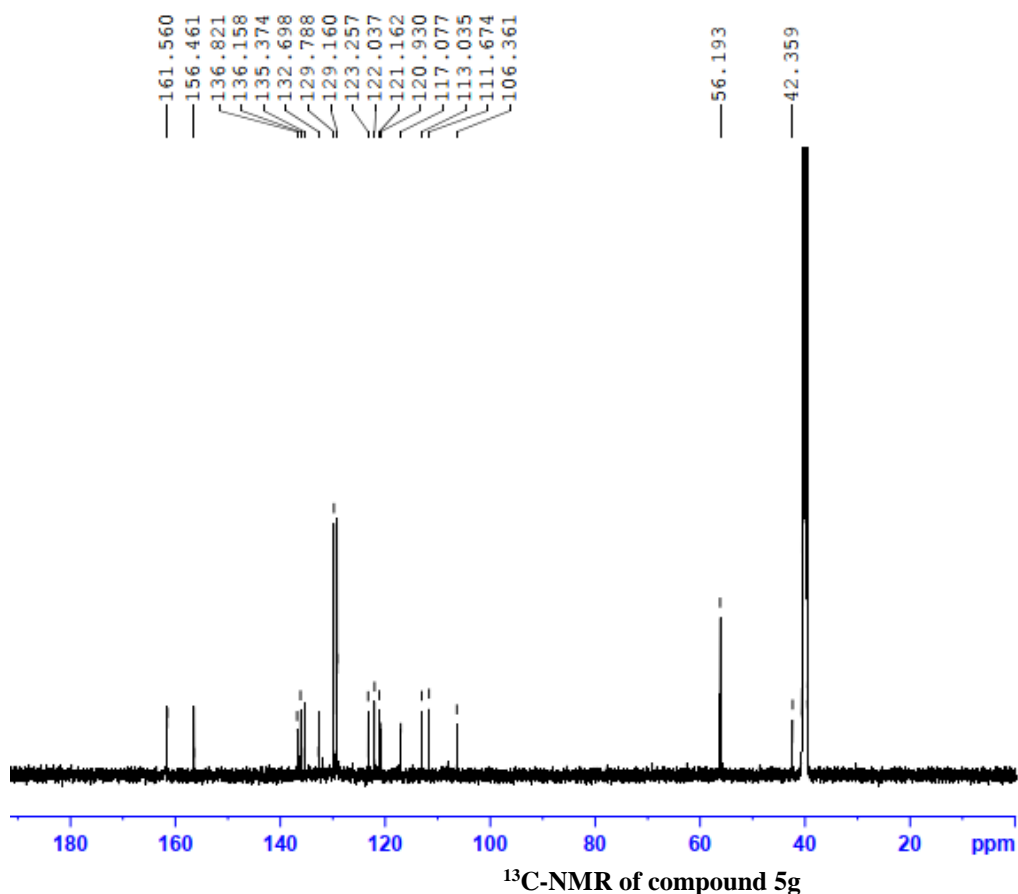


Current Data Parameters
 NAME Tien Anh-1046
 EXPNO 40
 PROCNO 1

FC - Acquisition Parameters:
 Date_ 20200118
 Time 0.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.182388 Hz
 AQ 3.2767999 sec
 RG 191.38
 DW 50.000 usec
 DE 6.50 usec
 TE 299.8 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL #1 =====
 SF01 500.1330885 MHz
 NUC1 1H
 P1 9.80 usec
 PLW1 24.00000000 W

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



Current Data Parameters
 NAME Tien Anh-1046
 EXPNO 41
 PROCNO 1

FC - Acquisition Parameter:
 Date_ 20200118
 Time 2.26
 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 1.04885760 sec
 RG 191.38
 DW 16.000 usec
 DE 6.50 usec
 TE 299.8 K
 D1 2.00000000 sec
 D11 0.02000000 sec
 TDO 1

===== CHANNEL #1 =====
 SF01 125.7703697 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 90.00000000 W

===== CHANNEL #2 =====
 SF02 500.1320005 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 80.00 usec
 PLW2 24.00000000 W
 PLW12 0.26015001 W
 PLW13 0.23050000 W

FC - Processing parameters
 SI 65536
 SF 125.7577888 MHz
 WDW EM
 SSB 0