

## Synthesis, cytotoxicity, apoptosis-inducing activity and molecular docking studies of novel isatin-podophyllotoxin hybrids

Ha Thanh Nguyen,<sup>a,b</sup> Ket Tran Van,<sup>\*,b,d</sup> Hai Pham-The,<sup>c</sup> Quang-Bao Le,<sup>c</sup> Giang Le-Nhat-Thuy,<sup>a,b</sup> Tuyet Anh Dang Thi,<sup>a,b</sup> Phuong Hoang Thi,<sup>a,b</sup> Quynh Giang Nguyen Thi,<sup>a</sup> Anh Nguyen Tuan,<sup>a,b</sup> Doan Vu Ngoc,<sup>d</sup> and Tuyen Van Nguyen<sup>\*,a,b</sup>

<sup>a</sup>Institute of Chemistry, Vietnam Academy of Science and Technology (VAST), 18 Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

<sup>b</sup>Graduate University of Science and Technology, VAST, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

<sup>c</sup>University of Science and Technology of Hanoi, VAST, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

<sup>d</sup>Military Technical Academy, 236 Hoang Quoc Viet, Bac Tu Liem, Hanoi, Vietnam

\* Corresponding author

E-mail addresses: [ngvtuyen@hotmail.com](mailto:ngvtuyen@hotmail.com), [tranvket@gmail.com](mailto:tranvket@gmail.com)

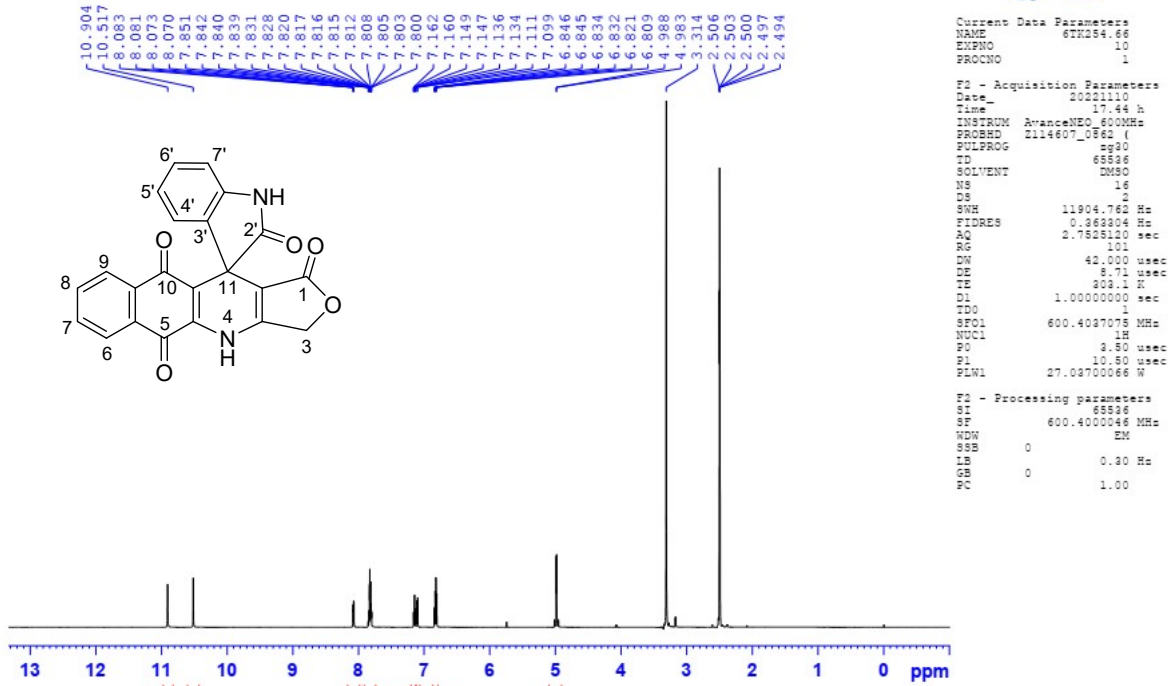
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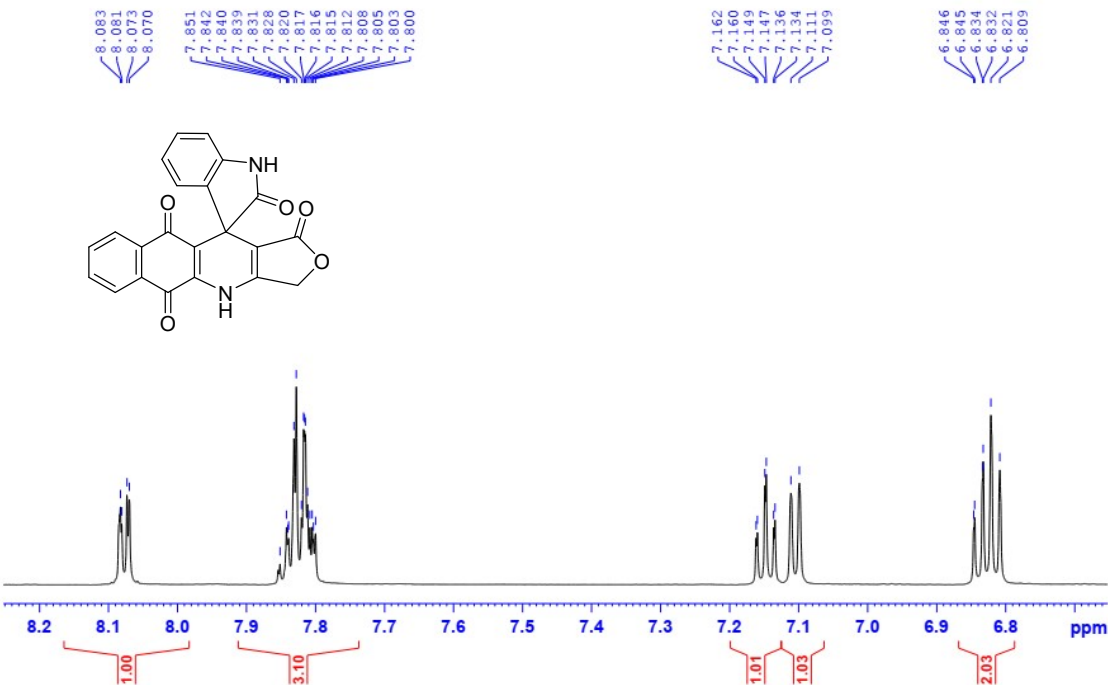
# SPECTRAL SECTION

## 3H-Spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7a)

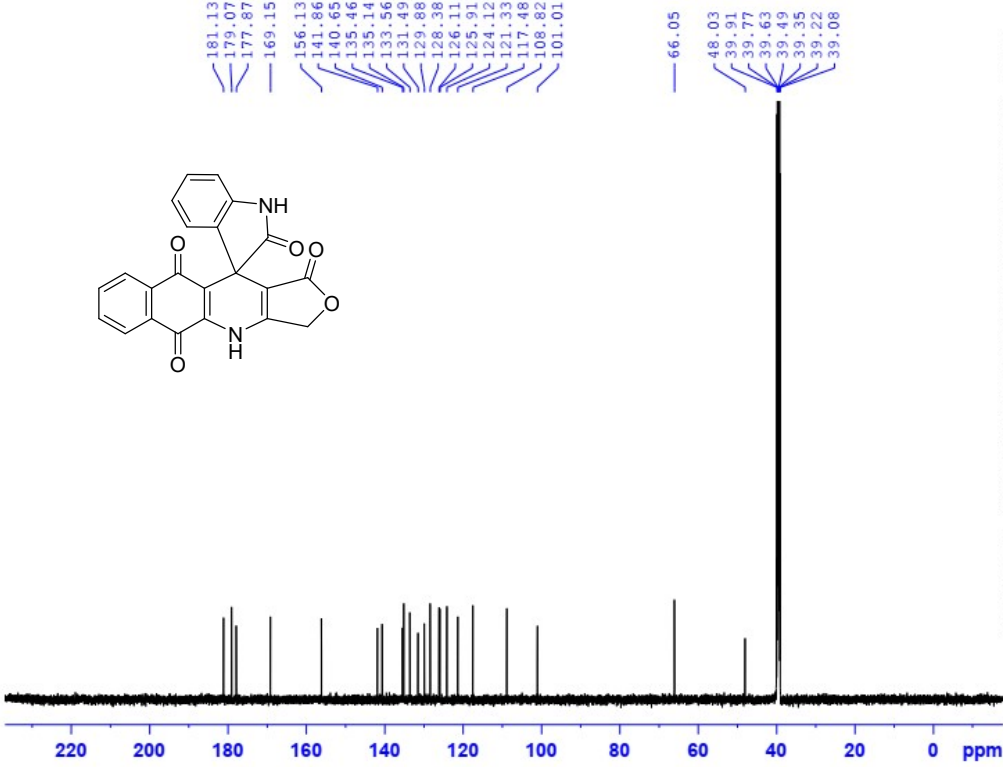
TK254.66-DMSO-1H



TK254.66-DMSO-1H



TK254.66-DMSO-C13CPD

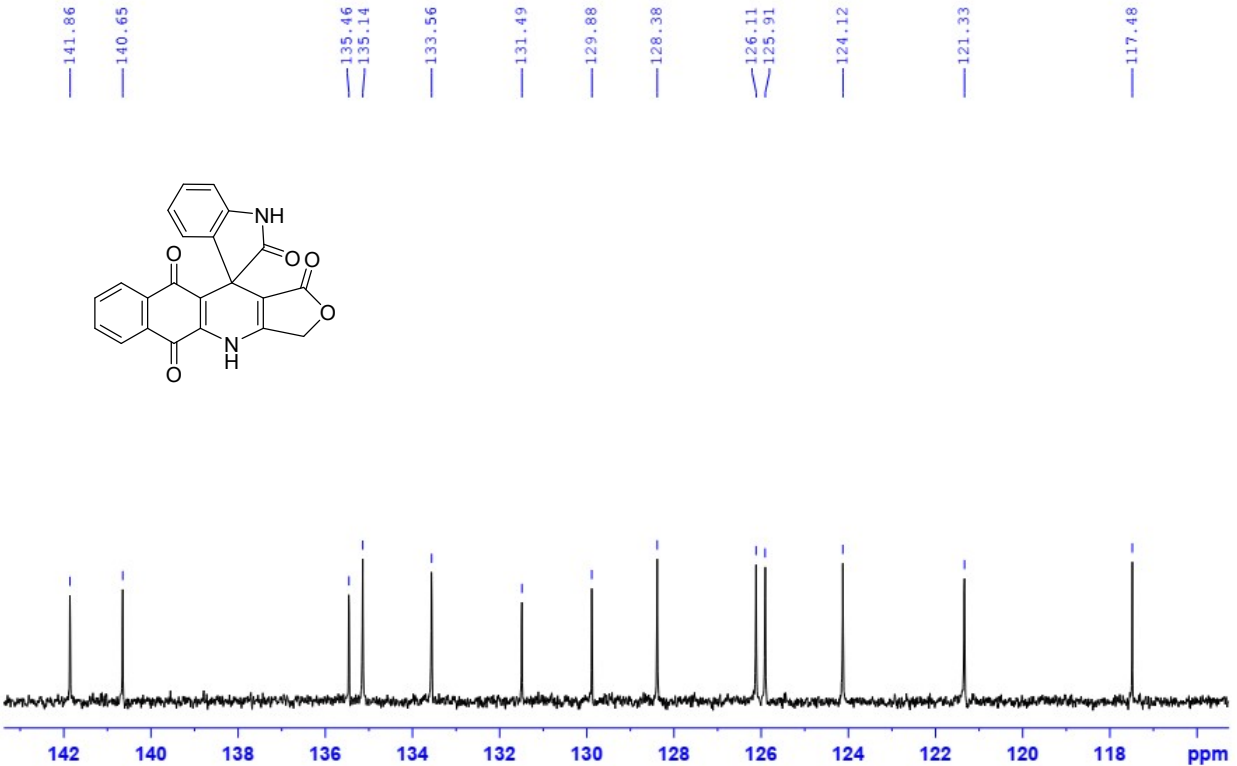


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 EXPNO 2  
 PROCNO 1

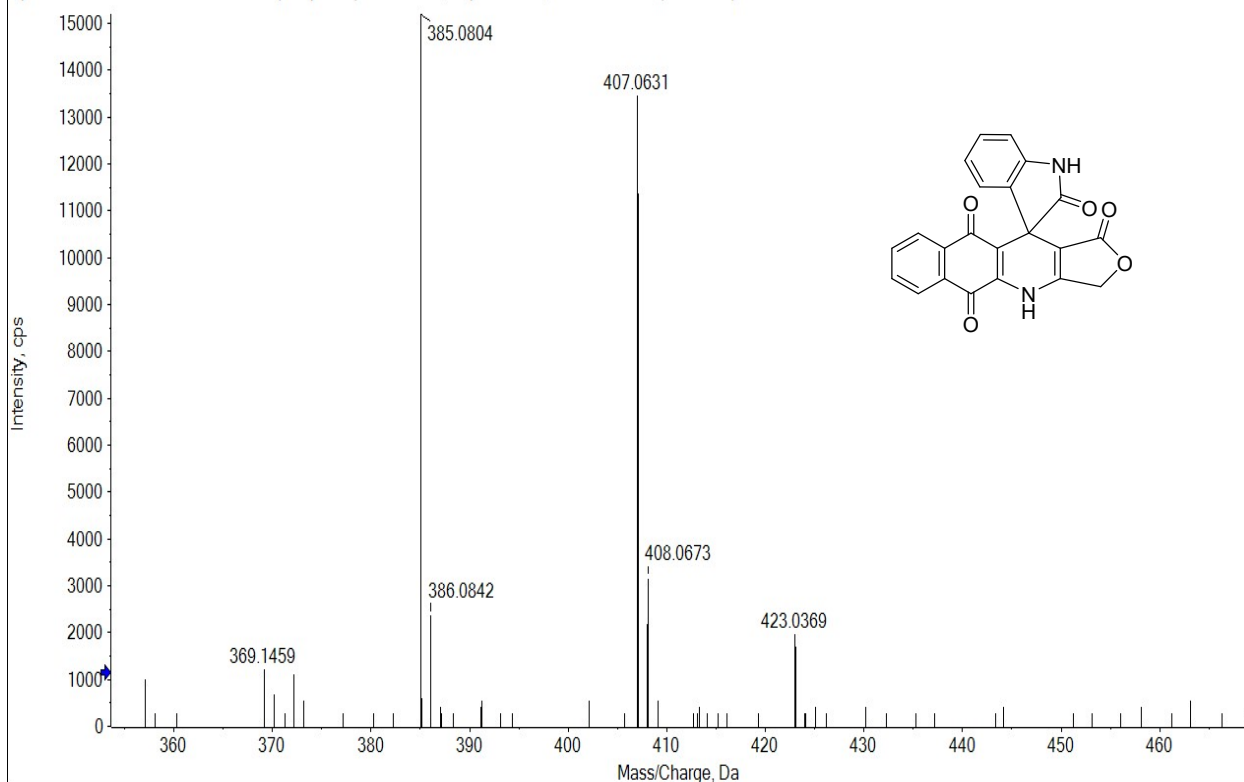
F2 - Acquisition Parameters  
 Date\_ 20221112  
 Time 9.18 h  
 INSTRUM AvanceNEO 600MHz  
 PROBHD D114607\_0862 (4  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2048  
 DS 4  
 SWH 38461.589 Hz  
 FIDRES 1.173752 Hz  
 AQ 0.8519680 sec  
 RG 101  
 DW 13.000 usec  
 DE 6.50 usec  
 TE 303.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 150.9873069 MHz  
 NUC1 13C  
 P1 4.20 usec  
 PL1 12.60 usec  
 PLM1 86.32800293 W  
 SFO2 600.4024016 MHz  
 NUC2 1H  
 CPDPRG12 waltz168  
 PCPD2 80.00 usec  
 PLM2 27.03700066 W  
 PLM12 0.46575001 W  
 PLM13 0.30599001 W

F2 - Processing parameters  
 SI 32768  
 SF 150.9707787 MHz  
 WDW EM  
 SSB 0  
 GB 0 1.00 Hz  
 PC 1.40

TK254.66-DMSO-C13CPD

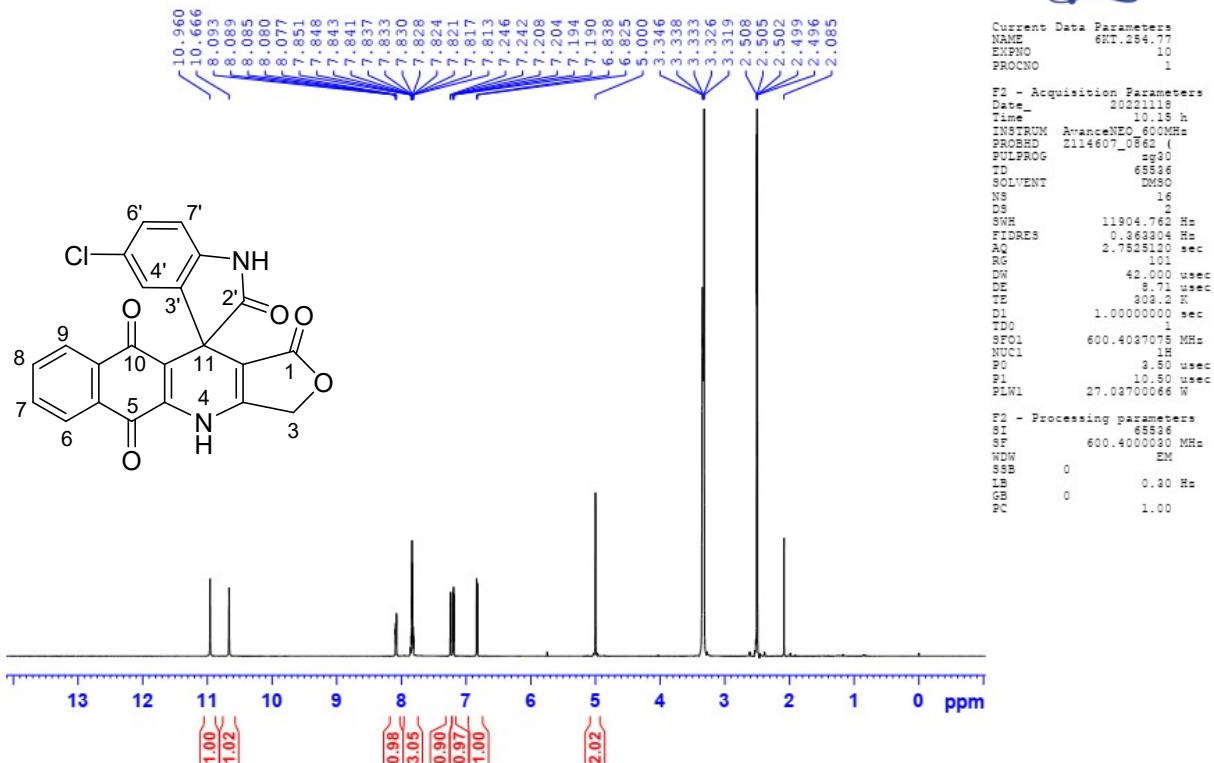


Spectrum from 20230208HANG.wiff2 (sample 20) - TK254.66, Experiment 1, +IDA TOF MS (20 - 4500) from 0.240 min

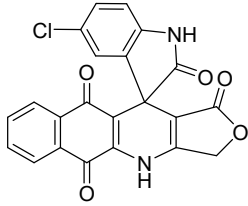
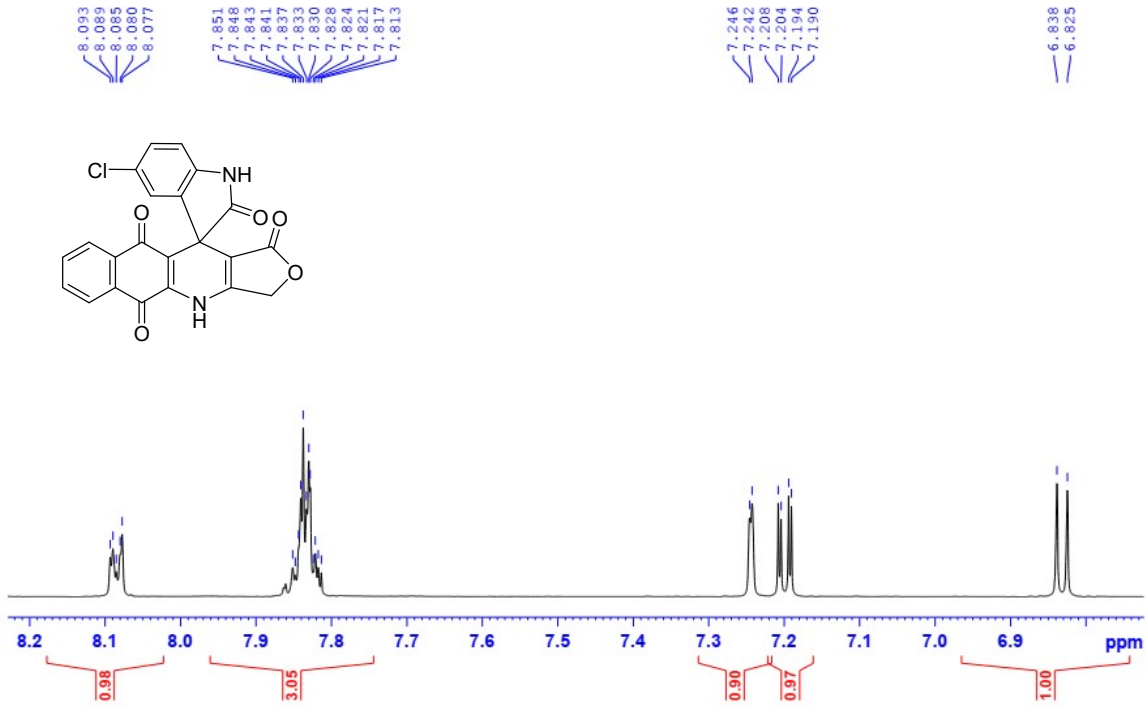


**4'-Chloro-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7b)**

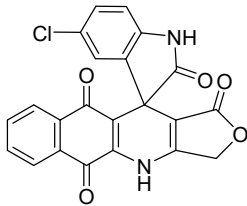
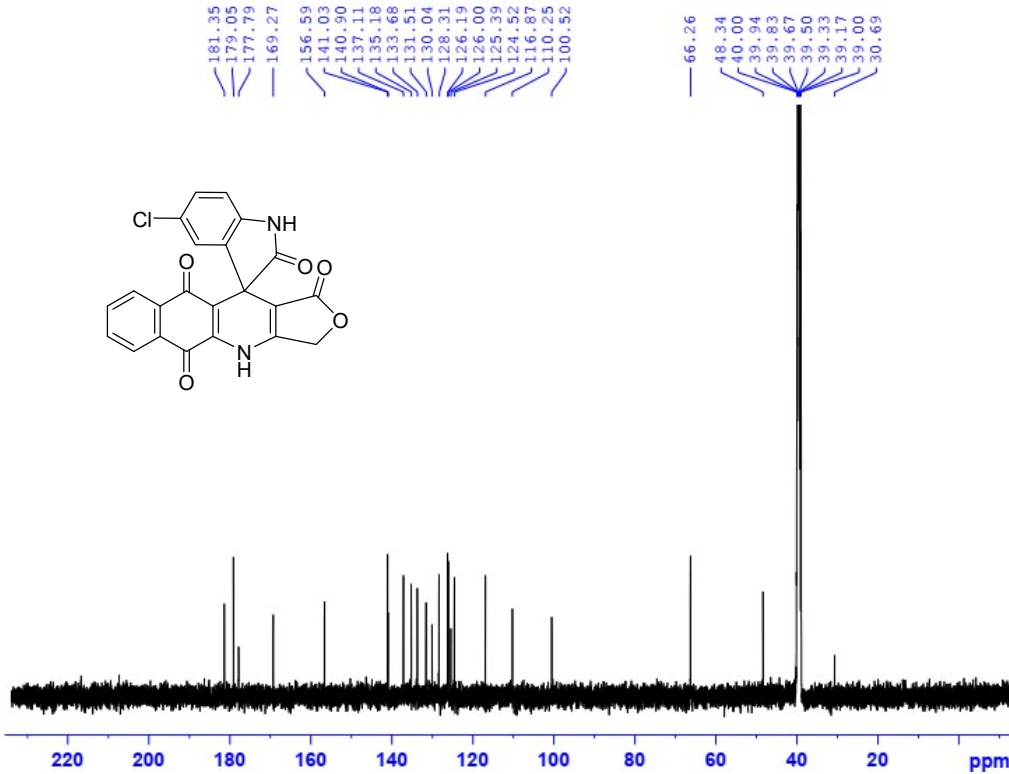
**TK254.77-DMSO-1H**



TK254.77-DMSO-1H



KT254.77-DMSO-C13CPD



Current Data Parameters  
NAME 6KT254.77  
EXPNO 2  
PROCNO 1

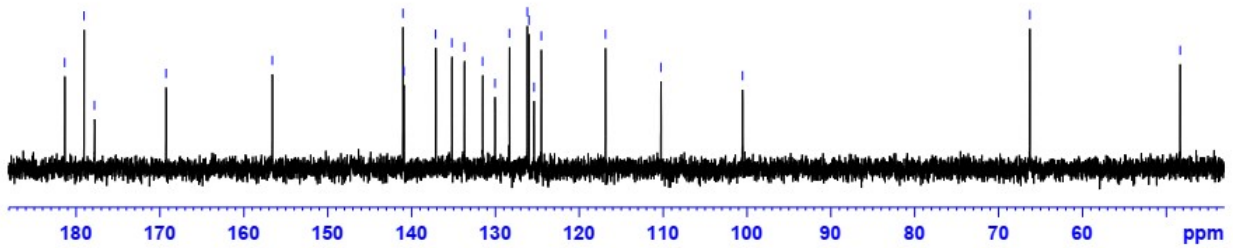
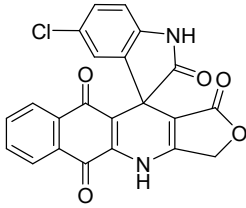
F2 - Acquisition Parameters  
Date\_ 20231122  
Time 4.34  
INSTRUM spect  
PROBHD 5 mm PABBO BBI  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1024  
DS 4  
SWH 31250.000 Hz  
FIDRES 0.476827 Hz  
AQ 1.0485760 sec  
RG 198.57  
DN 16.000 usec  
DE 8.50 usec  
TE 301.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 125.7990220 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 88.00000000 W

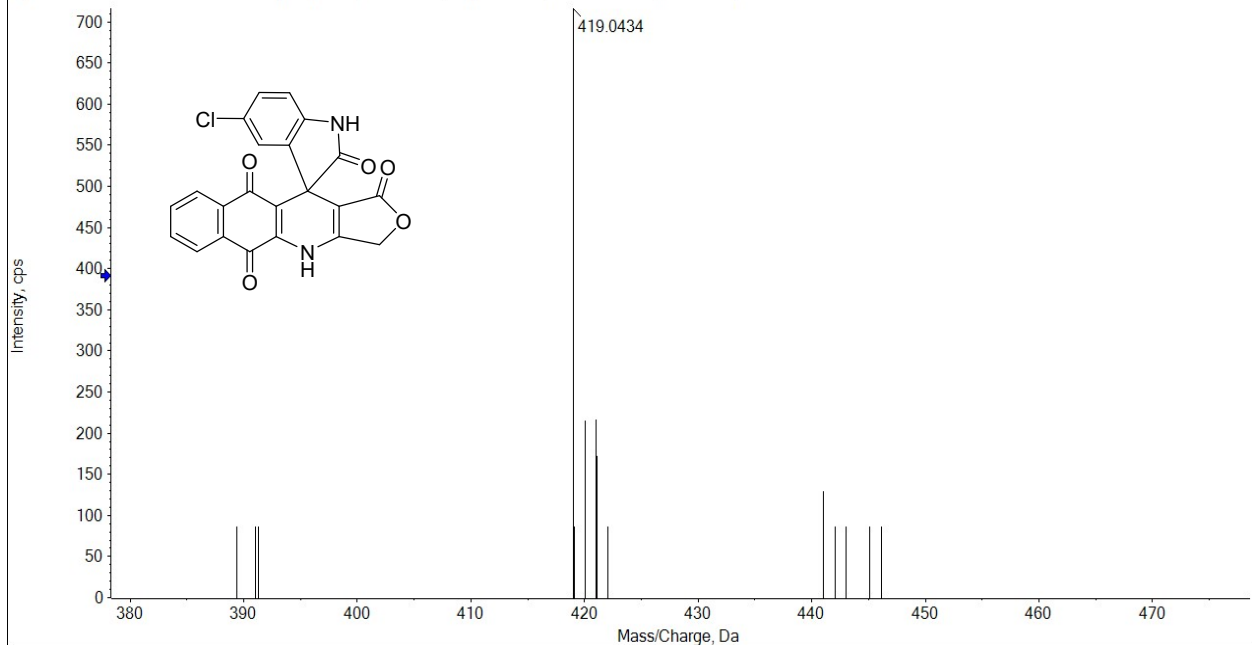
===== CHANNEL f2 =====  
SF02 500.2410010 MHz  
NUC2 1H  
CPDPRG12 waltz16  
PCPD2 80.00 usec  
P1M2 22.00000000 W  
PLW12 0.35764000 W  
PLW13 0.17989001 W

F2 - Processing parameters  
SI 32768  
SF 125.7652339 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

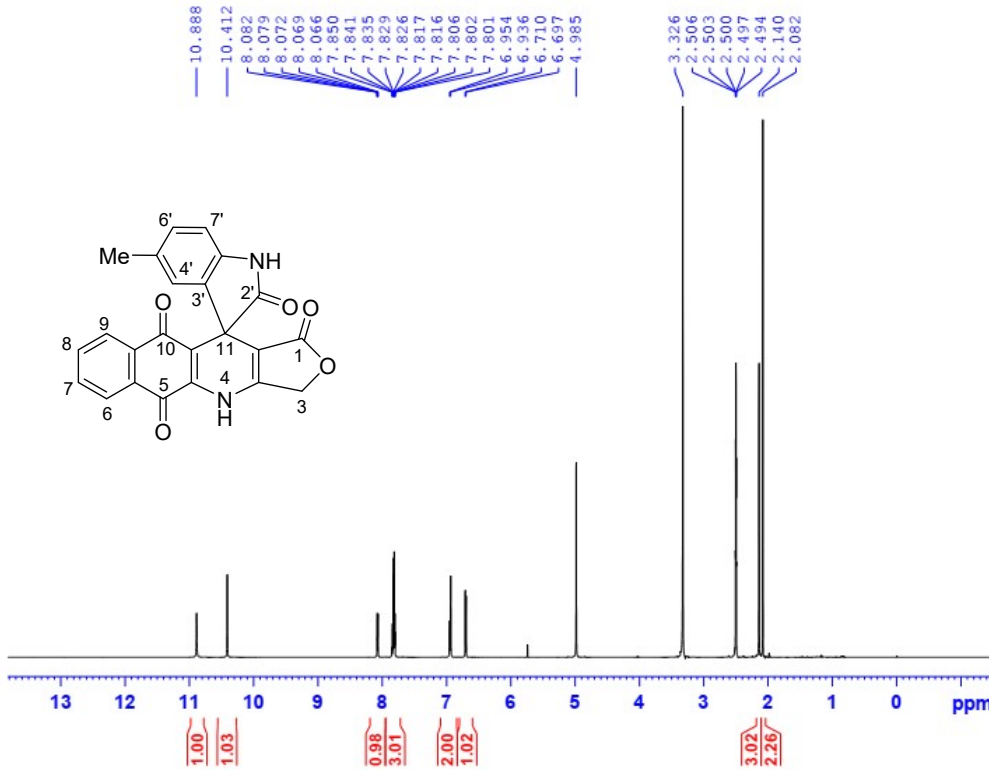
KT254.77-DMSO-C13CPD



Spectrum from 20230208HANG.wiff2 (sample 22) - TK254.77, Experiment 1, +IDA TOF MS (20 - 4500) from 0.186 min



**4'-Methyl-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7c)**  
**TK254.85-DMSO-1H**



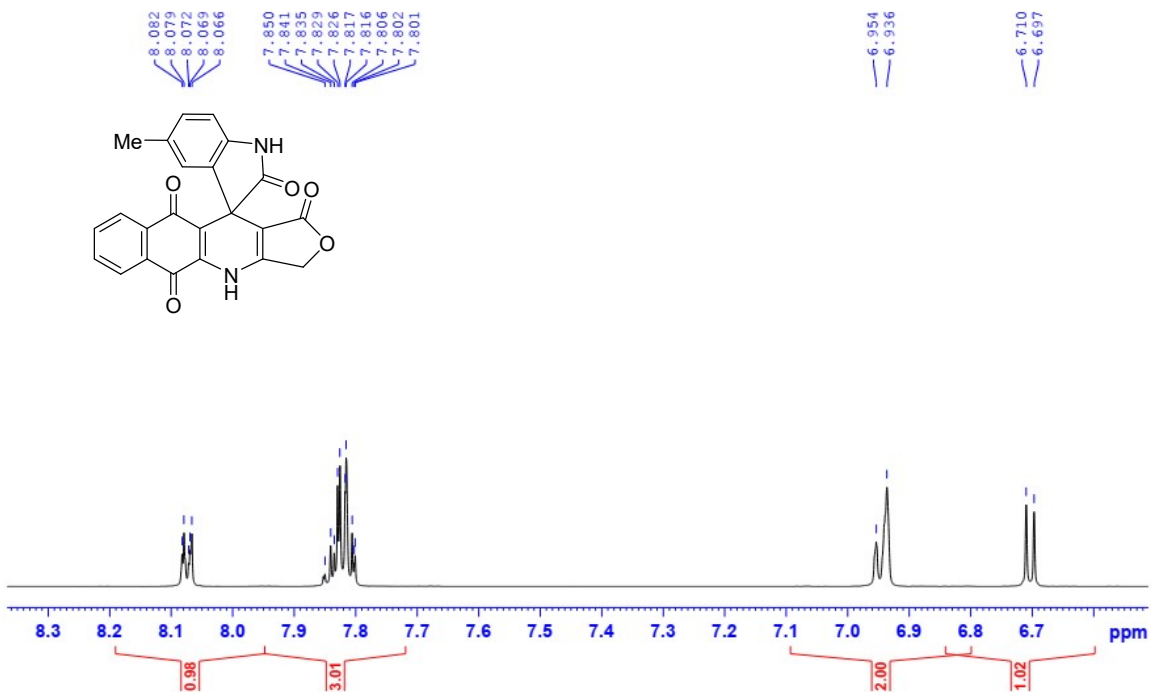
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Current Data Parameters
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EXPNO    10
PROCNO   1

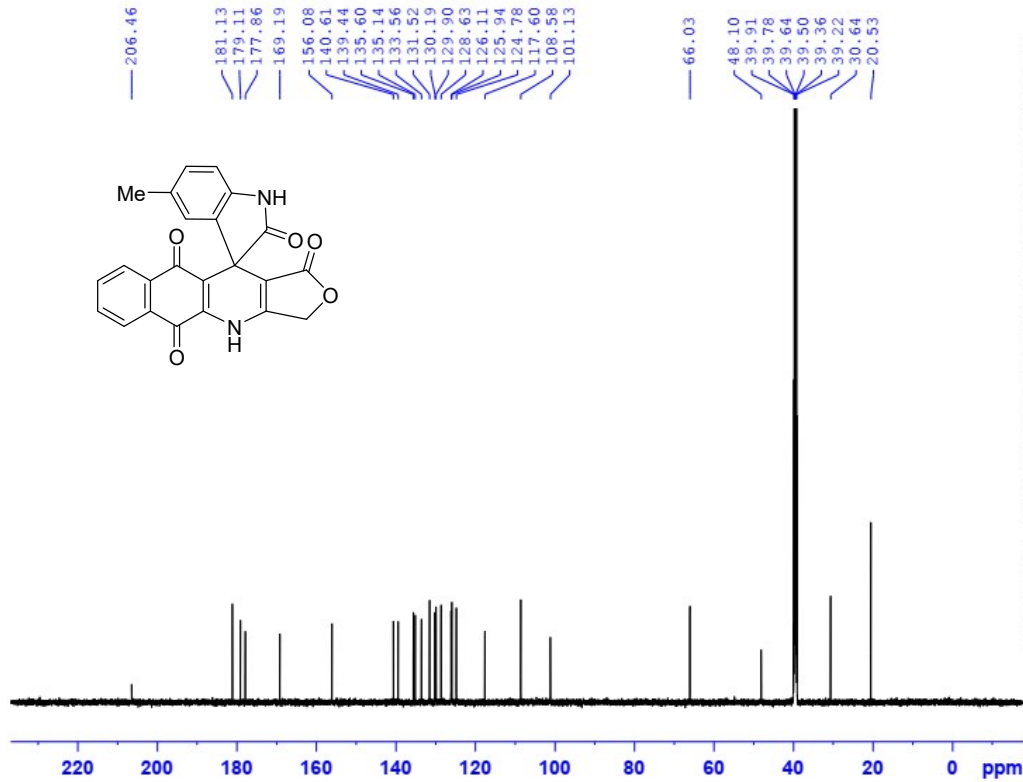
F2 - Acquisition Parameters
Date_    20221123
Time     5.54 h
INSTRUM  AvanceNeo_600MHz
PROBHD   1H14607_0862
PULPROG  zg30
TD        65526
SOLVENT  DMSO
NS        2
DS        2
SWMH     11904.762 Hz
FIDRES   0.362204 Hz
AQ        2.7525120 sec
RG         97.971
SM        42.000 usec
DE        8.71 usec
TE        303.1 K
D1        1.00000000 sec
ZD0
SFO1     600.4027071 MHz
NUC1      1H
PC        3.50 usec
PI        10.50 usec
PLW1     27.02700066 W

F2 - Processing parameters
SI        65526
SF        600.4000047 MHz
WDW       EM
SSB       0
GB        0
PC        1.00
    
```

TK254.85-DMSO-1H



TK254.85-DMSO-C13CPD

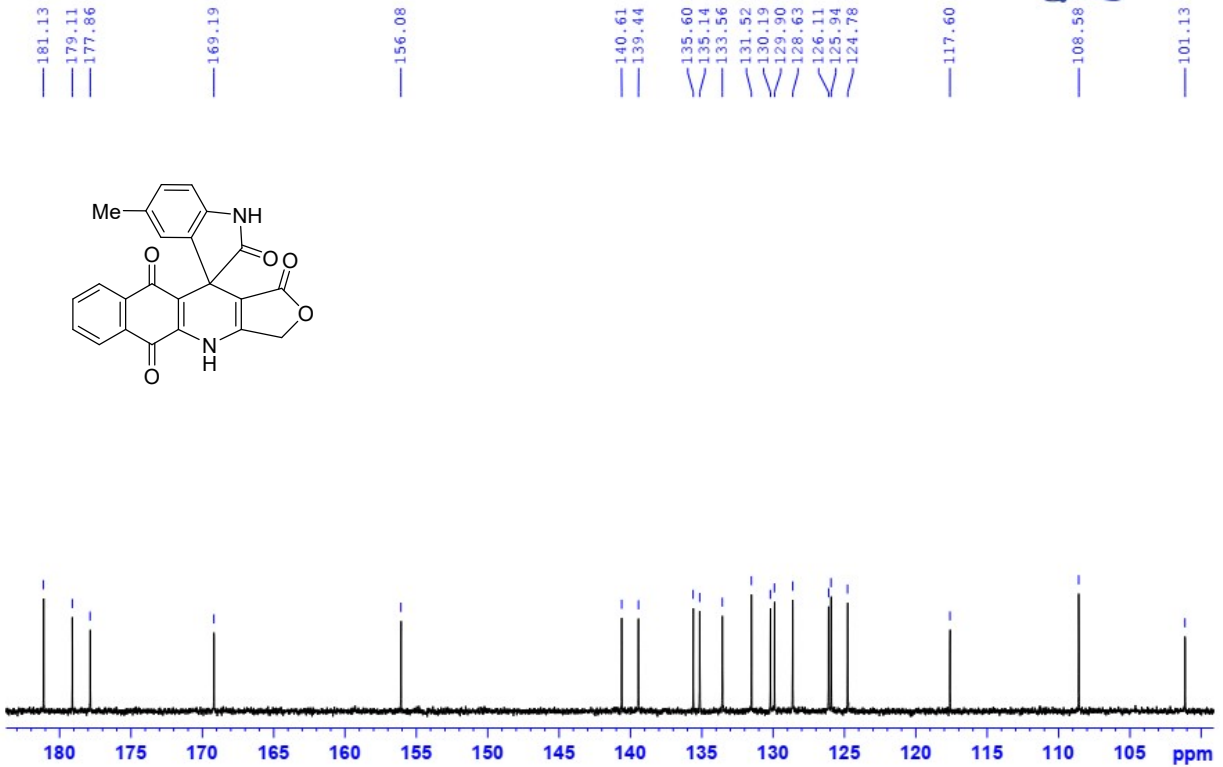


Current Data Parameters  
 NAME 6TH254.85  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
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 Time 19.14 h  
 INSTRUM AvanceNeo 600MHz  
 PROBEID zll4607\_0362 (1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1024  
 DS 4  
 SWH 38461.529 Hz  
 FIDRES 1.173754 Hz  
 AQ 0.8519680 sec  
 RG 101  
 DW 13.000 usec  
 DE 8.50 usec  
 TE 303.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1  
 SFO1 150.9878069 MHz  
 NUC1 13C  
 P0 4.20 usec  
 P1 12.60 usec  
 PLW1 86.32800293 W  
 SFO2 600.4024016 MHz  
 NUC2 1H  
 CPDPRG2 waltz165  
 PCPD2 80.00 usec  
 PLW2 27.03700066 W  
 PLW12 0.46575001 W  
 PLW13 0.30599001 W

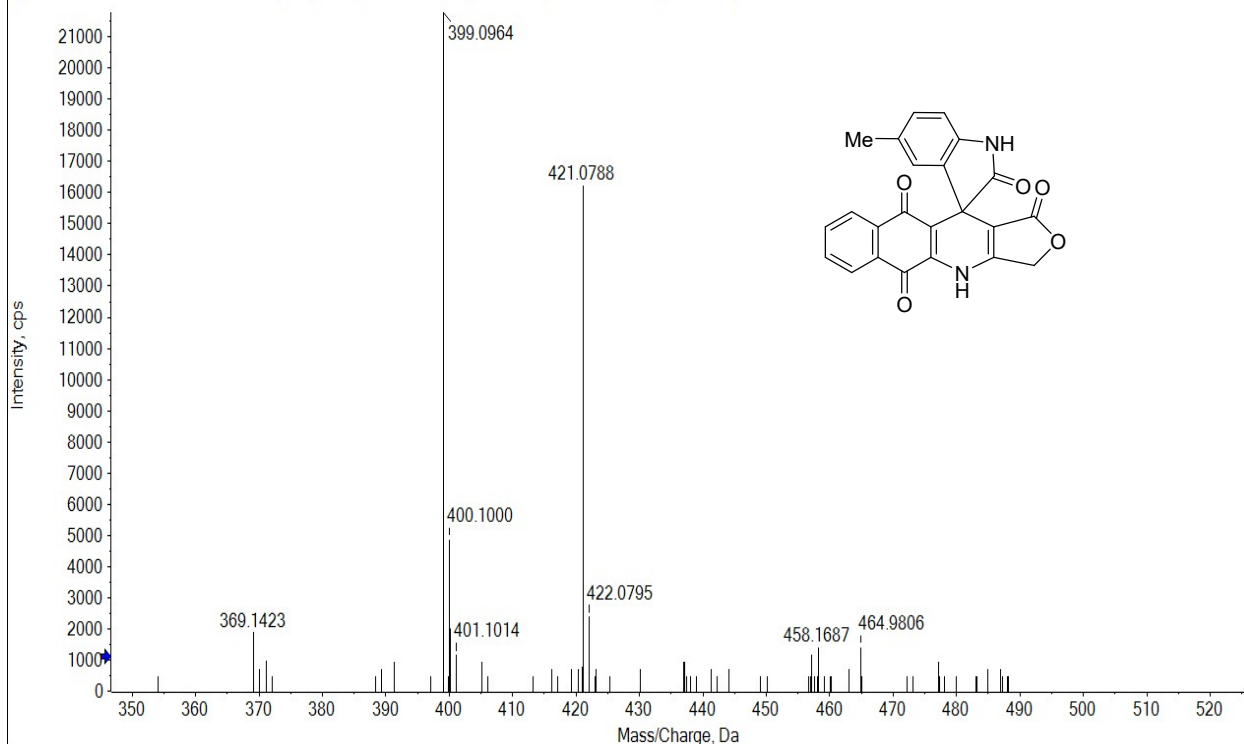
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 SF 150.9707761 MHz  
 NDNW EM  
 SSB 0 1.00 Hz  
 LB 0  
 GB 0  
 PC 1.40

TK254.85-DMSO-C13CPD

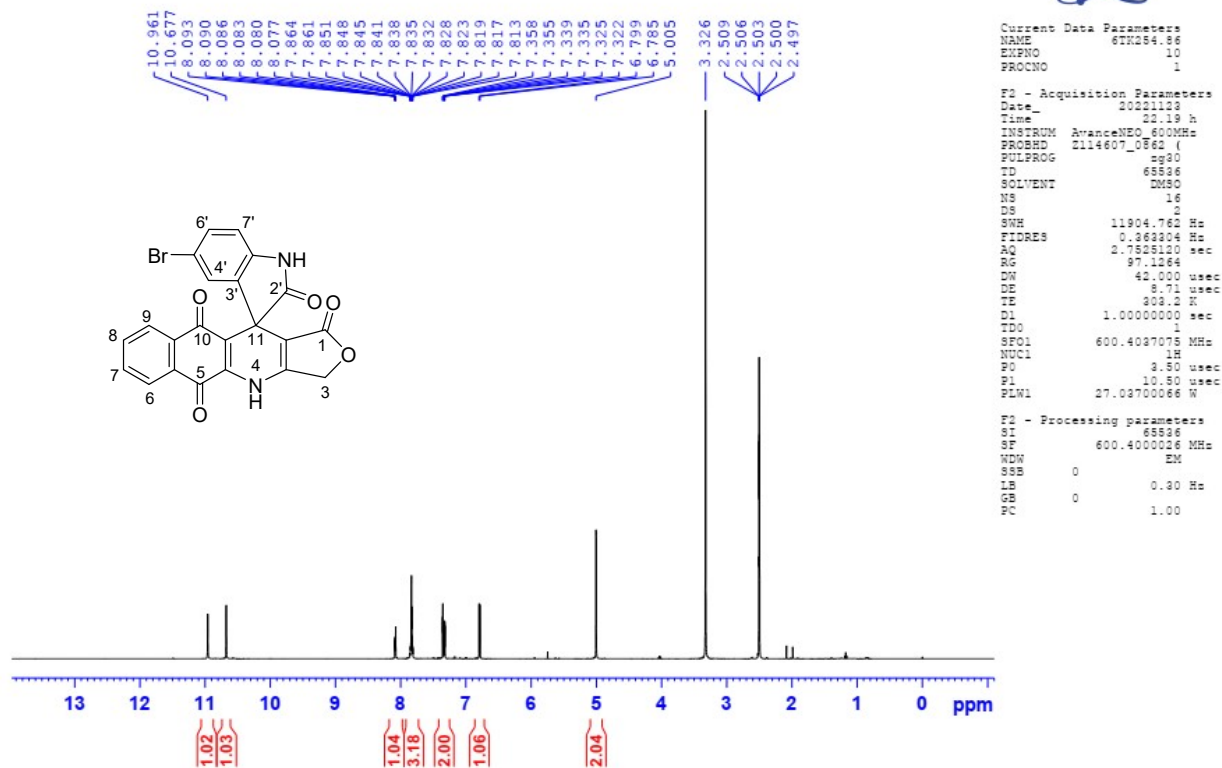




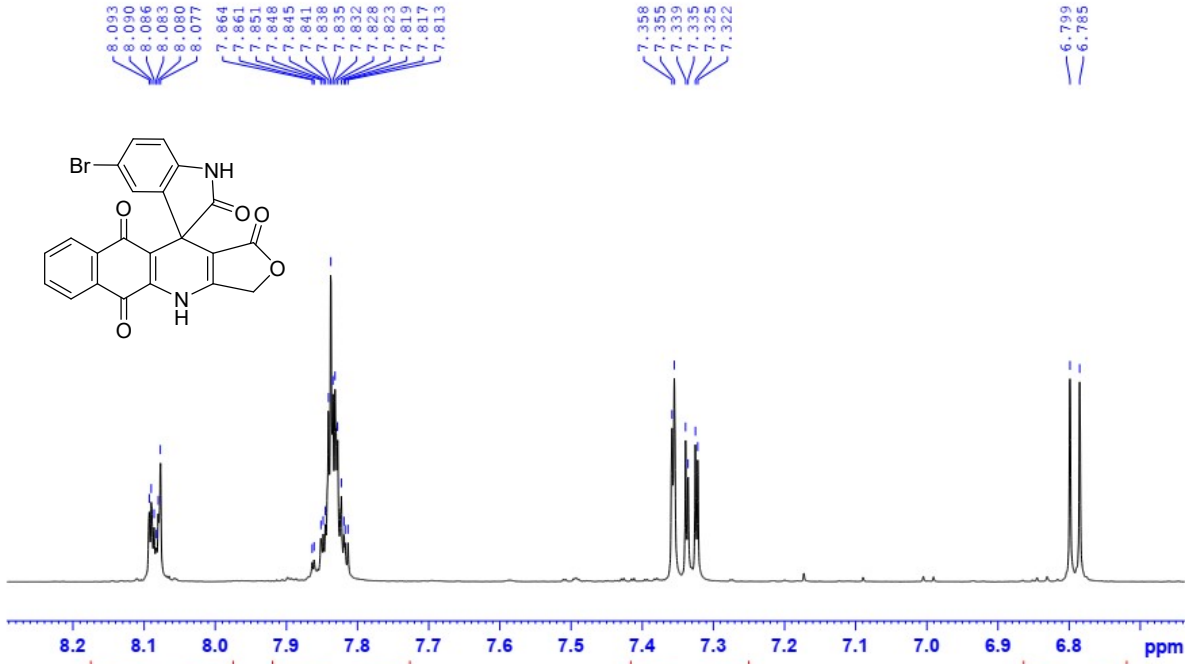
Spectrum from 20230208HANG.wiff2 (sample 23) - TK254.85, Experiment 1, +IDA TOF MS (20 - 4500) from 0.189 min



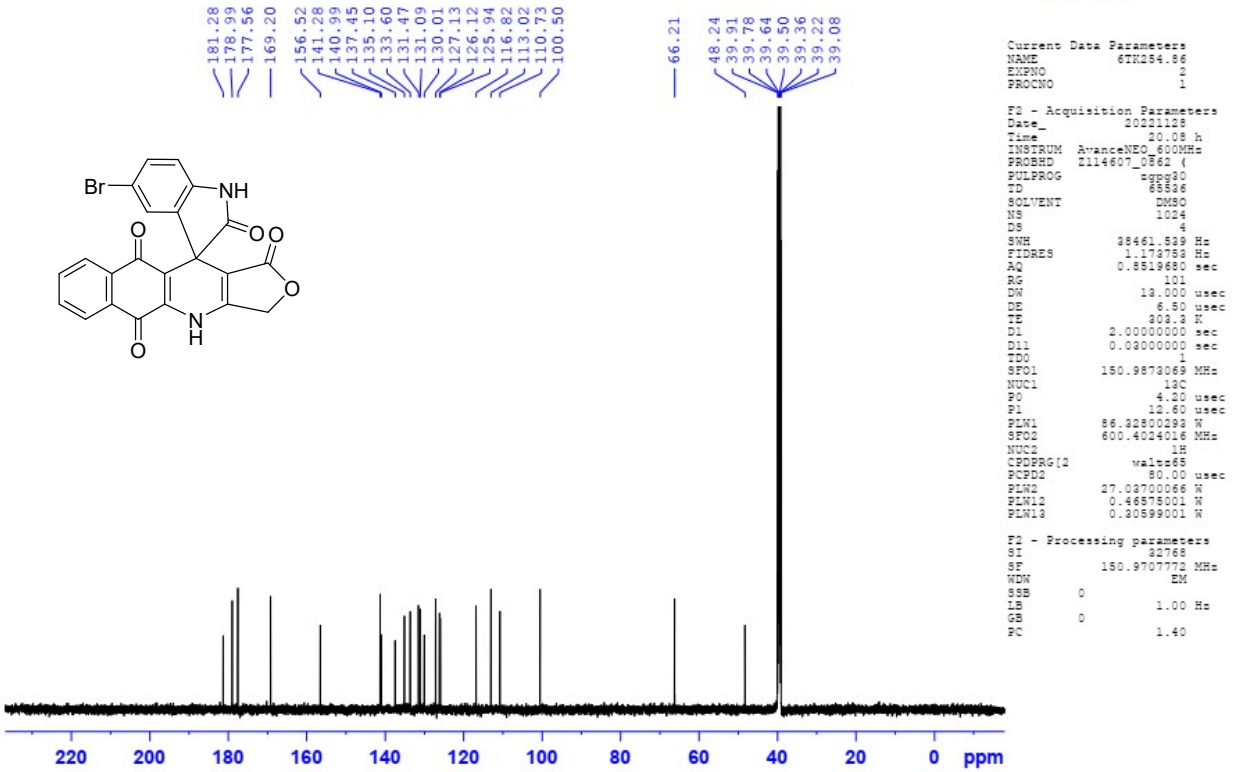
**4'-Bromo-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7d)**  
**TK254.86-DMSO-1H**



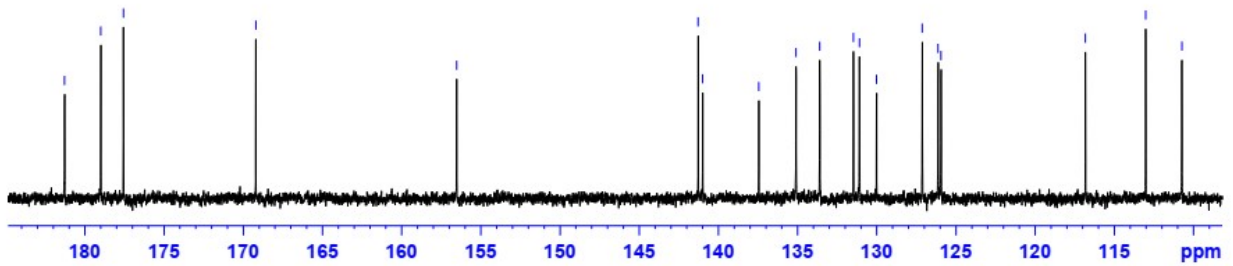
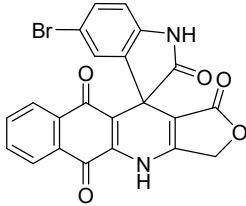
TK254.86-DMSO-1H



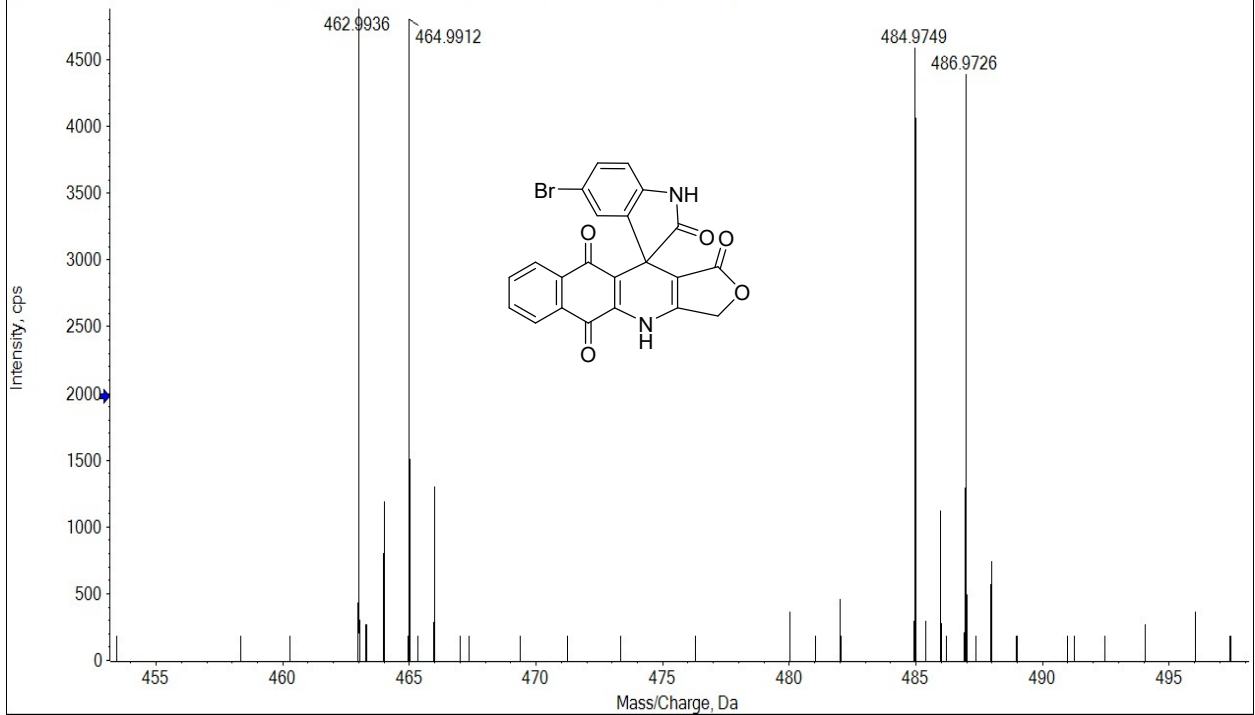
TK254.86-DMSO-C13CPD



TK254.86-DMSO-C13CPD

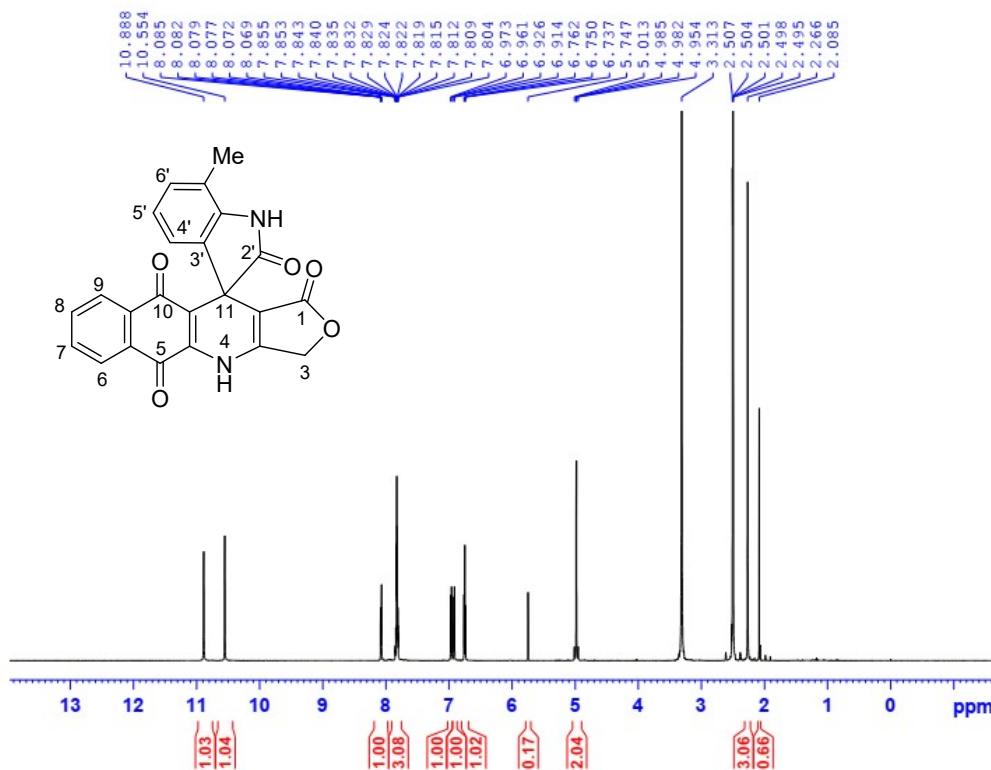


Spectrum from 20230208HANG.wiff2 (sample 24) - TK254.86, Experiment 1, +IDA TOF MS (20 - 4500) from 0.203 min



**6'-Methyl-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7e)**

TK254.98-DMSO-1H



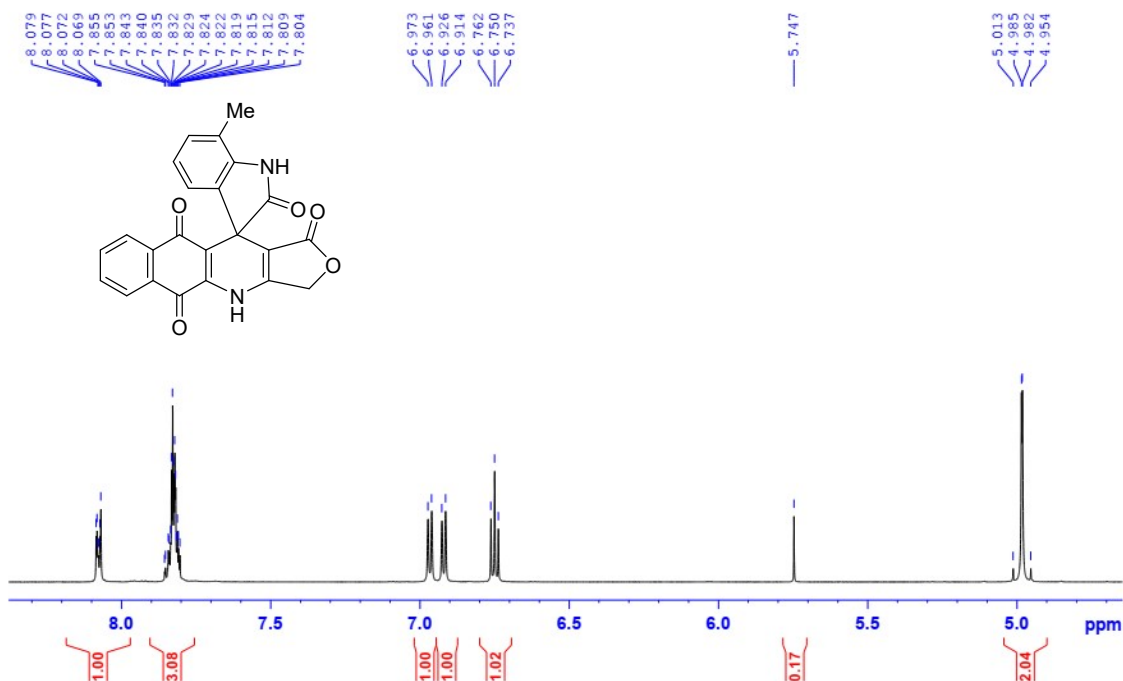
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Current Data Parameters
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EXPNO    10
PROCNO   1

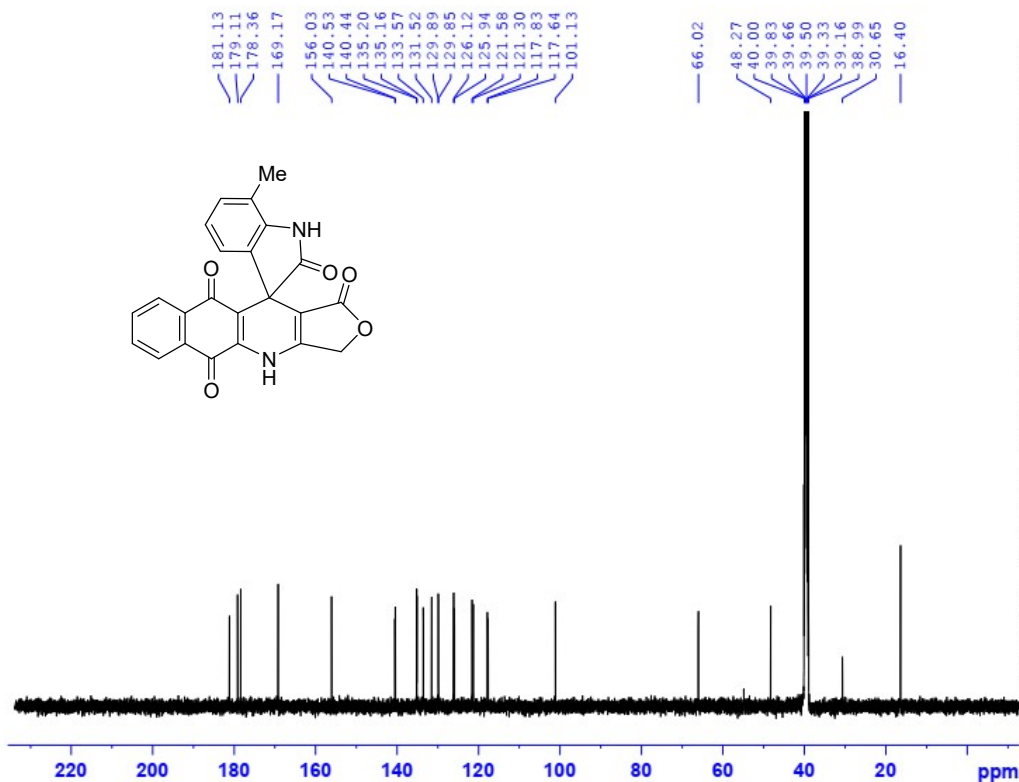
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Date_    20221206
Time     18.00 h
INSTRUM  AvanceNeo 600MHz
PROBHD   zll4607_0863
PULPROG  zg30
TD        65526
SOLVENT  DMSO
NS        16
DS        2
SMA       11904.762 Hz
FIDRES    0.362204 Hz
AQ        2.7525120 sec
RG         101
SM        42.000 usec
DE        8.71 usec
TE        303.1 K
D1        1.00000000 sec
TDO
SFO1     600.4027075 MHz
NUC1      1H
PC        3.50 usec
PI        10.50 usec
PLMW     27.02700066 W

F1 - Processing parameters
SI        65526
SF        600.4000039 MHz
WDW       EM
SSB       0
GB        0
PC        1.00
    
```

TK254.98-DMSO-1H



NTA254.98-DMSO-C13CPD



```

Current Data Parameters
NAME      6TH254.98
EXPNO    2
PROCNO   1

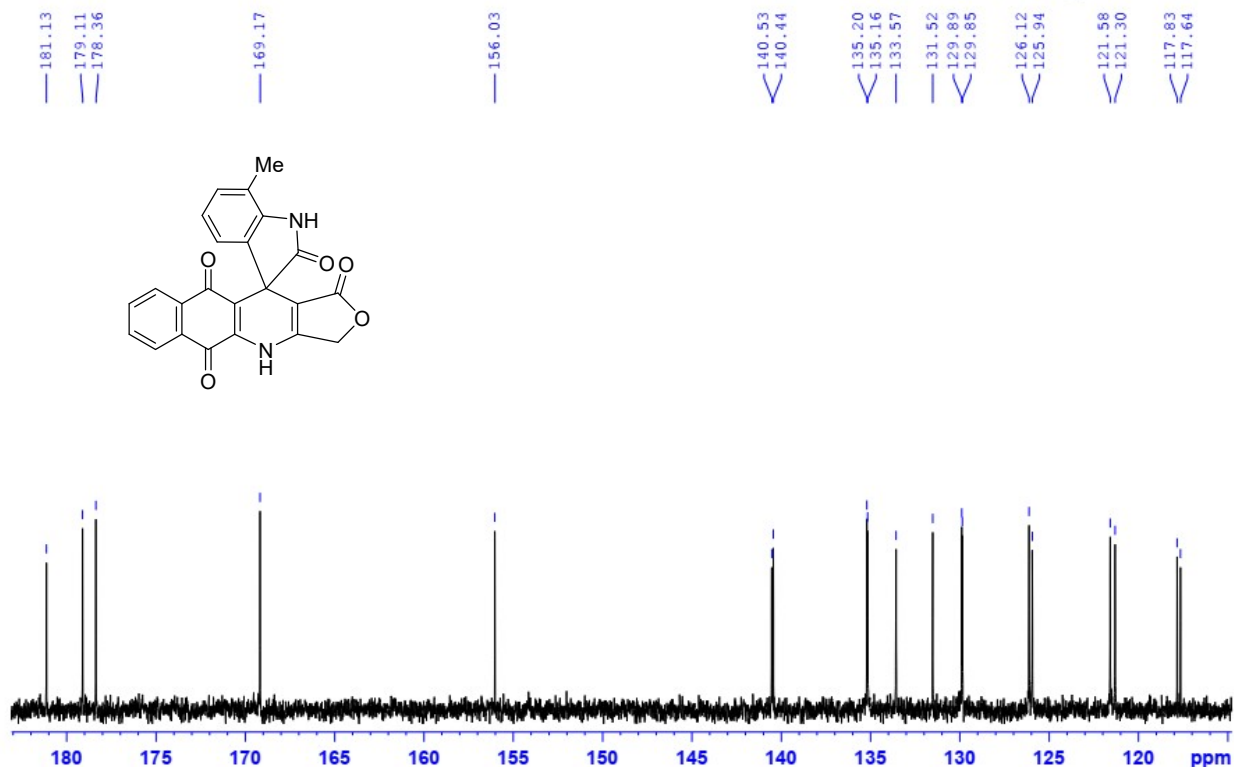
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Time     2.55
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65528
SOLVENT  DMSO
NS       2048
DS       4
SWH      31250.000 Hz
FIDRES   0.476637 Hz
AQ       1.0485760 sec
RG       188.57
DW       16.000 usec
DE       6.50 usec
TE       300.2 K
D1       2.00000000 sec
d11      0.03000000 sec
TDO      1

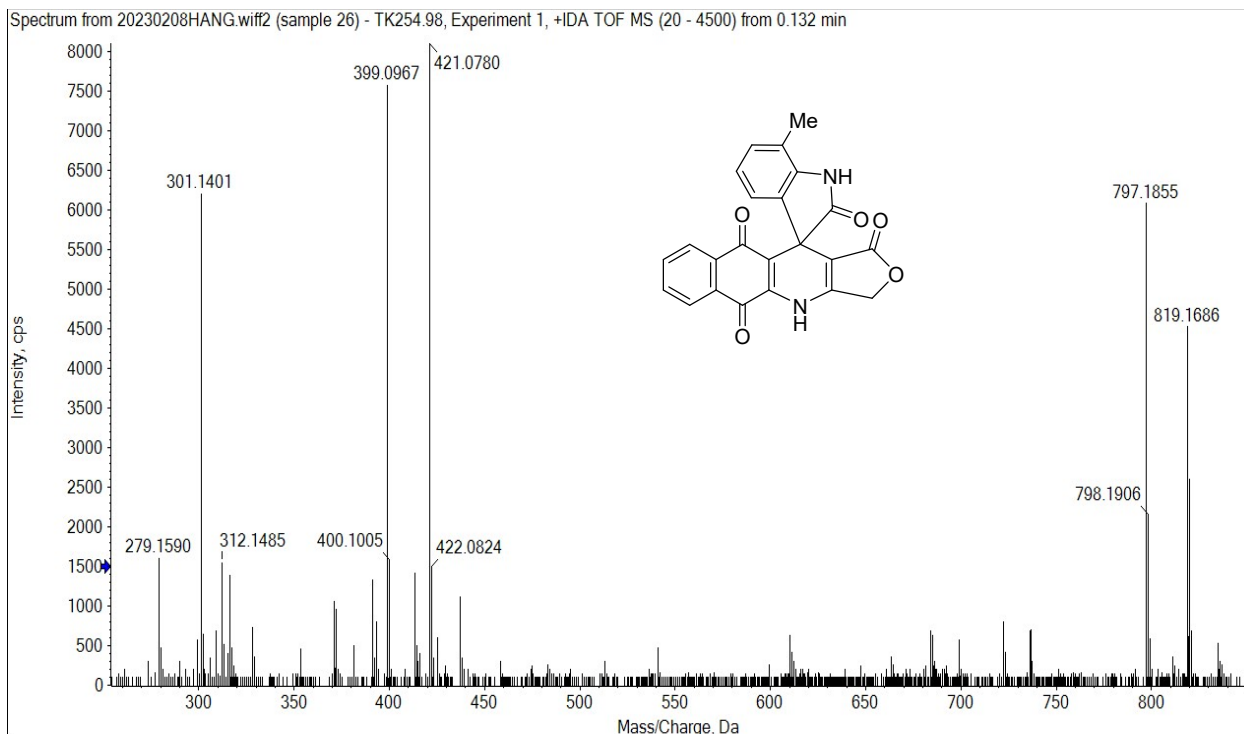
===== CHANNEL f1 =====
SFO1    125.7690380 MHz
NUC1    13C
P1      10.00 usec
PLM1    88.00000000 W

===== CHANNEL f2 =====
SFO2    500.2410010 MHz
NUC2    1H
PCPDPRG2  waltz16
PCPD2    80.00 usec
PLM2     23.00000000 W
PLM12    0.38764000 W
PLM13    0.17989001 W

F2 - Processing parameters
SI      32768
SF      125.7652603 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
    
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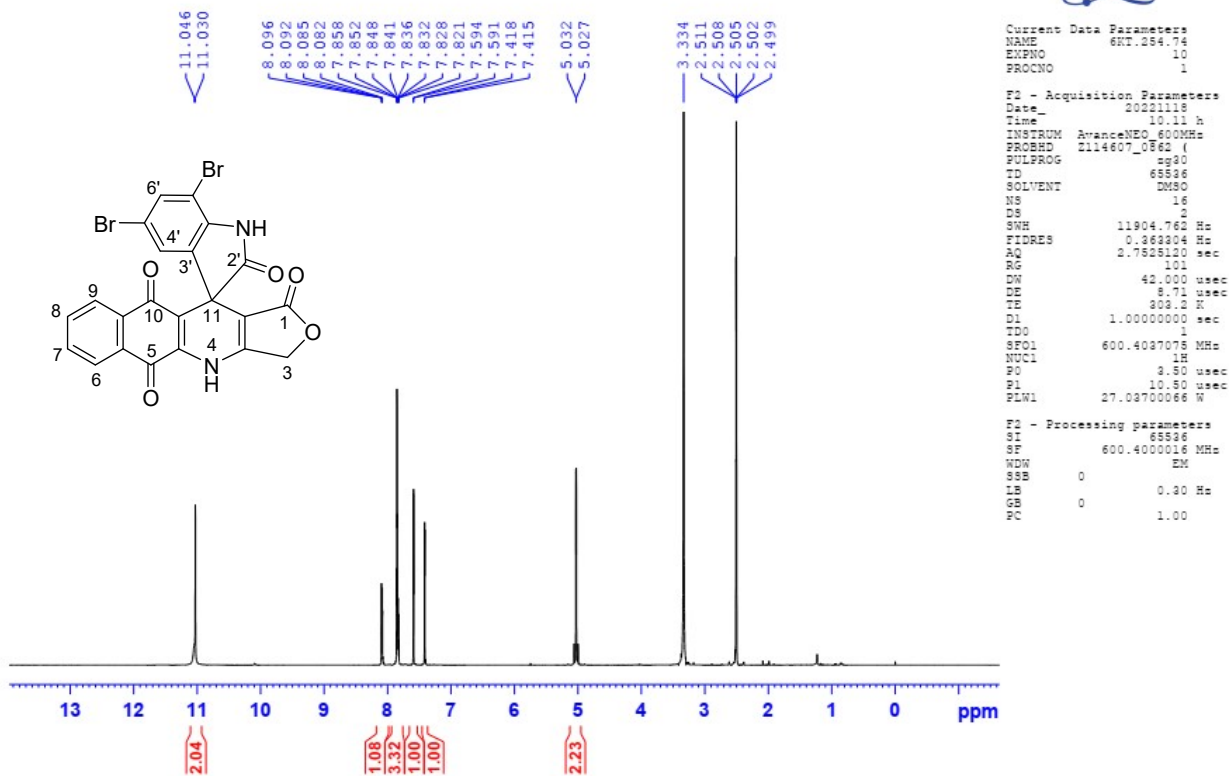
NTA254.98-DMSO-C13CPD



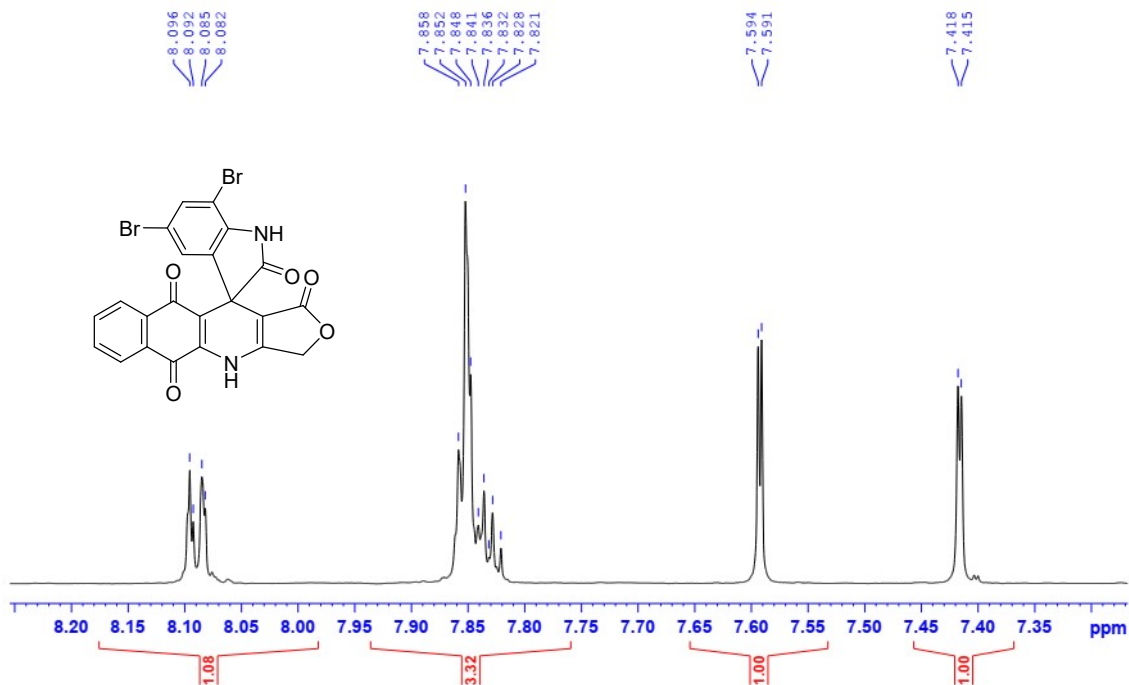


**4',6'-Dibromo-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2,5,10(4H)-tetraone (7f)**

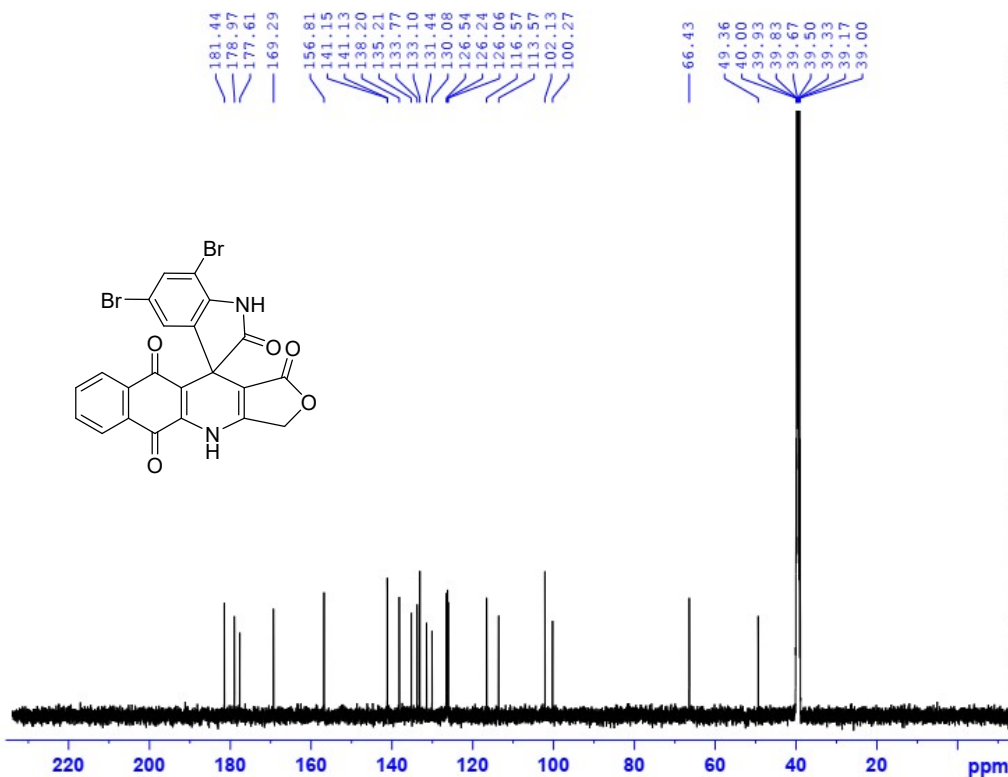
TK254.74-DMSO-1H



TK254.74-DMSO-1H



KT254.74-DMSO-C13CPD



```

Current Data Parameters
NAME          6KT254.74
EXPNO         1
PROCNO        1

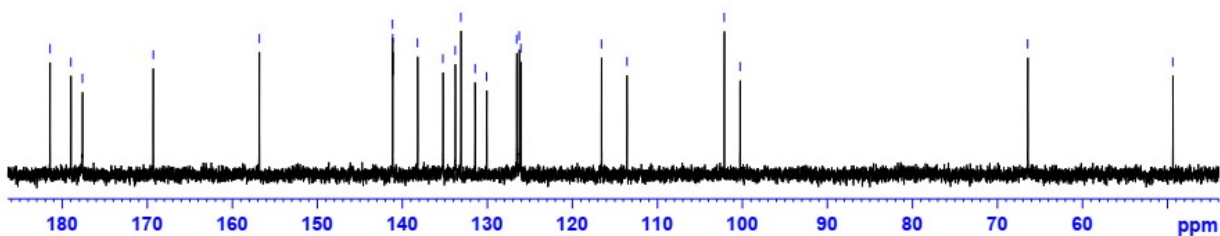
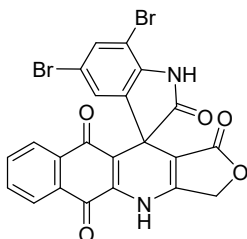
F2 - Acquisition Parameters
Date_         20221122
Time          3.38
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            512
DS            4
SWH           31250.000 Hz
FIDRES        0.476827 Hz
AQ            1.0485760 sec
RG            198.87
SM           16.000 usec
DE            6.50 usec
TE            301.9 K
DL            2.00000000 sec
Dl1           0.02000000 sec
TD0           1

===== CHANNEL f1 =====
SF01          125.7990220 MHz
NUC1          13C
P1            10.00 usec
PLM1          88.00000000 W

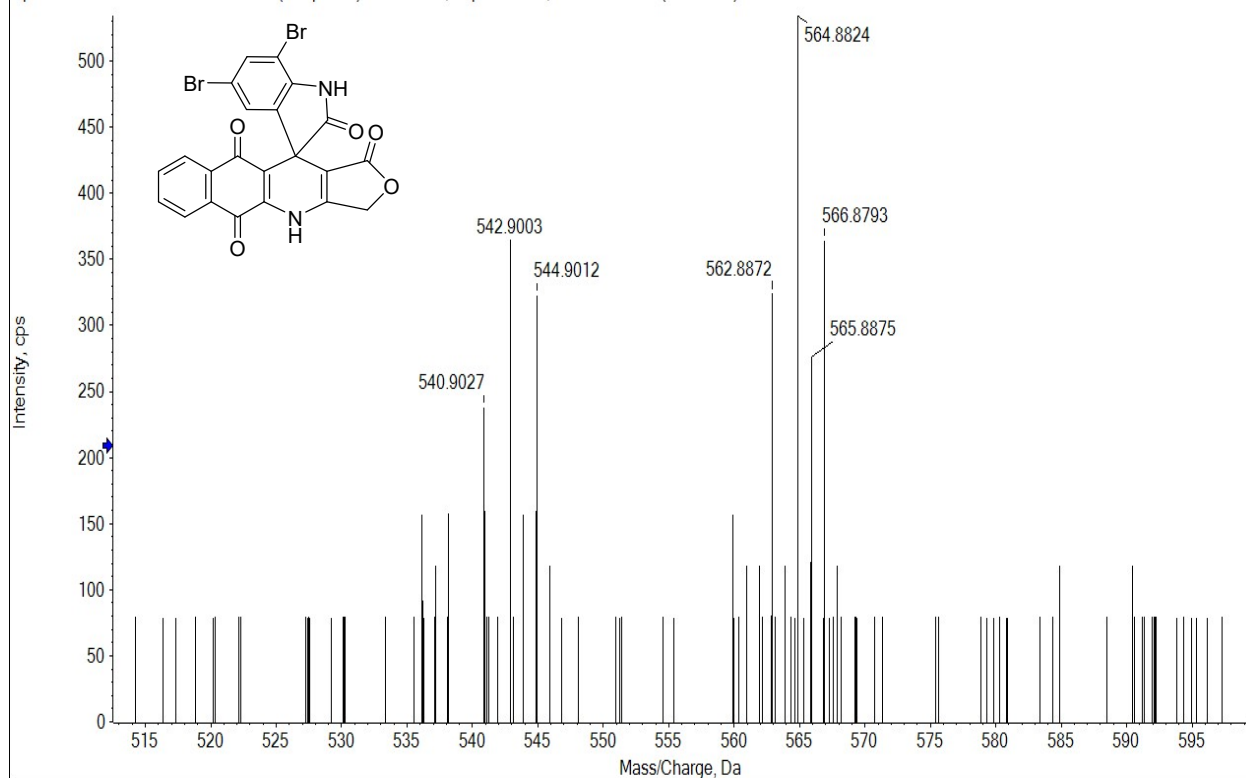
===== CHANNEL f0 =====
SF02          800.2410010 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         80.00 usec
PLM2          22.00000000 W
PLM12         0.35764000 W
PLM13         0.17989001 W

F2 - Processing parameters
SI            32768
SF           125.7852548 MHz
WDW           EM
SSB           0
GB            0
PC            1.40
    
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KT254.74-DMSO-C13CPD



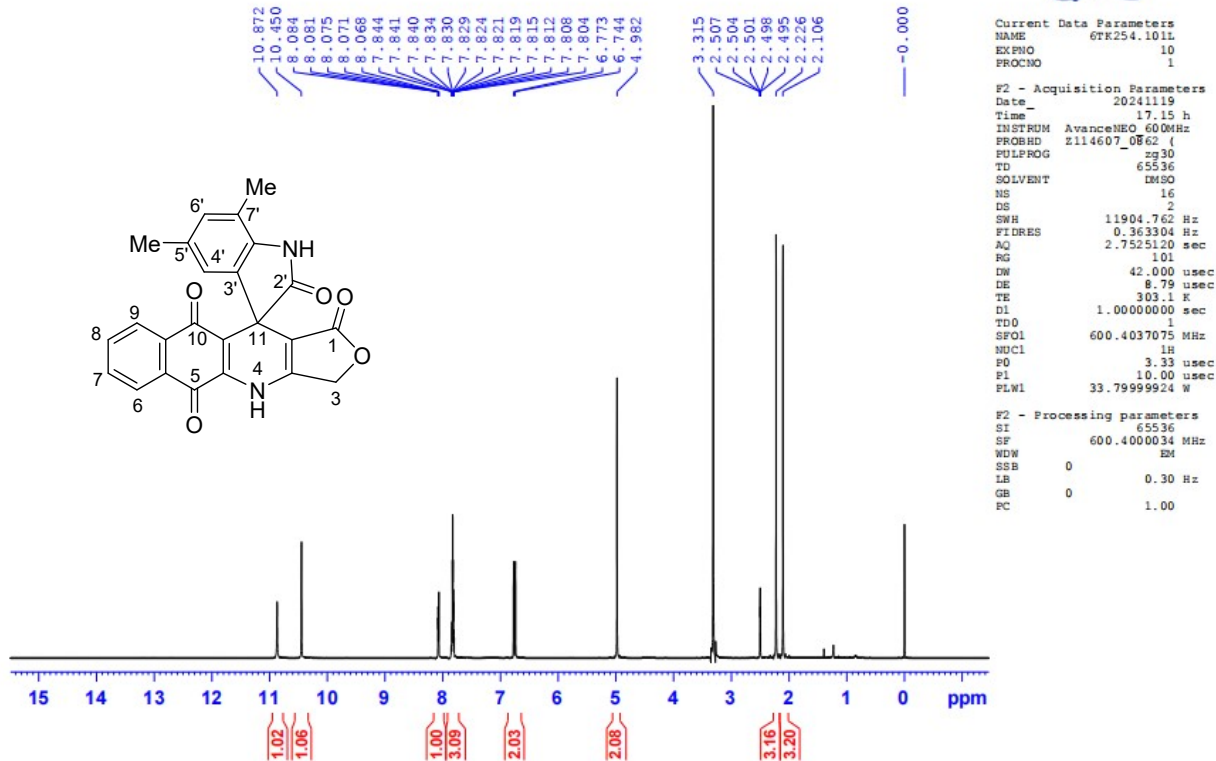
Spectrum from 20230208HANG.wiff2 (sample 21) - TK254.74, Experiment 1, +IDA TOF MS (20 - 4500) from 0.243 min





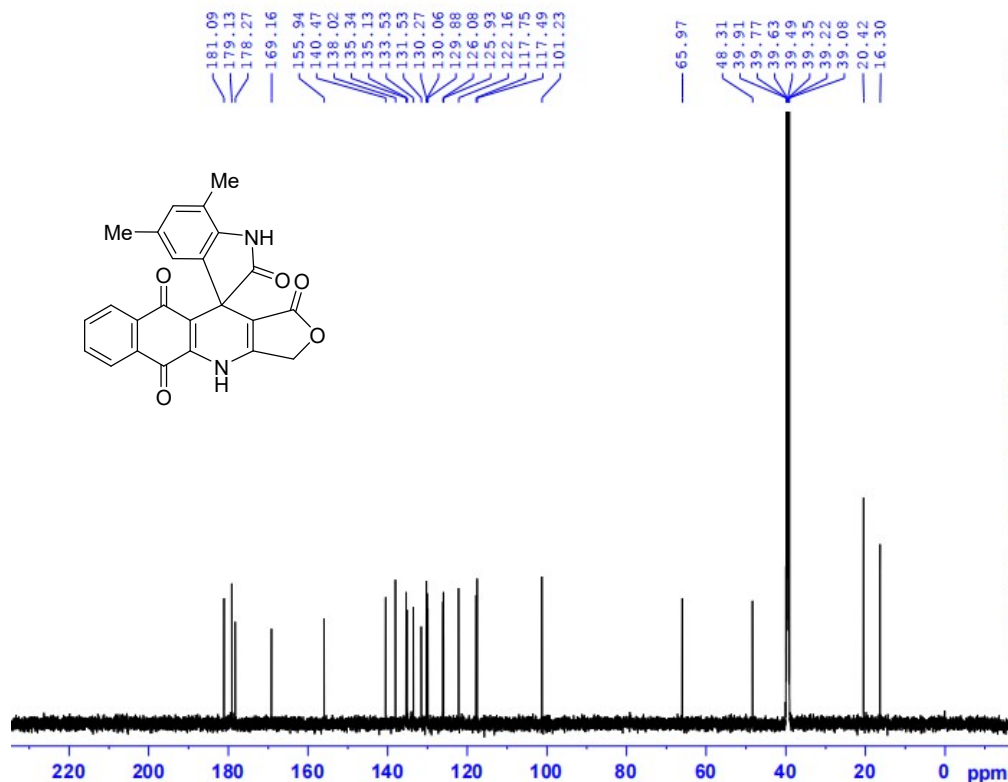
**4',6'-Dimethyl-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7g)**

TK254.101L-DMSO-1H





TK254.101L-DMSO-C13CPD

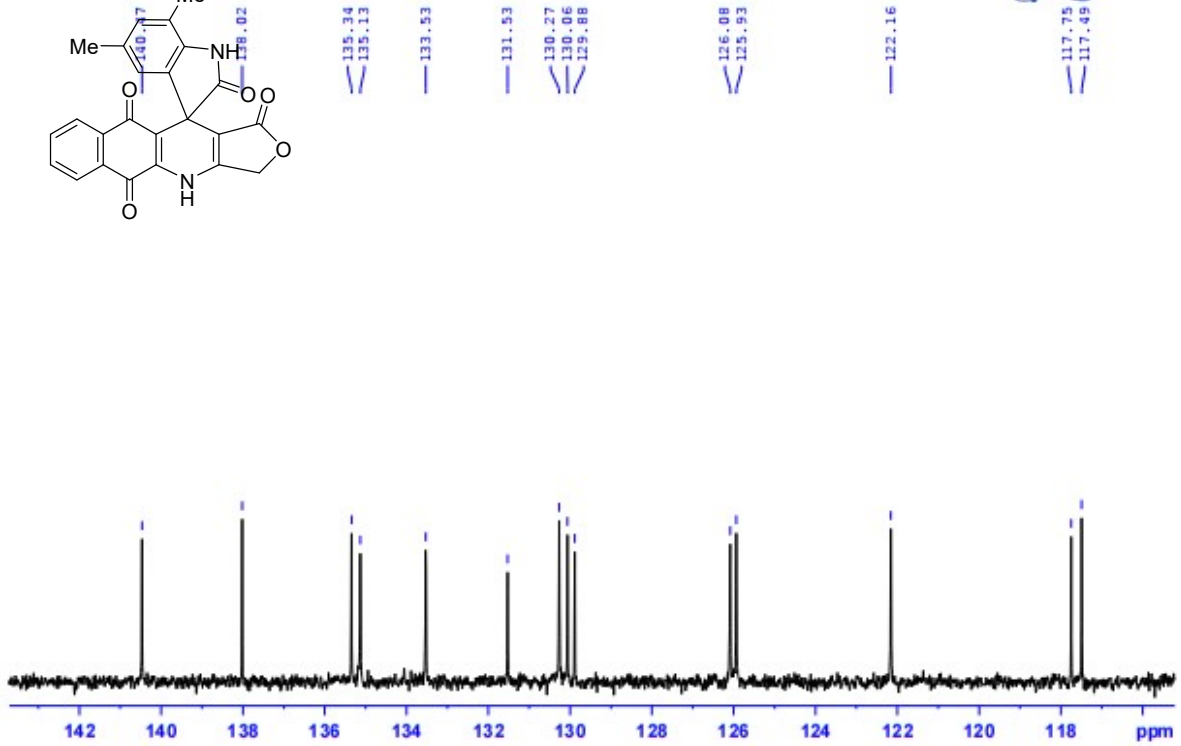
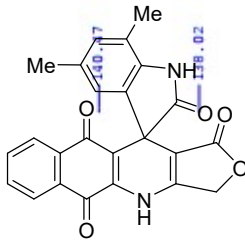


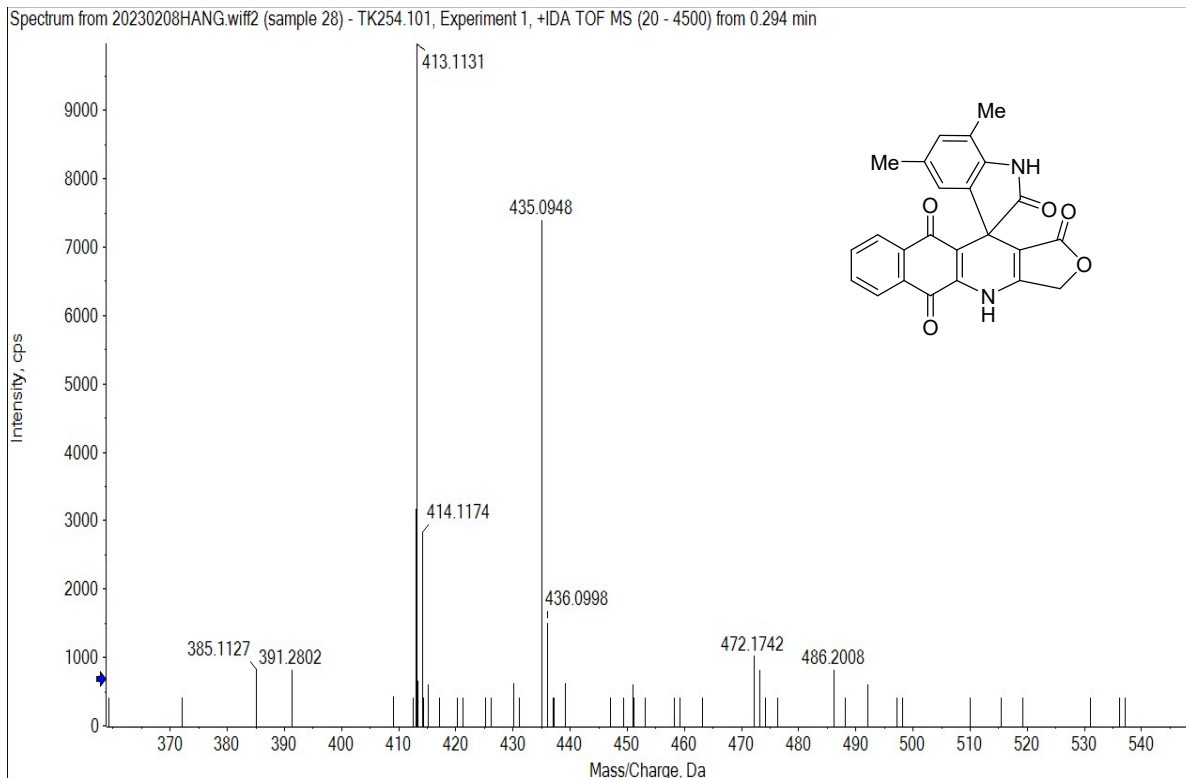
Current Data Parameters  
 NAME 6TK254.101L  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20241120  
 Time 9.57 h  
 INSTRUM AvanceNBO 600MHz  
 PROBHD Z114607 0862 (zggg30  
 FULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1024  
 DS 4  
 SWH 38461.539 Hz  
 FIDRES 1.173753 Hz  
 AQ 0.6519680 sec  
 RG 101  
 DW 13.000 usec  
 DE 6.50 usec  
 TE 303.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDD 1  
 SFO1 150.9873069 MHz  
 NUC1 13c  
 P0 4.00 usec  
 F1 12.00 usec  
 PLW1 115.00000000 W  
 SFO2 600.4024016 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 FCPD2 80.00 usec  
 PLW2 33.79999924 W  
 PLW12 0.52812999 W  
 PLW13 0.34696001 W

F2 - Processing parameters  
 SI 32768  
 SF 150.9707788 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40

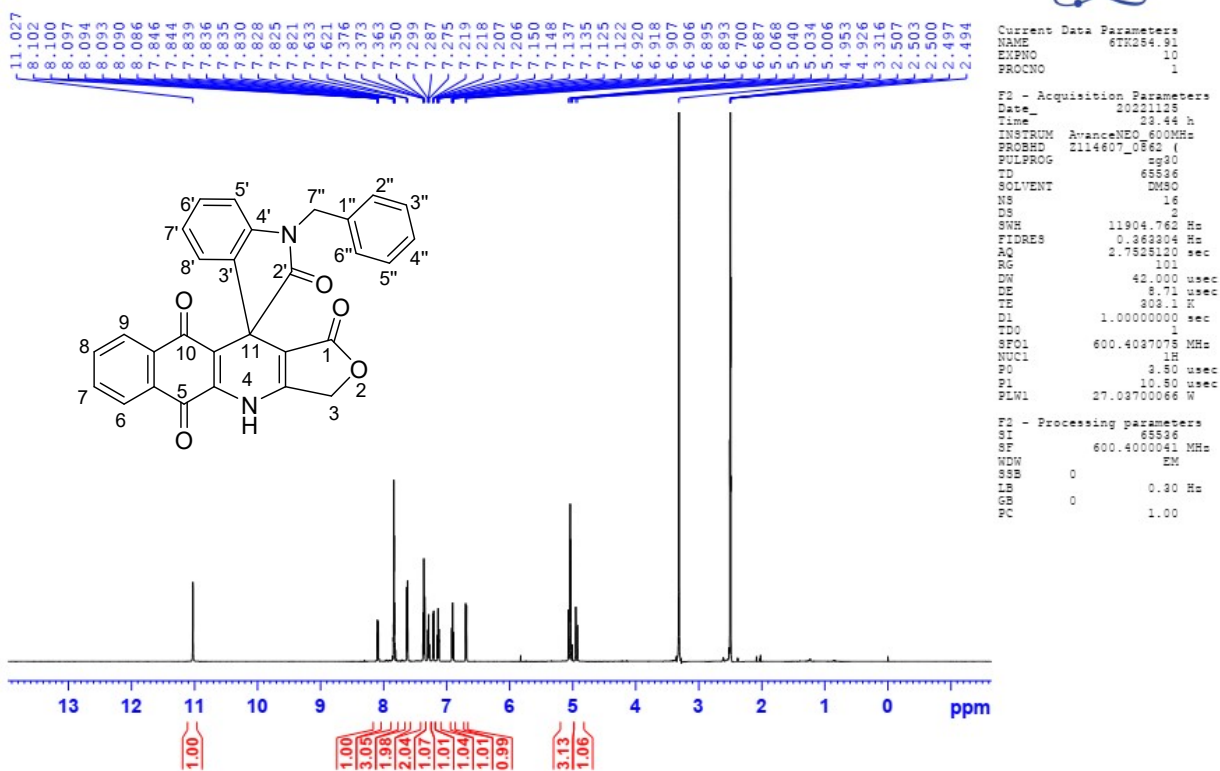
TK254.101L-DMSO-C13CPD



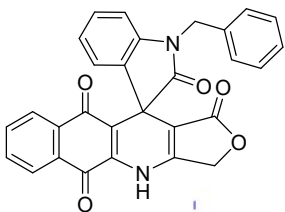
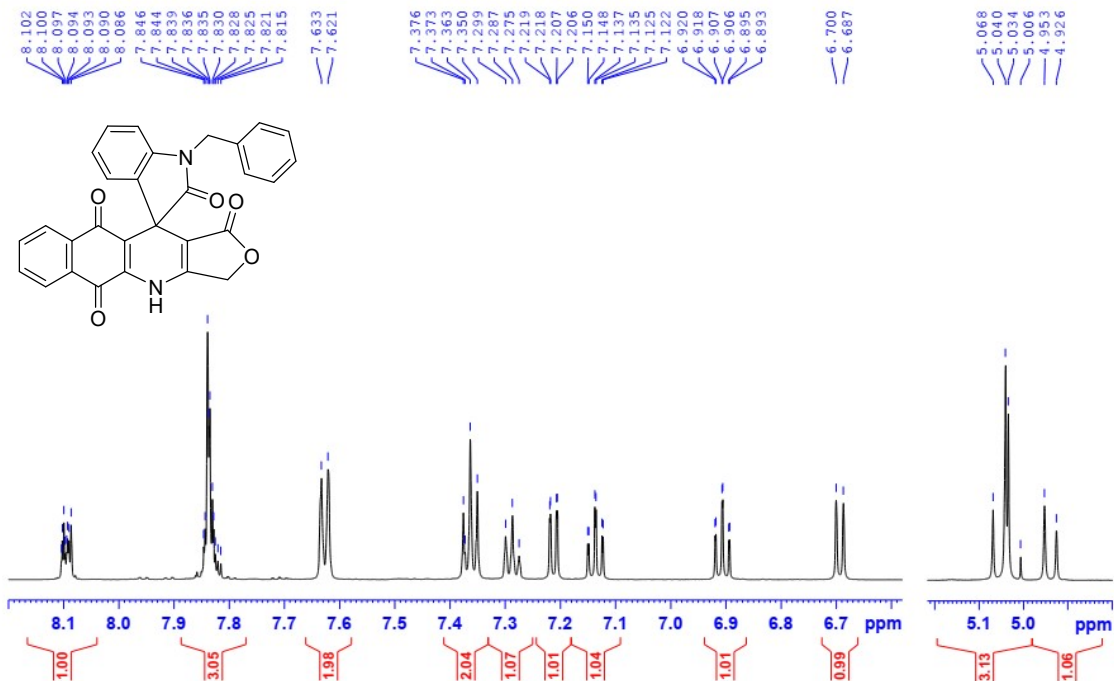


**1'-Benzyl-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7h)**

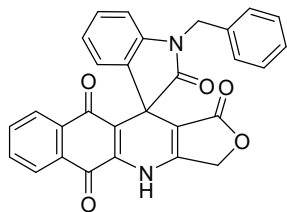
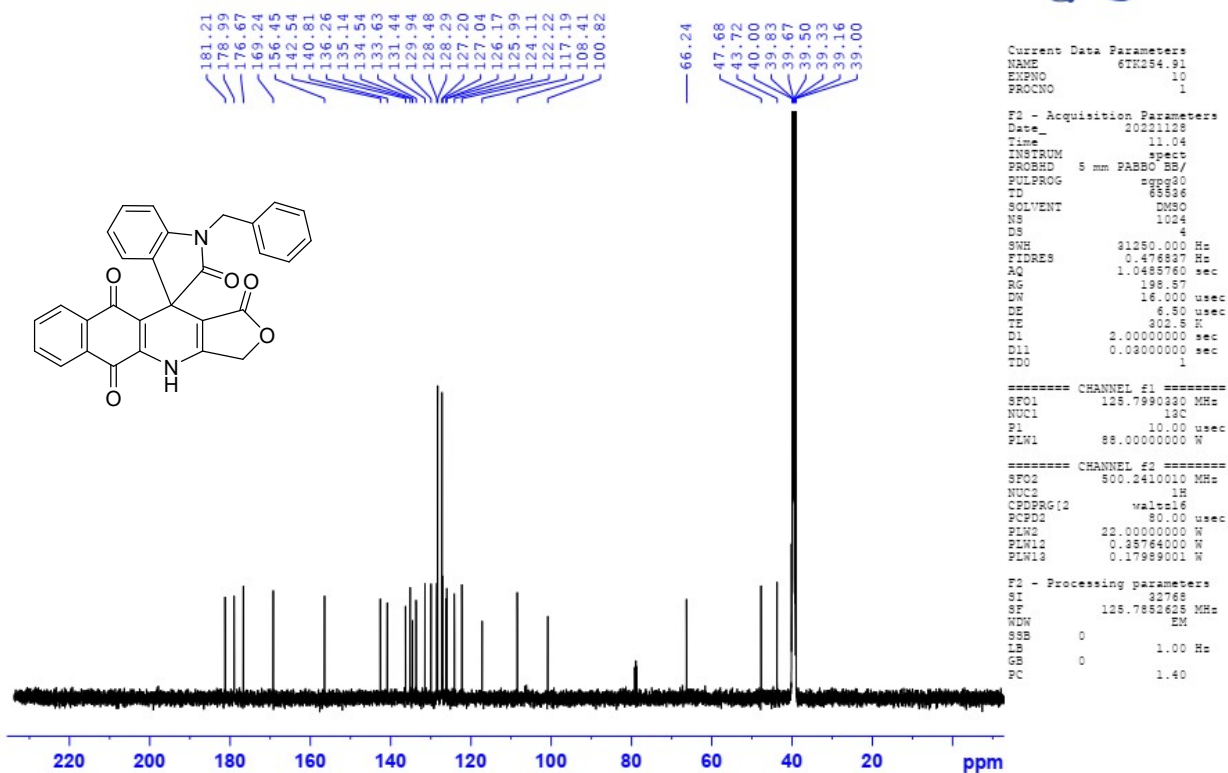
**TK254.91-DMSO-1H**



TK254.91-DMSO-1H



TK254.91-DMSO-C13CPD



```

Current Data Parameters
NAME      TK254.91
EXPNO    10
PROCNO   1

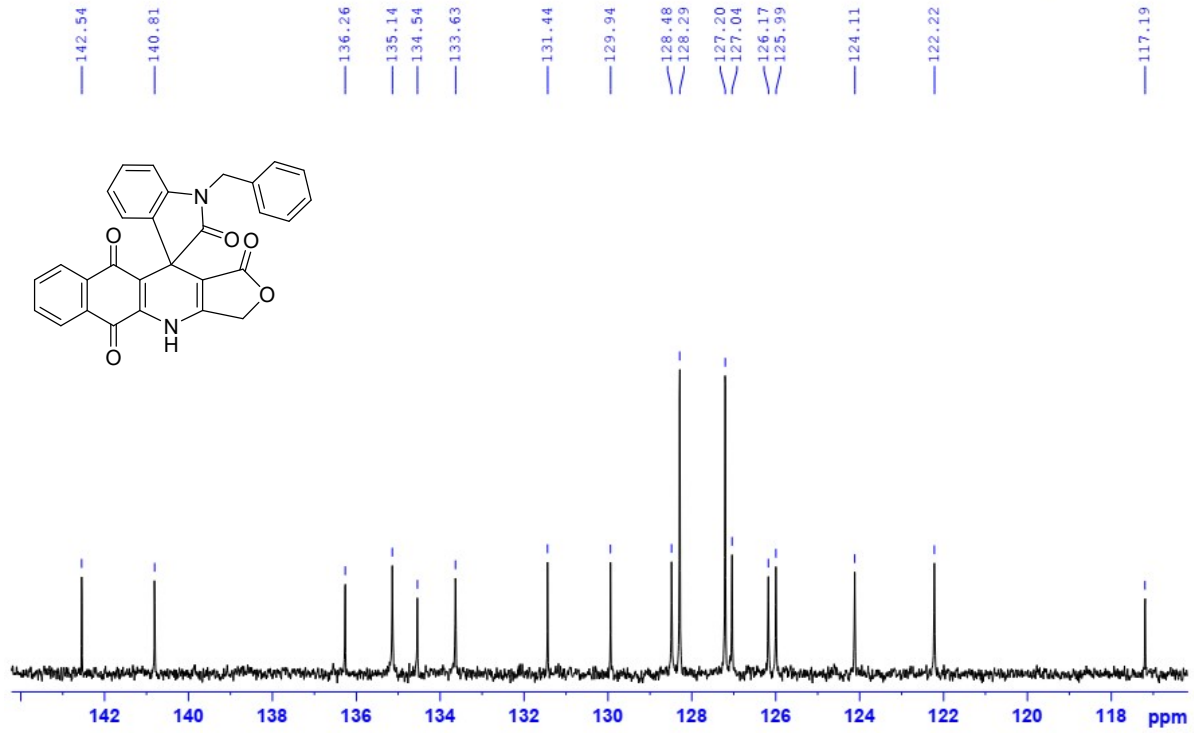
F2 - Acquisition Parameters
Date_    20211128
Time     11.04
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       1024
DS       4
SWH      31260.000 Hz
FIDRES   0.476837 Hz
AQ       1.0483760 sec
RG       198.87
DN       16.0000 usec
DE       6.50 usec
TE       302.5 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

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

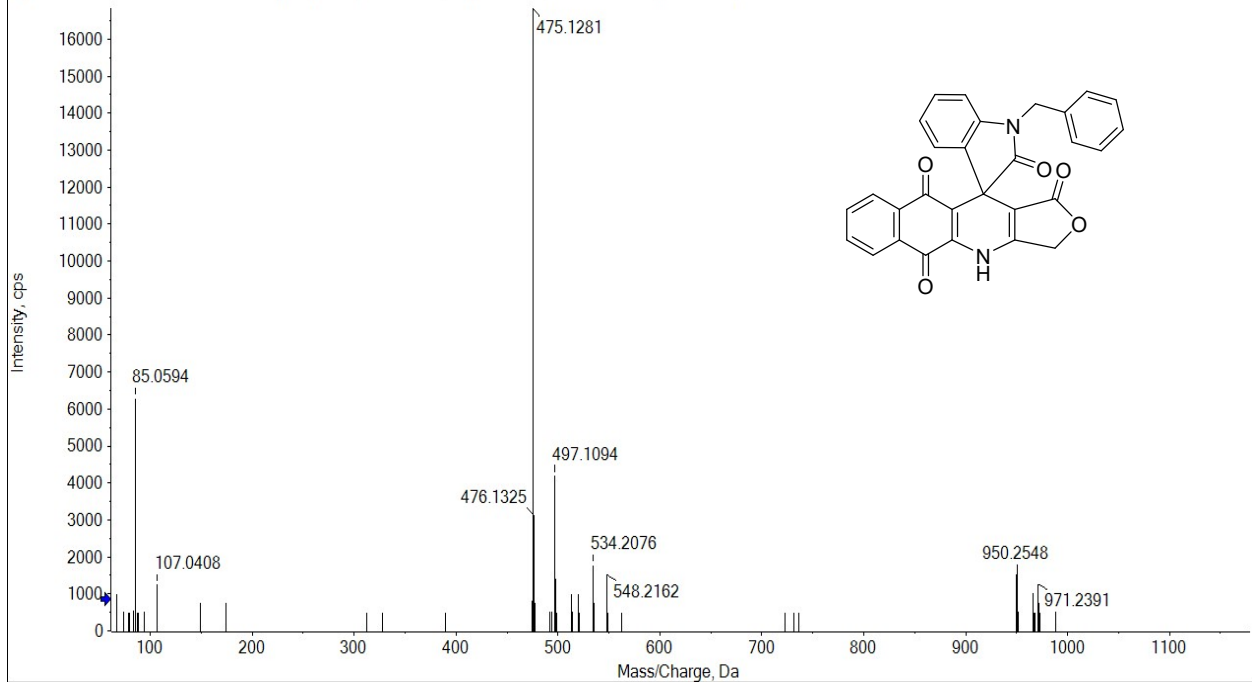
===== CHANNEL f2 =====
SF02     500.2410010 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLW2     22.00000000 W
PLM12    0.95764000 W
PLM13    0.17989001 W

F2 - Processing parameters
SI       32768
SF       125.7852625 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
FC       1.40
    
```

TK254.91-DMSO-C13CPD

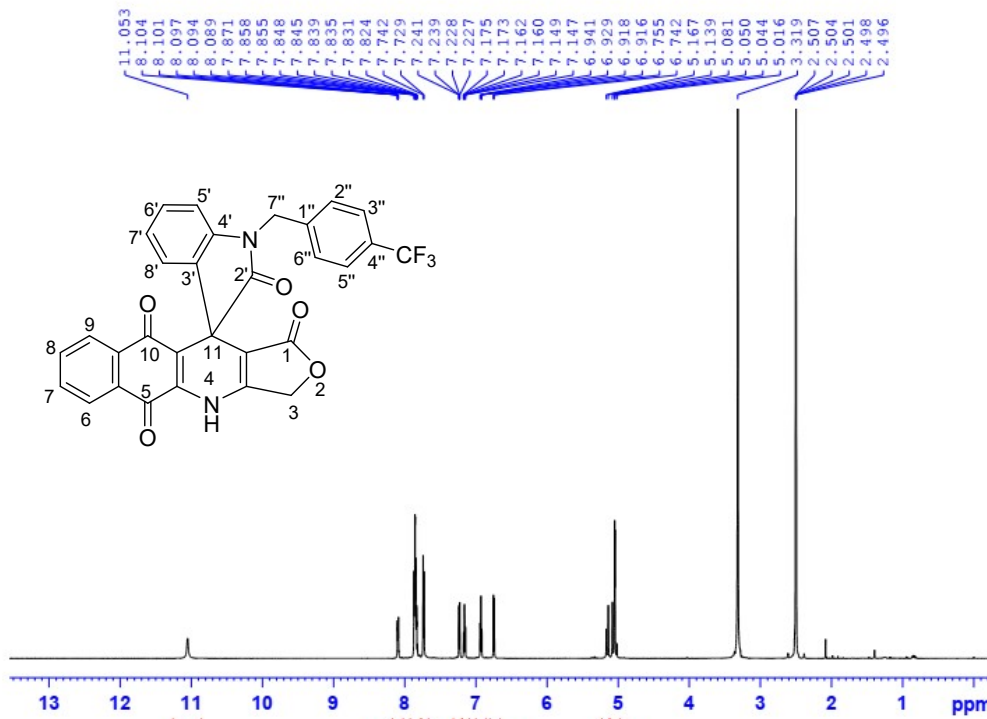


Spectrum from 20230208HANG.wiff2 (sample 25) - TK254.91, Experiment 1, +IDA TOF MS (20 - 4500) from 0.143 min



**1'-(4-(Trifluoromethyl)benzyl)-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7i)**

**TK254.100-DMSO-1H**



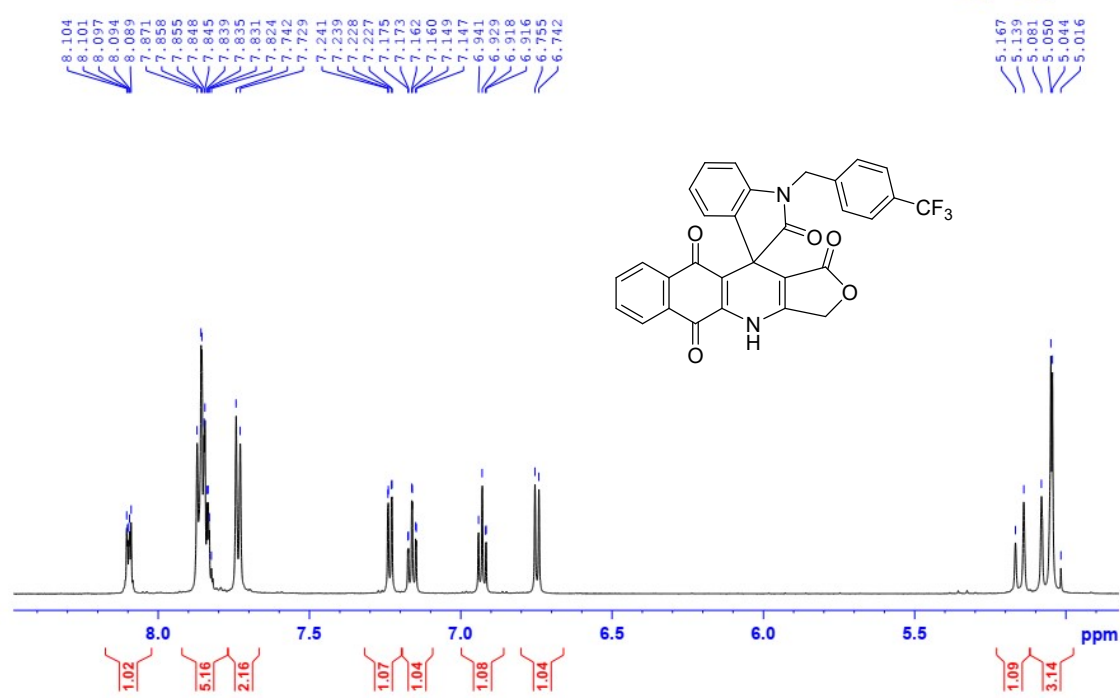
```

Current Data Parameters
NAME          TK254.100
EXPNO        10
PROCNO       1

F2 - Acquisition Parameters
Date_        20221206
Time         18.08 h
INSTRUM      AvanceNeo 800MHz
PROBHD       Z114607_0862 (
PULPROG      zgpg30
TD           65536
SOLVENT      DMSO
NS           16
DS           4
SWH          11904.762 Hz
FIDRES       0.362304 Hz
AQ           2.7828120 sec
RG           101
AQ           101
DN           42.000 usec
DE           9.71 usec
TE           300.2 K
D1           1.00000000 sec
ID0          1
SFO1         600.4037075 MHz
NUC1         1H
PS           2.50 usec
PI           10.50 usec
PLWL        27.03700066 W

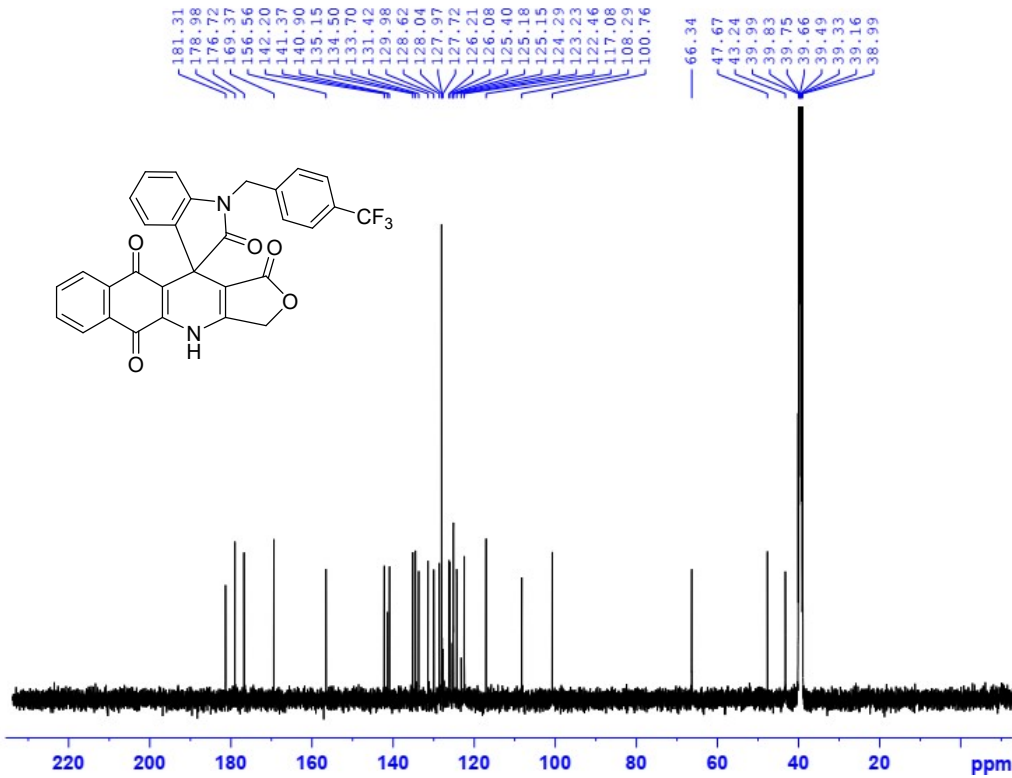
F2 - Processing parameters
scf1         65536
sf          600.4000025 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
    
```

**TK254.100-DMSO-1H**





TK254.100-DMSO-C13CPD



Current Data Parameters  
 NAME: TK254.100  
 F1FNO: 2  
 PROCNO: 1

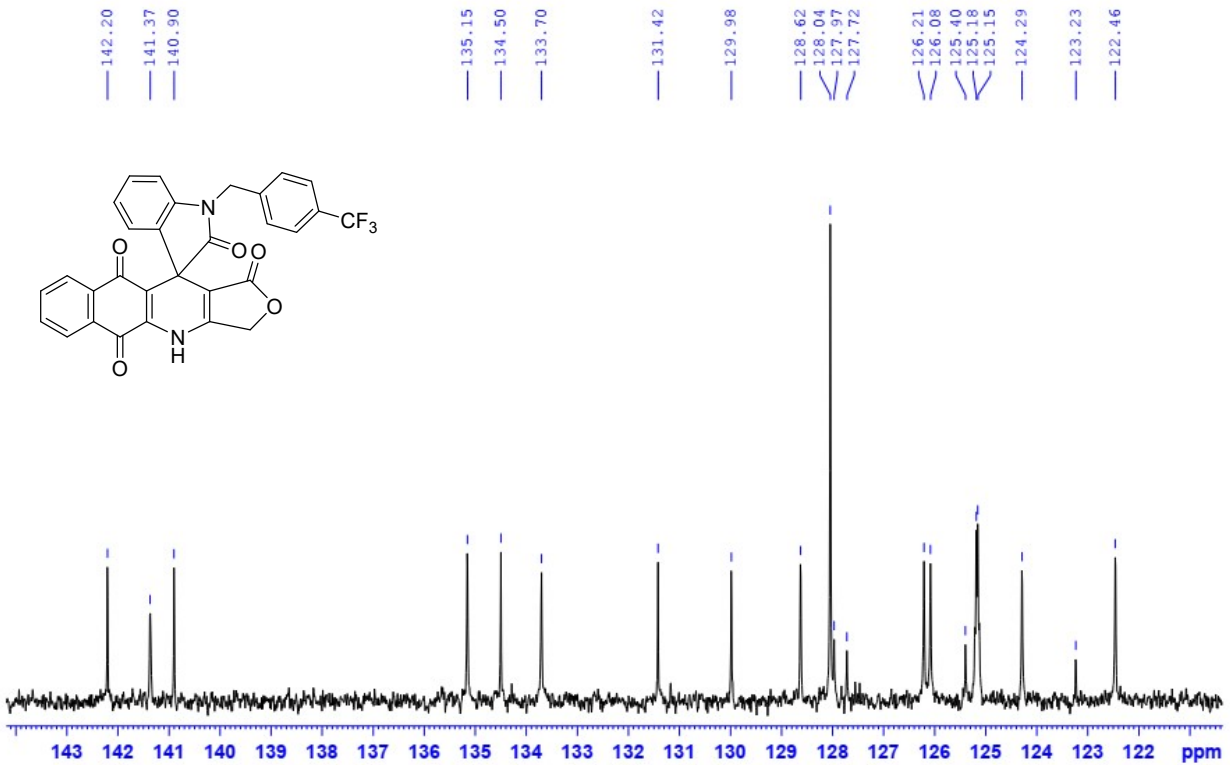
F2 - Acquisition Parameters  
 Date\_: 20221208  
 Time: 4.44  
 INSTRUM: spect  
 PROBHD: 5 mm PABBO BB/  
 PULPROG: zgpg30  
 TD: 65536  
 SOLVENT: DMSO  
 NS: 2048  
 DS: 4  
 SWH: 31250.000 Hz  
 FIDRES: 0.476827 Hz  
 AQ: 1.0485760 sec  
 RG: 198.57  
 DM: 16.000 usec  
 DE: 6.50 usec  
 TE: 300.4 K  
 D1: 2.00000000 sec  
 D11: 0.03000000 sec  
 TDO: 1

===== CHANNEL f1 =====  
 SFO1: 125.7990330 MHz  
 NUCL1: 13C  
 P1: 10.00 usec  
 PLW1: 88.00000000 W

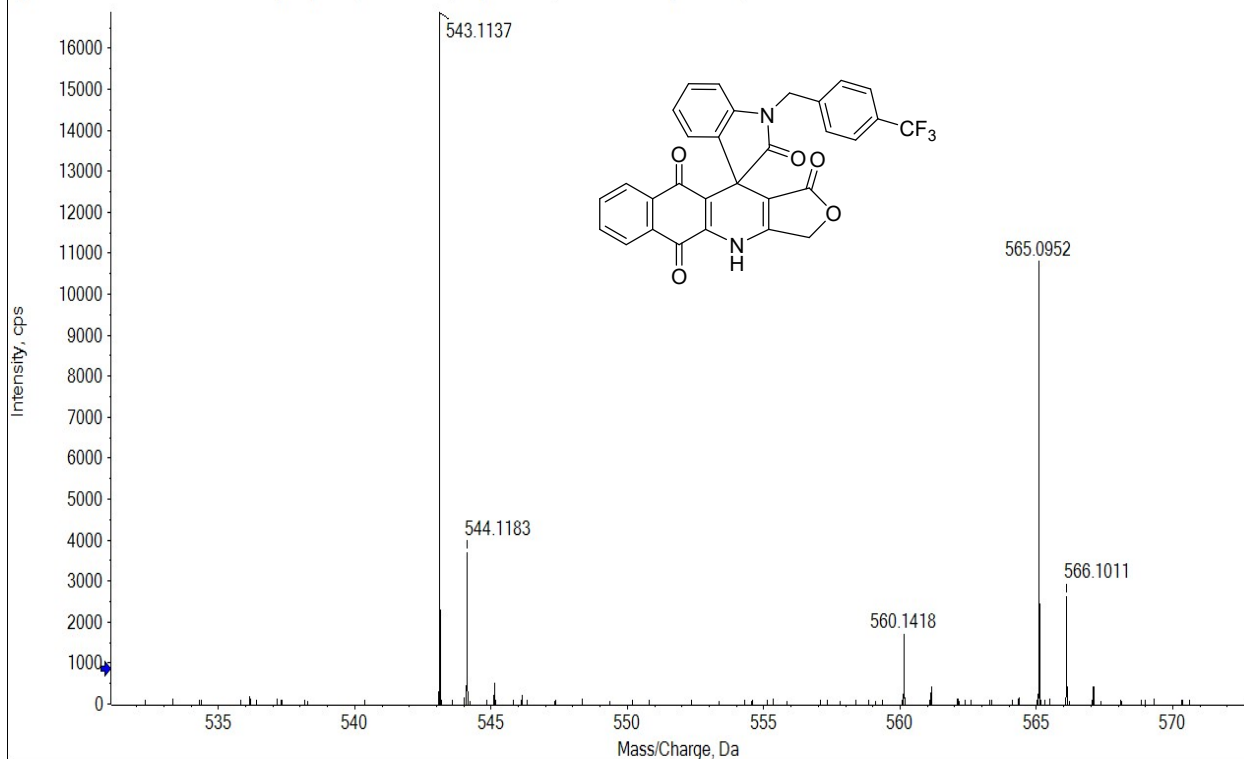
===== CHANNEL f2 =====  
 SFO2: 500.2410010 MHz  
 NUCL2: 1H  
 CPDPRG2: waltz16  
 PCPD2: 80.00 usec  
 PLW2: 22.00000000 W  
 PLW3: 0.28764000 W  
 PLW4: 0.17989001 W

F2 - Processing parameters  
 SI: 32768  
 SF: 125.7852602 MHz  
 WDM: EM  
 SSB: 0  
 GB: 1.00 Hz  
 PC: 1.40

TK254.100-DMSO-C13CPD

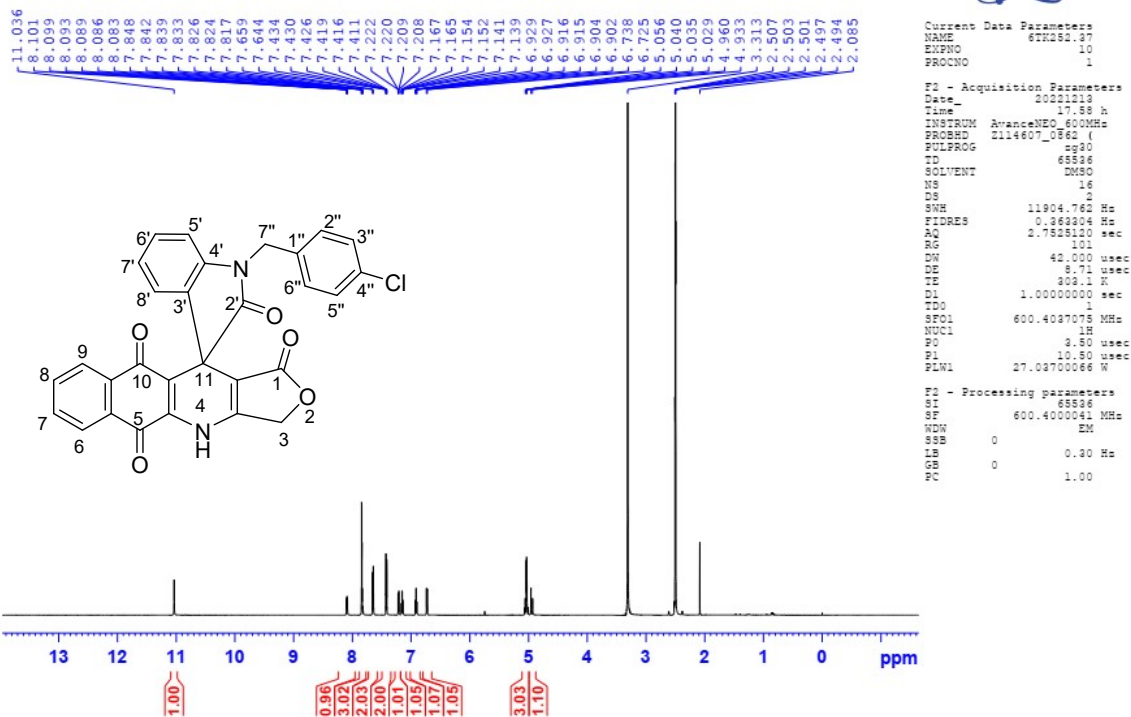


Spectrum from 20230208HANG.wiff2 (sample 27) - TK254.100, Experiment 1, +IDA TOF MS (20 - 4500) from 0.123 min

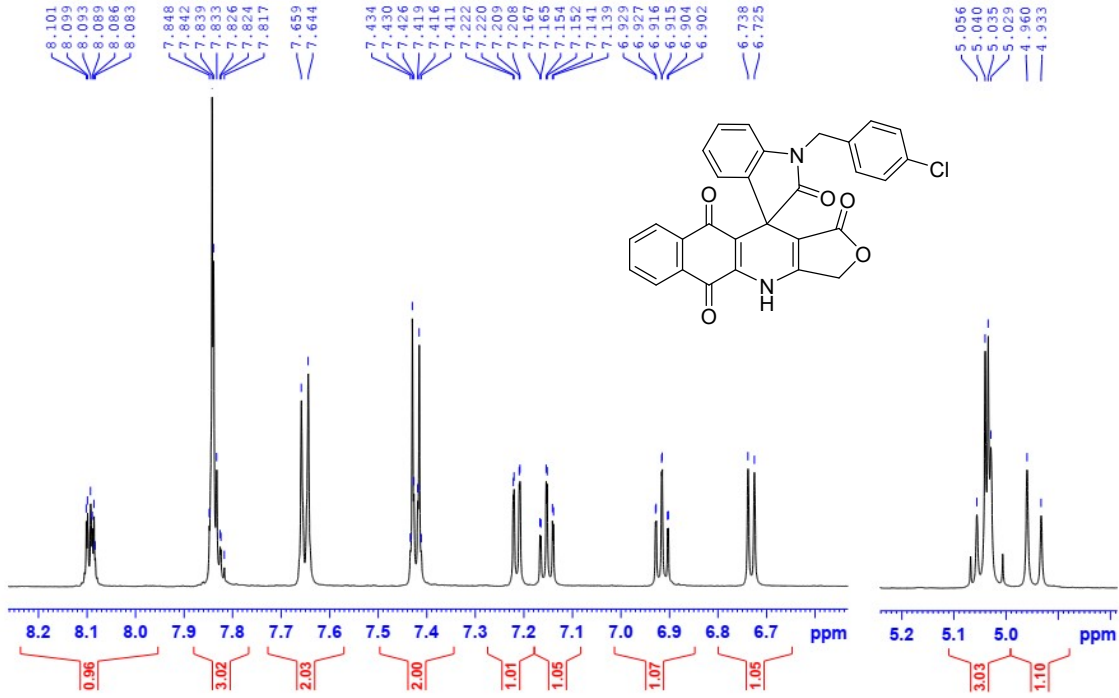


**1'-(4-Chlorobenzyl)-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7j)**

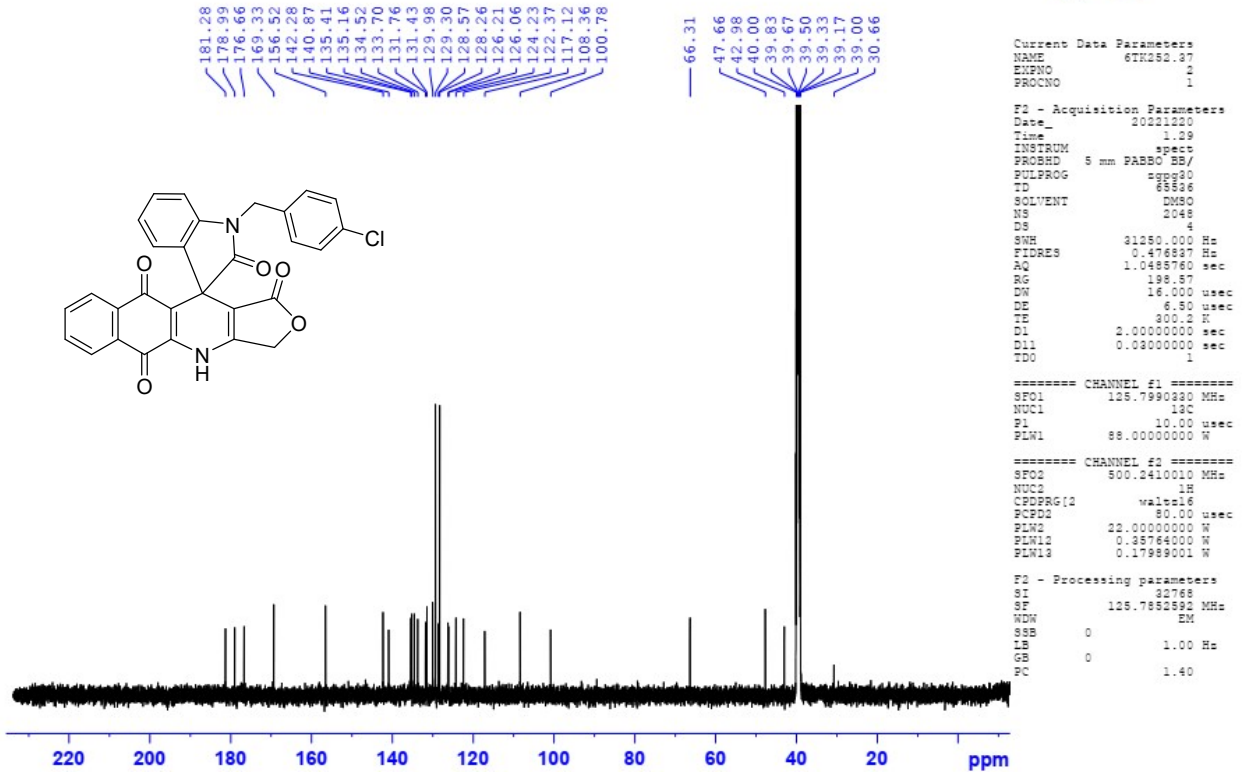
TK252.37-DMSO-1H



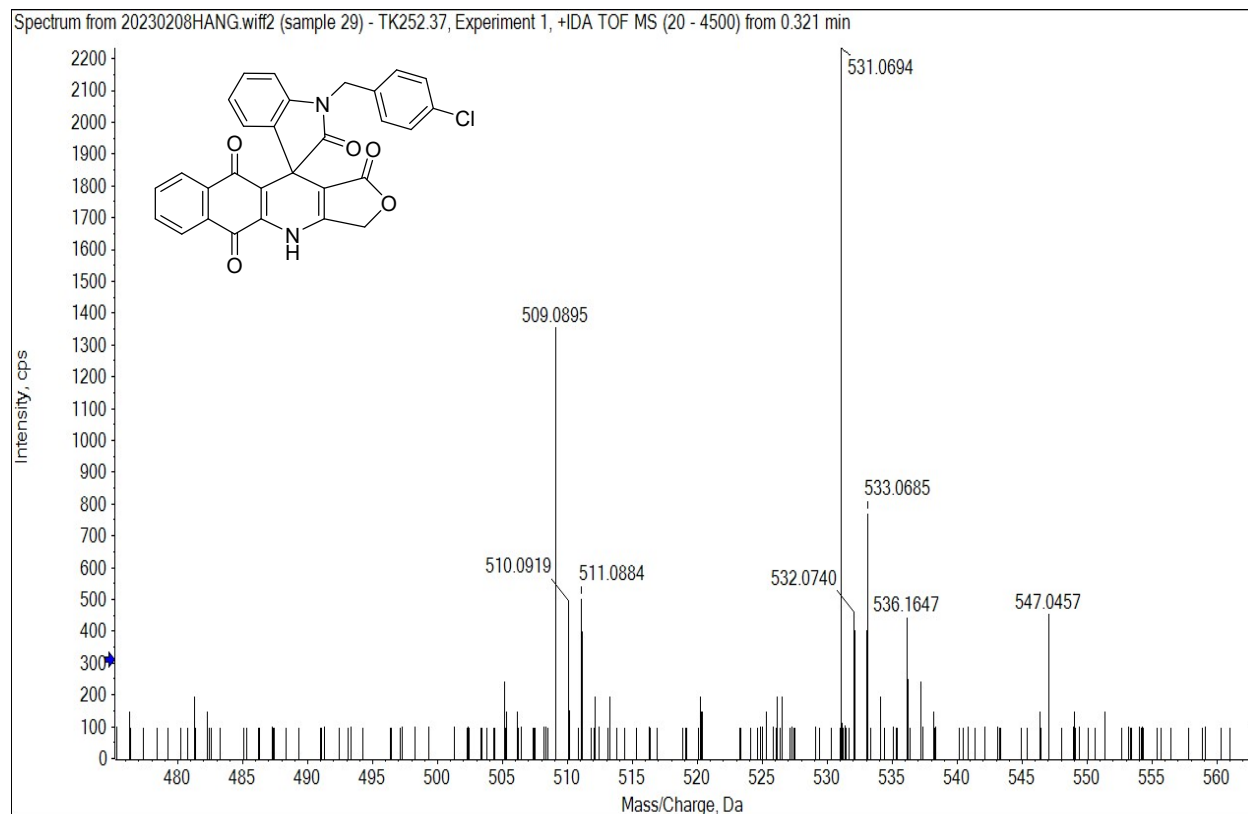
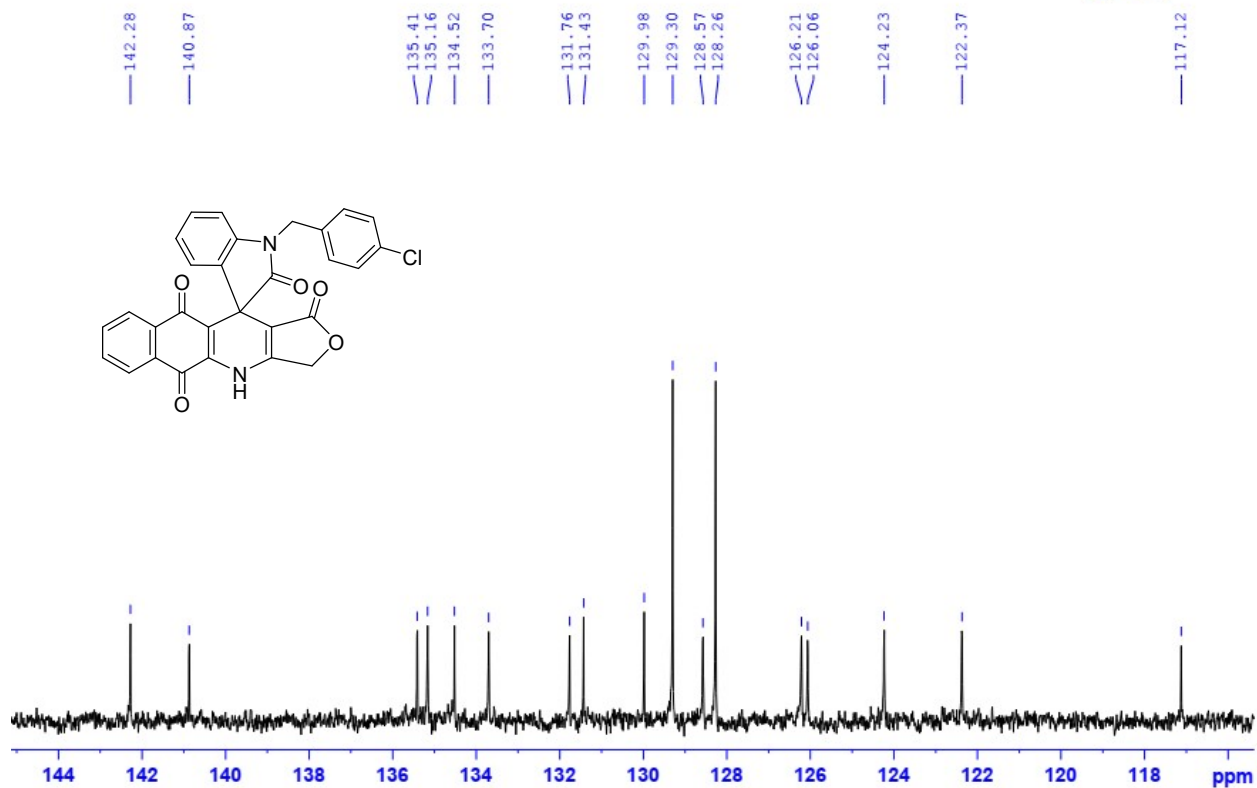
TK252.37-DMSO-1H



TK252.37-DMSO-C13CPD

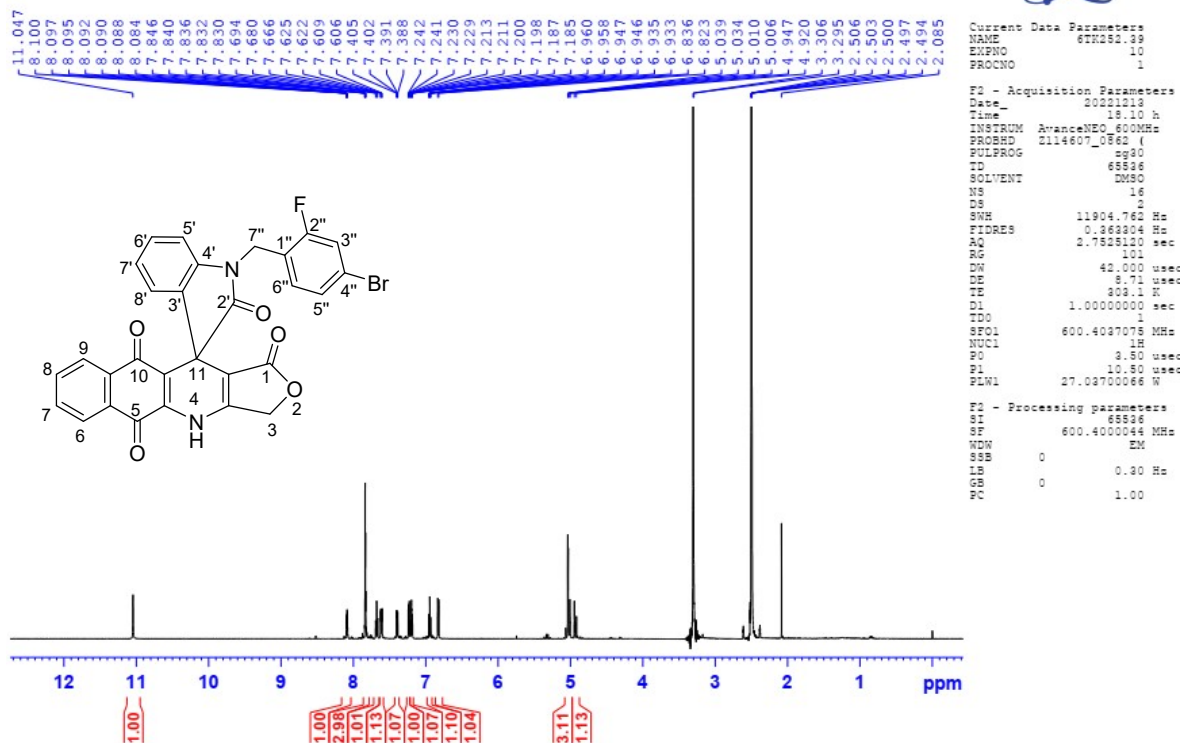


TK252.37-DMSO-C13CPD

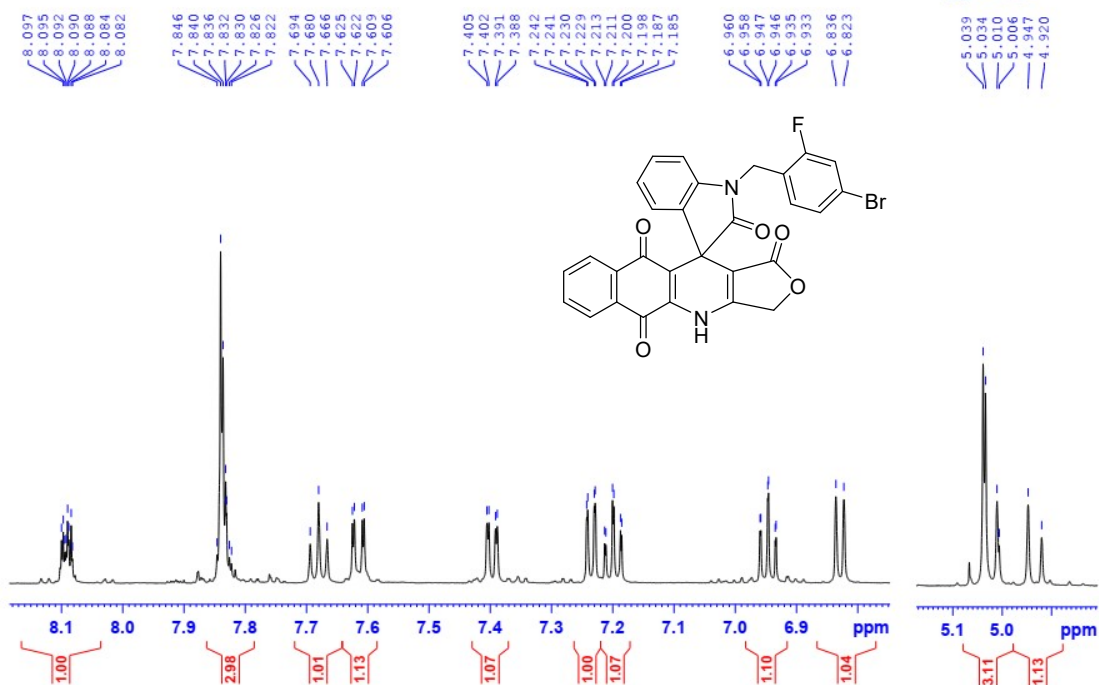


**1'-(4-Bromo-2-fluorobenzyl)-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7k)**

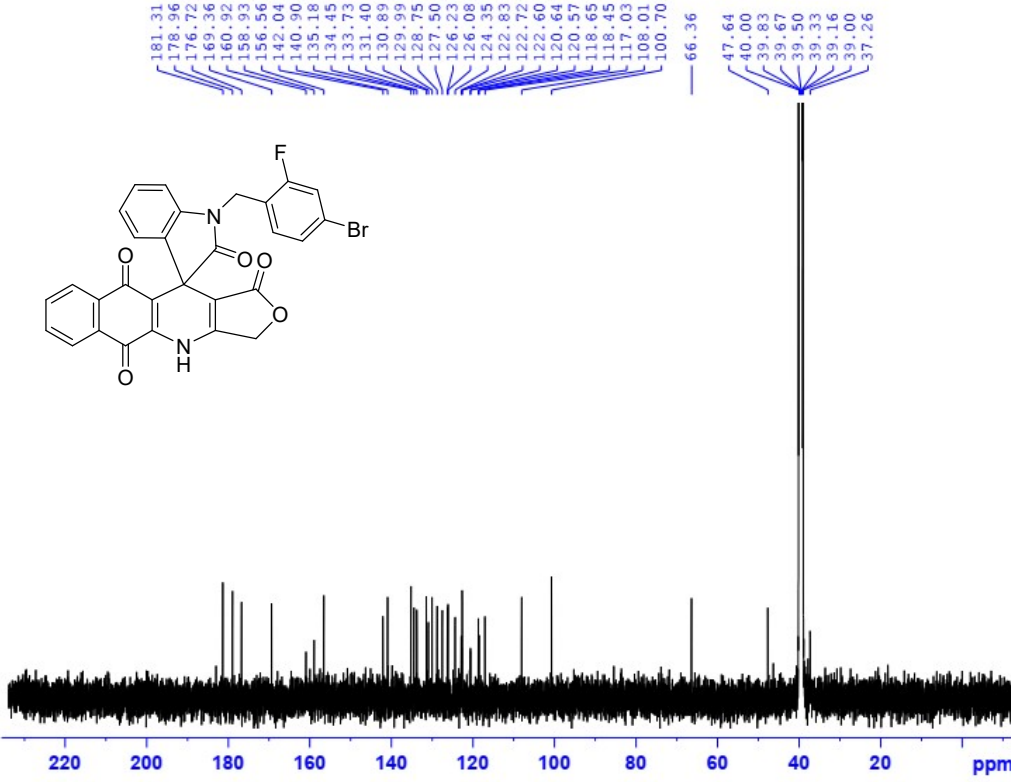
TK252.39-DMSO-1H



TK252.39-DMSO-1H



TK252.39-DMSO-C13CPD



Current Data Parameters  
 NAME TK252.39  
 EXPNO 2  
 PROCNO 1

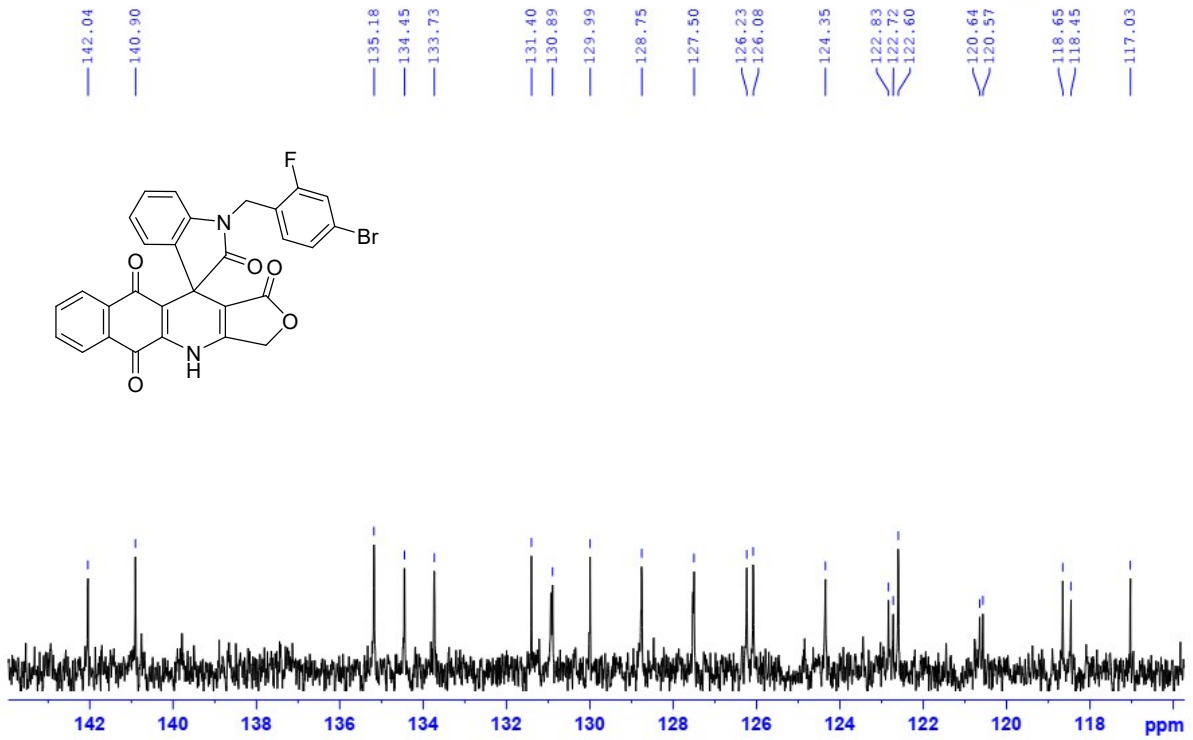
F2 - Acquisition Parameters  
 Date\_ 20211220  
 Time 5.04  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 4096  
 DS 4  
 SWH 31250.000 Hz  
 FIDRES 0.476887 Hz  
 AQ 1.0488760 sec  
 RG 198.57  
 DW 16.000 usec  
 DE 6.50 usec  
 TE 300.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 ID0 1

===== CHANNEL f1 =====  
 SFO1 125.7990320 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 88.00000000 W

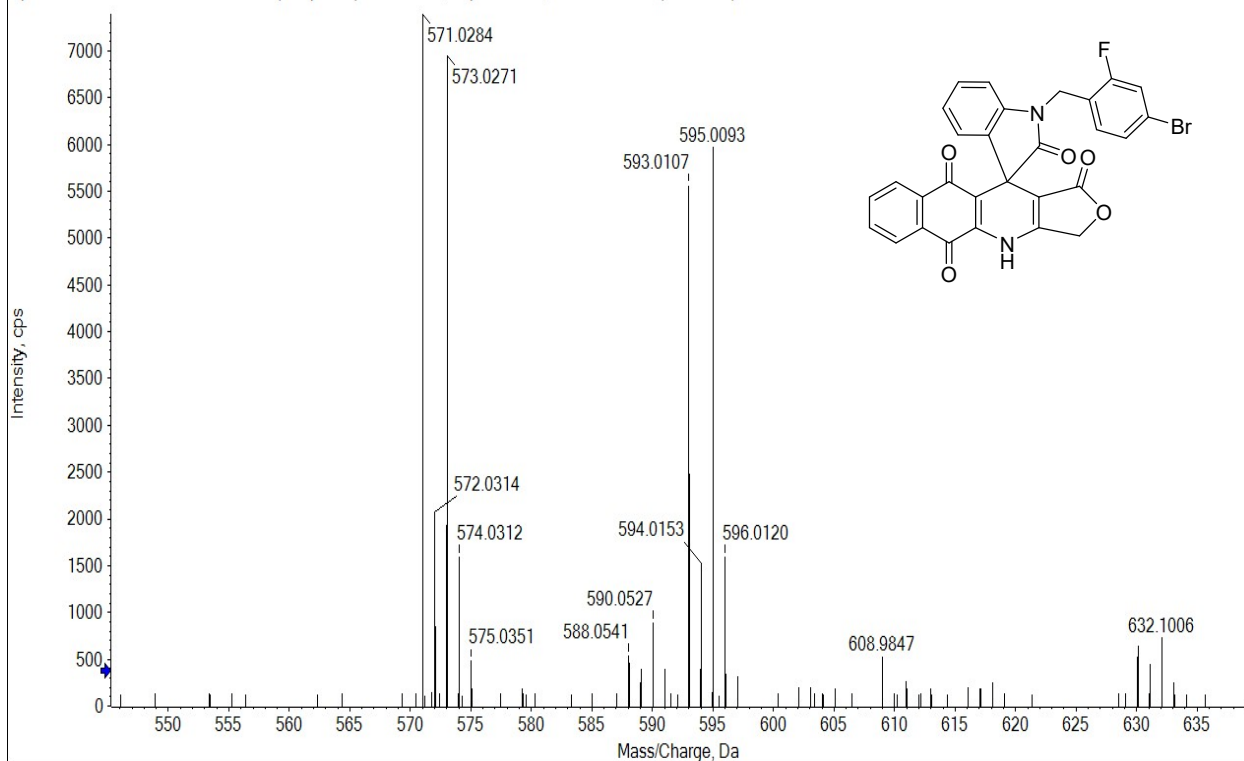
===== CHANNEL f2 =====  
 SFO2 500.2410010 MHz  
 NUC2 1H  
 CPDPRG12 waltz16  
 PCPD2 80.00 usec  
 PLW2 22.00000000 W  
 PLW3 0.25764000 W  
 PLW4 0.17989001 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7852583 MHz  
 WDN EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

TK252.39-DMSO-C13CPD

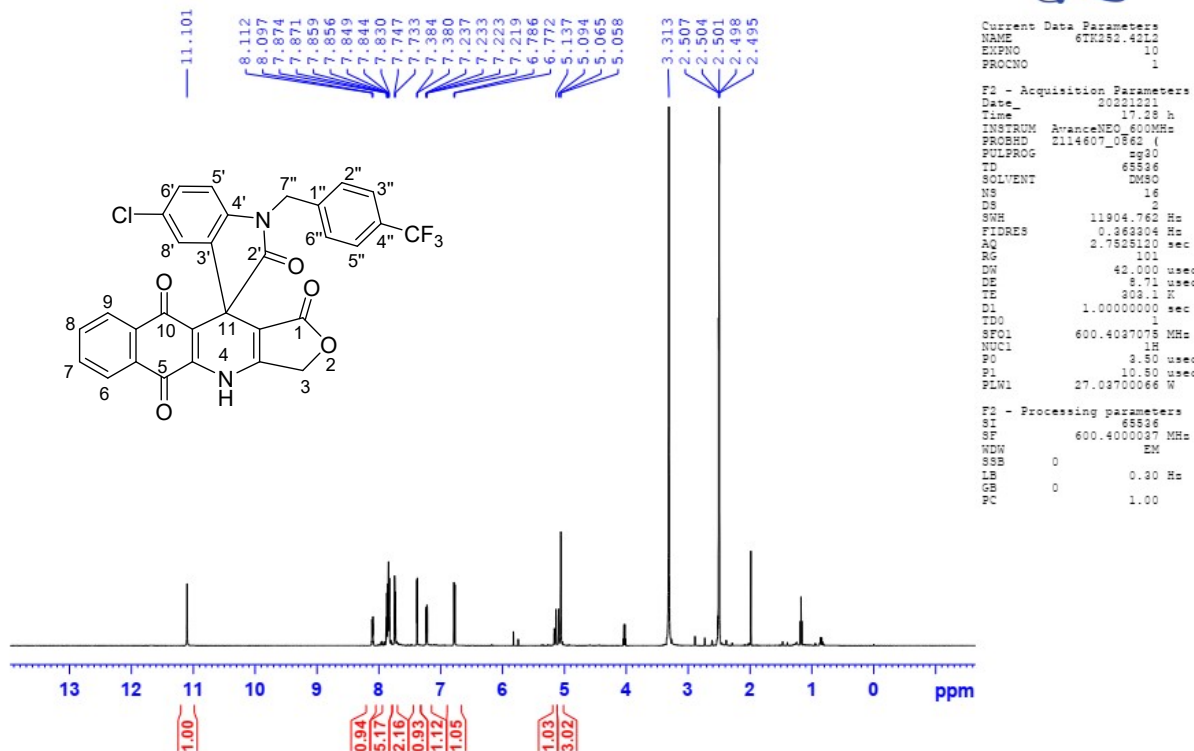


Spectrum from 20230208HANG.wiff2 (sample 30) - TK252.39, Experiment 1, +IDA TOF MS (20 - 4500) from 0.319 min

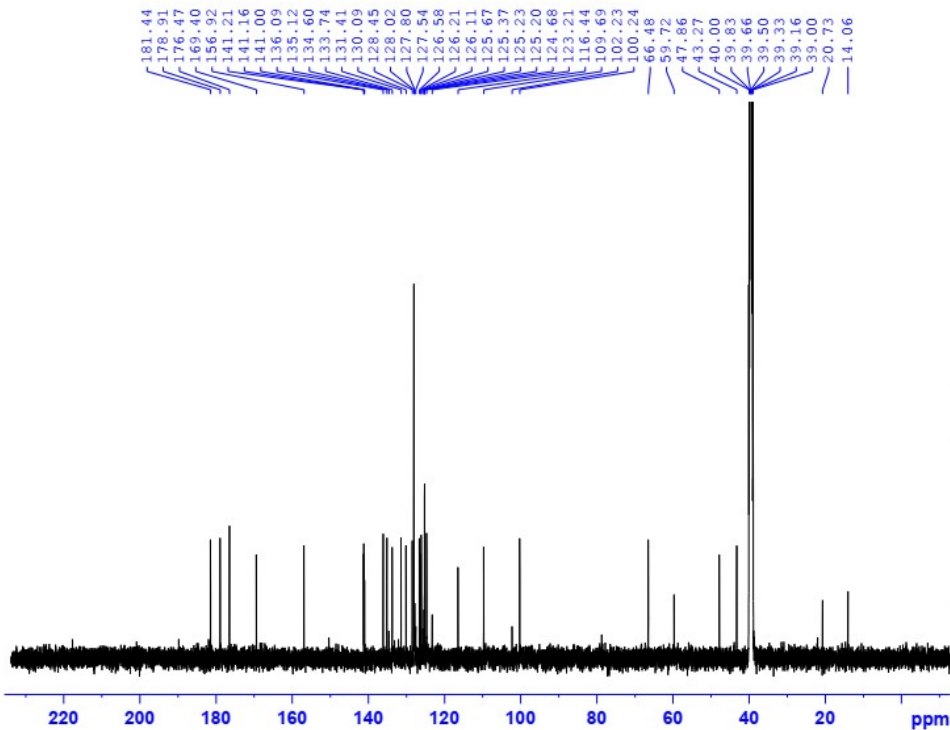


**5'-Chloro-1'-(4-(trifluoromethyl)benzyl)-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7l)**

**TK252.42L2-DMSO-1H**



TK252.42L2-DMSO-C13CPD



```

Current Data Parameters
NAME      671252.42L2
EXPNO    1
PROCNO   1

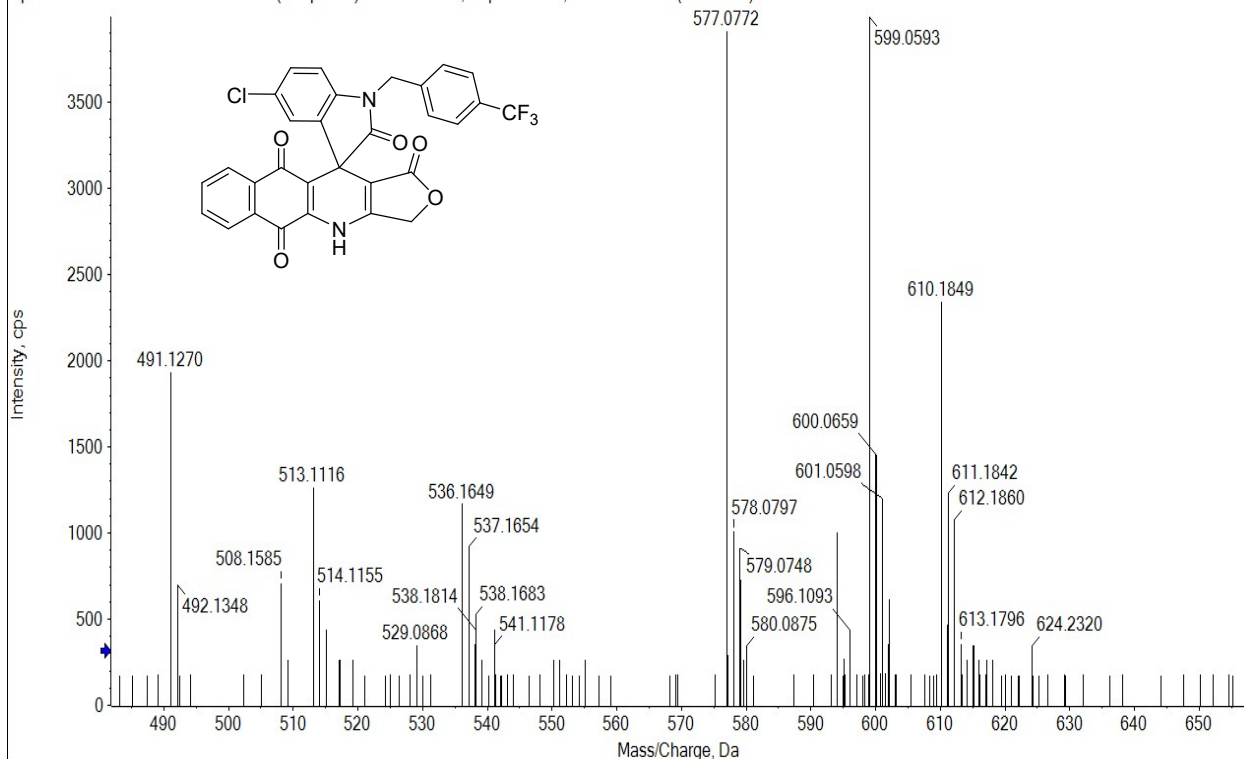
F2 - Acquisition Parameters
Date_    20231222
Time     22.14
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        4096
DS         4
SNH       31250.000 Hz
FIDRES    0.476597 Hz
AQ        1.0485760 sec
RG         198.57
DSH        16.000 usec
DE         6.50 usec
TE        300.6 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.769030 MHz
NUC1       13C
P1         10.00 usec
PLW1      88.00000000 W

===== CHANNEL f2 =====
SFO2      500.2410010 MHz
NUC2       1H
CPDPRG12  waltz16
PCPD2      80.00 usec
PLW2      22.00000000 W
PLW12     0.38764000 W
PLW13     0.17989001 W

F2 - Processing parameters
SI         32768
SF         125.7682596 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

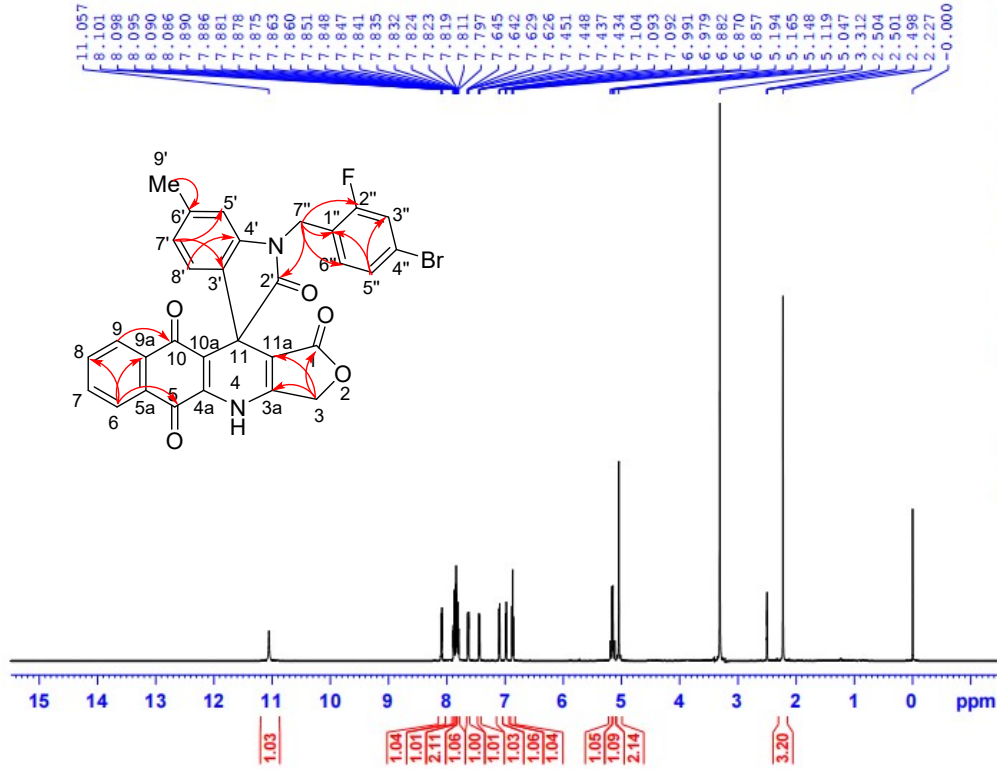
Spectrum from 20230208HANG.wiff2 (sample 31) - TK252.42L2, Experiment 1, +IDA TOF MS (20 - 4500) from 0.279 min





**1'-(4-Bromo-2-fluorobenzyl)-6'-methyl-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7m)**

**TK252.44L2-DMSO-1H**



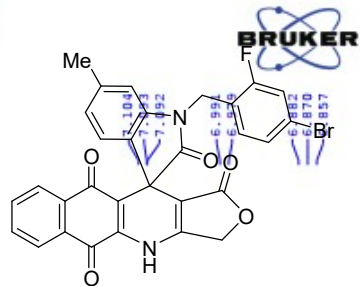
Current Data Parameters  
NAME TK252.44L2  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241119  
Time\_ 17.20 h  
INSTRUM Avance NEO 600MHz  
PROBHD Z114607 0862 (4  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 11904.762 Hz  
FIDRES 0.363304 Hz  
AQ 2.7525120 sec  
RG 101  
DW 42.000 usec  
DE 8.79 usec  
TE 303.1 K  
D1 1.00000000 sec  
TDO 1  
SF01 600.4037075 MHz  
NUC1 1H  
P0 3.33 usec  
F1 10.00 usec  
FLW1 33.79999924 W

F2 - Processing parameters  
SI 65536  
SF 600.4000035 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

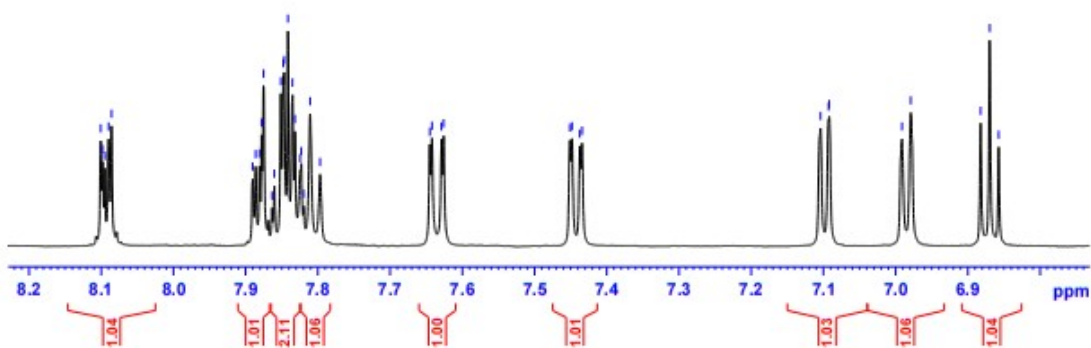
TK252.44L2-DMSO-1H

BRUKER

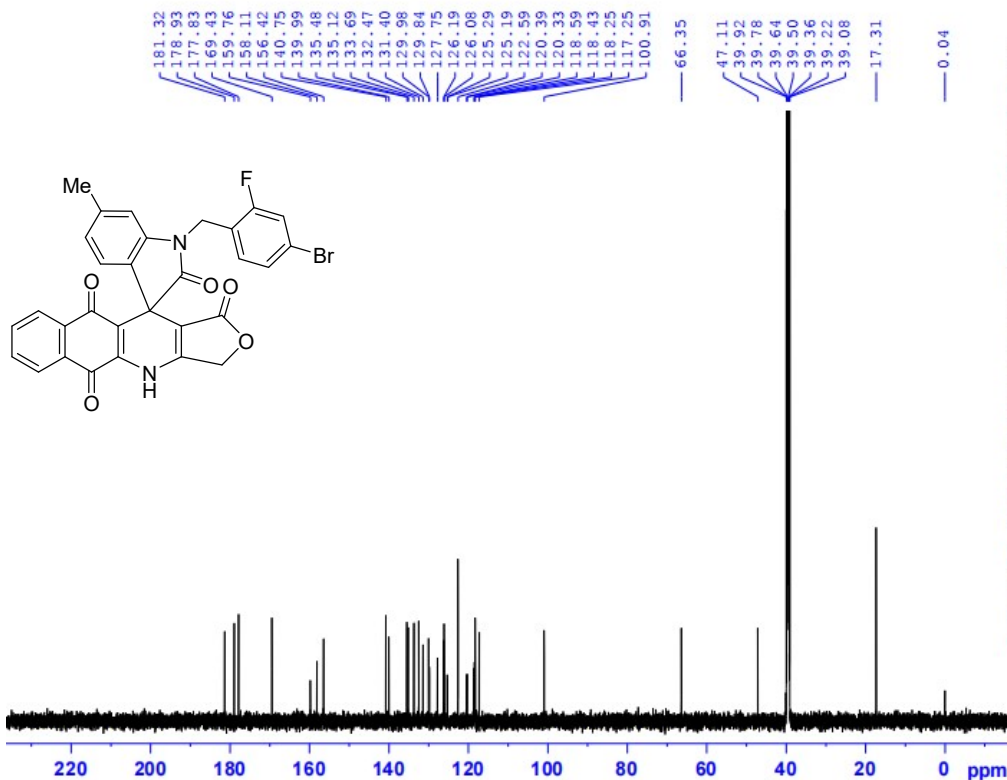


8.101  
8.098  
8.095  
8.050  
8.066  
7.880  
7.886  
7.881  
7.878  
7.875  
7.863  
7.860  
7.851  
7.849  
7.847  
7.841  
7.835  
7.832  
7.823  
7.819  
7.811  
7.797  
7.645  
7.642  
7.629  
7.626

7.451  
7.448  
7.437  
7.434



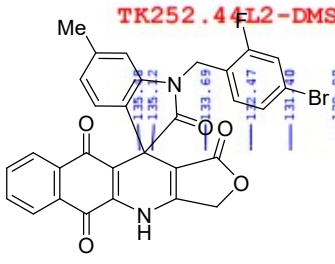
TK252.44L2-DMSO-C13CPD



Current Data Parameters  
 NAME 6TK254.44L  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20241119  
 Time\_ 20.00 h  
 INSTRUM AvanceNEO 600MHz  
 PROBHD Z114607\_0B62 (zpg30)  
 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 303.1 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDD 1  
 SFO1 150.9873069 MHz  
 NUC1 13C  
 P0 4.00 usec  
 P1 12.00 usec  
 PLW1 115.0000000 W  
 SFO2 600.4024016 MHz  
 NUC2 1H  
 CPDPRG2 waltz65  
 FCPD2 80.00 usec  
 PLW2 33.79999924 W  
 PLW12 0.52812999 W  
 PLW13 0.34696001 W

F2 - Processing parameters  
 SI 32768  
 SF 150.9707001 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



TK252.44L2-DMSO-C13CPD



140.75  
139.99

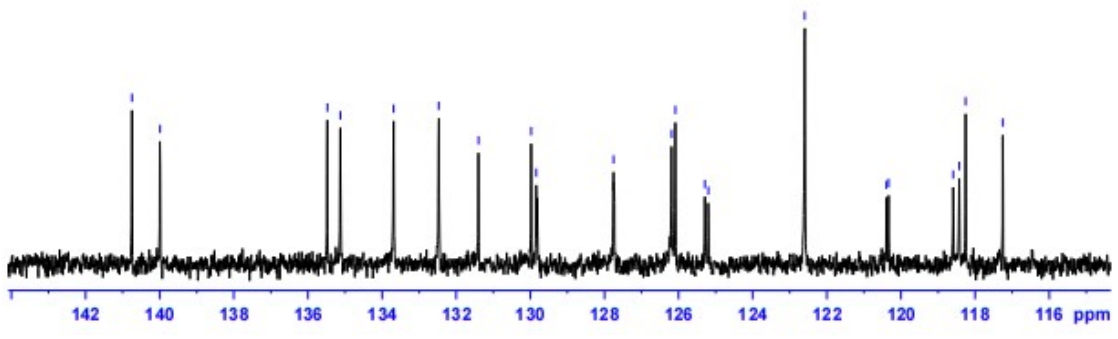
135.78  
135.72  
135.72

133.69  
129.88  
129.84

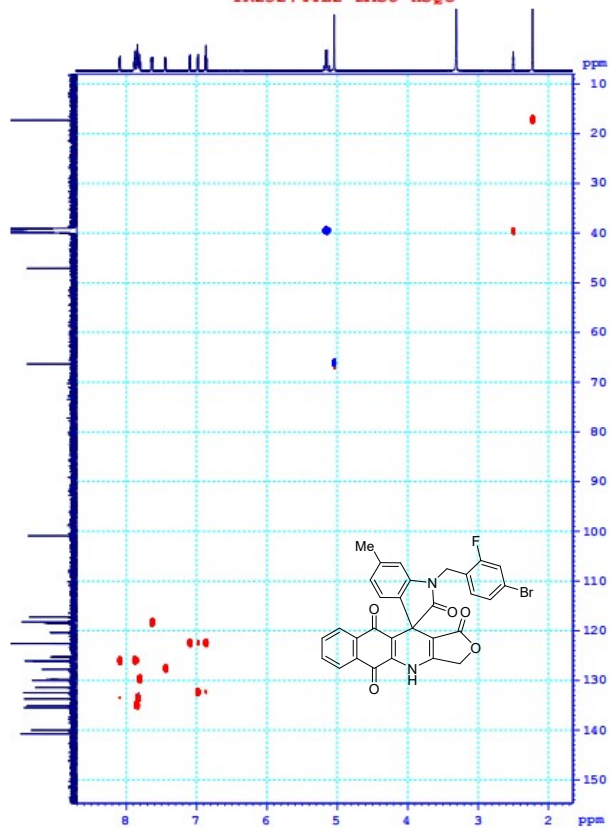
127.75  
126.19  
126.08  
125.79  
125.19

122.59  
120.39  
120.33

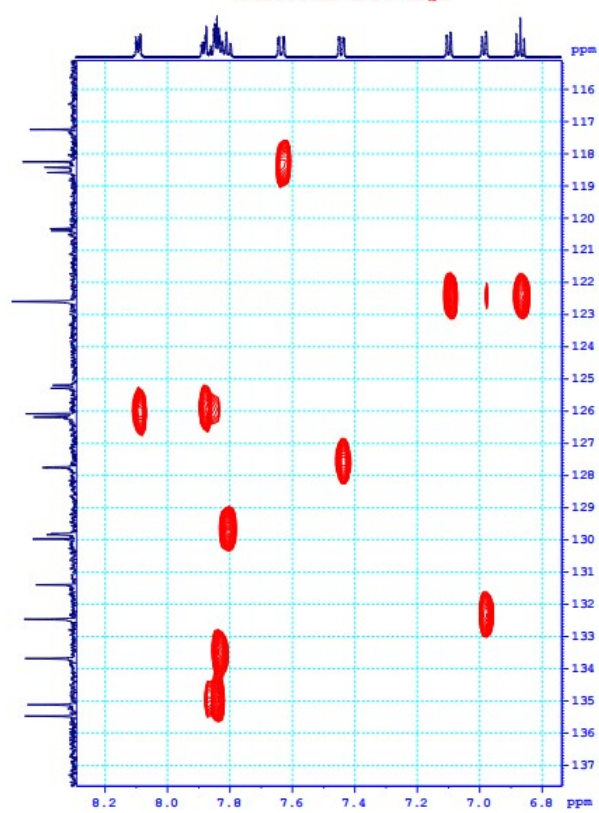
118.59  
118.43  
118.25  
117.25



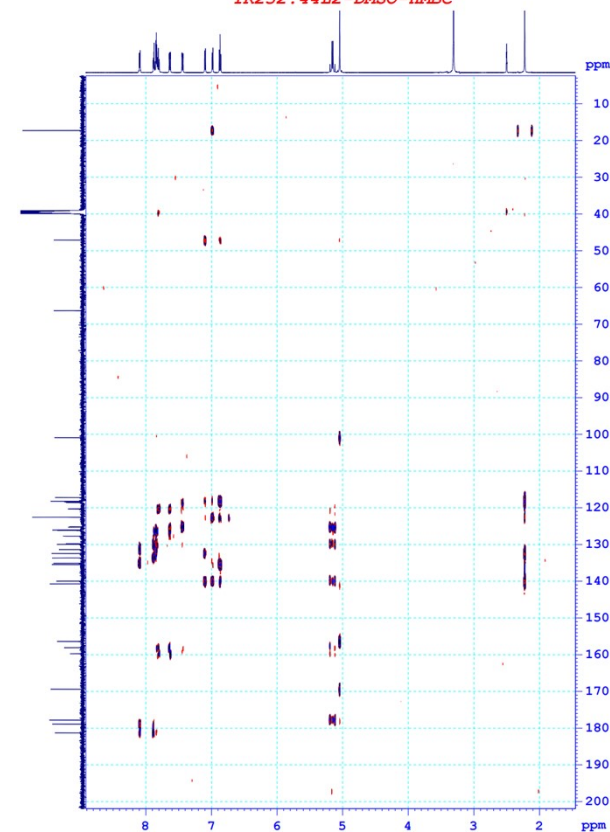
TK252. 44L2-DMSO-HSQC



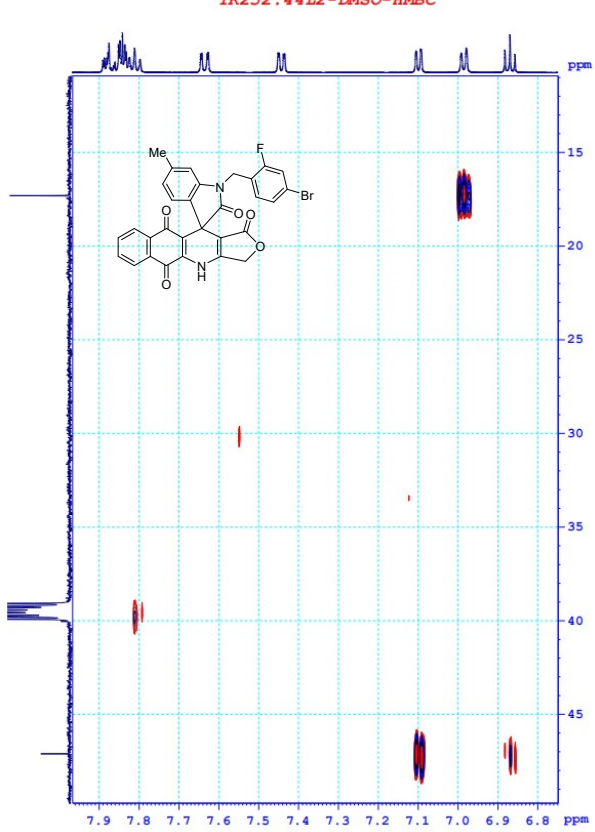
TK252. 44L2-DMSO-HSQC



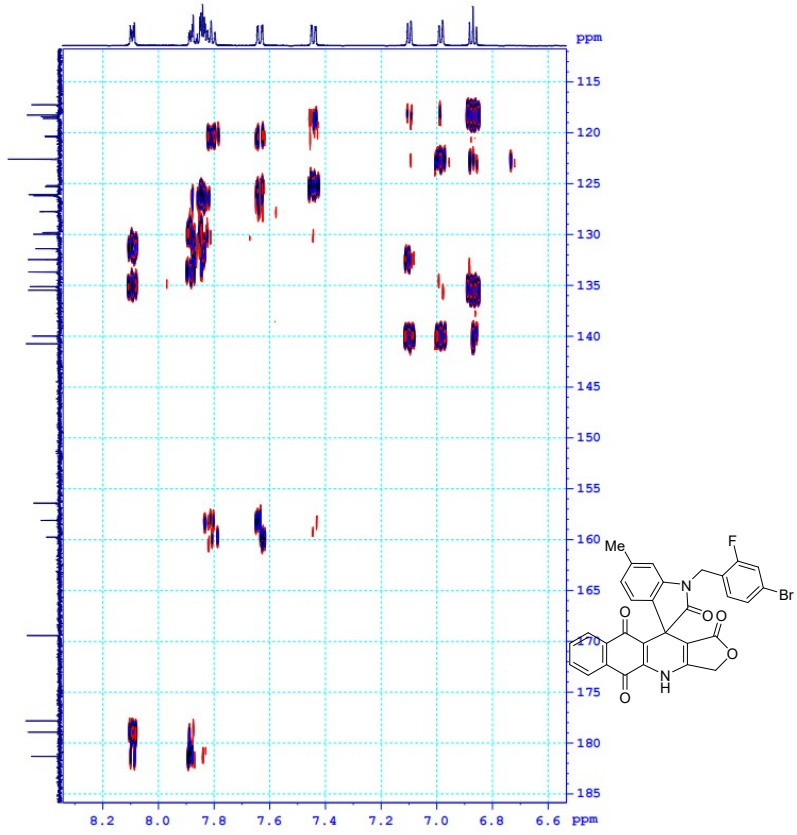
TK252. 44L2-DMSO-HMBC

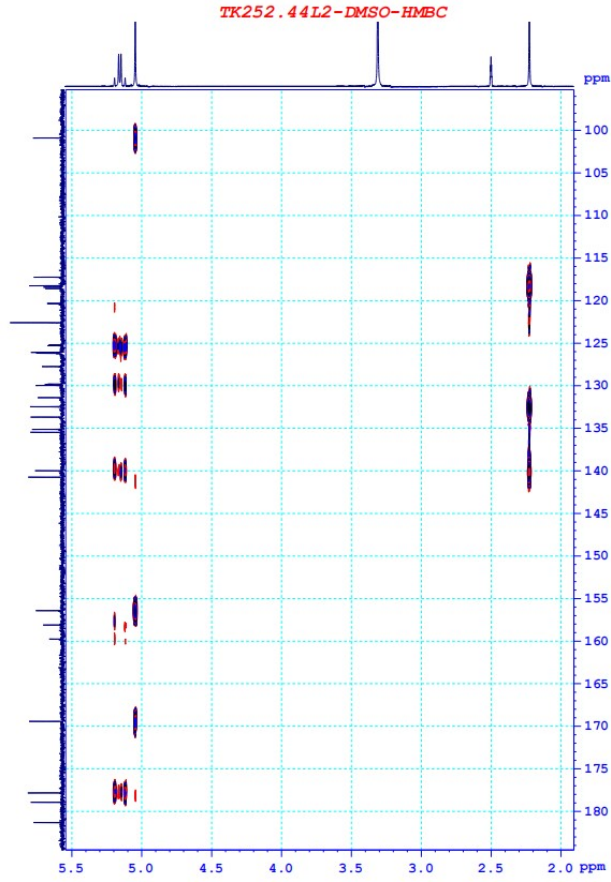


TK252. 44L2-DMSO-HMBC

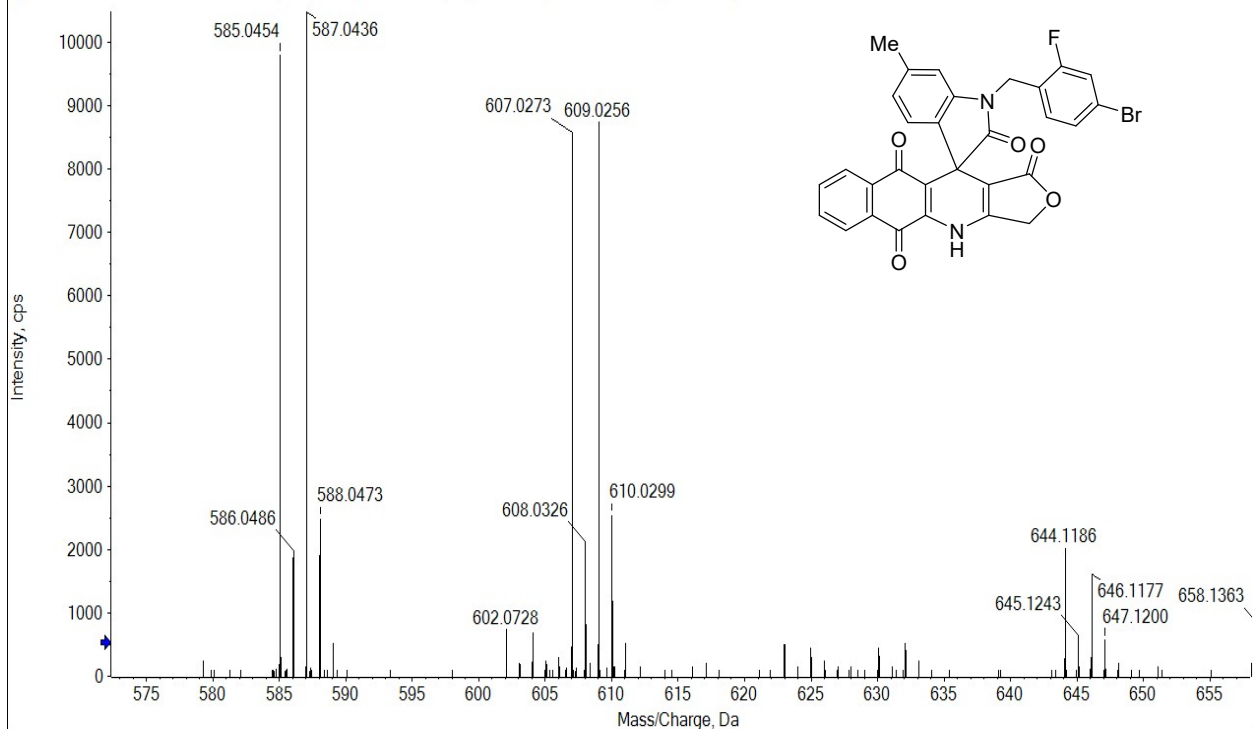


TK252.44L2-DMSO-HMBC





Spectrum from 20230208HANG.wiff2 (sample 32) - TK252.44, Experiment 1, +IDA TOF MS (20 - 4500) from 0.122 min



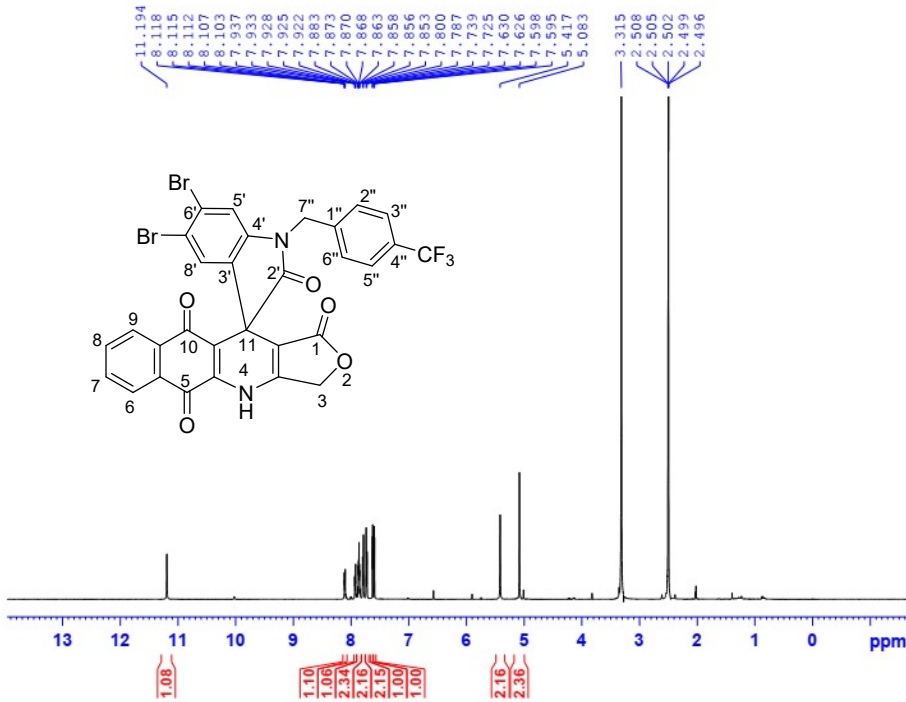
***The structural elucidation of compound 7m:***

The HR-ESI-MS of **7m** showed quasi-molecular ion peaks at  $m/z$  585.04564 and 587.0436 [ $M+H$ ]<sup>+</sup> (calcd. for  $[C_{30}H_{19}BrFN_2O_5]^+$ : 585.0456 and 587.0436) and  $m/z$  607.0273 and 609.0256 [ $M+Na$ ]<sup>+</sup> (calcd. for  $[C_{30}H_{18}BrFN_2NaO_5]^+$ : 607.0276 and 609.0255). IR spectrum revealed the presence of NH bond ( $3314\text{ cm}^{-1}$ ), carbonyl group of  $\gamma$ -butyrolactone ( $1762\text{ cm}^{-1}$ ), carbonyl group of naphthoquinone ( $1726\text{ cm}^{-1}$ ) and carbonyl group of an amide ( $1655\text{ cm}^{-1}$ ). The <sup>1</sup>H-NMR spectrum showed signals characteristic of one NH proton ( $\delta_H$  11.06 (1H, s)), four protons of quinone system { $\delta_H$  8.09 (1H, m, H-6),  $\delta_H$  7.89–7.88 (1H, m, H-9), 7.86–7.83 (2H, m, H-7, H-8)}, three benzyl aromatic protons { $\delta_H$  7.81 (1H, t,  $J = 8.4\text{ Hz}$ , H-6''), 7.64 (1H, dd,  $J = 9.6, 1.8\text{ Hz}$ , H-3''), 7.44 (1H, dd,  $J = 8.4\text{ Hz}, J = 1.8\text{ Hz}$ , H-5'')}, three indoline protons { $\delta_H$  7.09 (1H, d,  $J = 7.2\text{ Hz}$ , H-8'), 6.99 (1H, d,  $J = 7.2\text{ Hz}$ , H-5'), 6.87 (1H, t,  $J = 7.2\text{ Hz}$ , H-7')}, two benzylic methylene protons { $\delta_H$  5.18 and 5.13 (1H each, d,  $J = 17.4\text{ Hz}$ , H-7'')}, methylene group of  $\gamma$ -lactone ring { $\delta_H$  5.05 (2H, d,  $J = 16.8\text{ Hz}$ , H-3)) and methyl group at  $\delta_H$  2.23 (3H, s). The <sup>13</sup>C-NMR spectrum confirmed the presence of carbonyl carbons at  $\delta_C$  181.3 (C-10), 178.9 (C-5), 177.8 (C-2'), and 169.4 (C-1). A fluorine-coupled carbon 158.9 (d,  $J = 247.5\text{ Hz}$ , C-F) along with 10 CH carbons, 11 C<sub>q</sub> aromatic carbons, 2 CH<sub>2</sub> carbons (butyrolactone and benzyl carbon), 1 CH<sub>3</sub> carbon and 1 spiro carbon were observed. Detailed analysis of the HSQC spectrum confirmed the direct correlations between protons and carbons. Notable assignments included  $\delta_H/\delta_C$  correlations at 5.05/66.4 (H-3/C-3) and 5.18, 5.13/39.92 (H-7''/C-7''), further supporting the spiro connectivity. The aromatic regions showed expected correlations such as  $\delta_H$  7.64/118.6 (H-3''/C-3'') and  $\delta_H$  7.44/127.8 (H-5''/C-5''). The structure was further elucidated by the HMBC spectrum, which revealed long-range correlations supporting the connectivity of the spiro system and the substitution patterns. Correlations from H-3 to C-3a, C-4', and C-6', as well as from H-7'' to C-1 and C-11, confirmed the spiro connection and the placement of the benzyl substituent. The methyl group at C-9' was verified by correlations from H-9 to C-8, C-10, and C-11. These analyses conclusively determined the structure of product **7m** as 1'-(4-bromo-2-fluorobenzyl)-6'-methyl-3*H*-spiro[benzo[*g*]furo[3,4-*b*]quinoline-11,3'-indoline]-1,2',5,10(4*H*)-tetraone.



14. 5',6'-Dibromo-1'-(4-(trifluoromethyl)benzyl)-3H-spiro[benzo[g]furo[3,4-b]quinoline-11,3'-indoline]-1,2',5,10(4H)-tetraone (7n)

TK252.51L2-DMSO-1H



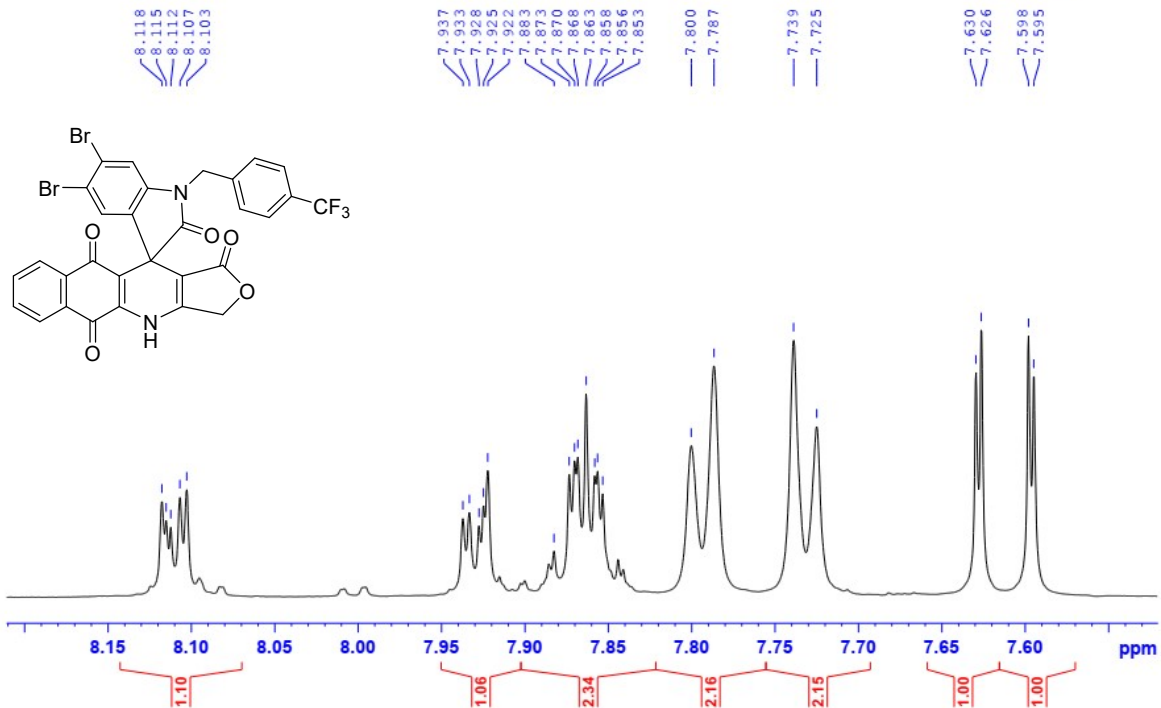
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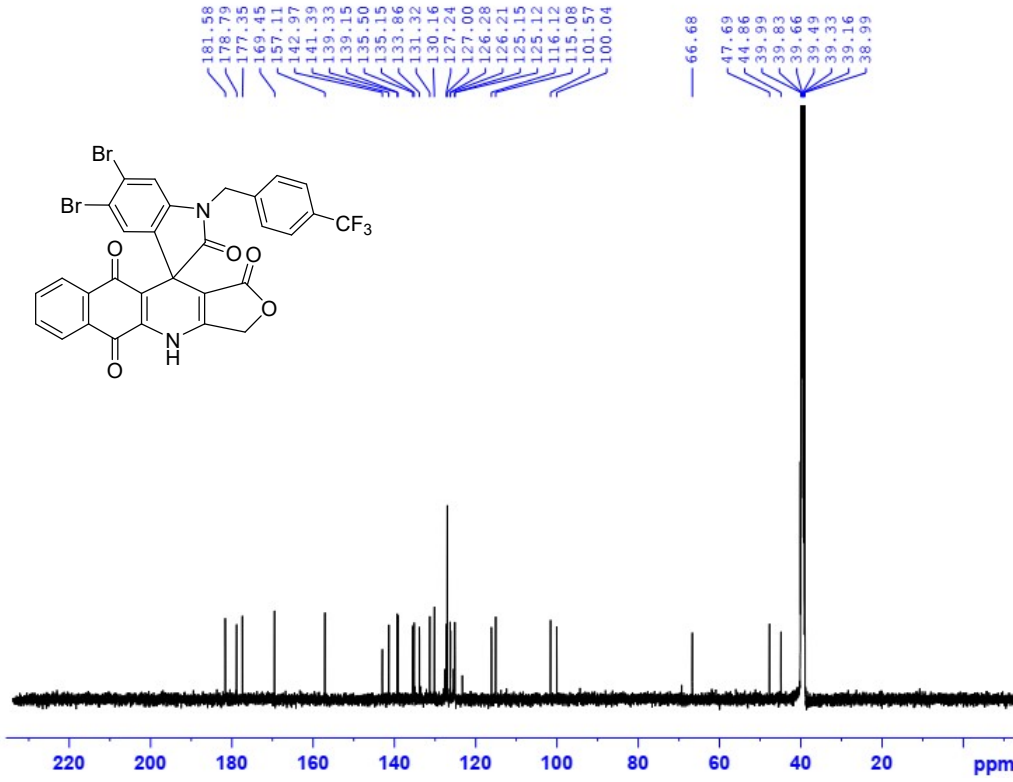
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TK252.51L2-DMSO-1H



TK252.51L2-DMSO-C13CPD



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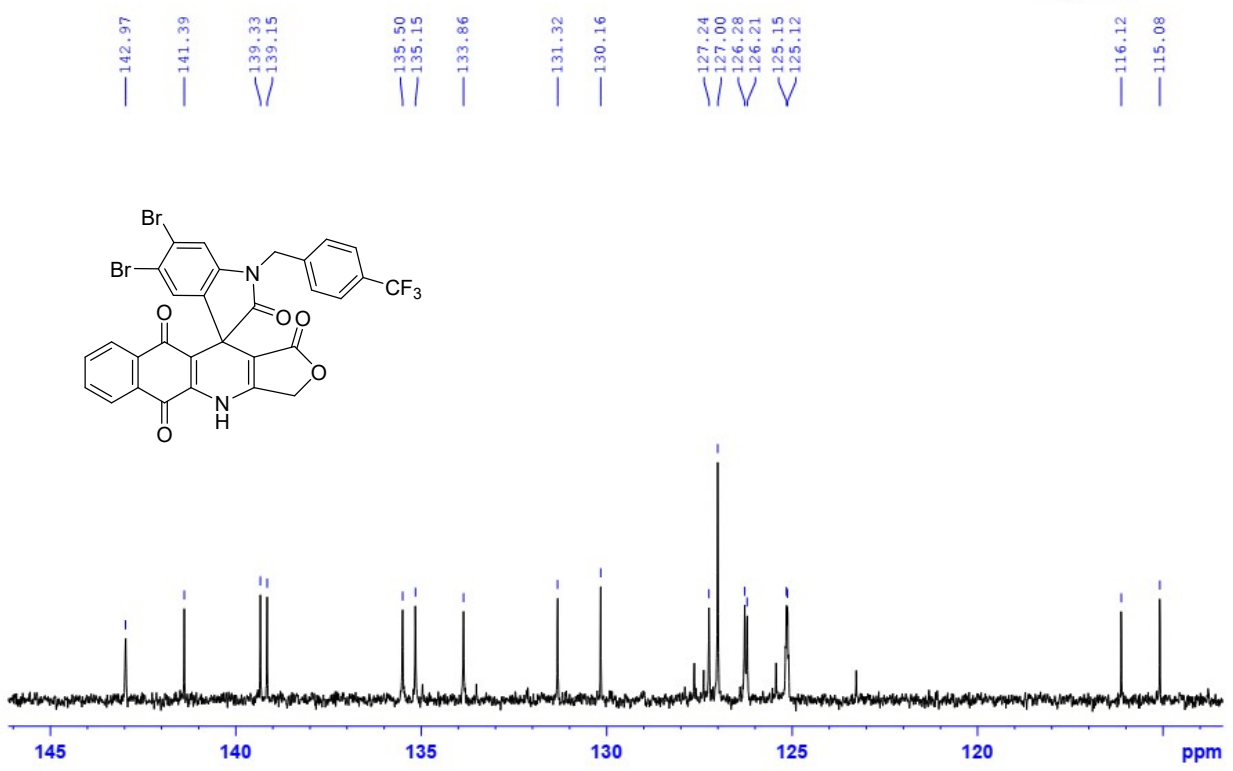
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F2 - Processing parameters  
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TK252.51L2-DMSO-C13CPD



Spectrum from 20230208HANG.wiff2 (sample 33) - TK252.51L2, Experiment 1, +IDA TOF MS (20 - 4500) from 0.295 min

