

**Synthesis and biological activity, and molecular modelling studies of potent cytotoxic podophyllotoxin–naphthoquinone compounds**

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*Dr.* Ha Thanh Nguyen

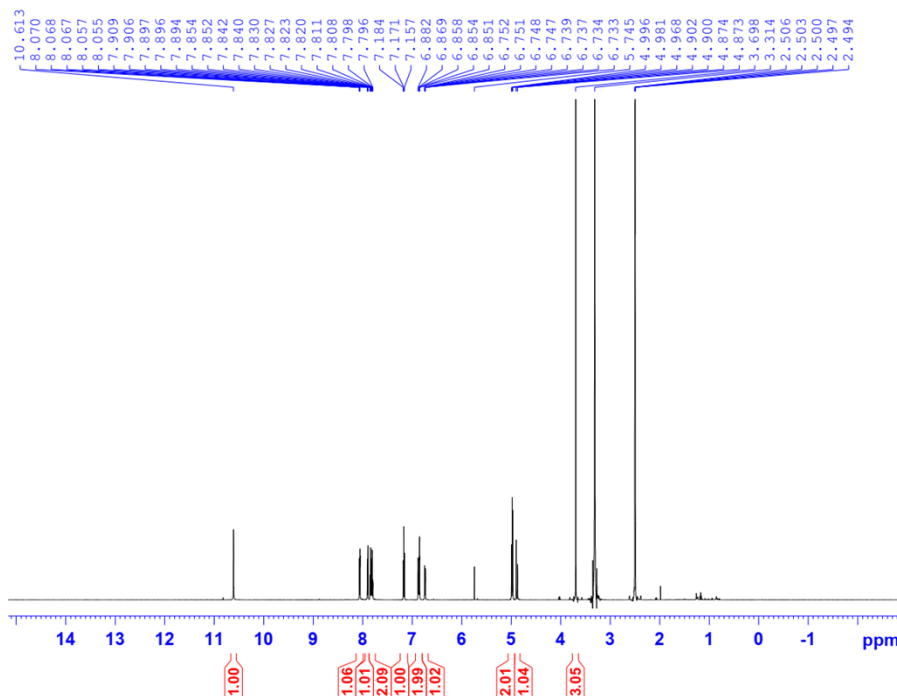
E-mail: [hathanhnguyen1512@gmail.com](mailto:hathanhnguyen1512@gmail.com) (H. T. Nguyen)

## Contents

|   |    |
|---|----|
| 11-(3-Methoxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione ( <b>5a</b> ).....          | 3  |
| 11-(3-Nitrophenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H) -trione ( <b>5b</b> ) .....          | 4  |
| 11-(3-Bromophenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H) -trione ( <b>5c</b> ). .....         | 5  |
| 11-(Phenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H) -trione ( <b>5d</b> ).....                  | 6  |
| 11-(2-Hydroxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione ( <b>5h</b> ).....          | 7  |
| 11-(4-Hydroxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione ( <b>5i</b> ).....          | 9  |
| 11-(4-Nitrophenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione ( <b>5j</b> ). .....          | 12 |
| 4-(1,5,10-Trioxo-1,3,4,5,10,11-hexahydrobenzo[g]furo[3,4-b]quinolin-11-yl)benzotrile ( <b>5k</b> ). .....   | 15 |
| 11-(3,4-Dimethoxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione ( <b>5l</b> ). .....    | 17 |
| 11-(3,4,5-Trimethoxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione ( <b>5m</b> ). ..... | 19 |
| 11-(Pyridin-3-yl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione ( <b>5n</b> ). .....           | 21 |
| 11-(5-Bromopyridin-2-yl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione ( <b>5o</b> ). .....    | 24 |

# 11-(3-Methoxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione (5a)

HP245.29-DMSO-1H

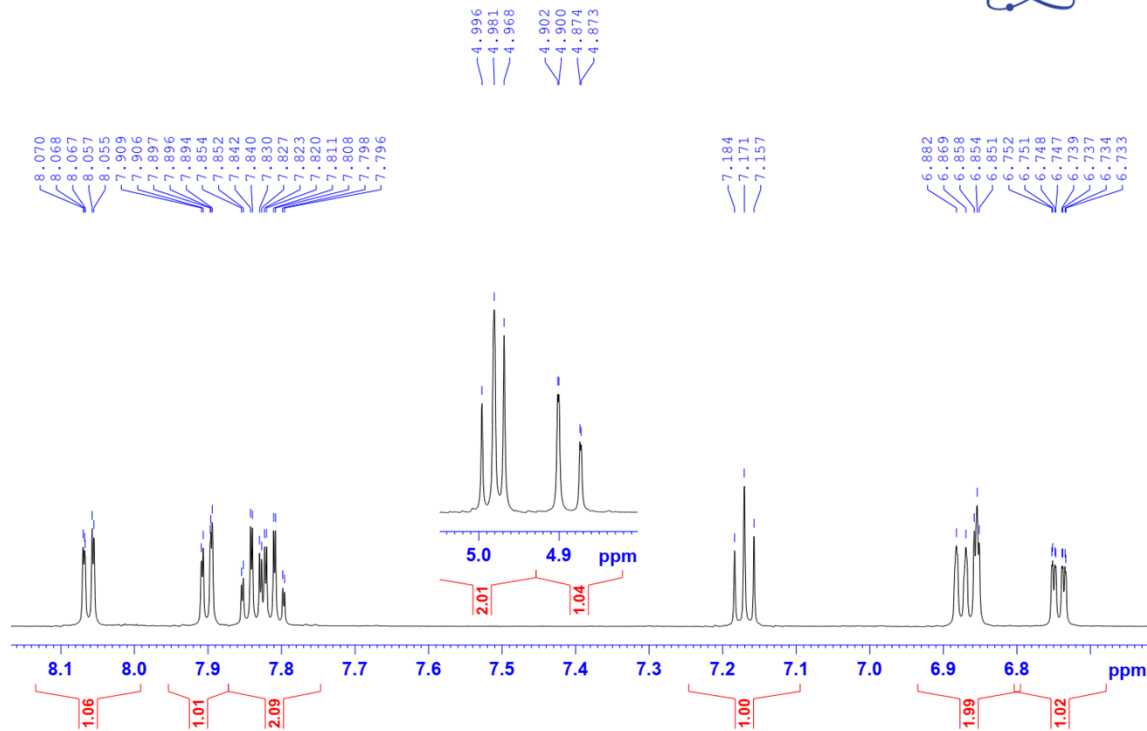


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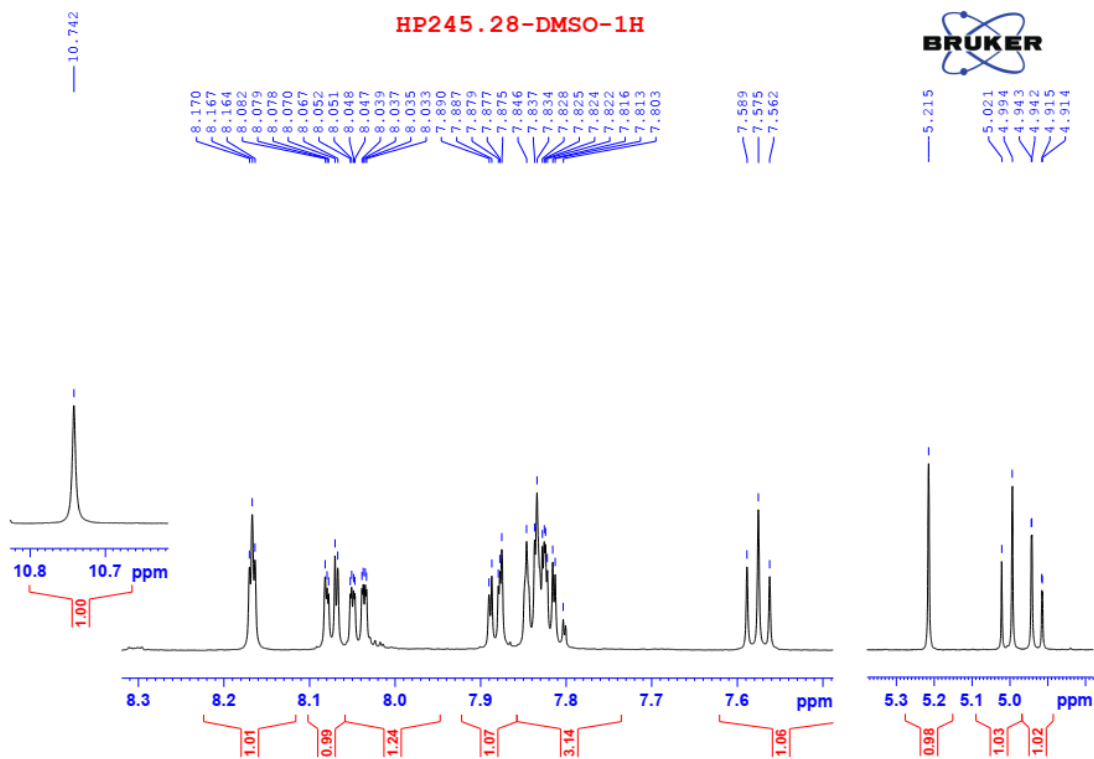
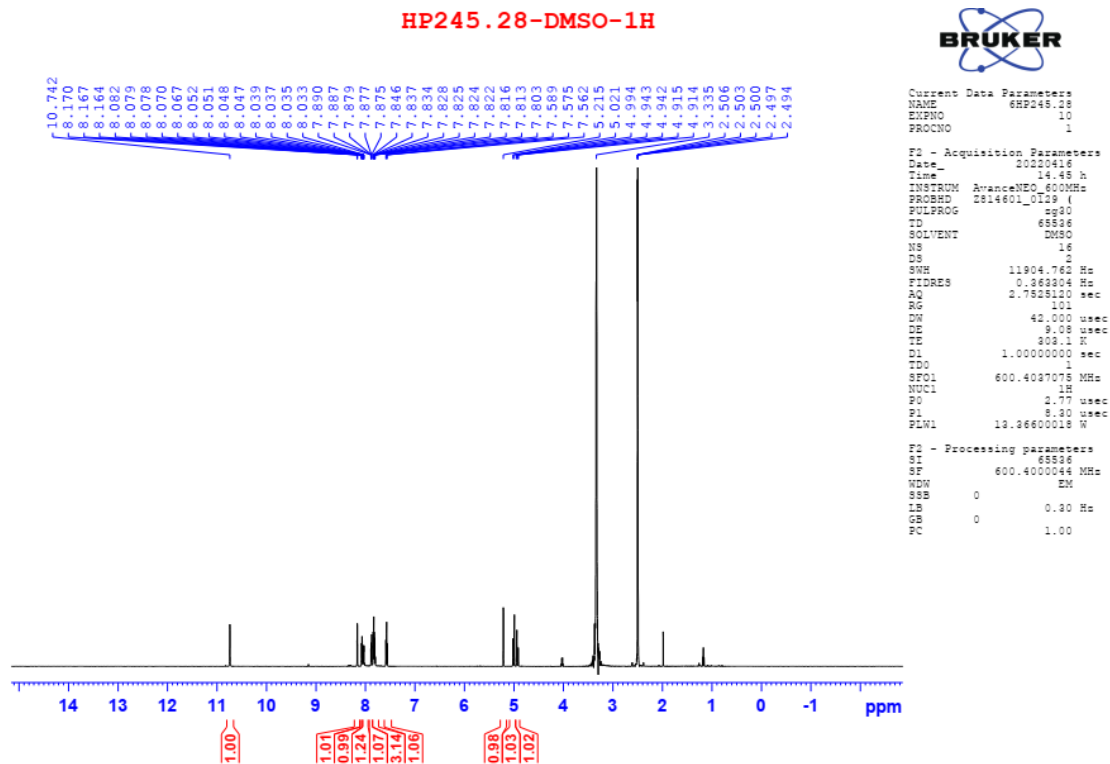
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 PROBHD: Z814601\_0129 ( )  
 PULPROG: zg30  
 TD: 65536  
 SOLVENT: DMSO  
 NS: 16  
 DS: 2  
 SWH: 11904.762 Hz  
 FIDRES: 0.368304 Hz  
 AQ: 2.7525120 sec  
 RG: 101  
 DW: 42.000 usec  
 DE: 9.08 usec  
 TE: 303.2 K  
 D1: 1.00000000 sec  
 TDO: 1  
 SFO1: 600.4037075 MHz  
 NUC1: 1H  
 P0: 2.77 usec  
 F1: 8.30 usec  
 PLW1: 13.36600018 W

F2 - Processing parameters  
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 PC: 1.00

HP245.29-DMSO-1H

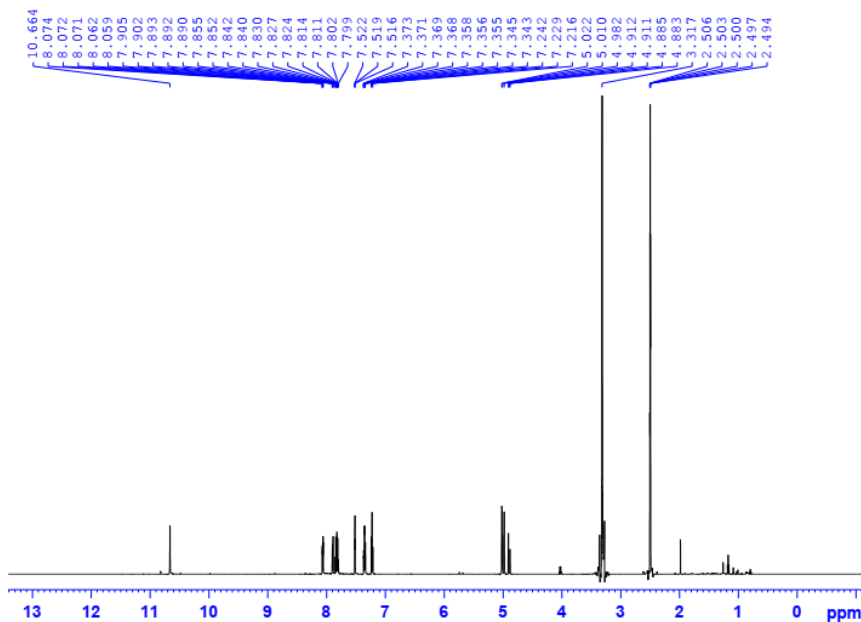


# 11-(3-Nitrophenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione (5b)



# 11-(3-Bromophenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H) -trione (5c).

HP245.14.01-DMSO-1H



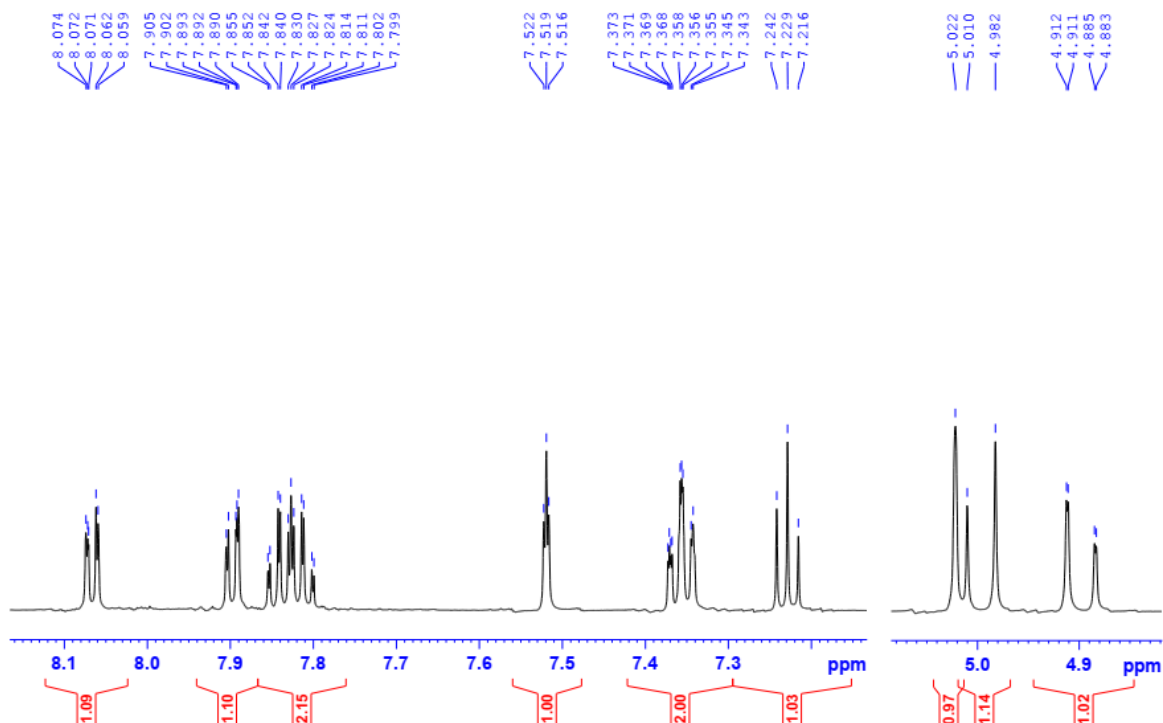
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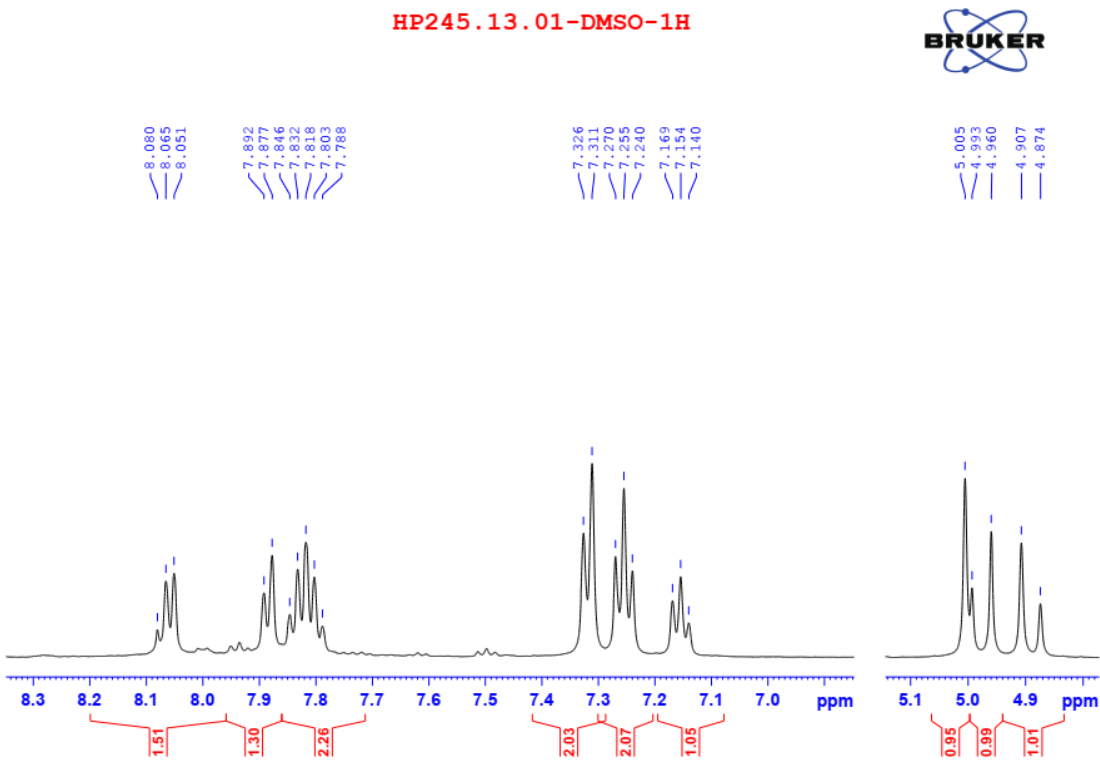
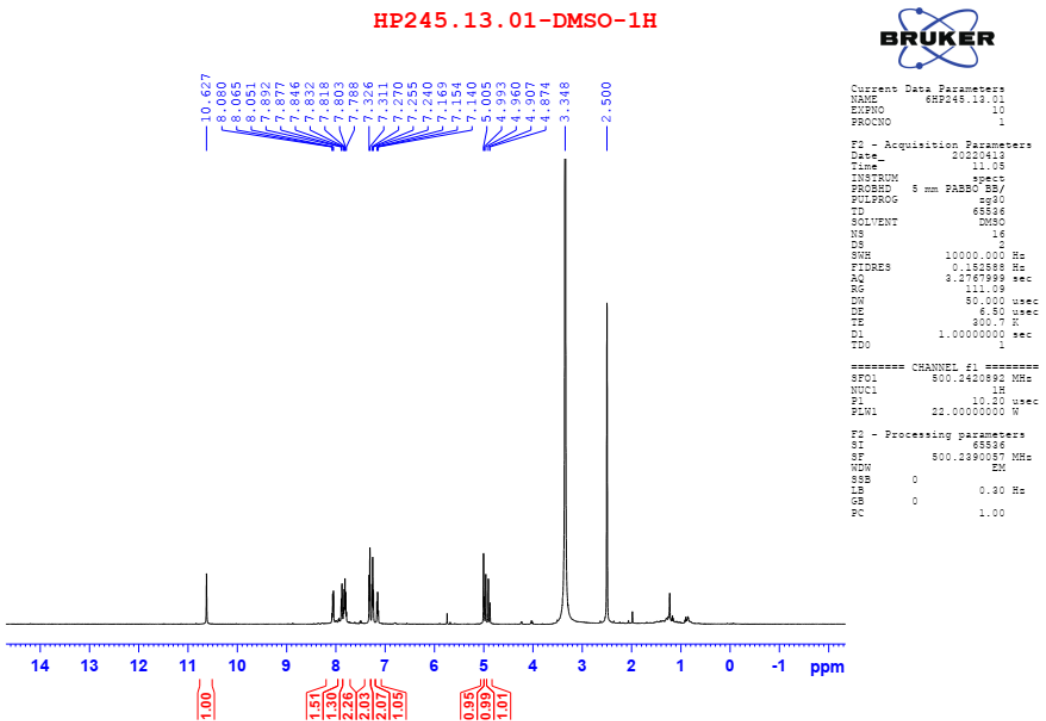
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DS       4
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FIDRES    0.268204 Hz
AQ         2.7525110 sec
RG         101
DM         42.0000 usec
DE         9.08 usec
TE        303.2 K
D1         1.00000000 sec
DELTA     0.00000000 sec
H1        600.4037071 MHz
NUC1      1H
P1         2.77 usec
PL1       0.00 usec
NUC2      13C
P2         12.26600018 sec
PL2       0.00 usec

Processing parameters
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SSB        0
GB         0
PC         0.20 Hz
RG         1.00
  
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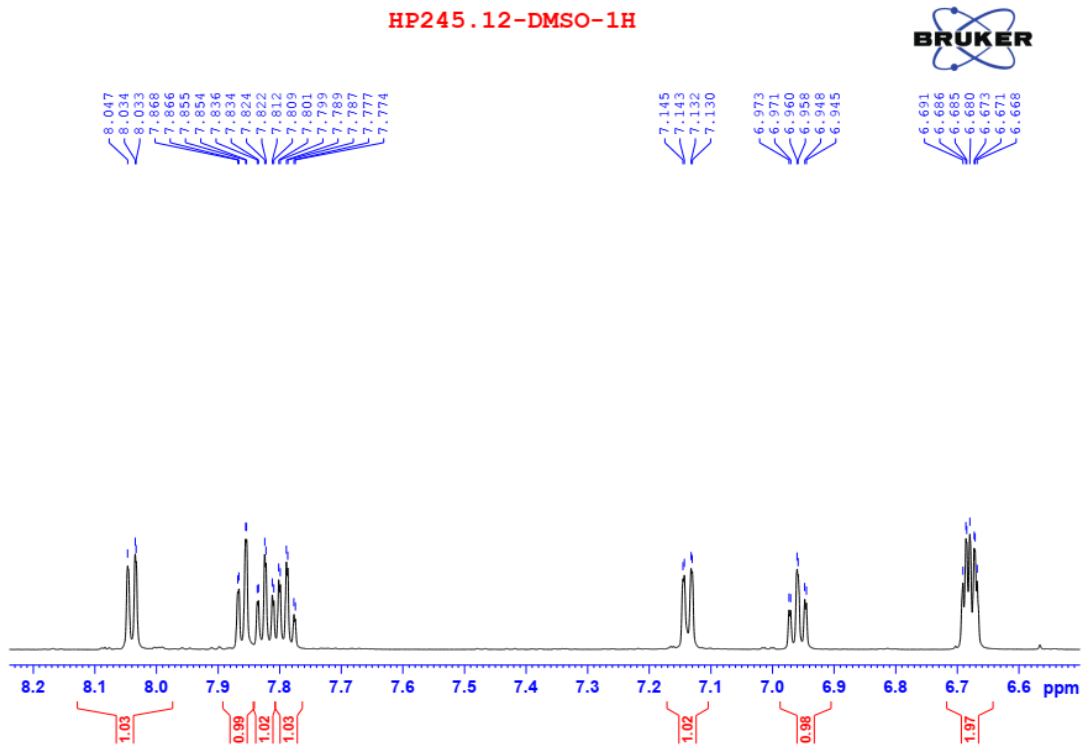
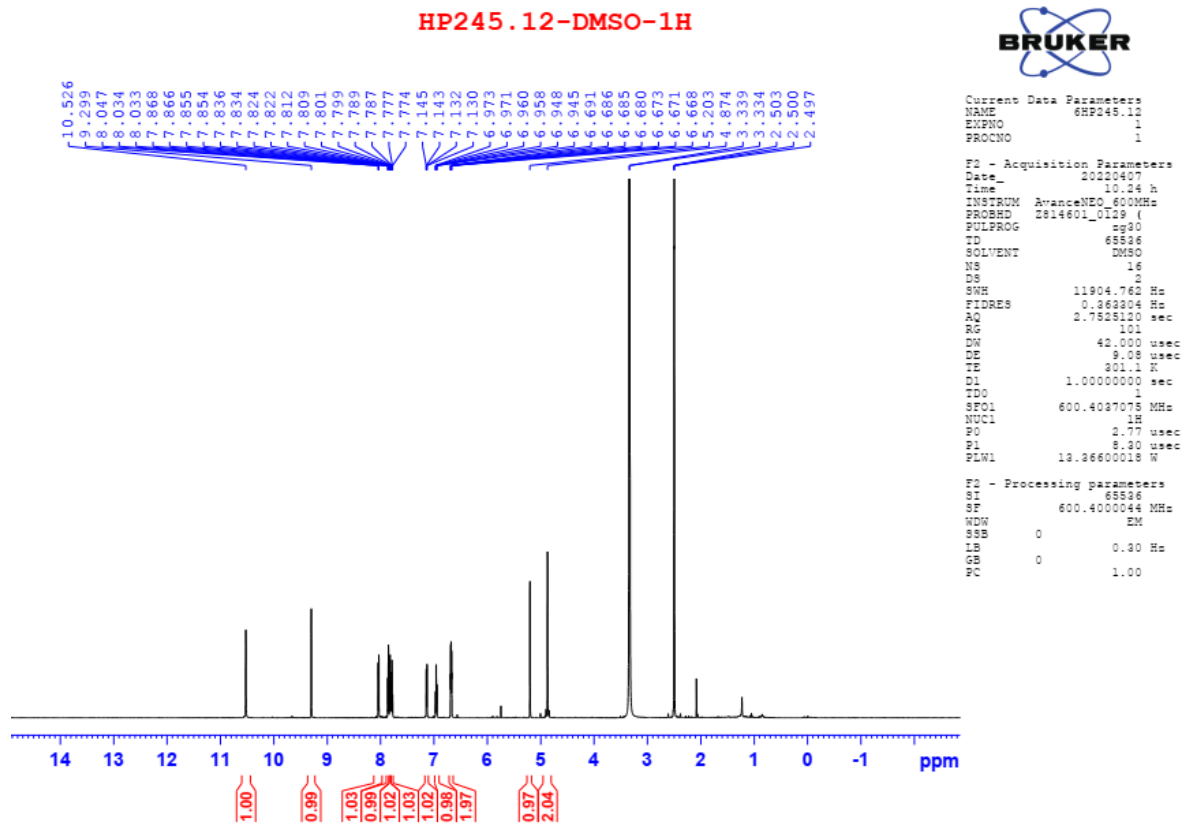
HP245.14.01-DMSO-1H



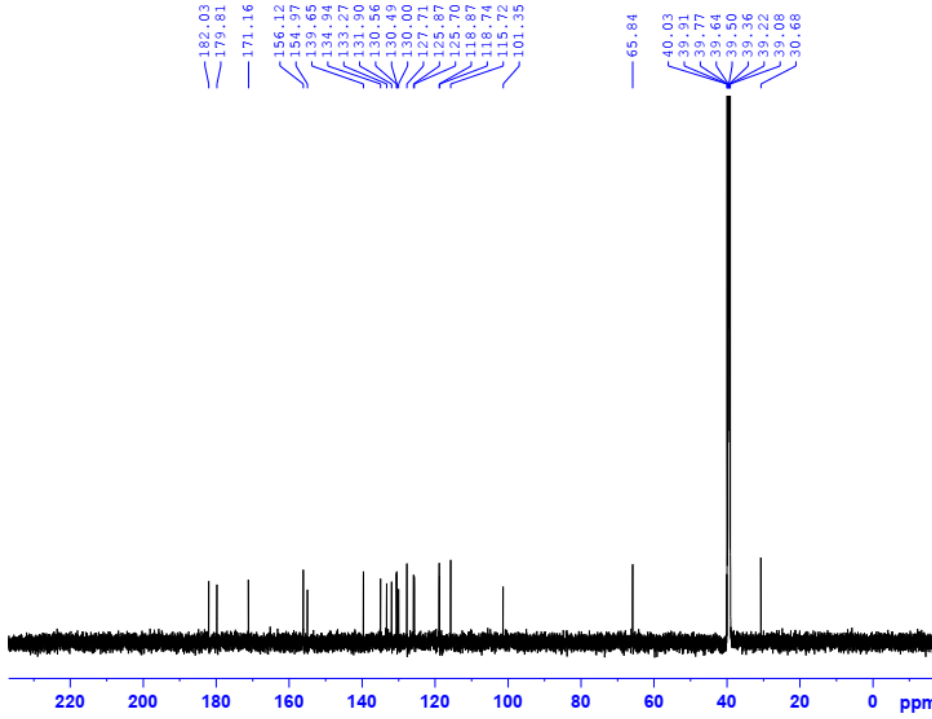
# 11-(Phenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H) -trione (5d)



# 11-(2-Hydroxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione (5h)

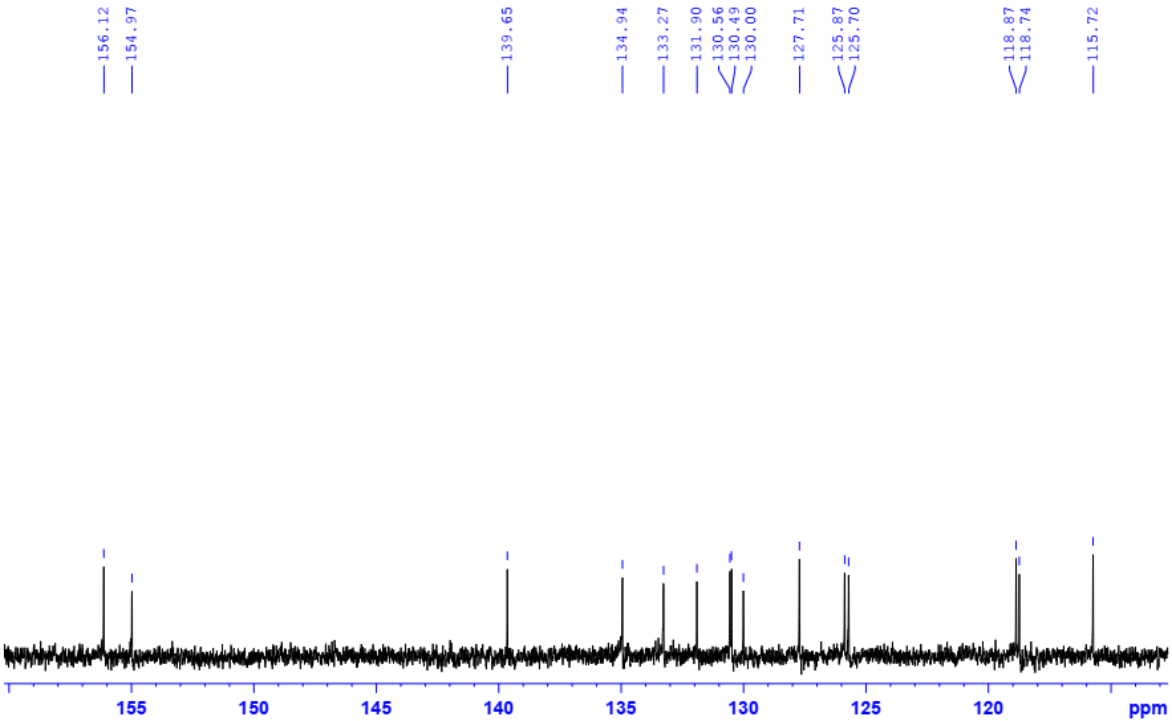


HP245.12-DMSO-C13CPD

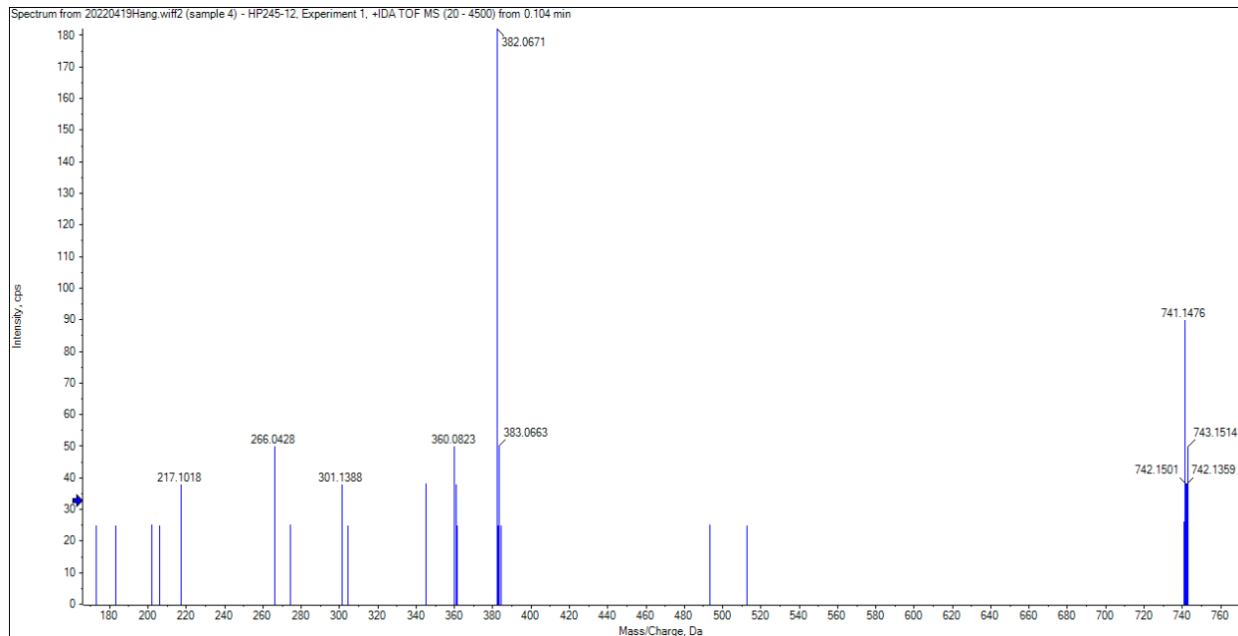


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 PROCNO 1  
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2048  
 DS 4  
 SWH 38461.80 Hz  
 FIDRES 1.173753 Hz  
 AQ 0.6519680 sec  
 RG 101  
 WM 13.200 usec  
 DE 6.50 usec  
 TE 302.4 K  
 DL 2.0000000 sec  
 D11 0.0300000 sec  
 TDD 1  
 SFO1 150.9873069 MHz  
 NUC1 13C  
 P0 5.29 usec  
 P1 16.00 usec  
 PLW1 112.9000153 W  
 SFO2 600.4024016 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 70.00 usec  
 PLW2 12.2660018 W  
 PLW3 0.1878200 W  
 PLW4 0.09482000 W  
 F2 - Processing parameters  
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 SF 150.9707748 MHz  
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 LB 1.00 Hz  
 GB 0  
 PC 1.40

HP245.12-DMSO-C13CPD

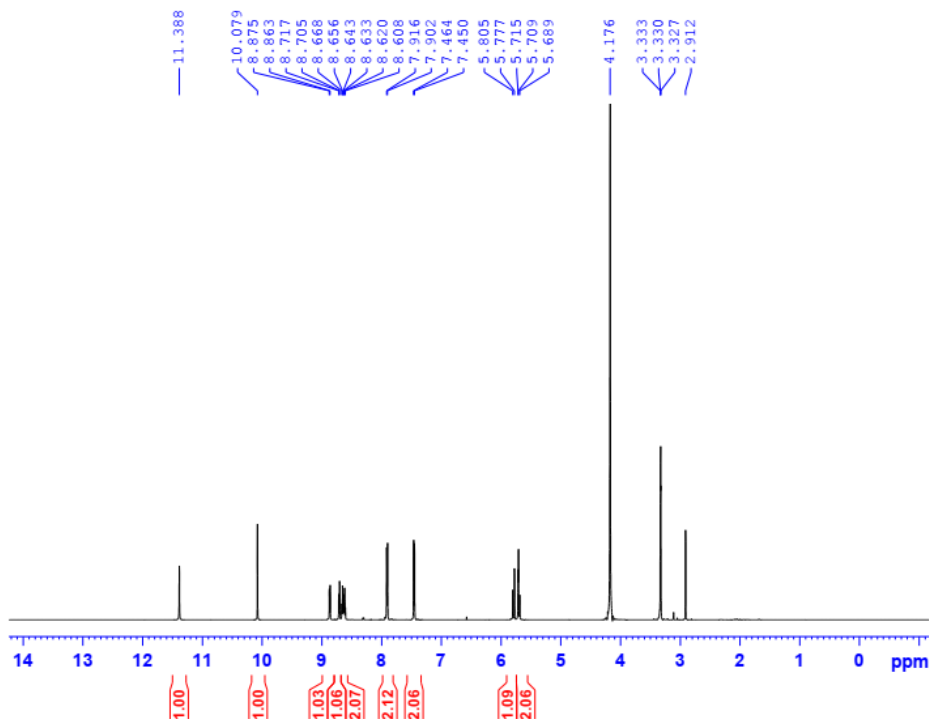






## 11-(4-Hydroxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione (5i)

HP245.17-DMSO-1H



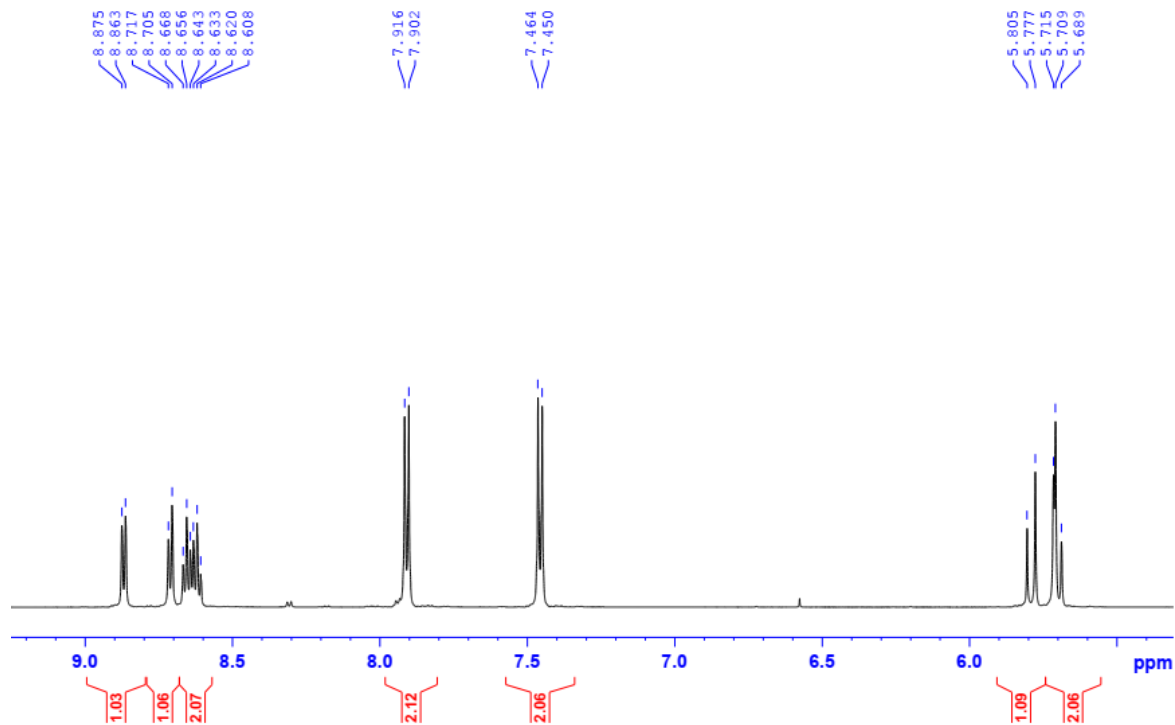
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PROCNO   1

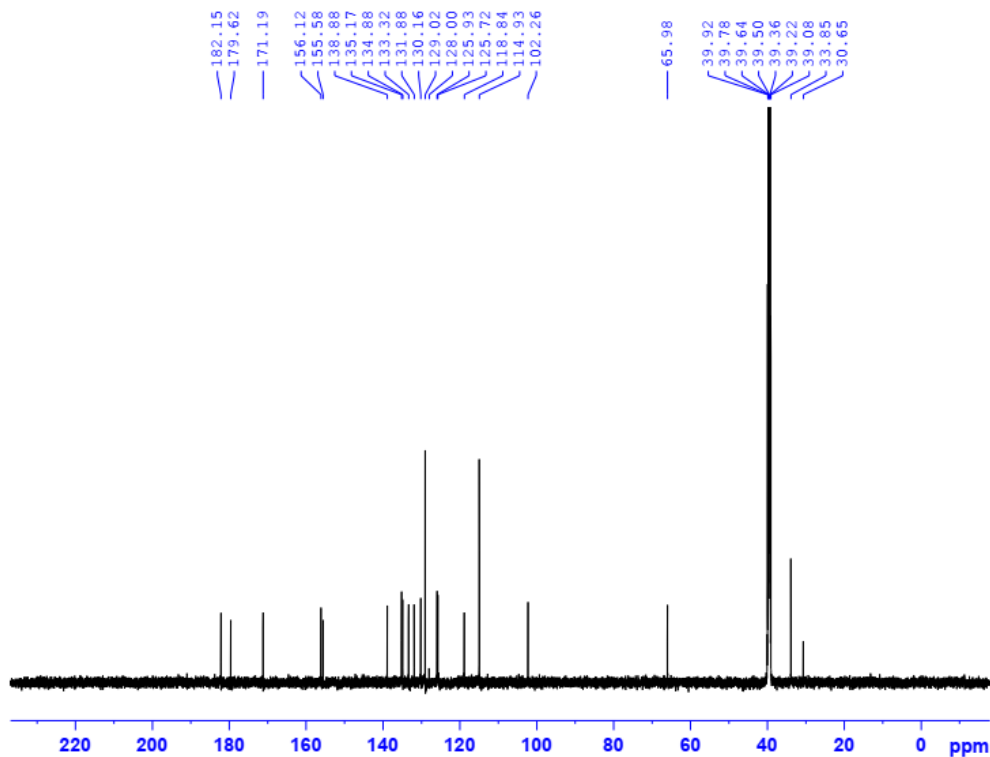
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PROBHD   ZB14601_0129 (
PULPROG  zgpg
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      11904.762 Hz
FIDRES   0.388304 Hz
AQ       2.7525120 sec
RG       101
DN       42.000 usec
DE       9.00 usec
TE       299.9 K
D1       1.00000000 sec
TDO      1
SFO1     600.4027075 MHz
NUC1     1H
PQ       2.77 usec
PI       8.30 usec
PLM1     13.36600018 W

F2 - Processing parameters
SI       65536
SF       600.3995065 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

HP245.17-DMSO-1H



HP245.17-DMSO-C13CPD

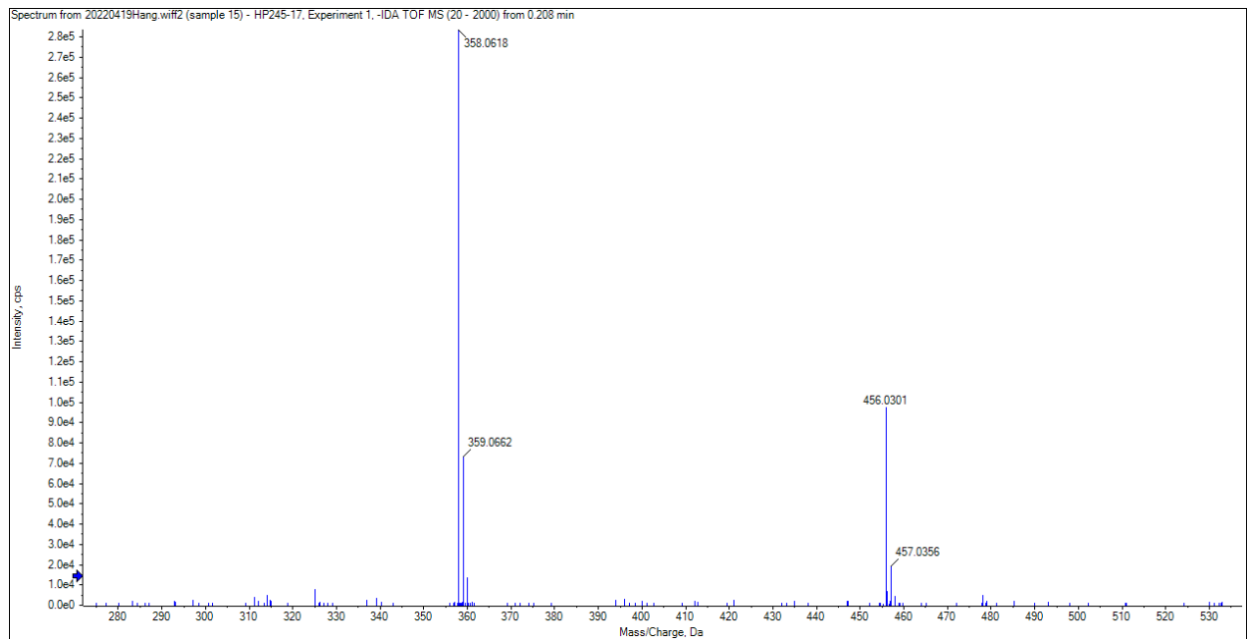
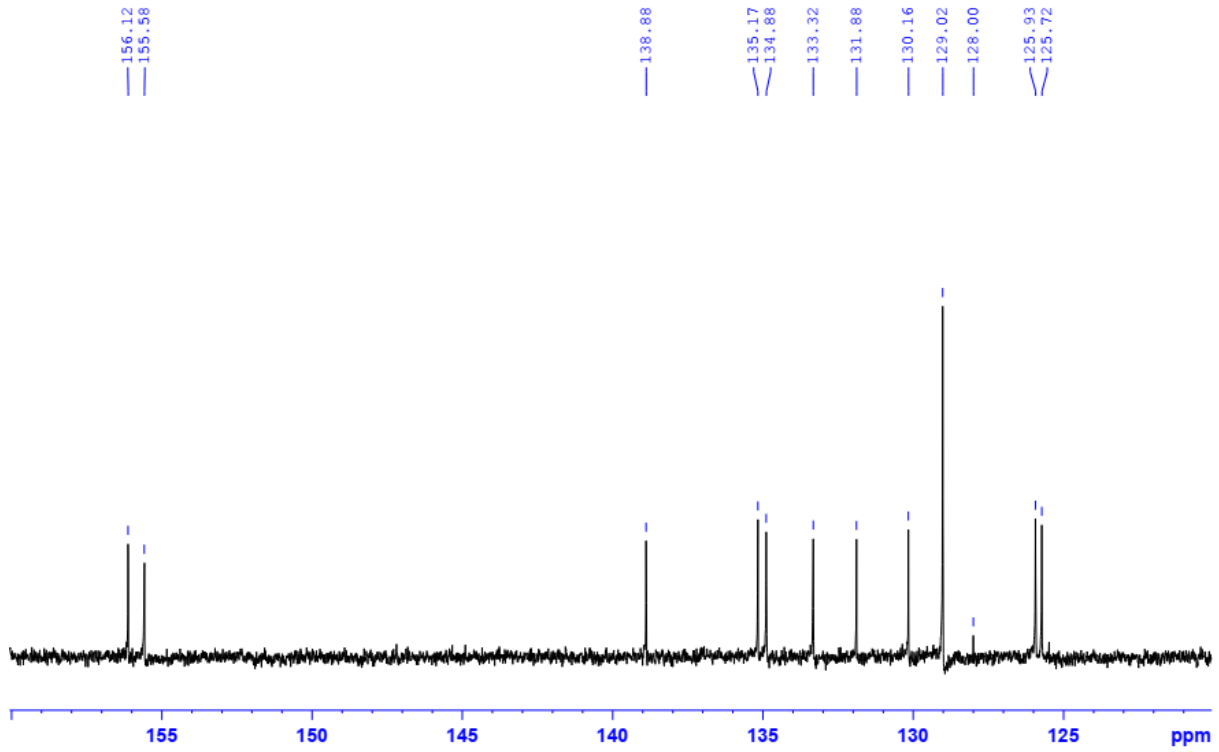


Current Data Parameters  
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 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
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 INSTRUM AvanceNeo\_500MHz  
 PROBRD zsl4601\_0129 (4  
 PULPROG zgpg30  
 TD 65536  
 ID 65536  
 SOLVENT DMSO  
 NS 1024  
 DS 4  
 SWH 38461.539 Hz  
 FIDRES 1.173753 Hz  
 AQ 0.8519680 sec  
 RG 101  
 DM 12.000 usec  
 DE 6.50 usec  
 TE 302.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD 1  
 SFO1 150.9873069 MHz  
 NUC1 13C  
 P0 5.33 usec  
 P1 14.00 usec  
 PLM1 113.90000182 W  
 SFO2 600.4024016 MHz  
 NUC2 1H  
 CPDPRG12 waltz65  
 PCPDG 70.00 usec  
 PLM2 13.36600018 W  
 PLM12 0.18792000 W  
 PLM13 0.09452000 W

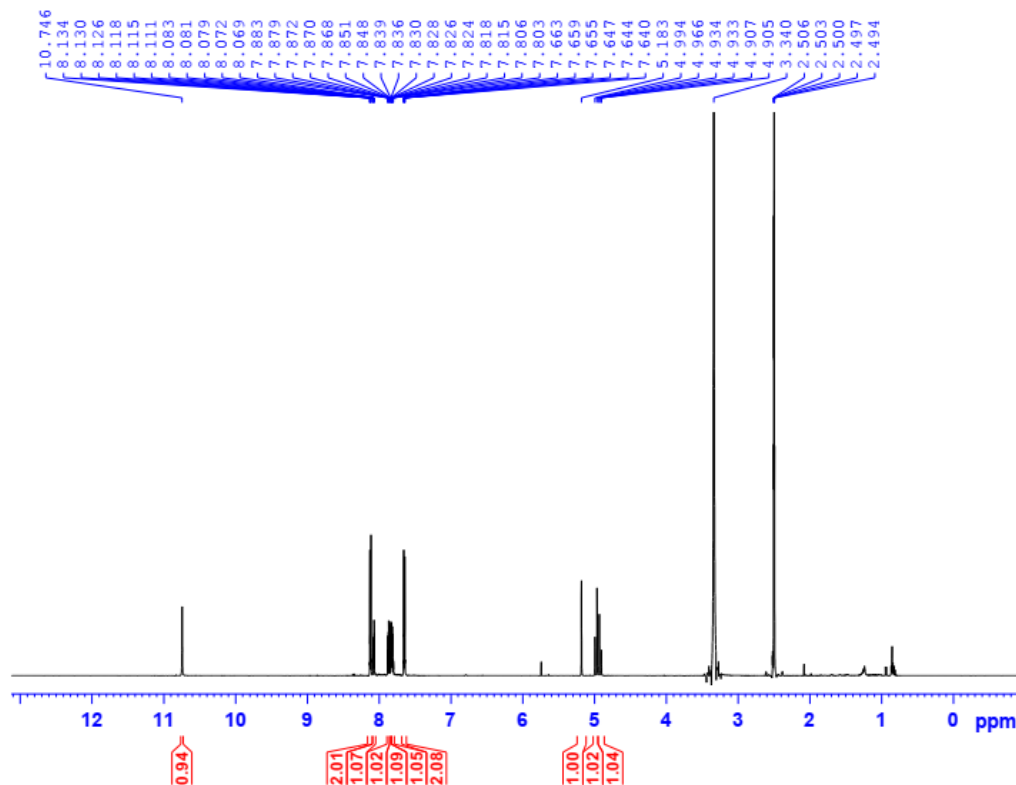
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 SF 150.9707749 MHz  
 WDM EM  
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 LB 1.00 Hz  
 GB 0  
 PC 1.40

HP245.17-DMSO-C13CPD



11-(4-Nitrophenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione (5j).

HP245.19-DMSO-1H

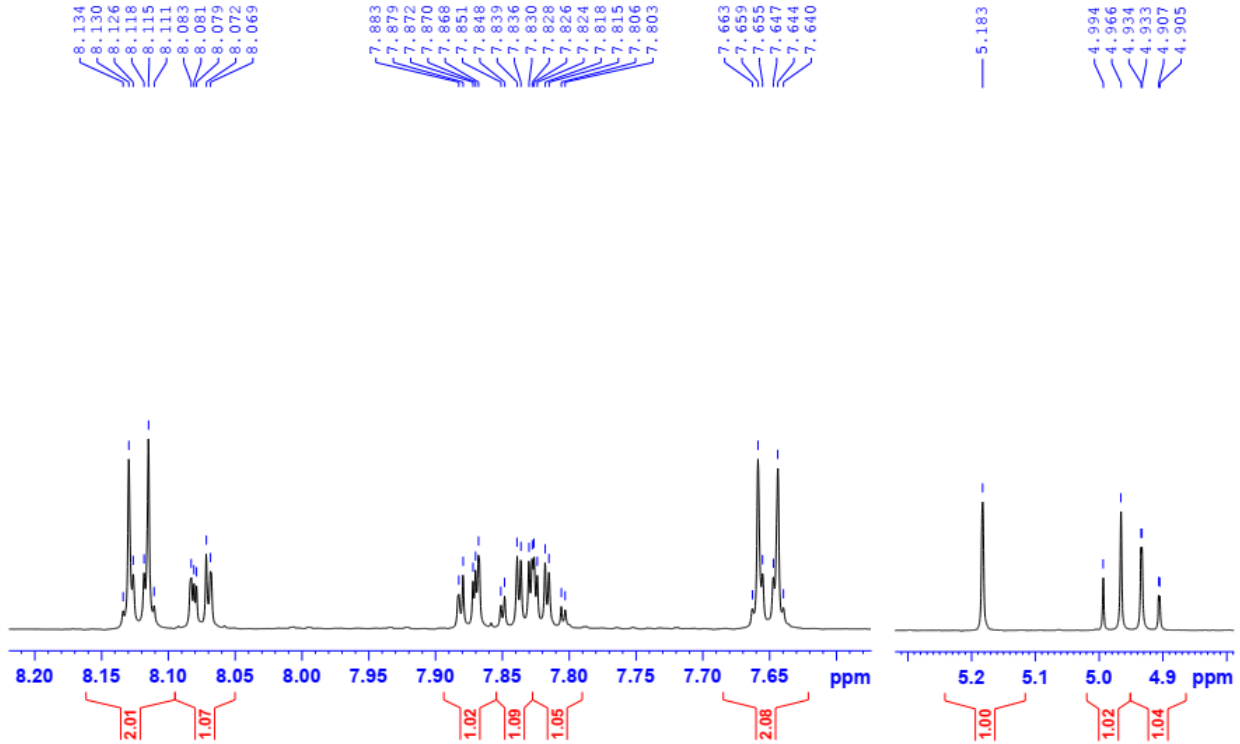


Current Data Parameters  
NAME HP245.19  
EXPNO 10  
PROCNO 1

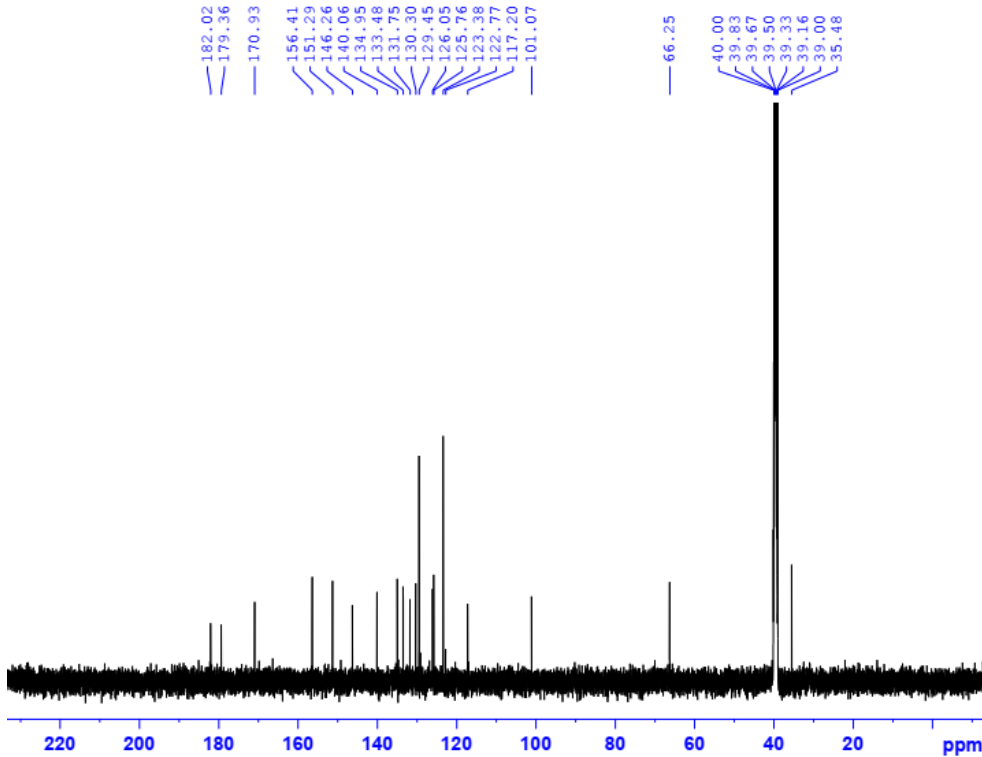
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Time 14.44 h  
INSTRUM AvanceNeo 600MHz  
PROBHD ZS14601-Q129 (1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 11904.762 Hz  
FIDRES 0.362204 Hz  
AQ 2.7525120 sec  
RG 101  
DN 42.000 usec  
DE 9.08 usec  
TE 302.1 K  
D1 1.00000000 sec  
TD0 1  
SFO1 600.4027075 MHz  
NUC1 1H  
FO 2.77 usec  
F1 8.30 usec  
PLM1 13.26600018 W

F2 - Processing parameters  
SI 65536  
SF 600.4000048 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

HP245.19-DMSO-1H



HP245.19-DMSO-C13CPD



```

Current Data Parameters
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PROCNO   1

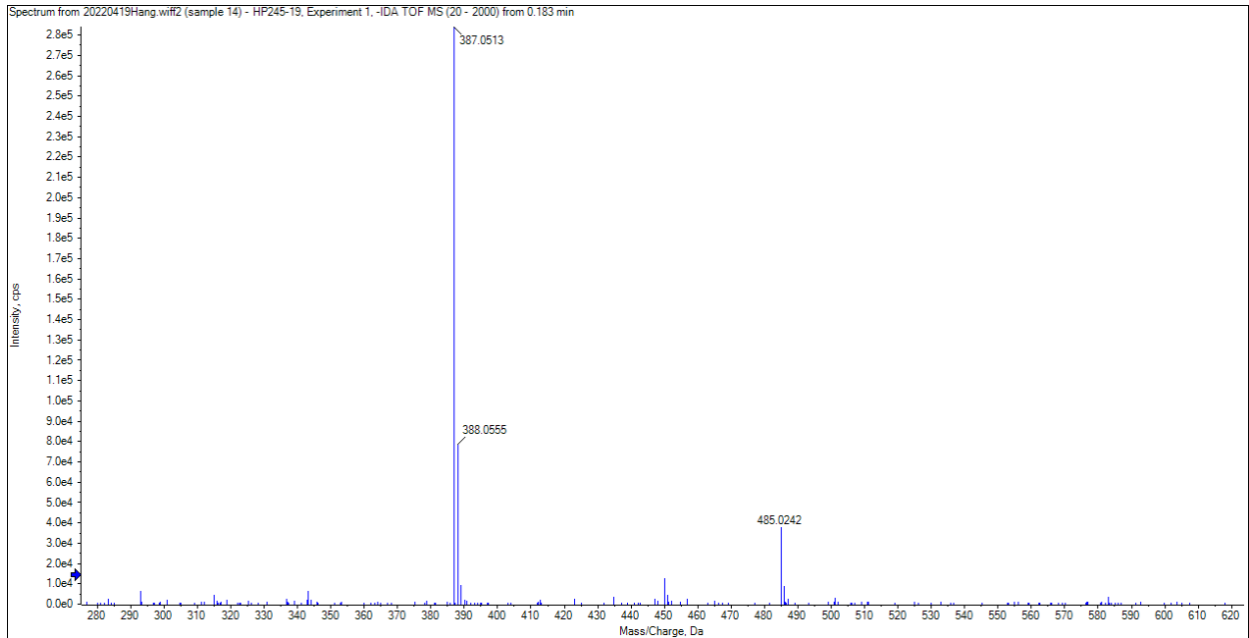
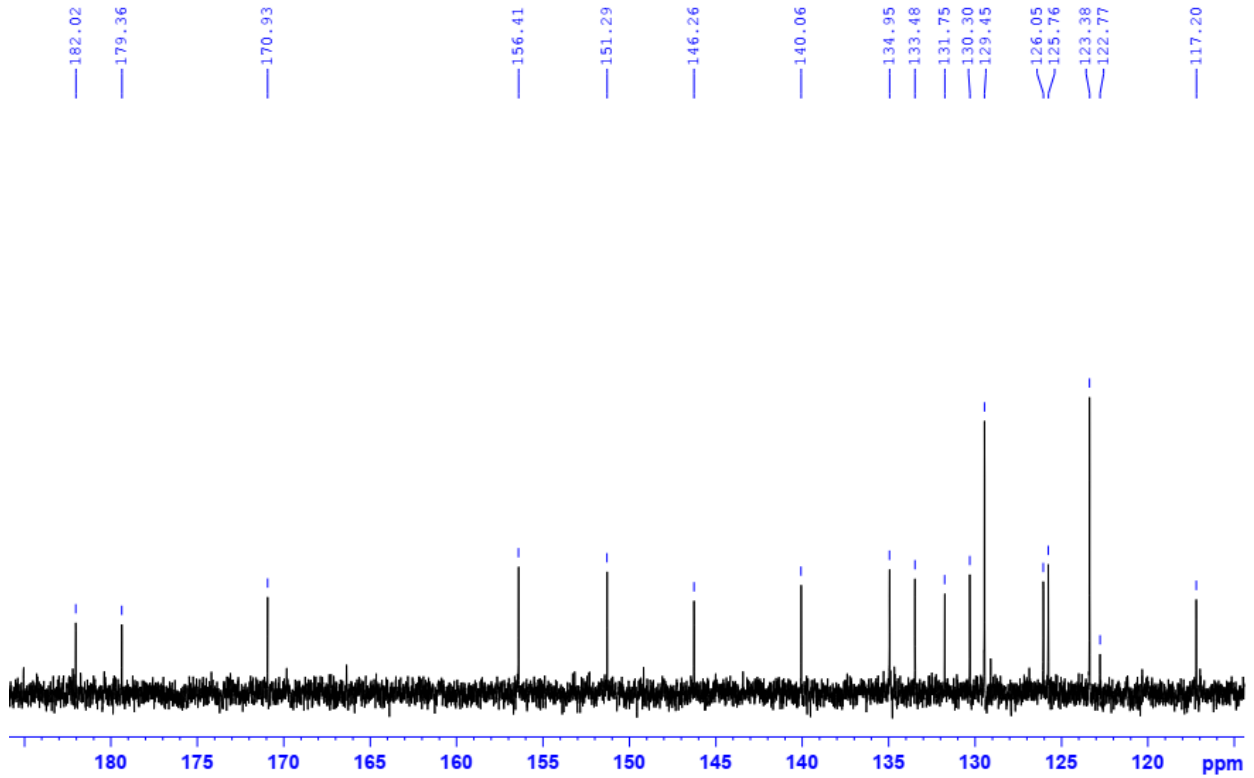
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PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       1024
DS       4
SWH      31250.000 Hz
FIDRES   0.476897 Hz
AQ       1.0485760 sec
RG       198.57
DW       16.000 usec
DE       6.50 usec
TE       302.6 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1

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SFO1    125.7690220 MHz
NUC1     13C
P1      10.00 usec
PLW1    88.0000000 W

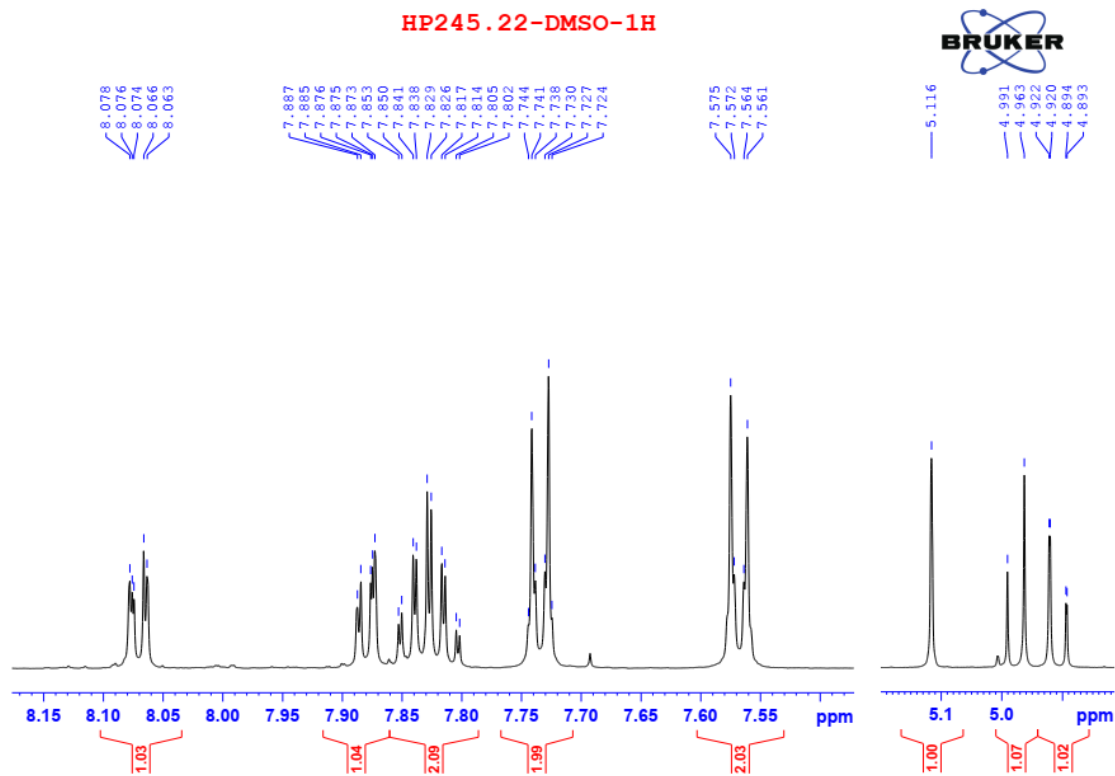
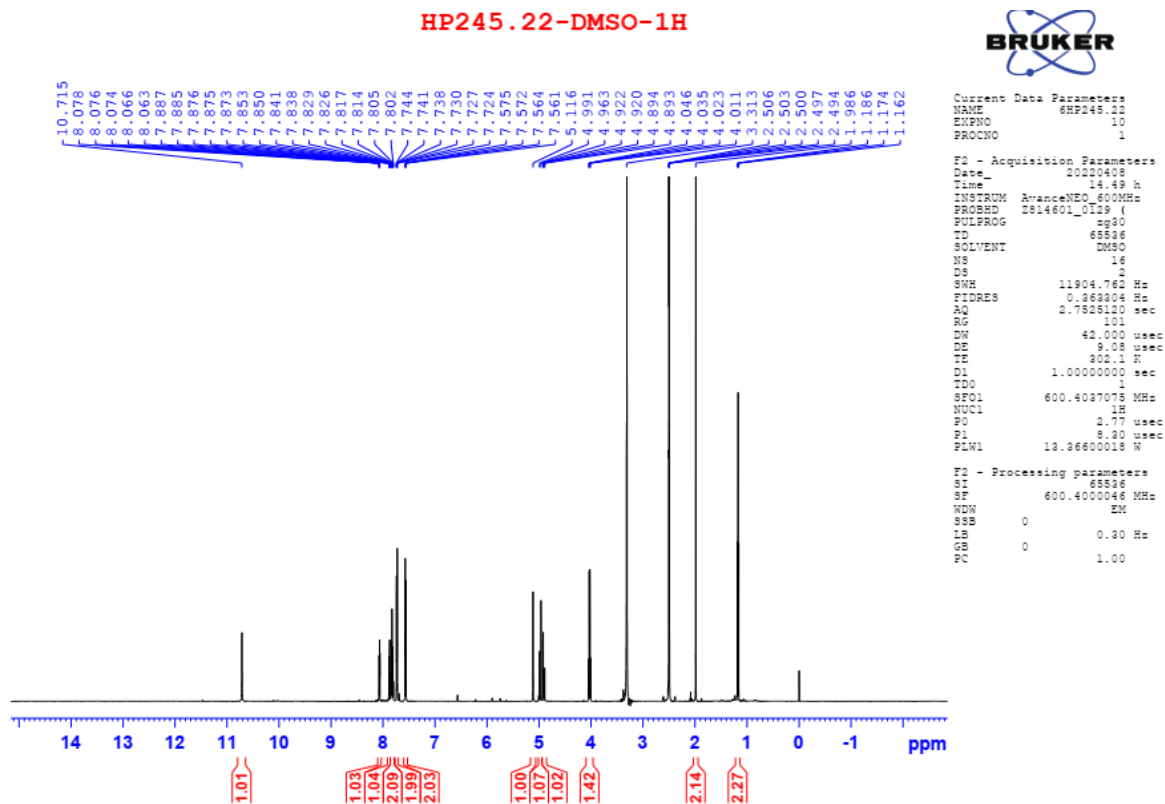
===== CHANNEL f2 =====
SFO2    500.2410010 MHz
NUC2     1H
CPDPRG2 waltz16
PCPD2   80.00 usec
PLW2    22.0000000 W
PLM12   0.28764000 W
PLM13   0.17989001 W

F2 - Processing parameters
SC      32768
SF      125.7652581 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
    
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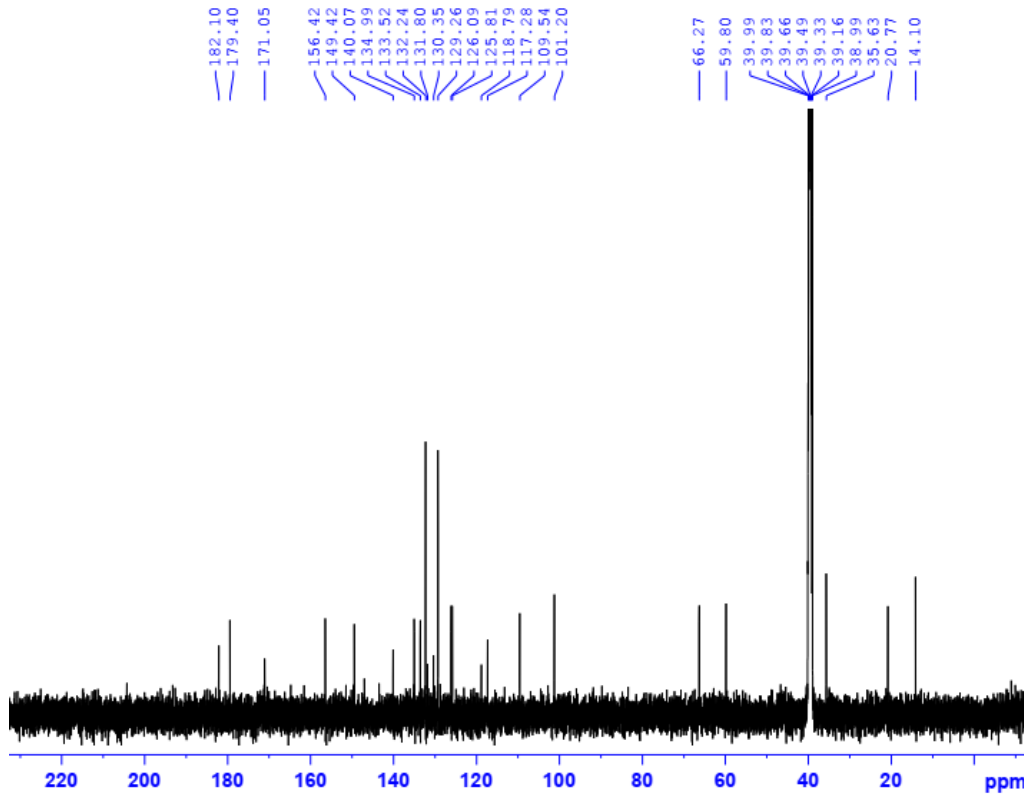
HP245.19-DMSO-C13CPD



4-(1,5,10-Trioxo-1,3,4,5,10,11-hexahydrobenzo[g]furo[3,4-b]quinolin-11-yl)benzotrile  
(5k).



HP245.22-DMSO-C13CPD



Current Data Parameters  
 NAME 6HP245.22  
 EXPNO 2  
 PROCNO 1

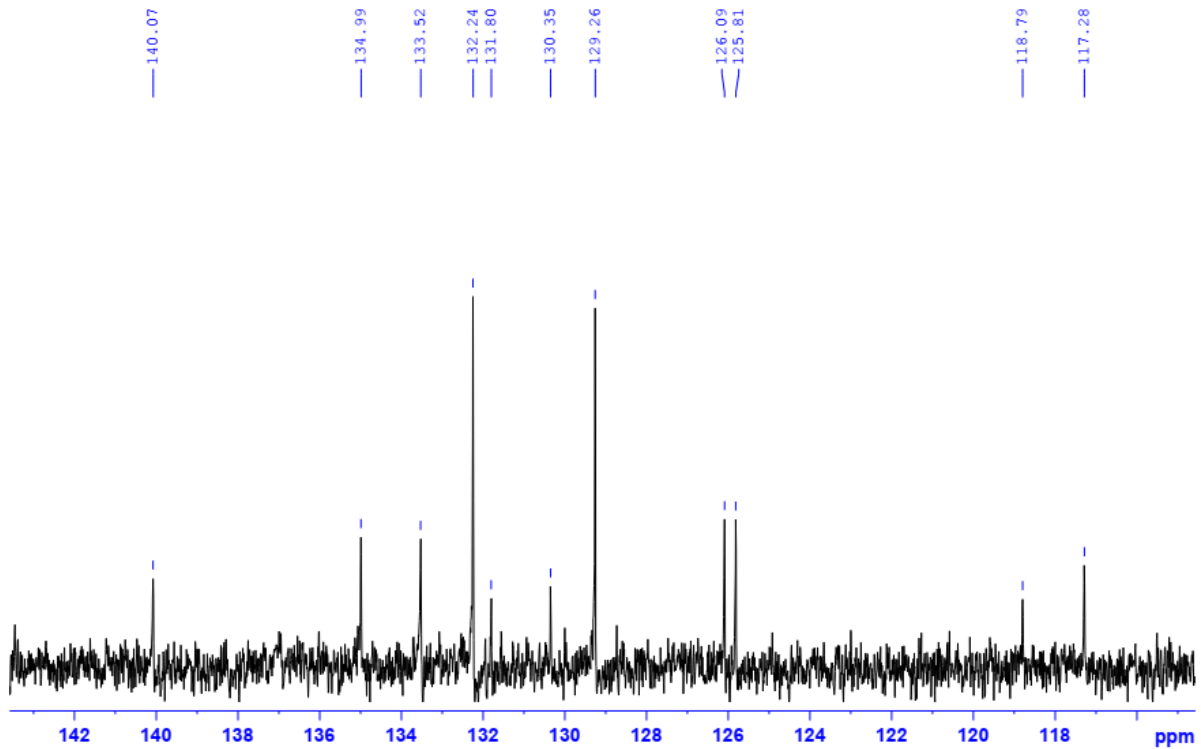
F2 - Acquisition Parameters  
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 Time 4.27  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 6526  
 SOLVENT DMSO  
 NS 1024  
 DS 4  
 SWH 31250.000 Hz  
 FIDRES 0.476837 Hz  
 AQ 1.0485760 sec  
 RG 198.57  
 DM 16.0000 usec  
 DE 6.50 usec  
 TE 303.0 K  
 DL 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 125.7990330 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 88.00000000 W

===== CHANNEL f2 =====  
 SF02 500.2410010 MHz  
 NUC2 1H  
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 PCPD2 80.00 usec  
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 PLW2 0.38764000 W  
 PLW3 0.17989001 W

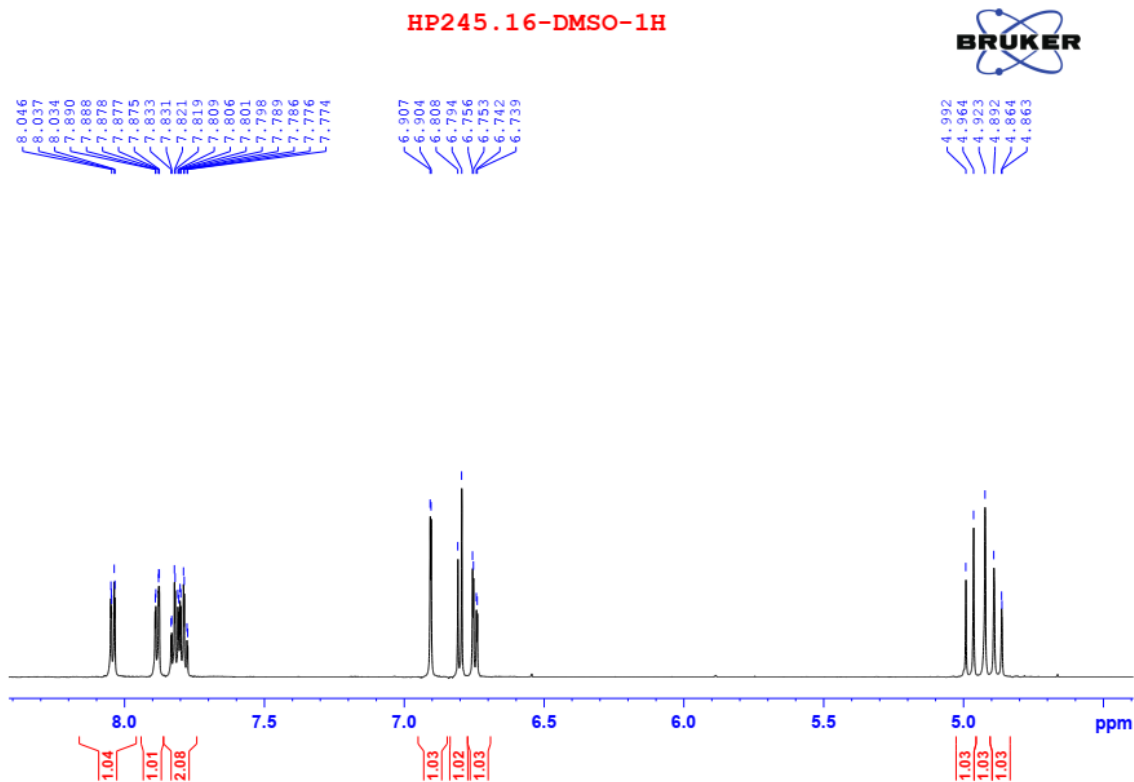
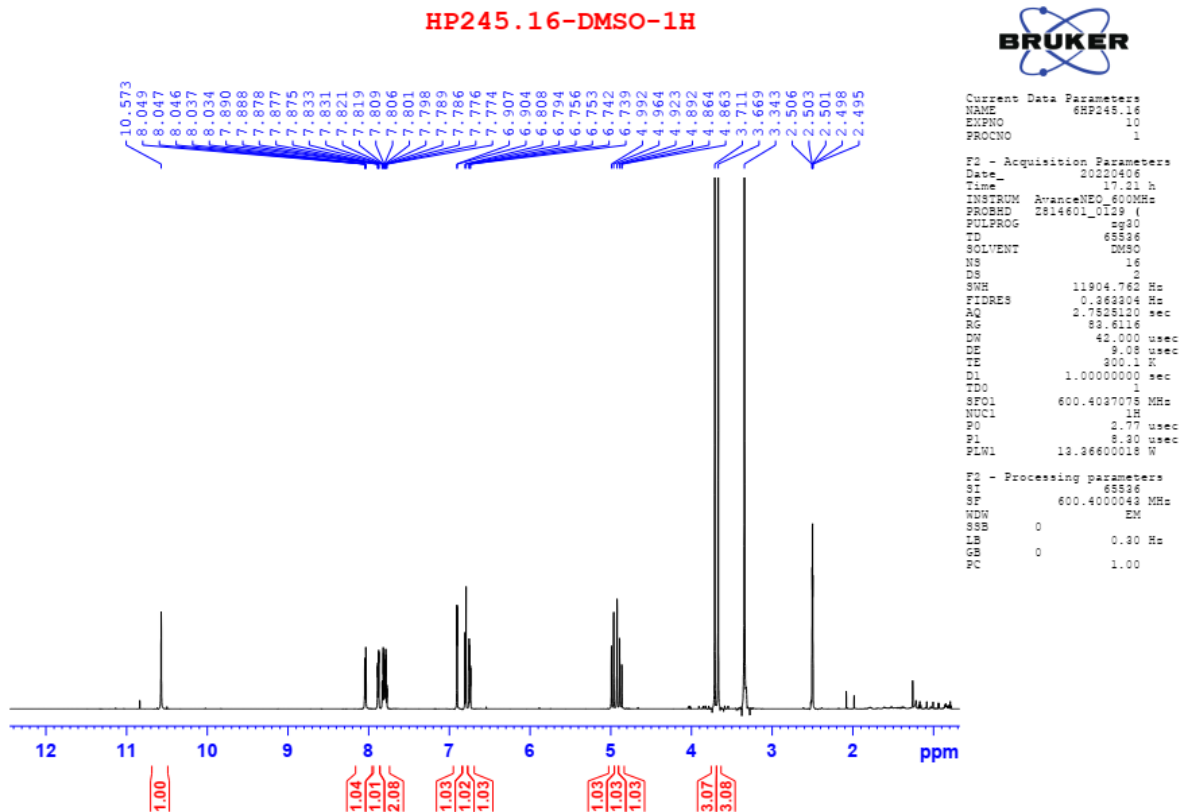
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 GB 0  
 PC 1.40

HP245.22-DMSO-C13CPD

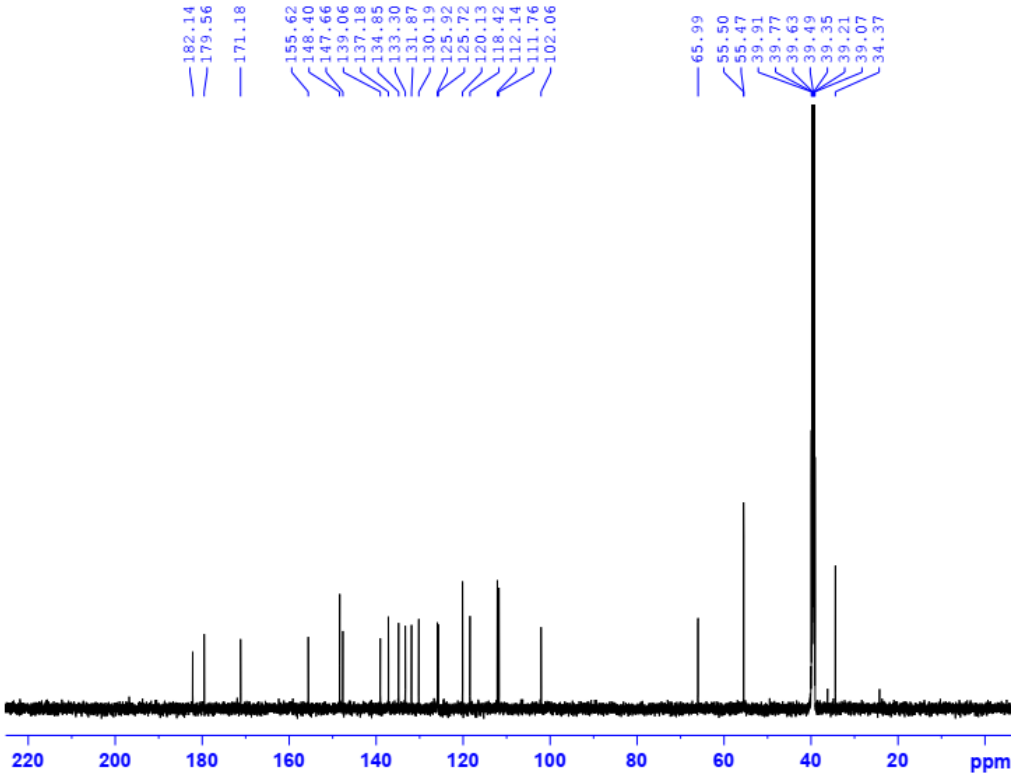




11-(3,4-Dimethoxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione (5l).



HP245.16-DMSO-C13CPD



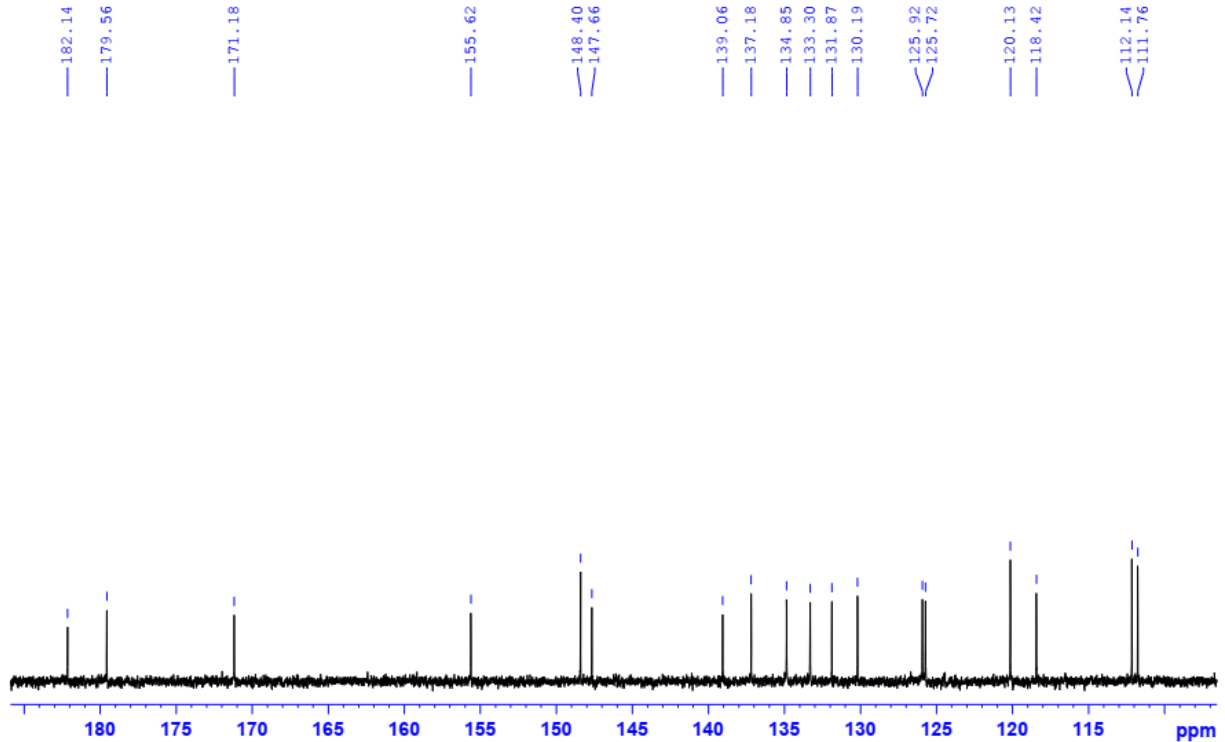
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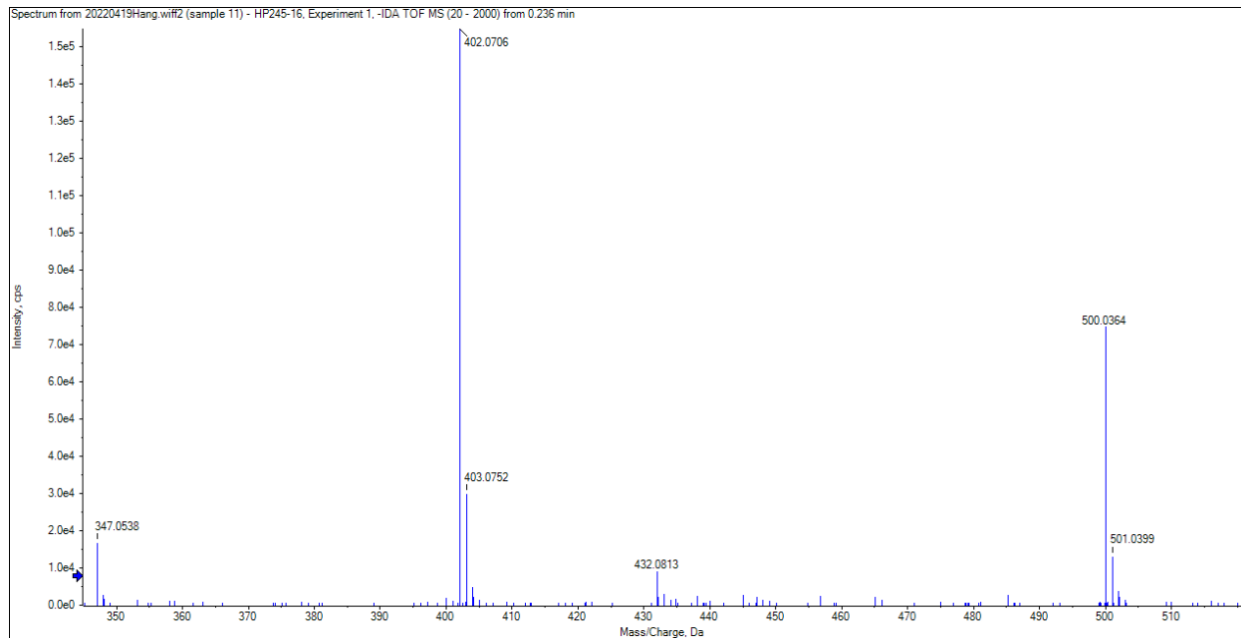
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EXPNO    1
PROCNO   1

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PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       512
DS       4
SWH      38461.539 Hz
FIDRES   1.173753 Hz
AQ       0.8519680 sec
RG       101
DW       13.000 usec
DE       6.50 usec
TE       302.6 K
D1       2.0000000 sec
D11      0.0300000 sec
TDO      0
SFO1     150.9873069 MHz
NUC1     13C
PC       5.33 usec
PI       16.00 usec
PLM1     112.8000015 W
SFO2     600.4024016 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    70.00 usec
PMD2     13.3660018 W
PLM2     0.18782000 W
PLM3     0.09452000 W

F2 - Processing parameters
SI       32768
SF       150.9707766 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
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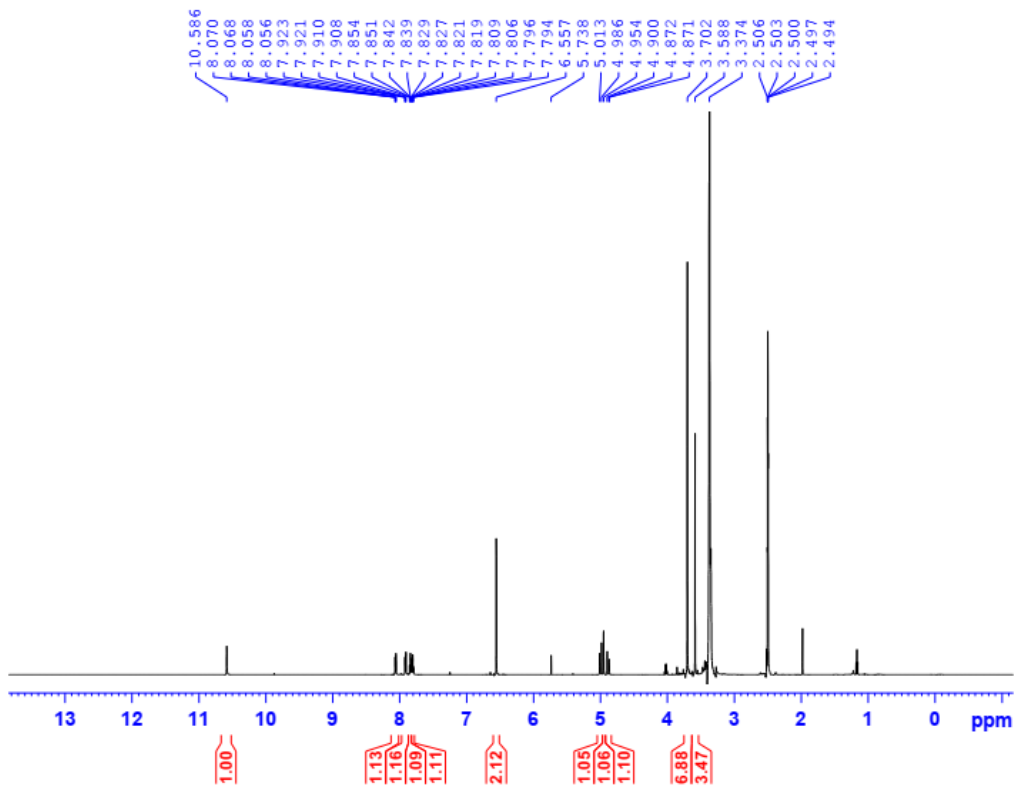
HP245.16-DMSO-C13CPD





**11-(3,4,5-Trimethoxyphenyl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione (5m).**

HP245.03-DMSO-1H



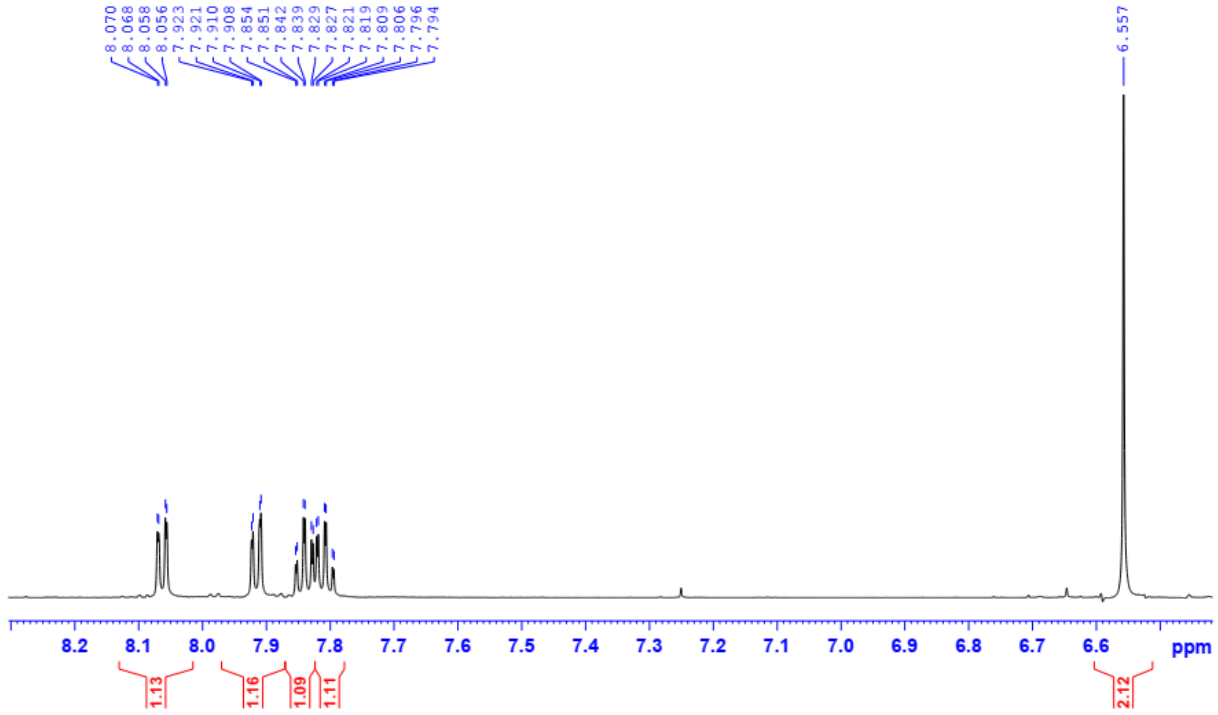
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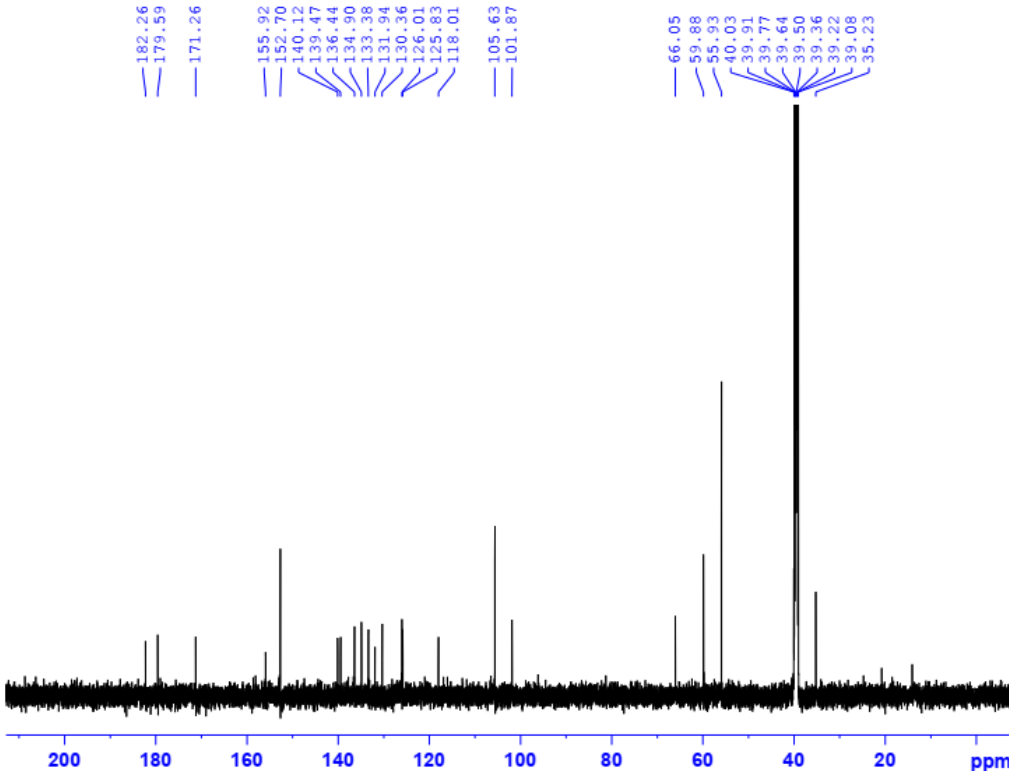
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PROBHD   zgpg30
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        16
DS        2
SWH       11904.762 Hz
FIDRES   0.362304 Hz
AQ        2.7828120 sec
RG        82.0467
DM        42.000 usec
DE        9.08 usec
TE        301.2 K
D1        1.00000000 sec
TDO       1
SFO1     600.4037075 MHz
NUC1     1H
FO       2.77 usec
F1       8.20 usec
PLW1     13.26600018 W

F2 - Processing parameters
SI        65536
SF        600.4000044 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
WC        1.00
  
```

HP245.03-DMSO-1H



HP245.03-DMSO-C13CPD

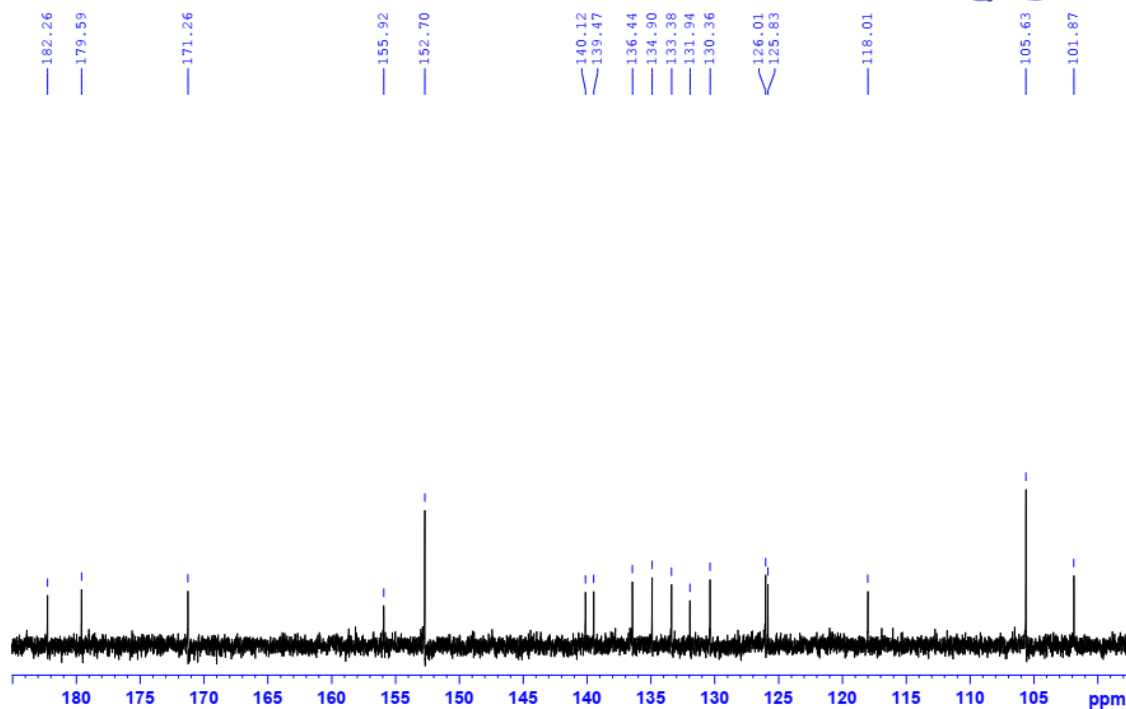


Current Data Parameters  
 NAME HP245.03  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220320  
 Time 19.26 h  
 INSTRUM AvanceNEO\_600MHz  
 PROBHD Z814601\_0129 (4  
 FULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1024  
 DS 4  
 SWH 35714.288 Hz  
 FIDRES 1.059913 Hz  
 AQ 0.9175040 sec  
 RG 101  
 DW 14.000 usec  
 DE 6.50 usec  
 TE 301.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SF01 150.9857972 MHz  
 NUC1 13C  
 PU 5.33 usec  
 P1 16.00 usec  
 PLN1 113.90000159 W  
 SF02 600.4024016 MHz  
 NUC2 1H  
 CPDPRG13 waltz168  
 PCPD2 70.00 usec  
 PLM2 13.26600018 W  
 PLN12 0.18792000 W  
 PLN13 0.09452000 W

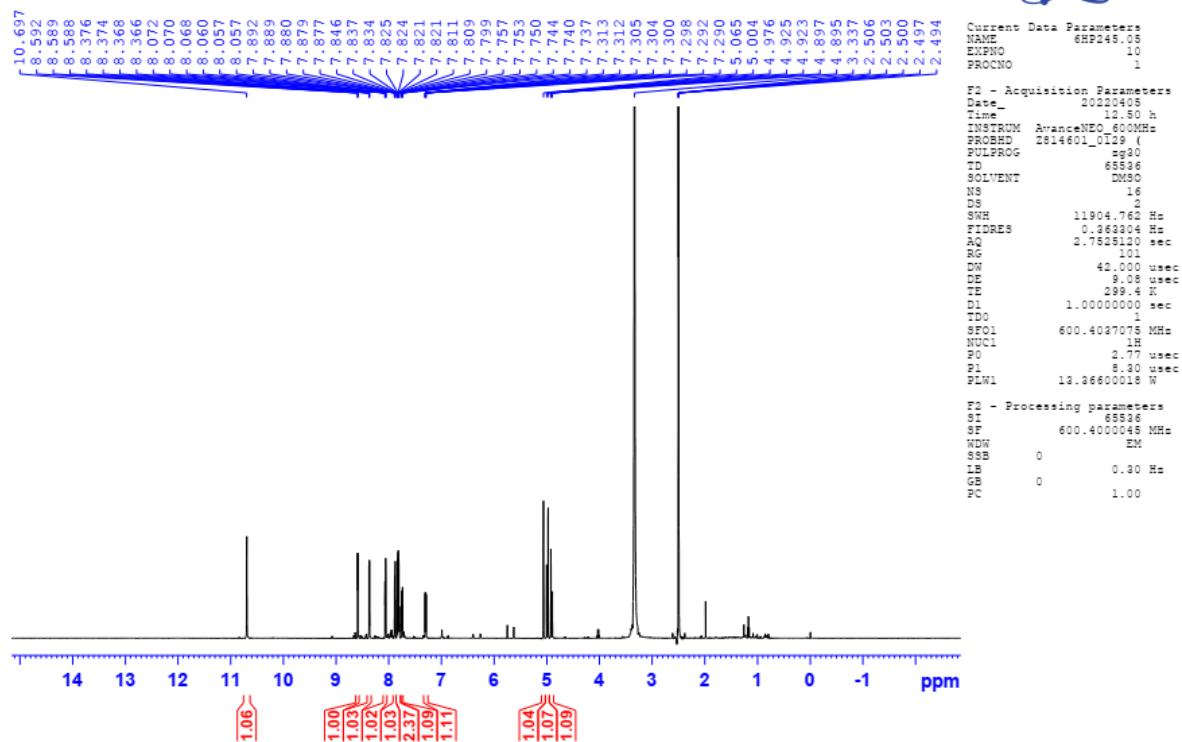
F2 - Processing parameters  
 SI 32768  
 SF 150.9707682 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

HP245.03-DMSO-C13CPD

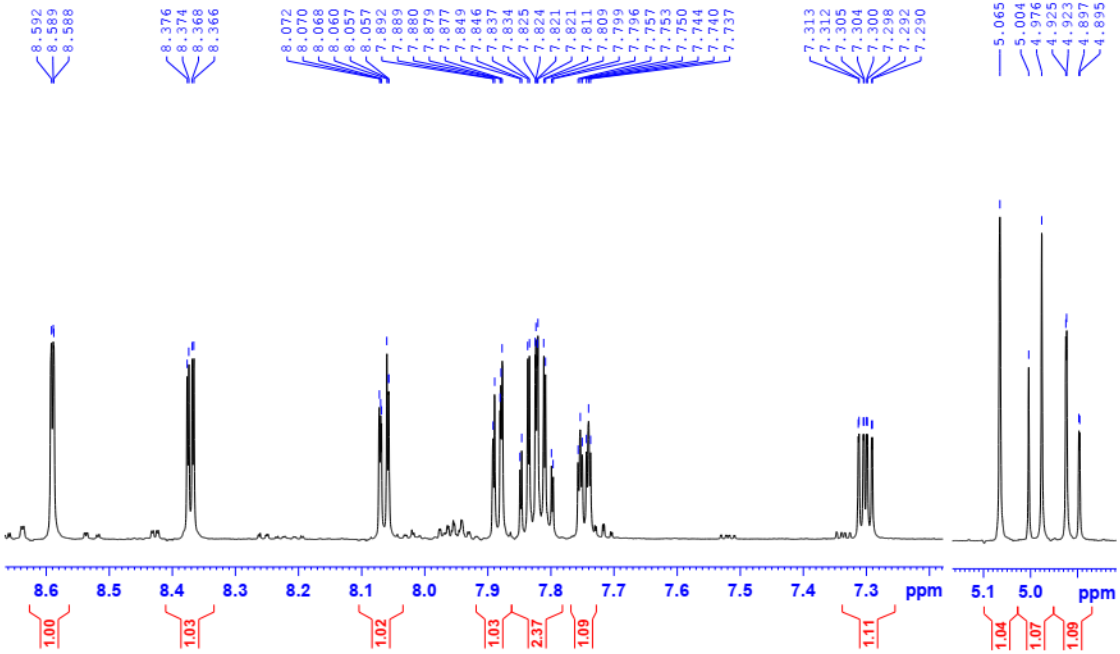


11-(Pyridin-3-yl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione (5n).

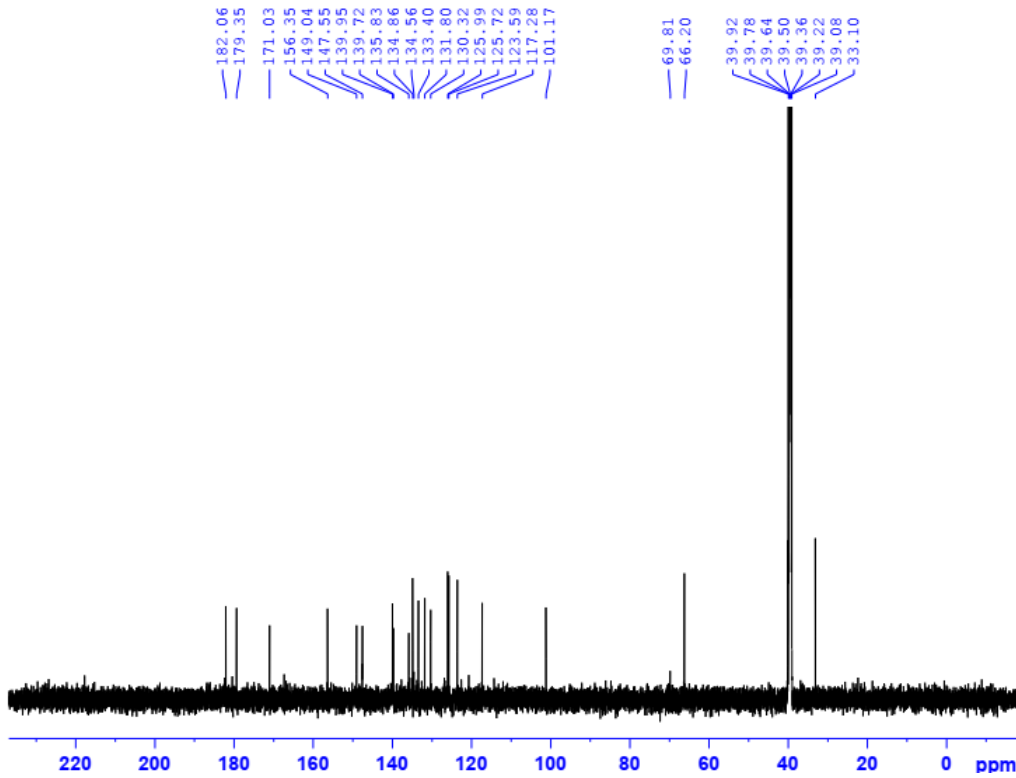
HP245.05-DMSO-1H



HP245.05-DMSO-1H



HP245.05-DMSO-C13CPD



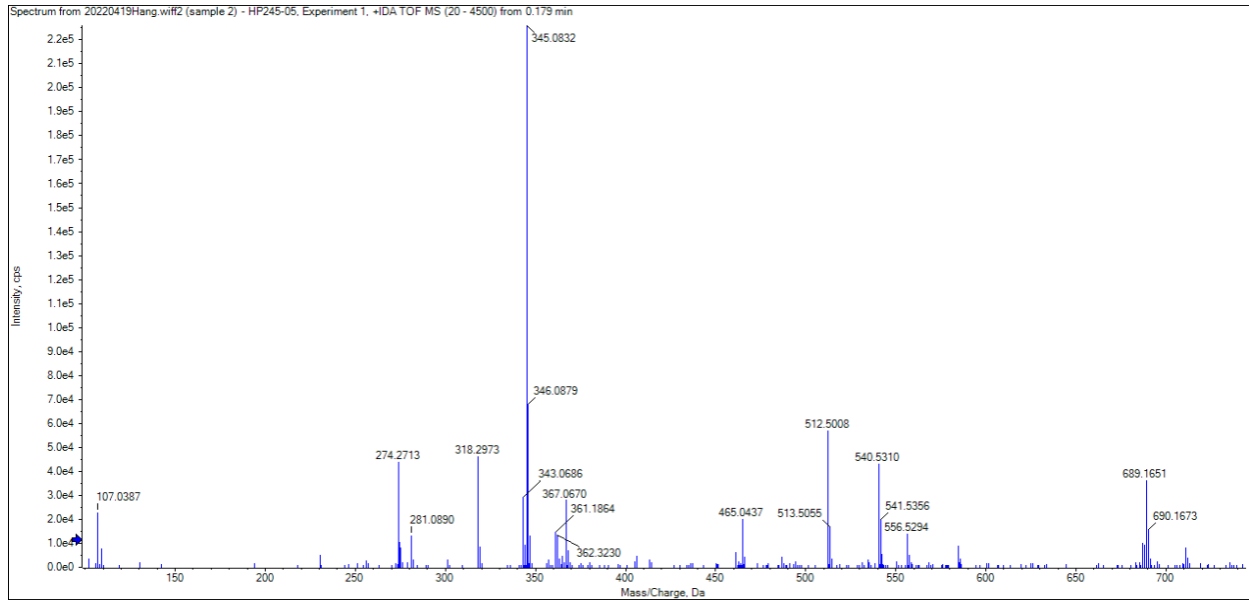
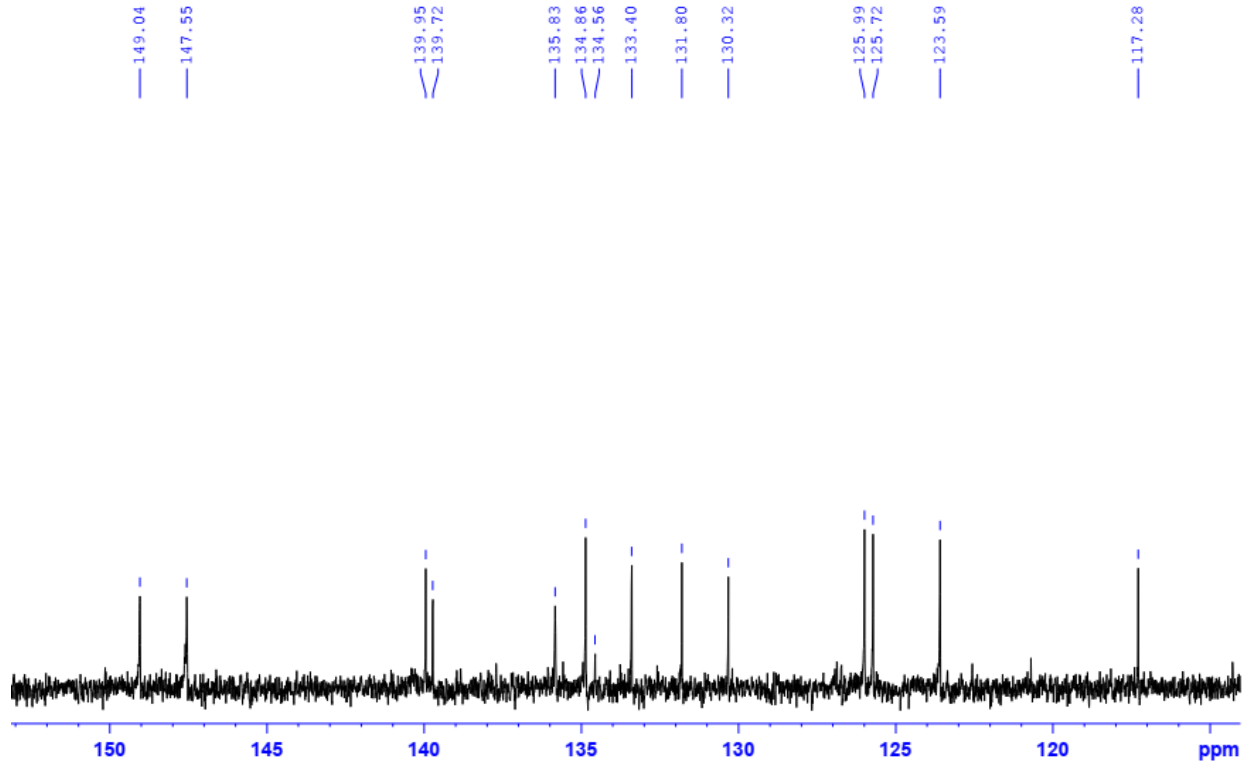
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Current Data Parameters
NAME      6HP245.05
EXPNO    2
PROCNO   1

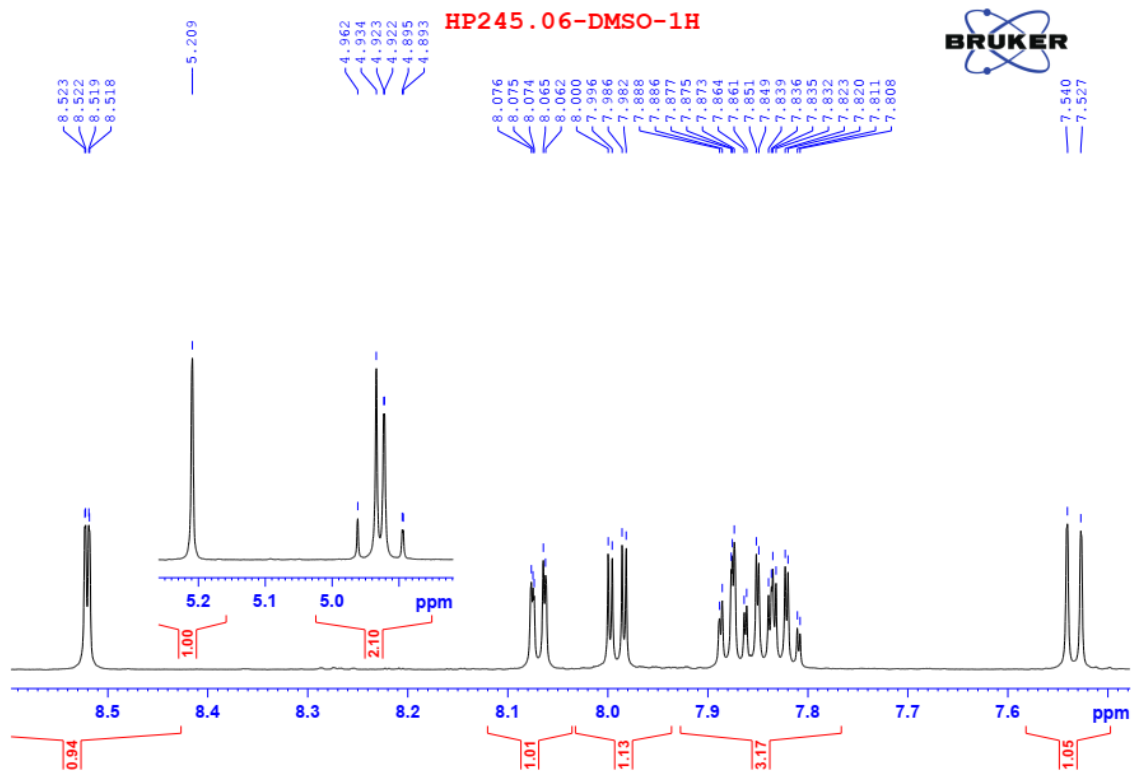
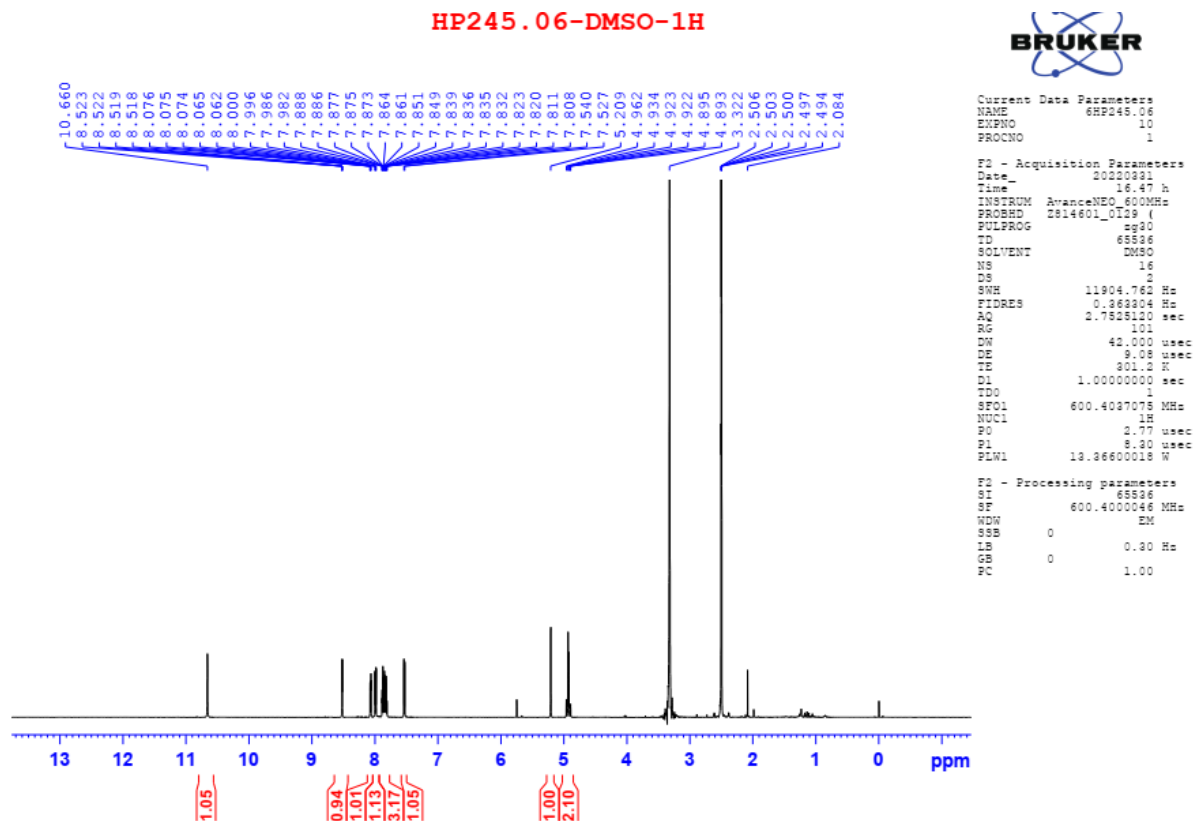
F2 - Acquisition Parameters
Date_    20220408
Time     20.23 h
INSTRUM  Avance NEO 600MHz
PROBHD   zgpg30
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       2072
DS       4
SWH      38461.539 Hz
FIDRES   1.173783 Hz
AQ       0.8519680 sec
RG       101
DN       13.000 usec
DE       8.50 usec
TE       302.6 K
D1       2.00000000 sec
D11      0.03000000 sec
TDO      1
SFO1     150.9873069 MHz
NUC1     13C
PC       5.22 usec
P1       16.00 usec
PLW1     113.90000153 W
SFO2     600.4024016 MHz
NUC2     1H
CPDPRG2  waltz165
PCPD2    70.00 usec
PLW2     13.36600018 W
PLW12    0.18792000 W
PLW13    0.09452000 W

F2 - Processing parameters
SI       32768
SF       150.9707760 MHz
WDW      EM
SSB      0
GB       0
PC       1.40
    
```

HP245.05-DMSO-C13CPD

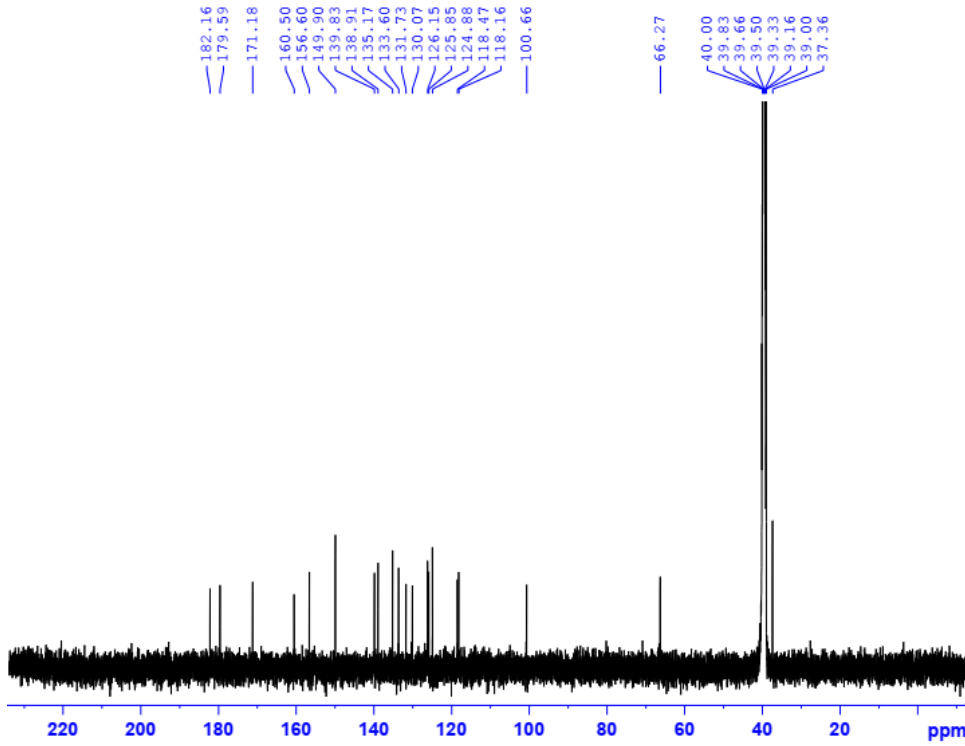


11-(5-Bromopyridin-2-yl)-4,11-dihydrobenzo[g]furo[3,4-b]quinoline-1,5,10(3H)-trione (5o).





HP245.06-DMSO-C13CPD



Current Data Parameters  
 NAME HP245.06  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220404  
 Time 19.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 NS 2048  
 DS 4  
 SWH 31250.000 Hz  
 FIDRES 0.476837 Hz  
 AQ 1.0483760 sec  
 RG 198.87  
 DW 16.000 usec  
 DE 6.50 usec  
 TE 300.2 K  
 D1 2.00000000 sec  
 D11 0.02000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 125.7990220 MHz  
 NUCL1 13C  
 P1 10.00 usec  
 PLW1 88.00000000 W

===== CHANNEL f2 =====  
 SF02 500.2410010 MHz  
 NUCL2 1H  
 CPDPRG12 waltz16  
 P2P21 80.00 usec  
 PLM2 22.00000000 W  
 PLM12 0.38764000 W  
 PLM13 0.17989001 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7852323 MHz  
 NDM EM  
 SSB 0  
 GB 1.00 Hz  
 PC 1.40

HP245.06-DMSO-C13CPD

