

## Supplementary Materials

# Design and Synthesis of (2-oxo-1,2-Dihydroquinolin-4-yl)-1,2,3-triazole Derivatives via Click Reaction: Potential Apoptotic Antiproliferative Agents

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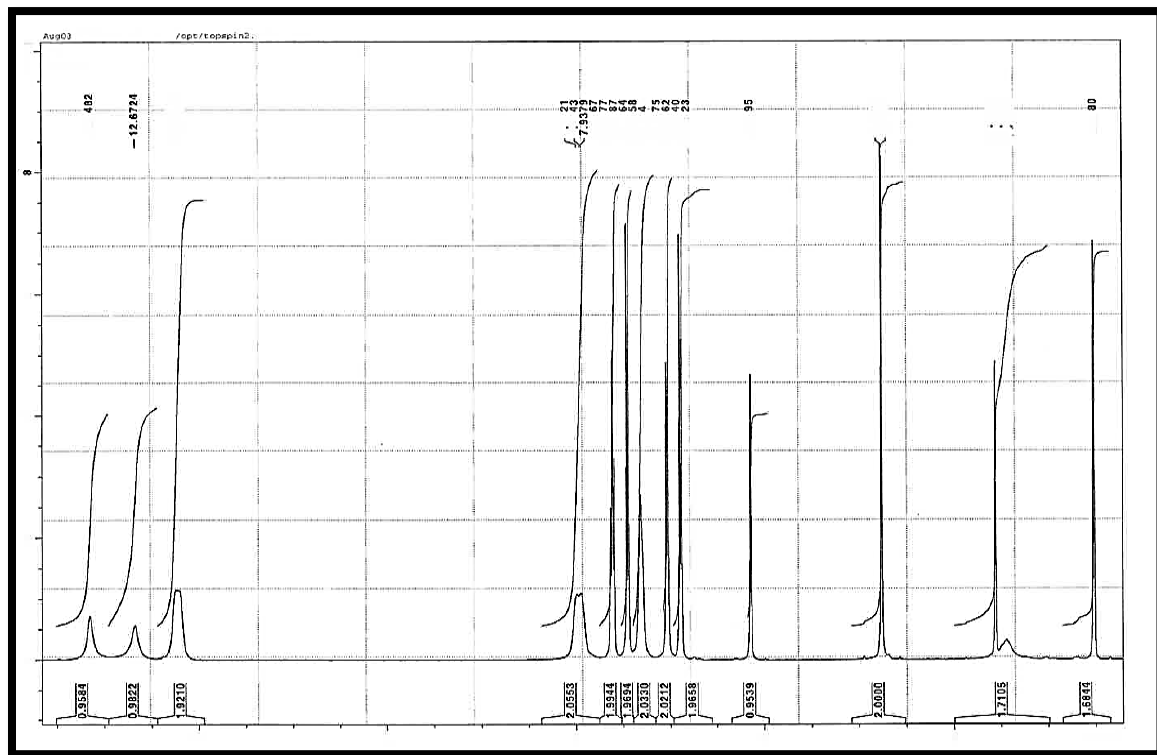
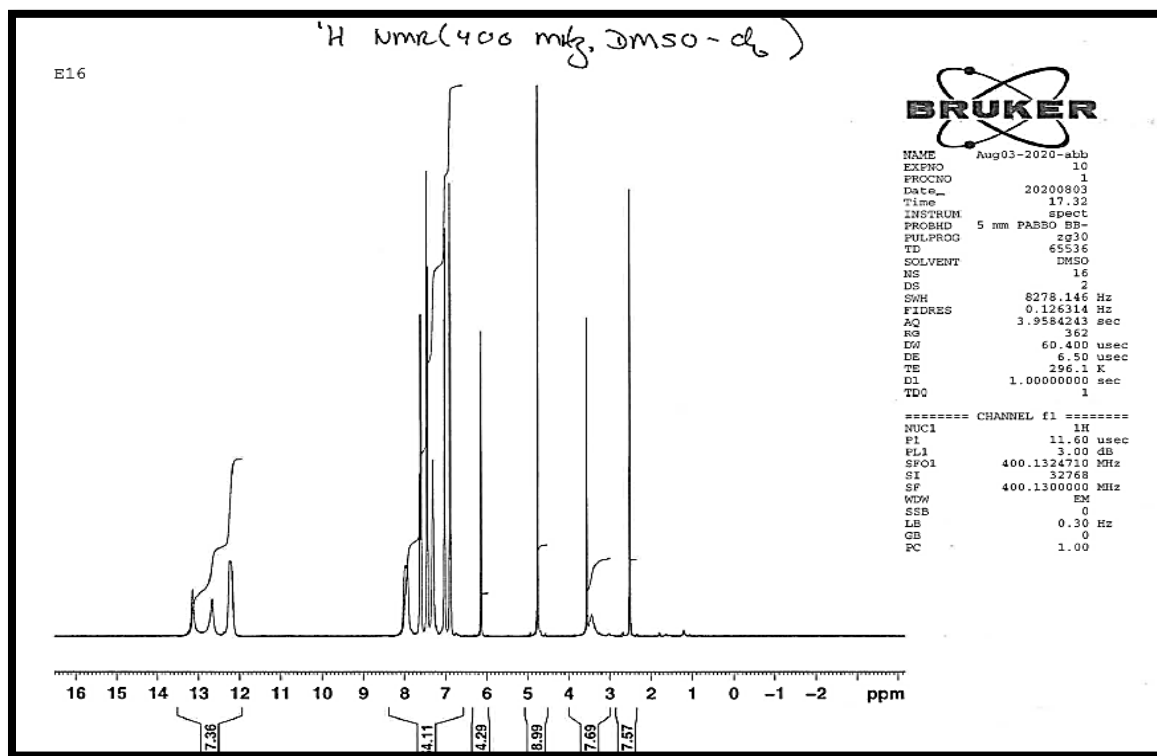
<sup>6</sup> Institute of Organic Chemistry, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

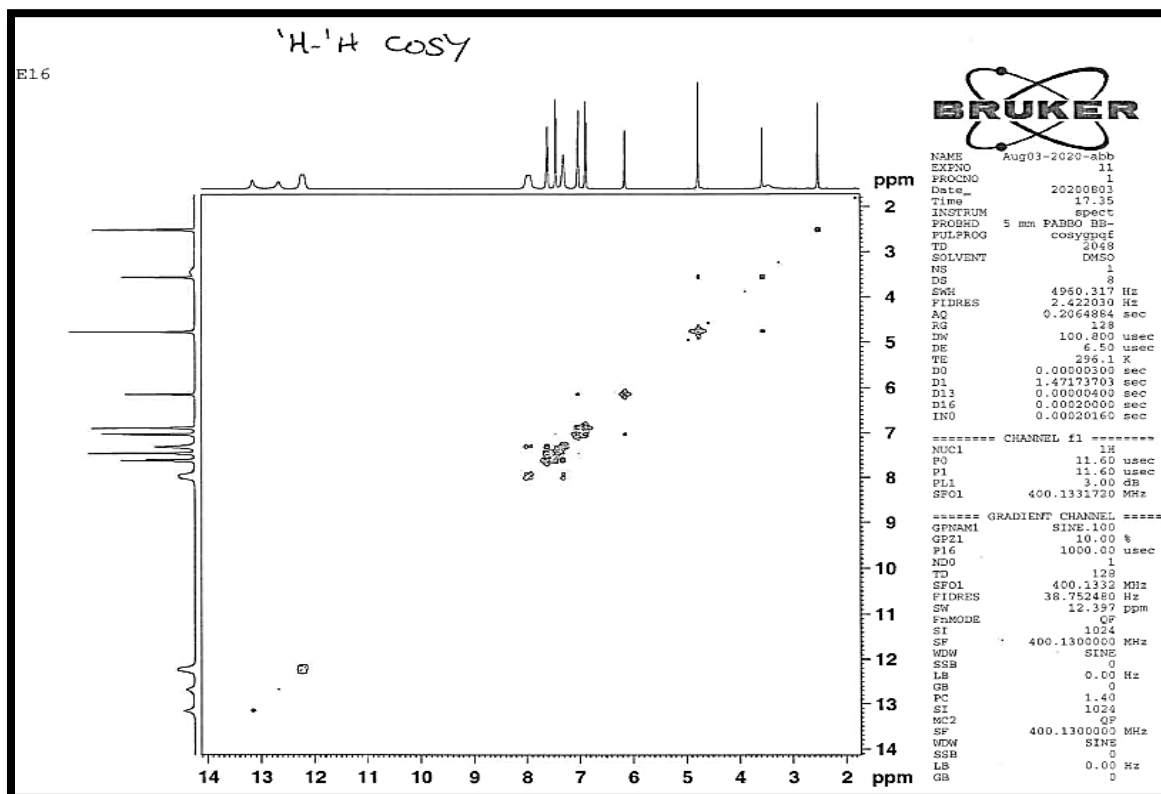
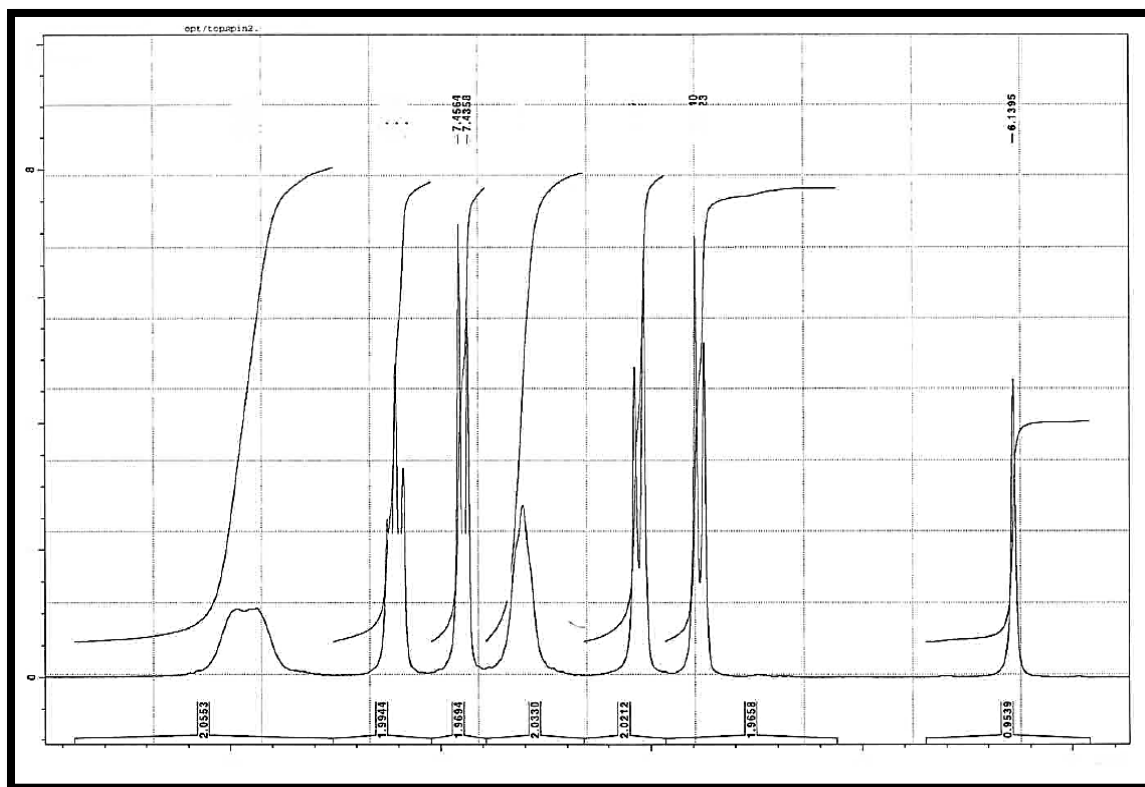
<sup>7</sup> Institute of Biological and Chemical Systems (IBCS-FMS), Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

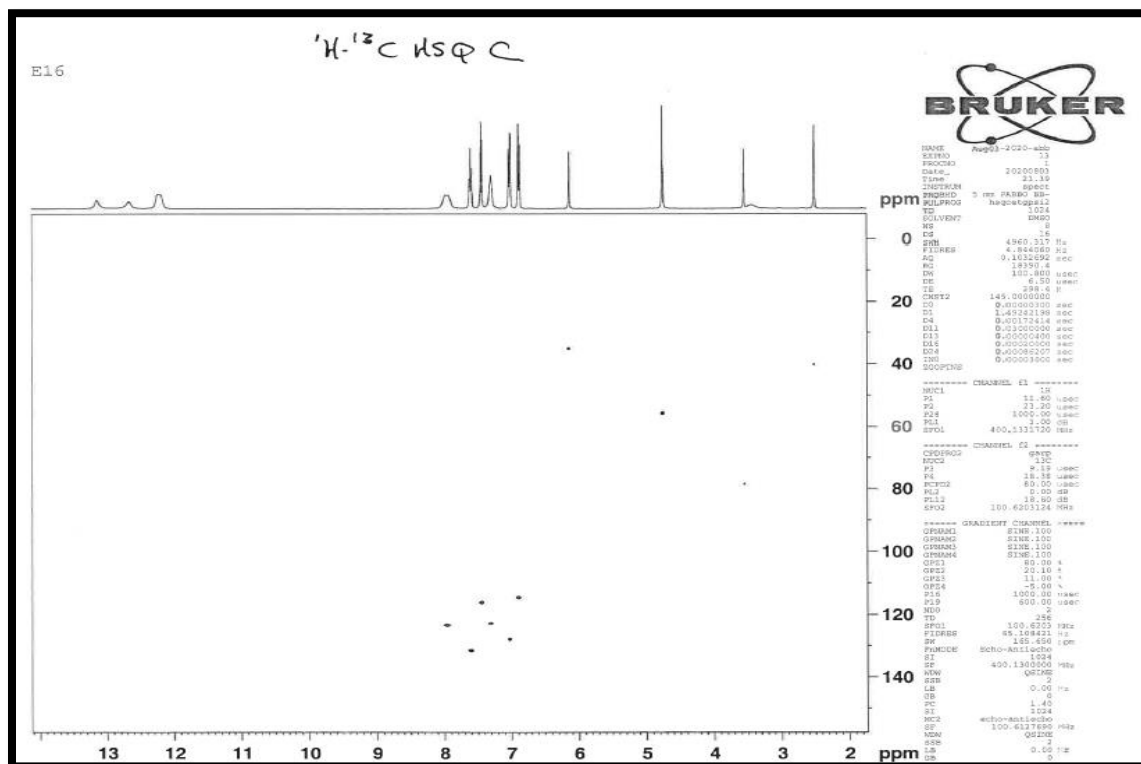
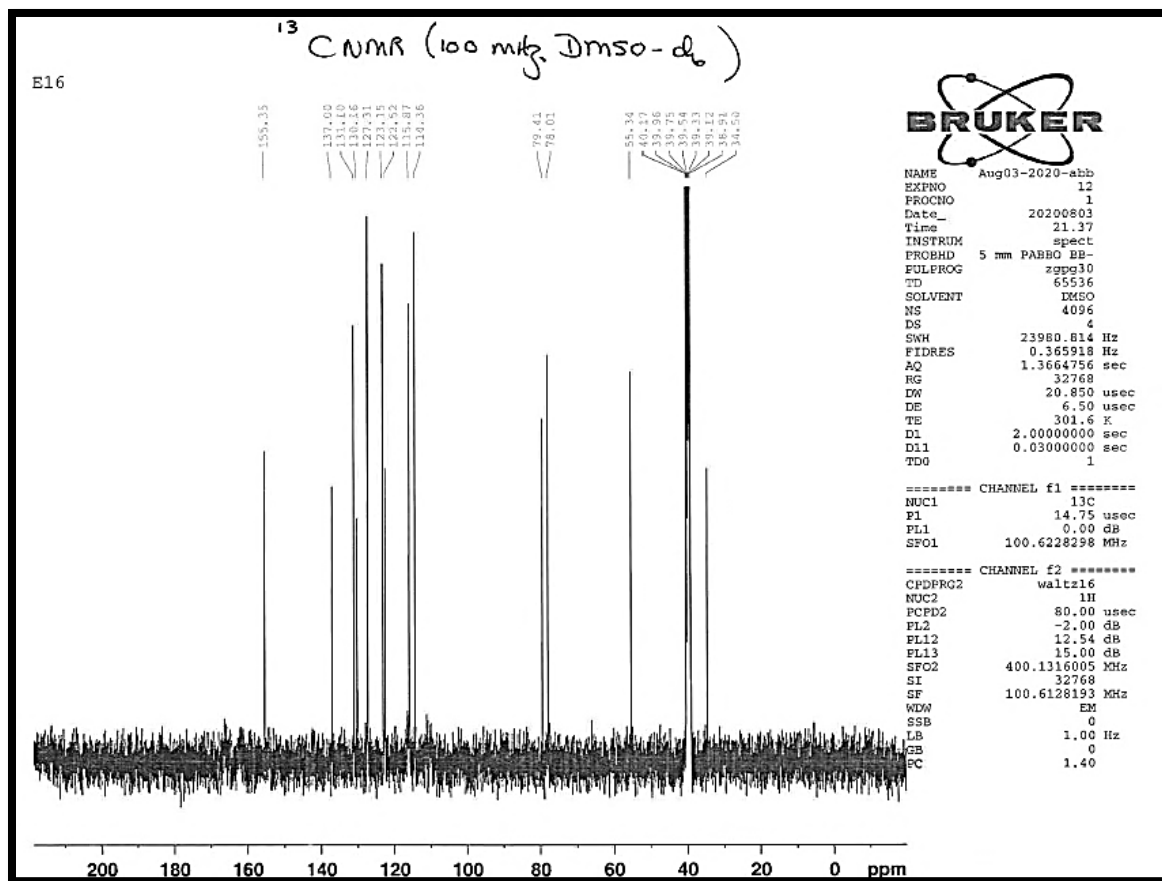
<sup>8</sup> Pharmaceutical Organic Chemistry Department, Faculty of Pharmacy, Assiut University, Assiut 71526, Egypt

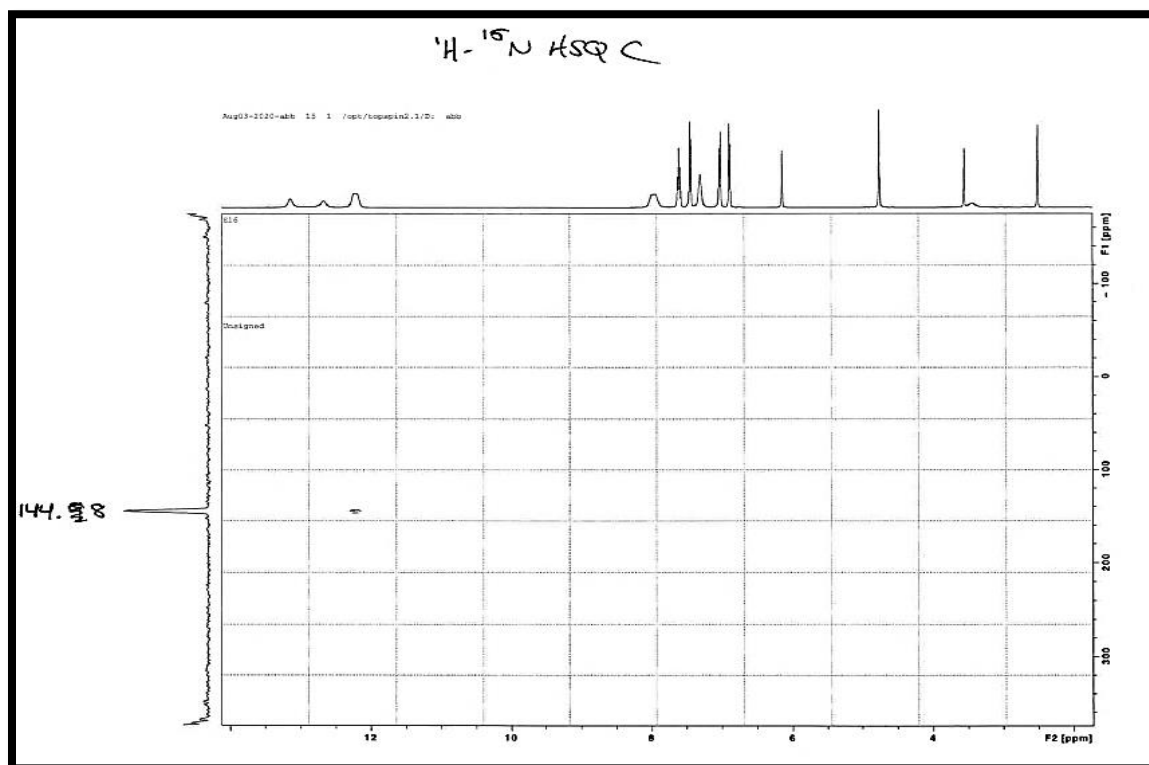
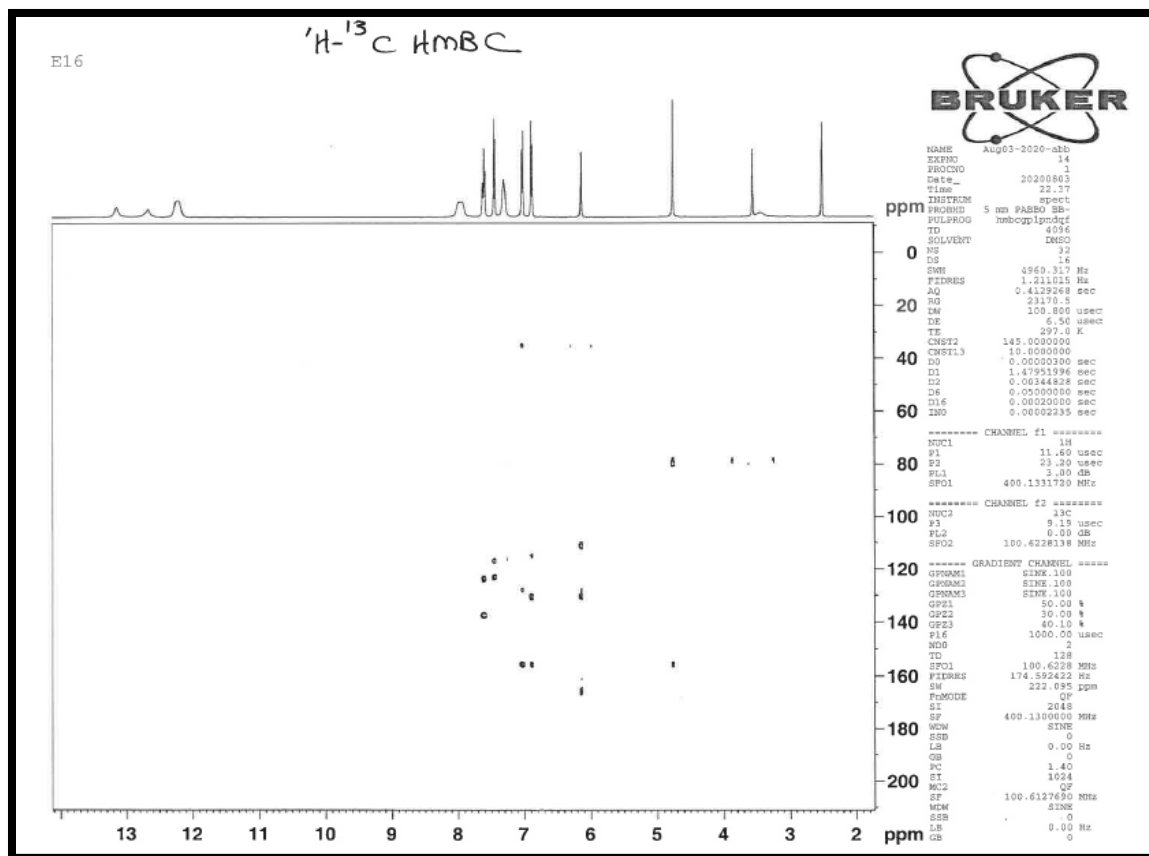
\* Correspondence: essmat\_elsheref@mu.edu.eg (E.M.E.-S.); braese@kit.edu (S.B.); bgyoussif@ju.edu.sa (B.G.M.Y.); Tel: +20-1064890489 (E.M.E.-S.); +49-721-608-42902 (S.B.); +20-1098294419 (B.G.M.Y.)

# Spectrum data for Compound 4a









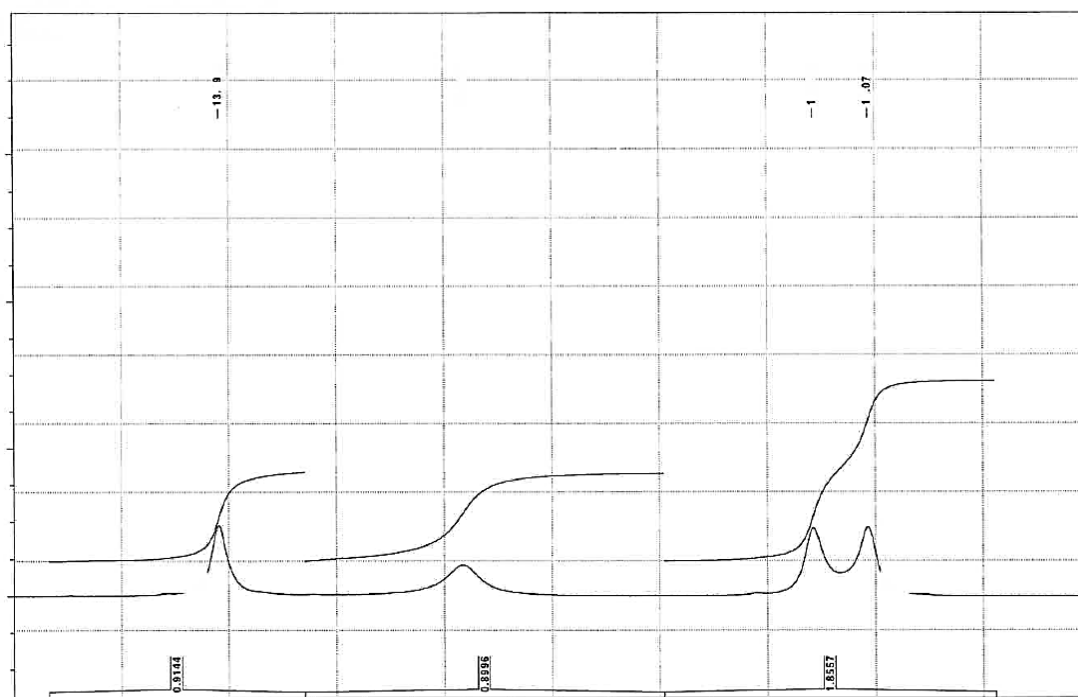
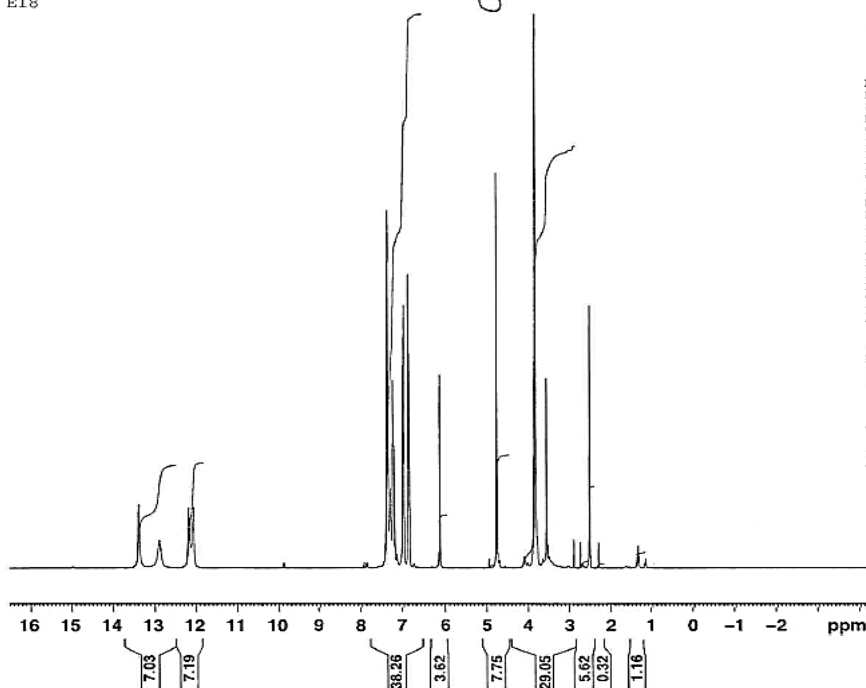
Spectrum data for Compound 4b

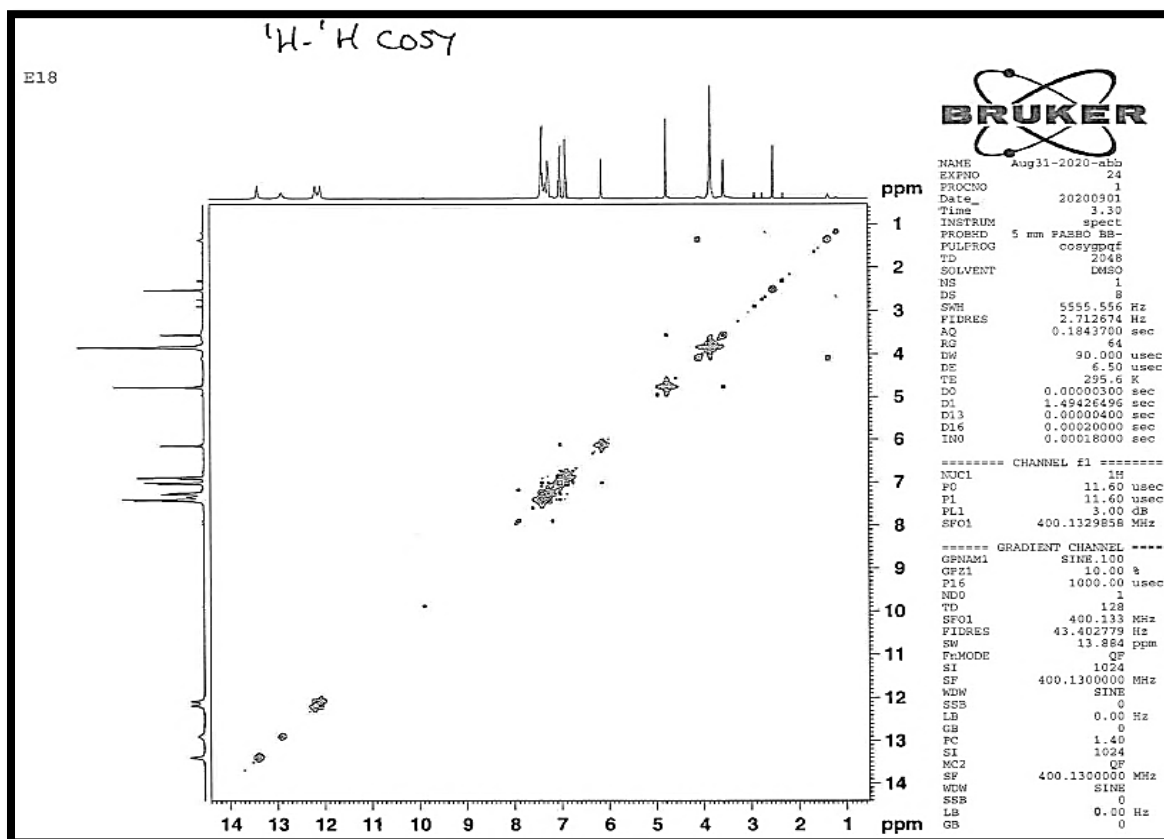
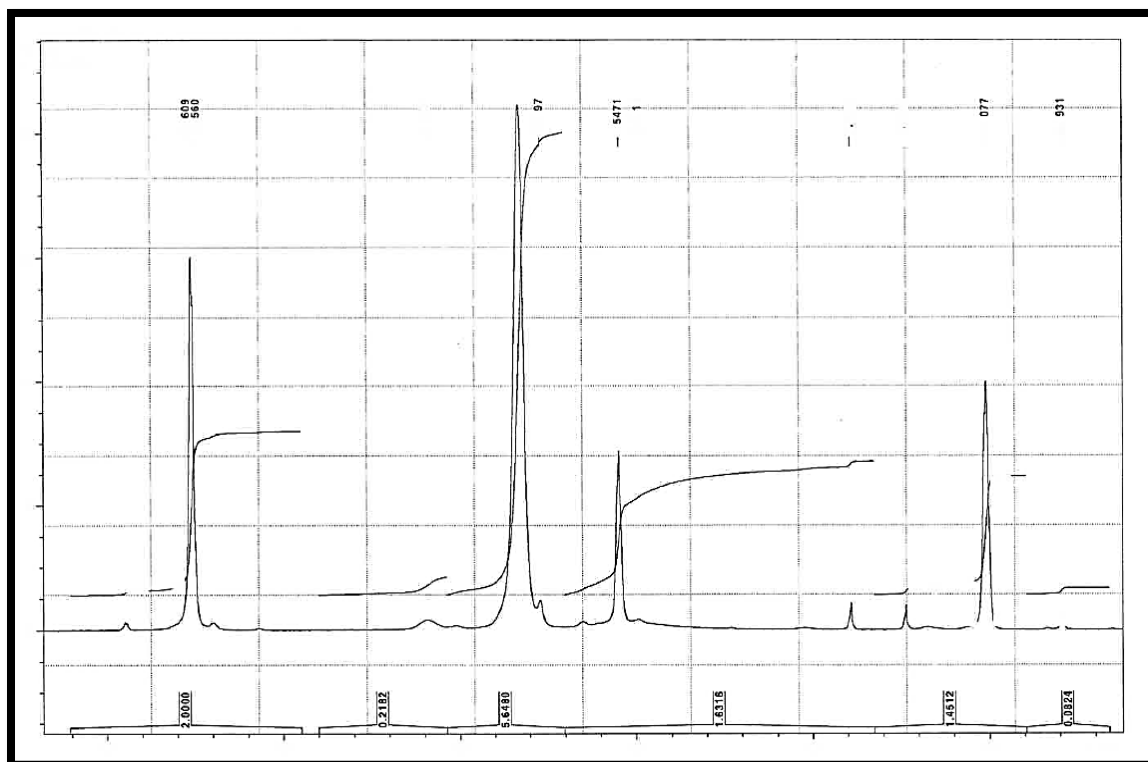
E18

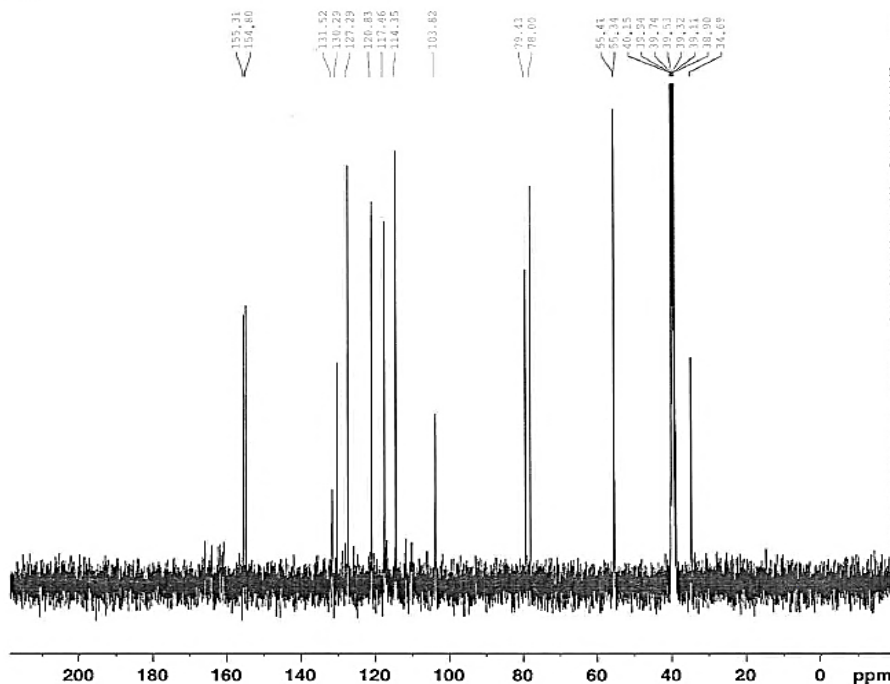
<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>)

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PROBHD 5 mm F400 EB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 181  
DW 60.400 usec  
DE 6.50 usec  
TE 297.4 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 11.60 usec  
PL1 3.00 dB  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )

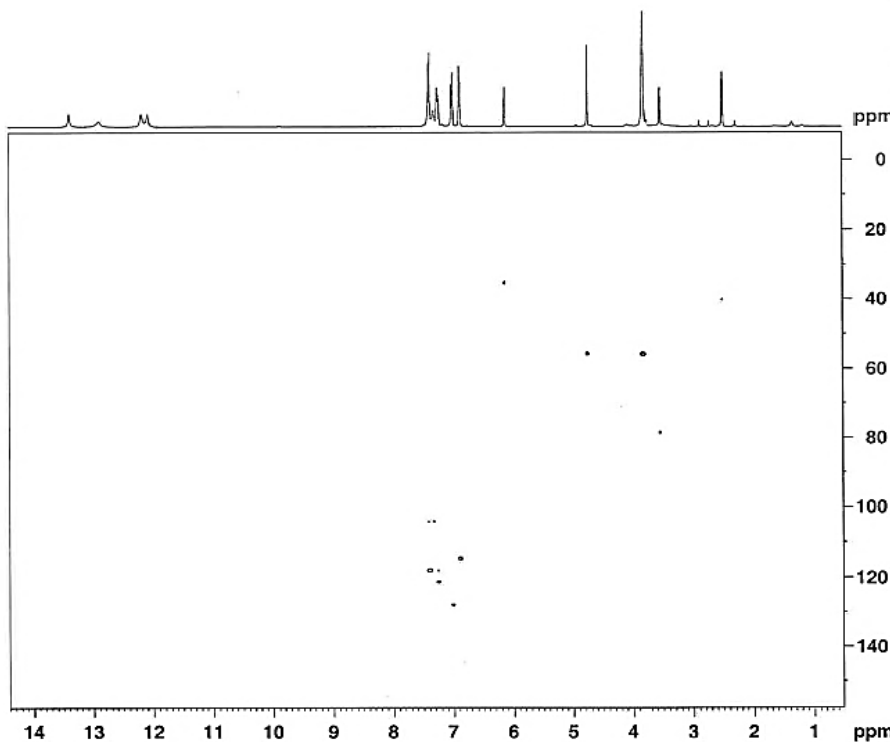
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|---------|----------------|
| NAME    | Aug31-2020-abb |
| EXPNO   | 20             |
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| Date_   | 20200901       |
| Time    | 0.12           |
| INSTRUM | spect          |
| PROBHD  | 5 mm PABBO BB- |
| PULPROG | zgpg30         |
| TD      | 65536          |
| SOLVENT | DMSO           |
| NS      | 4096           |
| DS      | 4              |
| SWH     | 23980.814 Hz   |
| FIDRES  | 0.365918 Hz    |
| AQ      | 1.3664756 sec  |
| RG      | 32768          |
| DW      | 20.850 usec    |
| DE      | 6.50 usec      |
| TE      | 300.6 K        |
| D1      | 2.00000000 sec |
| D11     | 0.03000000 sec |
| TD0     | 1              |

```
===== CHANNEL f1 =====
NUC1          13C
P1             14.75 usec
PL1            0.00 dB
SFO1          100.6228298 MHz
```

```

***** CHANNEL f2 *****
CPDPRG2          waltz16
NUC2              1H
PCPD2            80.00 usec
PL2              -2.00 dB
PL12             12.54 dB
PL13             15.00 dB
SFO2             400.1316005 MHz
SI               32768
SF              100.6128193 MHz
WDM              EM
SSB              0
LB               1.00 Hz
GB               0
PC               1.40

```

 ${}^1\text{H}-{}^{13}\text{C}$  HSQC

|         |                     |       |
|---------|---------------------|-------|
| NAME    | Aug 11 - 2020 - 880 | 23    |
| EXPNO   |                     | 2     |
| PROCNO  |                     | 1     |
| DATE_   | 20200901            |       |
| TIME    |                     | 0.18  |
| INSTRUM |                     | spect |
| PROBHD  | 5 mm PABBO BB-      |       |
| PULPROG | zgpg30              | 2     |
| TD      | 1624                |       |
| SOLVENT | IMSD                | 0     |
|         |                     | 0     |
| DW      | 555.55              | Hz    |
| F2      | 321.337             | Hz    |
| AQ      | 0.02218             | sec   |
| HG      | 13390.4             |       |
| TE      | 300.00              | TEMP  |
| DE      | 6.50                | mm    |
|         | 297.1               | K     |
| CHRG2   | 145.000000          |       |
| D0      | 0.00000000          | sec   |
| D1      | 0.04266953          | sec   |
| D2      | 0.07177414          | sec   |
| D11     | 0.23000000          | sec   |
| D12     | 0.00000400          | sec   |
| D13     | 0.00000000          | sec   |
| D14     | 0.00000000          | sec   |
| IMD     | 0.00000000          | sec   |

```
***** CHANNEL #1 *****
MUC1      1M
P1         11.50 used
P2         23.20 used
P28        1000.00 used
PFL        3.00 dB
SPOT1      400.1329858 MHz
```

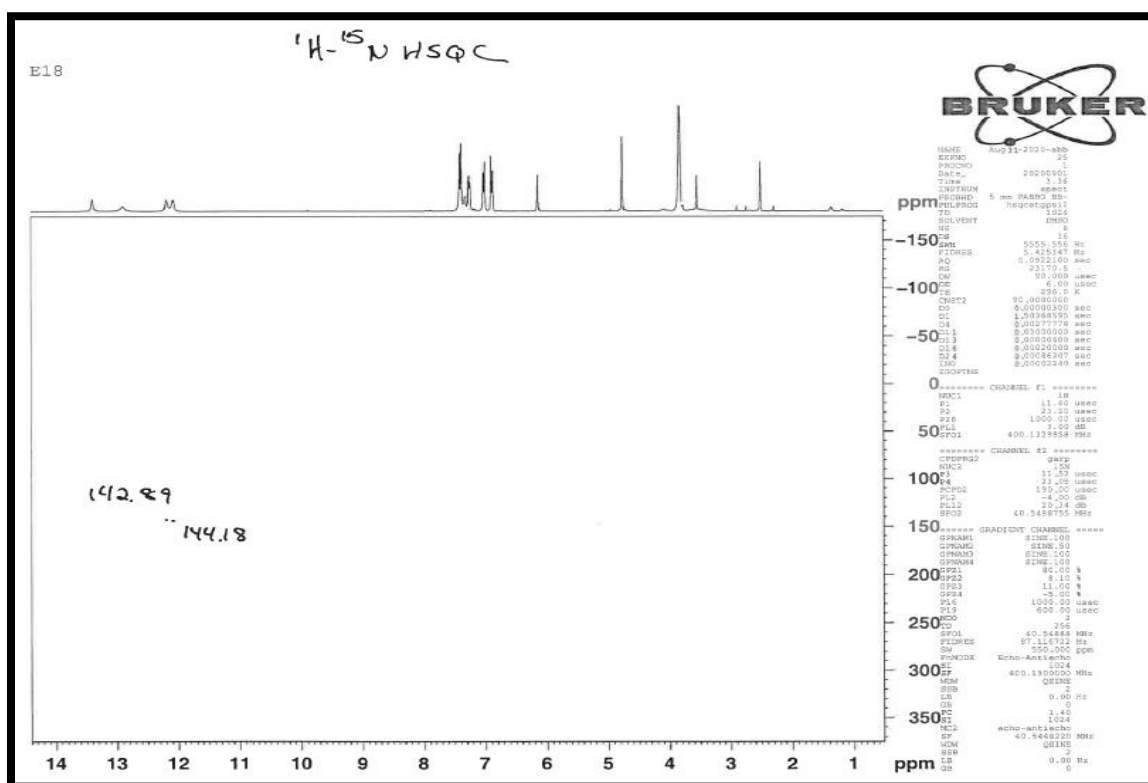
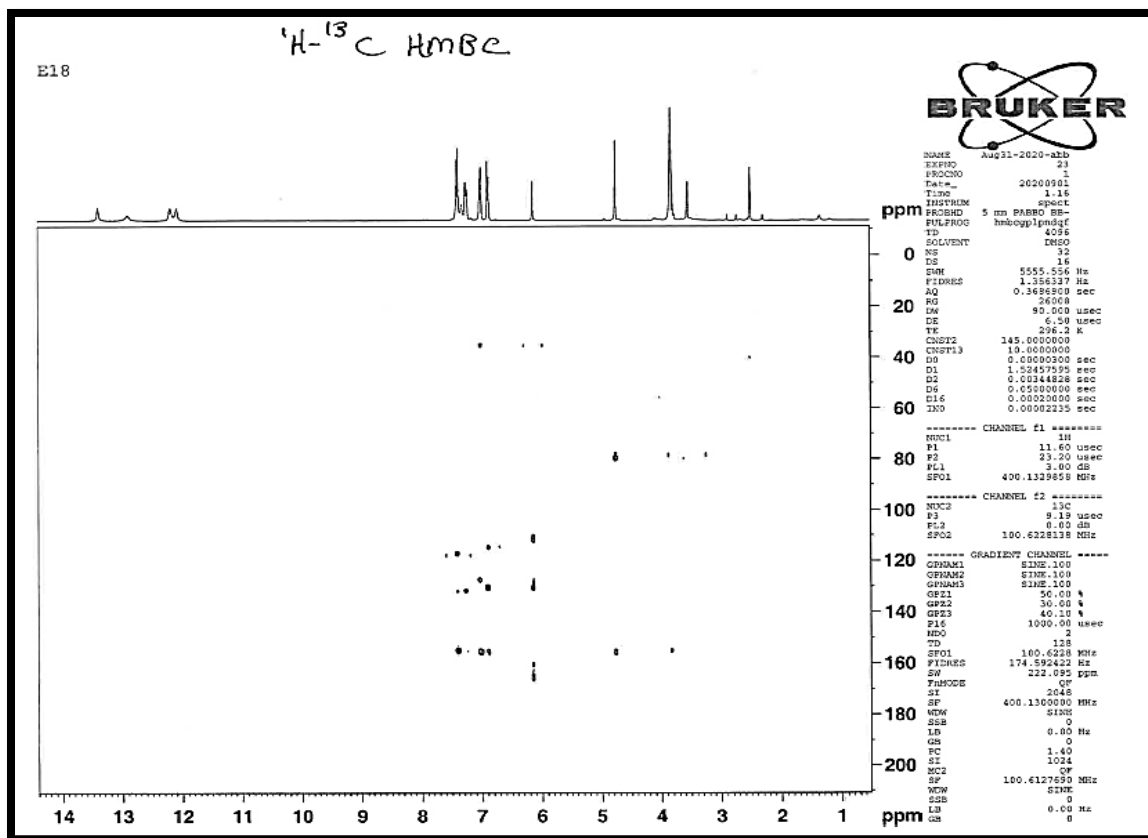
```
***** CHANNEL #2 *****
CPEPRG2      garp
NUC2          13C
P3            9.19 used
P4            18.36 used
PCPDG        80.00 used
FL2           0.00 dB
FL12          18.80 dB
SPG2         100.6203124 MHz
```

```

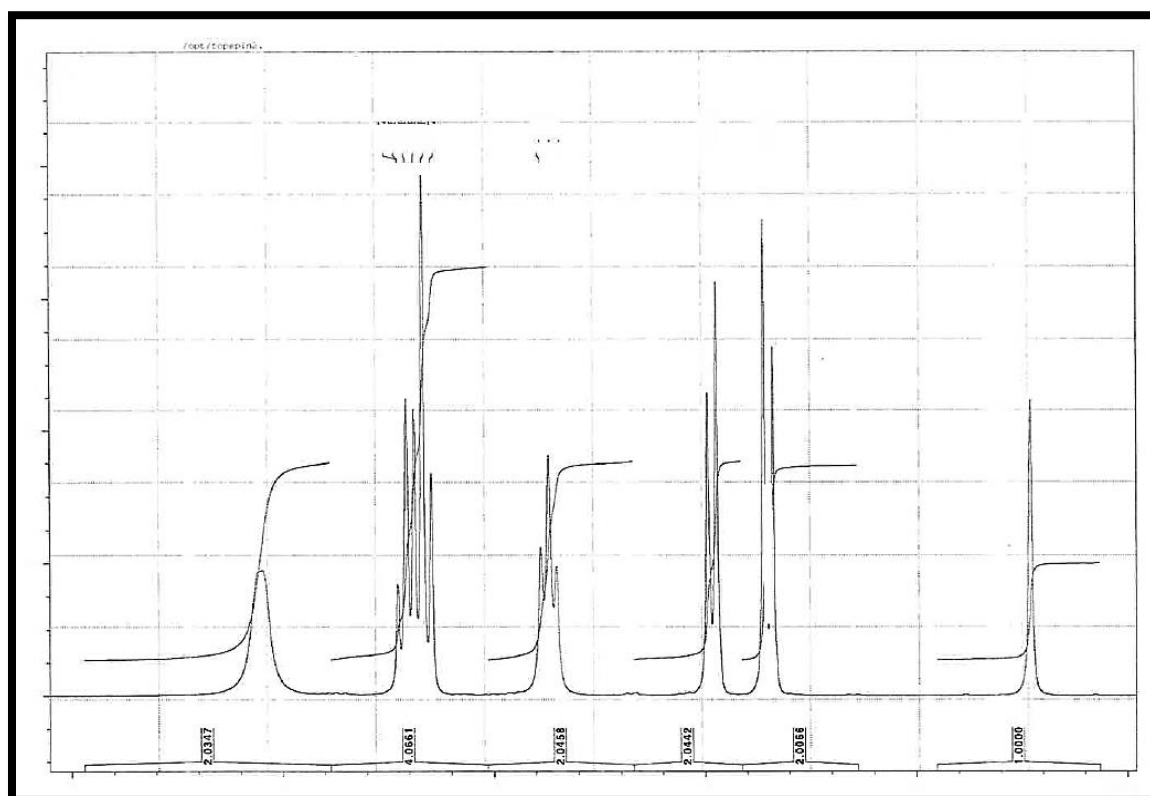
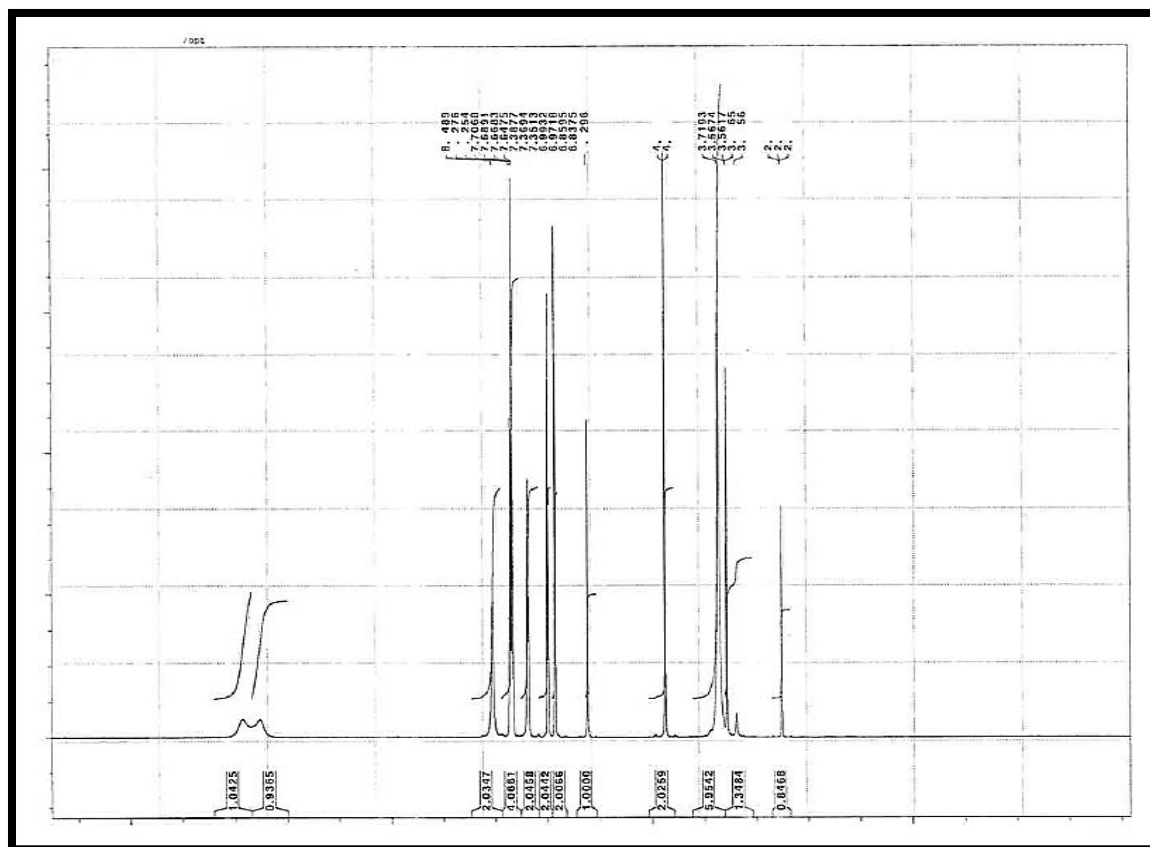
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CPNAME1      SINZ.100
CPNAME2      SINZ.100
CPNAME3      SINZ.100
CPNAME4      SINZ.100
GPZ1         80.00  t
GPZ2         20.10  t
GPZ3         11.00  t
GPZ4         -5.00  t
P16          1000.00  used
P19          600.00  used

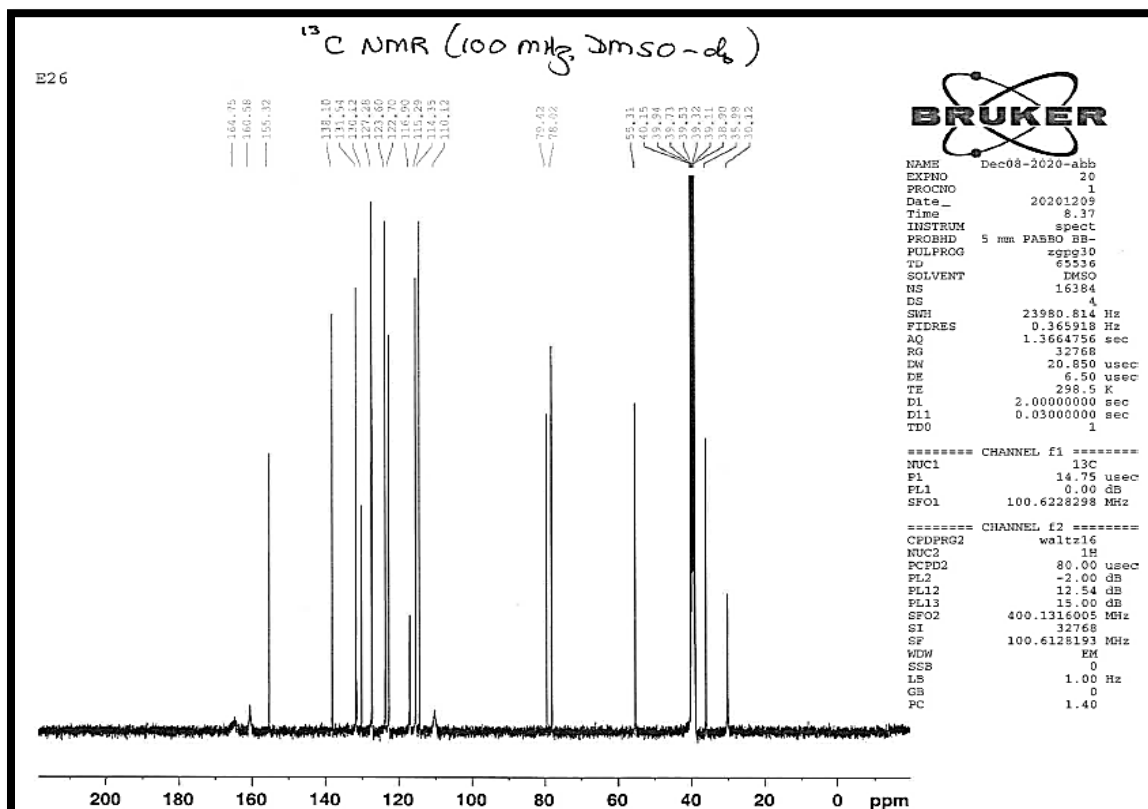
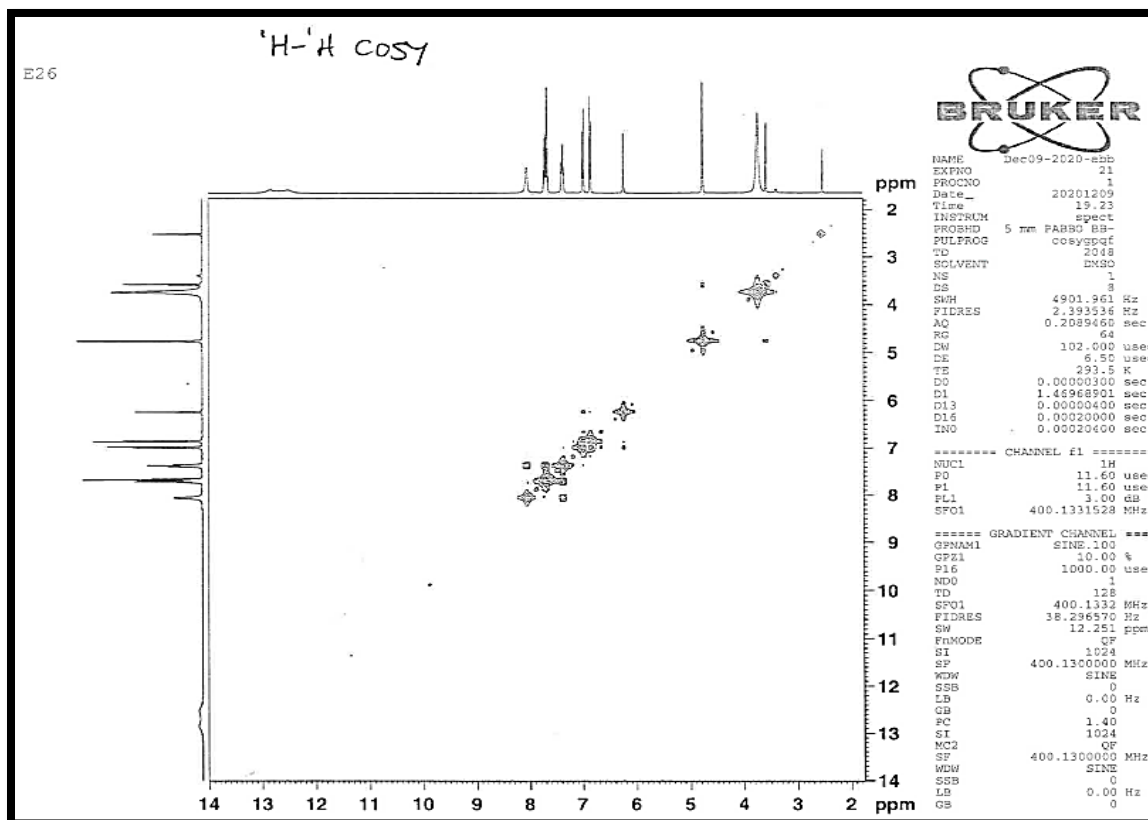
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|        |               |     |
|--------|---------------|-----|
| TO     | 255           |     |
| SP01   | 100.6203      | Hz  |
| FI0000 | 65.108421     | Hz  |
| SM     | 165.650       | pps |
| PR0000 | Echo-Antiecho |     |
| ST     | 1024          |     |
| SF     | 400.1300000   | MHz |
| MDM    | QTIME         |     |
| SDB    | 2             |     |
| LB     | 0.00          | Hz  |
| QR     | 0             |     |
| PC     | 1.40          |     |
| SI     | 1024          |     |
| MC2    | echo-antiecho |     |
| SF     | 100.6127693   | MHz |
| MDM    | QTIME         |     |
| SDB    | 2             |     |
| LB     | 0.00          | Hz  |
| QR     | 0             |     |





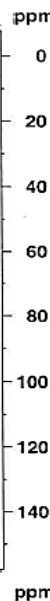
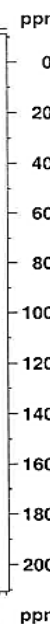


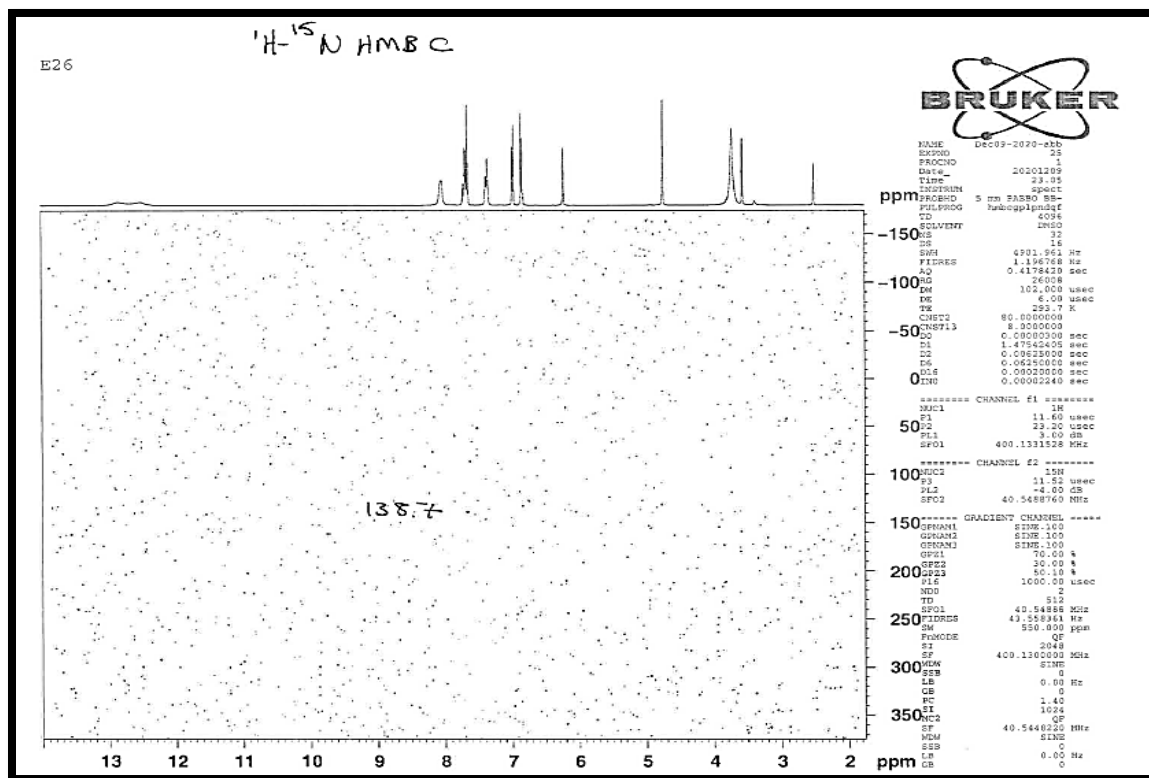


${}^1\text{H}-{}^{13}\text{C HSQC}$ 

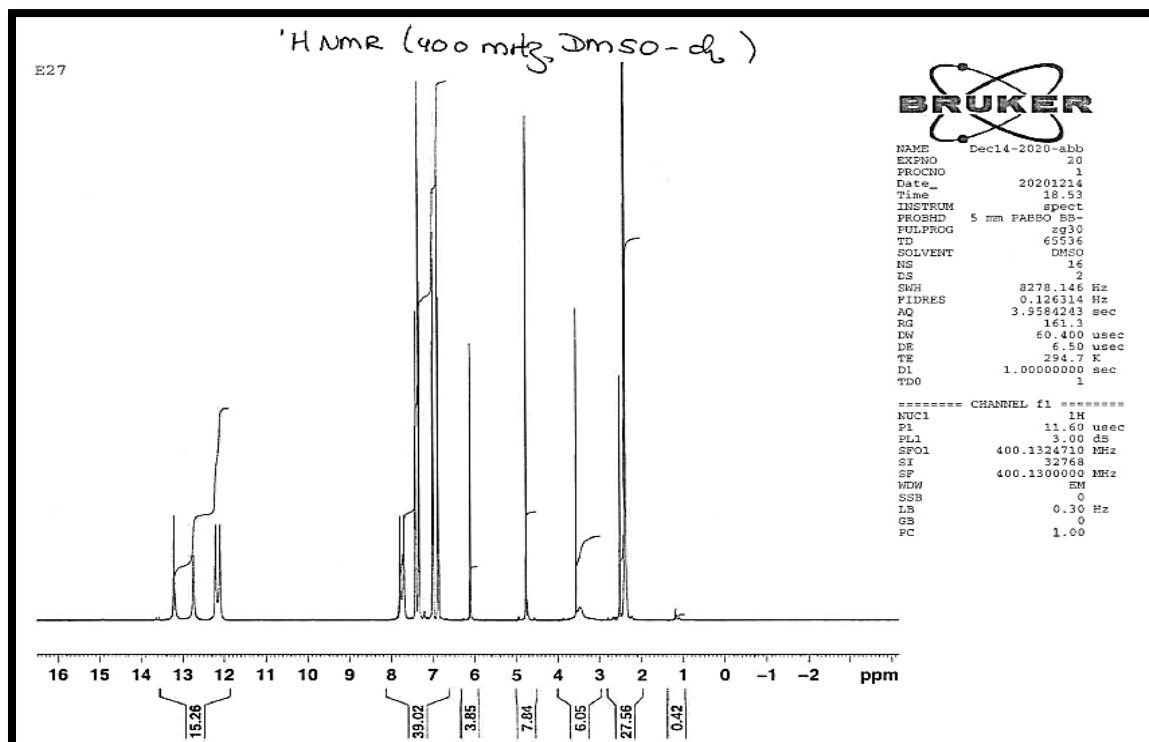
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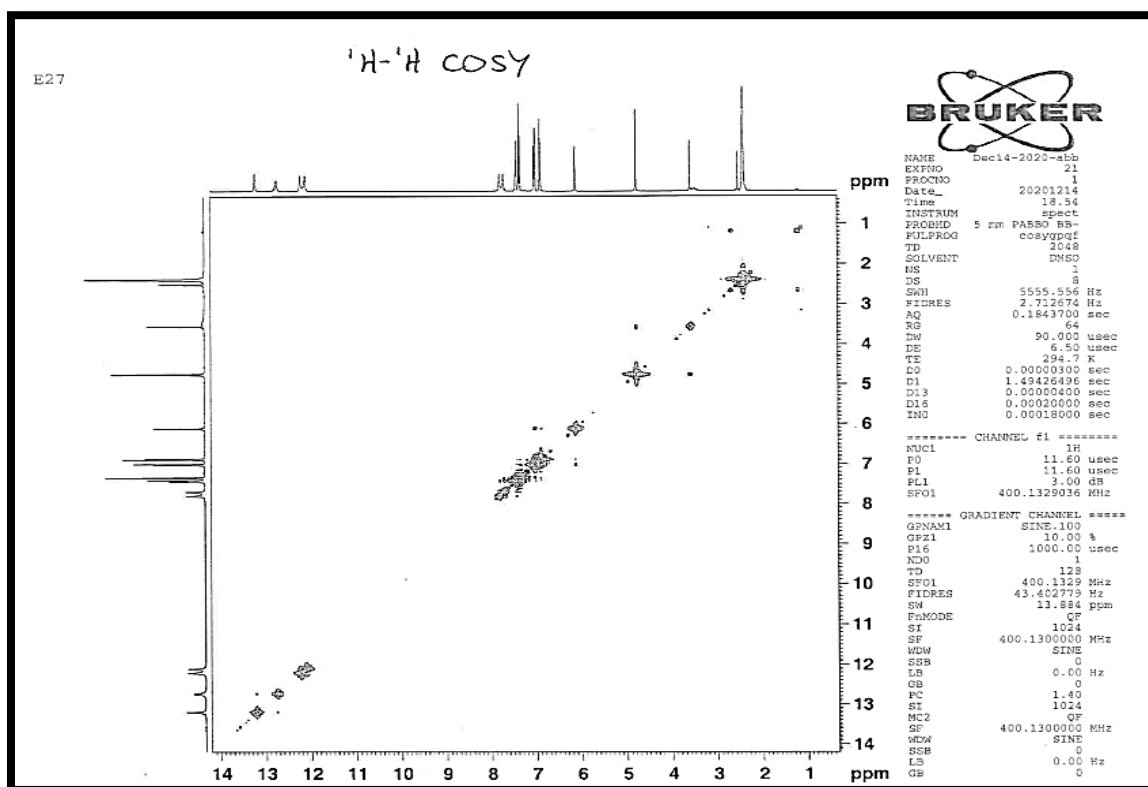
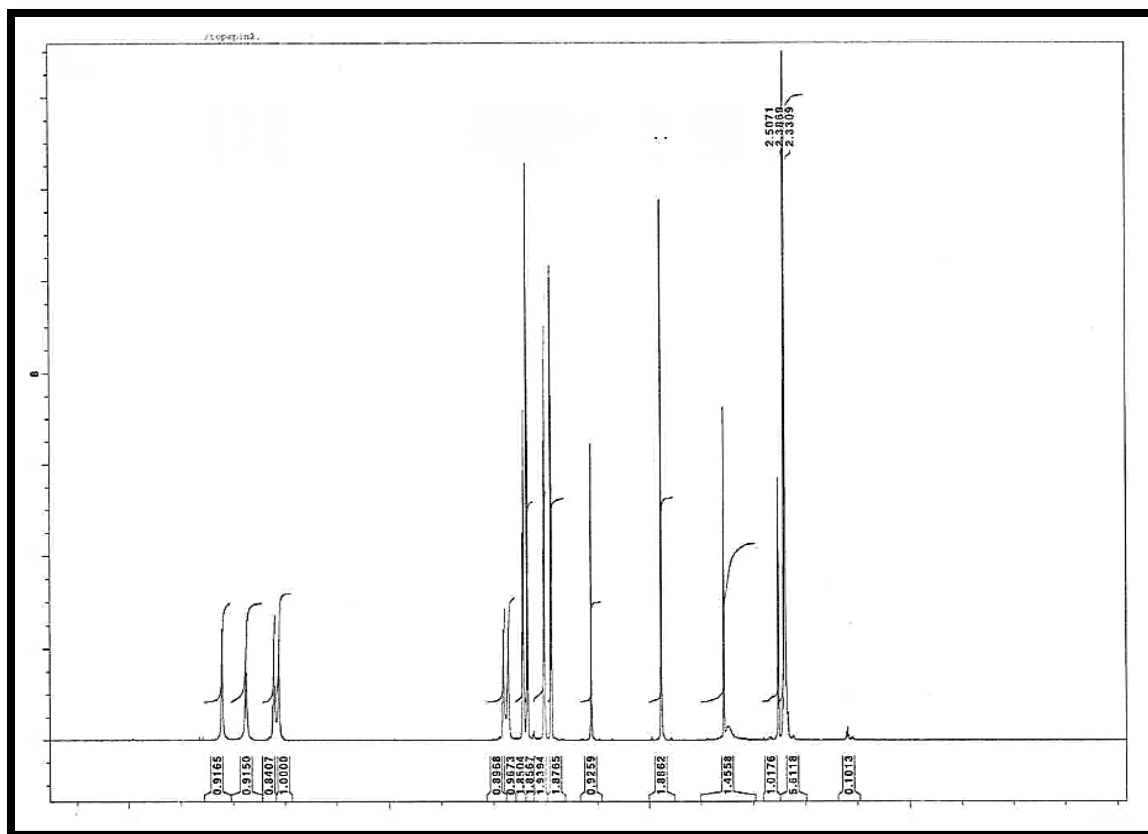
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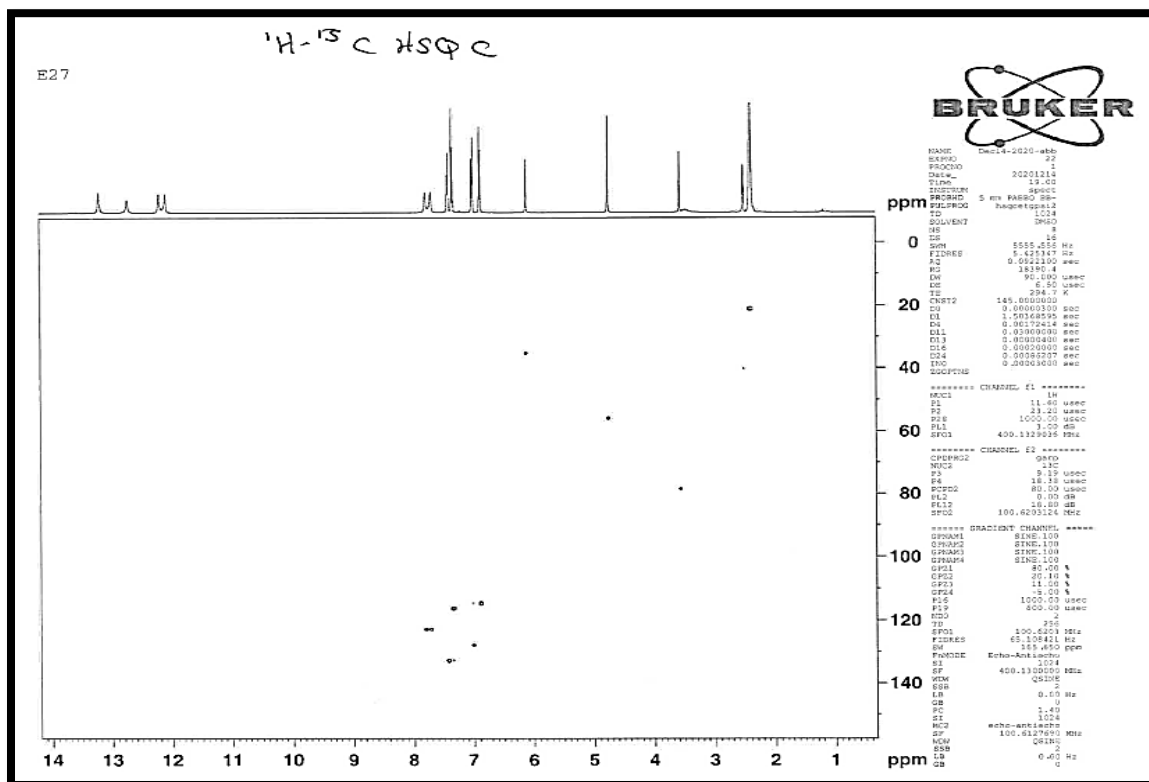
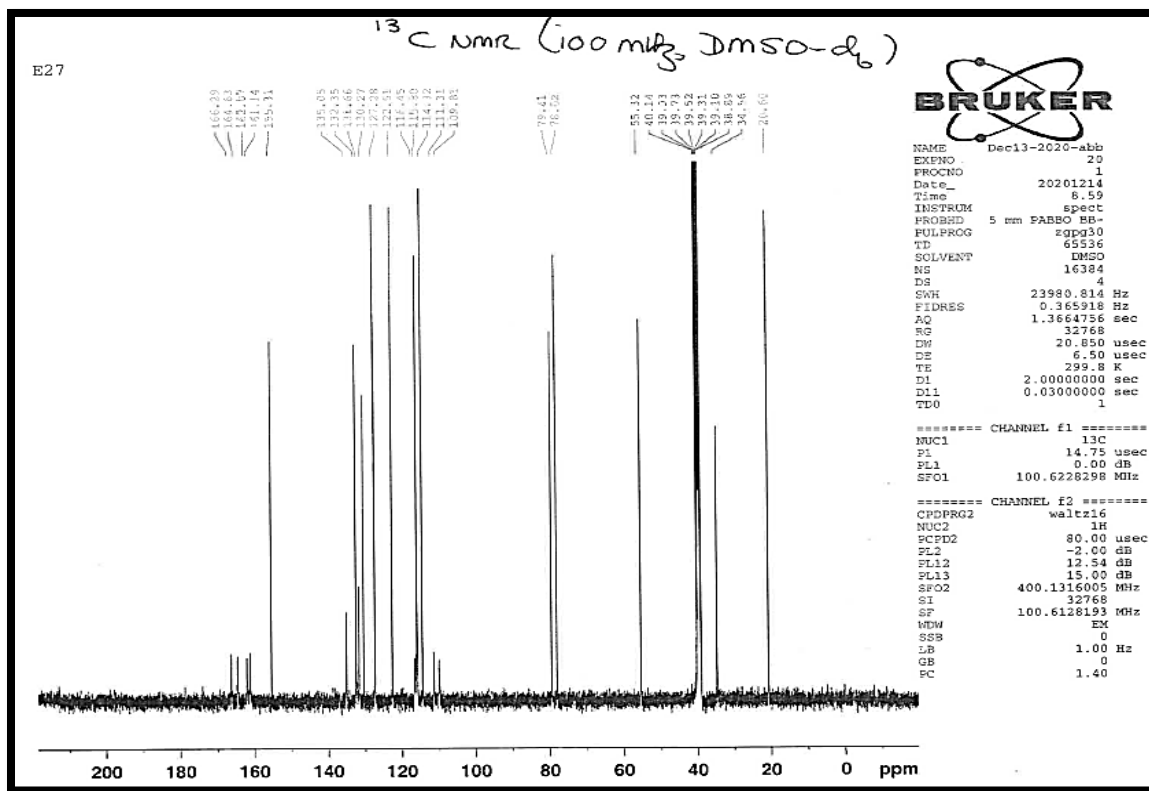

$$^1\text{H}-^{13}\text{C} \subset \text{HMB} \subset$$
[illegible]



Spectrum data for Compound 4d







E27

 $^1\text{H}-^{13}\text{C}$  HMB C

NAME Dec14-2020-abb  
EXPNO 23  
PROCNO 1  
Date\_ 20201214  
TIME 15:59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30p1pdg  
TD 4096  
SOLVENT H<sub>2</sub>O  
NS 32  
DS 16  
SWH 5555.556 Hz  
FIDRES 1.356337 Hz  
AQ 0.388820 sec  
RG 24008  
DW 90.900 usec  
DE 6.50 usec  
TE 294.9 K  
CHST2 145.000000  
CHST13 10.000000  
DO 0.0000300 sec  
DI 1.52457595 sec  
DQ 0.0034828 sec  
DE 0.0000000 sec  
D16 0.0002000 sec  
D10 0.0000235 sec

ppm

0

20

40

60

80

100

120

140

160

180

200

ppm

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 <sup>13</sup>C  
P1 11.60 usec  
P2 23.20 usec  
PL1 3.00 dB  
SFO1 400.1329036 MHz  
\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
NUC2 <sup>1</sup>H  
P3 9.19 usec  
P4 0.00 usec  
PL2 100.622818 MHz  
\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*  
GPMAX1 SINE:100  
GPMAX2 SINE:100  
GPMAX3 SINE:100  
CP1 50.00 %  
CP2 50.00 %  
CP3 40.10 %  
P16 1000.00 usec  
ND0 2  
TD 128  
SFO1 100.6228 MHz  
FIDRES 174.592422 Hz  
SW 222.055 ppm  
FQMODE OF  
SI 2048  
SF 400.1300000 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40  
SI 1024  
MC2 100.6127690 MHz  
SF SINE  
WDW 0  
LB 0.00 Hz  
GB 0

14 13 12 11 10 9 8 7 6 5 4 3 2 1

E27

 $^1\text{H}-^{15}\text{N}$  HSQ C

ppm

-150

-100

-50

0

50

100

150

200

250

300

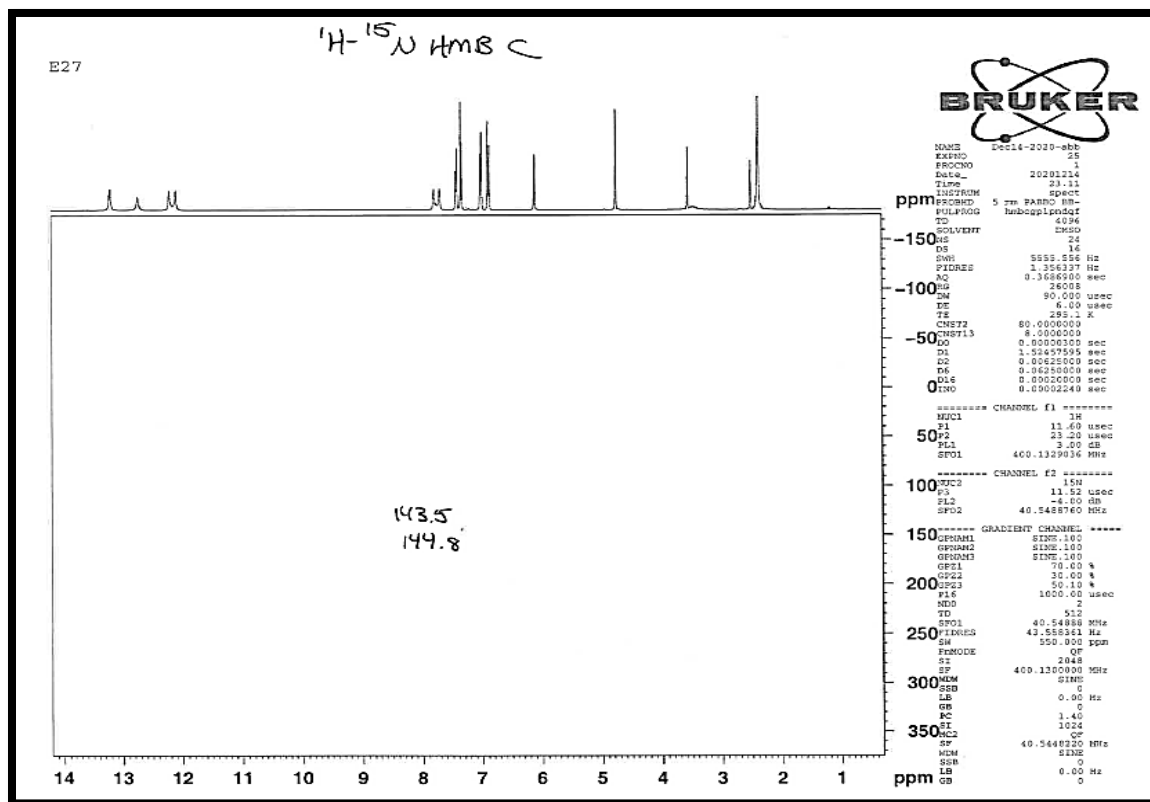
350

ppm

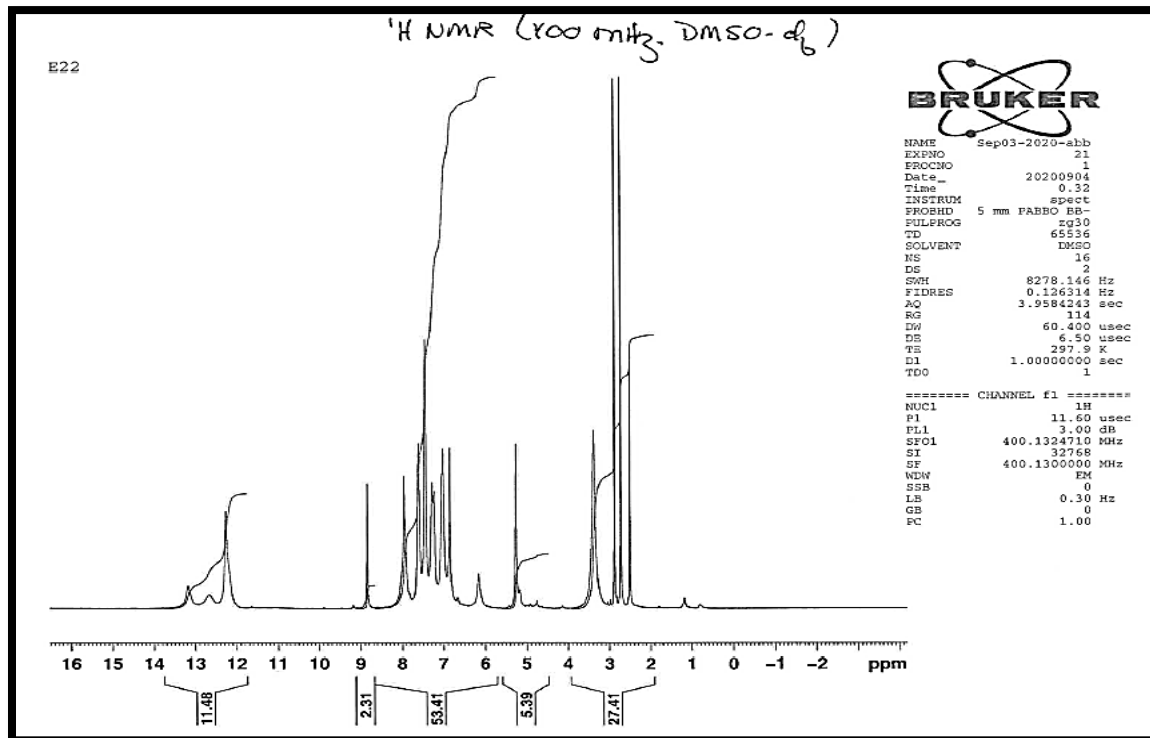
NAME Dec14-2020-abb  
EXPNO 14  
PROCNO 1  
Date\_ 20201214  
TIME 22:14  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30p1pdg  
TD 1024  
SOLVENT H<sub>2</sub>O  
NS 8  
DS 8  
SWH 5555.556 Hz  
FIDRES 5.403147 Hz  
AQ 0.0922100 sec  
RG 23170.5  
DW 59.000 usec  
DE 6.00 usec  
TE 295.1 K  
CHST2 82.000000  
DO 0.0000380 sec  
DI 1.5000000 sec  
DQ 0.00277575 sec  
D1 0.0000000 sec  
D11 0.0000000 sec  
D13 0.0000000 sec  
D16 0.0022000 sec  
D14 0.0000000 sec  
D10 0.0000240 sec  
\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 <sup>15</sup>N  
P1 11.60 usec  
P2 23.20 usec  
P3 1000.00 usec  
PL1 3.00 dB  
SFO1 400.1310018 MHz  
\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
NUC2 <sup>1</sup>H  
P4 9.19 usec  
P5 11.52 usec  
P6 11.00 usec  
P7 190.00 usec  
PL2 4.00 dB  
PL3 20.34 dB  
SFO2 40.5468755 MHz  
\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*  
GPMAX1 SINE:100  
GPMAX2 SINE:50  
GPMAX3 SINE:100  
GPMAX4 SINE:100  
CP1 80.00 %  
CP2 8.00 %  
CP3 11.00 %  
CP4 5.00 %  
P16 1000.00 usec  
P17 600.00 usec  
ND0 2  
TD 256  
SFO1 40.5468755 MHz  
FIDRES 81.116122 Hz  
SW 810.000 ppm  
FQMODE Echo-AntiEcho  
SI 1024  
SF 400.1300000 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40  
SI 1024  
MC2 Echo-AntiEcho  
SF 40.5468220 MHz  
WDW SINE  
LB 0.00 Hz  
GB 0

143.4  
144.6

14 13 12 11 10 9 8 7 6 5 4 3 2 1



Spectrum data for Compound 8a







$^1\text{H}-^{13}\text{C}$  HMBC

```

NAME          Sp33-2020-23
EXPNO         21
PROCNO        1
F2 - F1       2020090.4
TIME          1.33
INSTRUM       spect
PROBHD        5 mm PABBO-BB
PULPROG       zgpg30
TD            4096
SOLVENT       DMSO
DE            0.2
DS            16
AQ            57.74 162 Hz
FIDRES        1.287662 Hz
AQ           0.3883508 sec
D1            23170.5
D2            34.800 usec
D3            6.50 usec
D4            256.6
CN123        145.0000000
CNC123        10.0000000
D0            0.00000300 sec
D1            0.0449603 sec
D2            0.00344828 sec
D3            0.05040000 sec
D4            0.00000000 sec
60            0.00062235 sec
----- CHANNEL f1 -----
NUC1          1H
P1            11.60 usec
P2            23.20 usec
SFO1          3.00 dB
SF01          400.1331325 MHz
----- CHANNEL f2 -----
100           100
NUC2          13C
P1            3.19 usec
P2            0.20
SFO2          100.6228118 MHz
----- GRADIENT CHANNEL -----
=====
CPDPRG1       SINE.10
CPDPRG2       SINE.0
CPDPRG3       SINE.100
SF01          30.00 %
SF02          36.00 %
G203          40.10 %
G204          100.00 usec
RG0           2
RG1           128
SF01          100.6228 MHz
FIDRES        174.292428 ppm
FINPROG       zgpg30
AQ            0.48
SF            400.1300000 MHz
MDM           SINE
LB            0
GB            0
PC            0.90 Hz
SI            1024
SF            100.6127600 MHz
NUC1          13C
SSB           0
LB            0
000           0.00 Hz
ppm

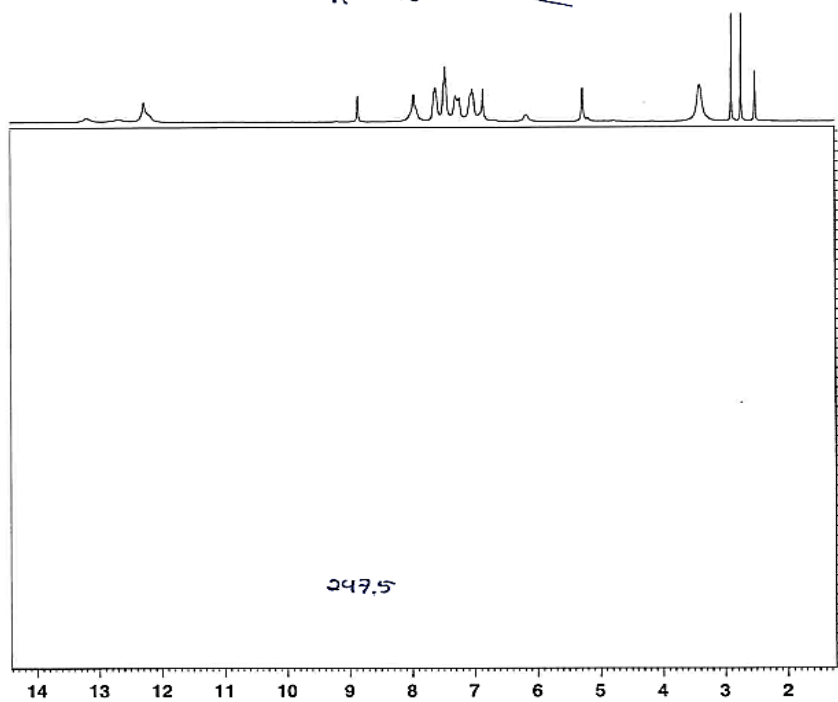
```

 ${}^1\text{H}-{}^{15}\text{N}$  HSQC

```

NAME          Sgpr3-2023-ahb
EXPNO         24
PROCNO        1
DATE_         2011_07
TIME          22:17
INSTRUM       spect
PROBHD        F5mm VQNP500
PULPROG       hsqzgpcg013
SOLVENT        DMSO
NS             15
DS             2
SWH            5717.013 Hz
FIDRES         0.11 Hz
AQ            0.091152 sec
RG             231.11
WDW            EM
SSB            0
LB             94.880 usec
GB            0.000
PC            256.4 K
=====
-150 MHz
P1            92.000000 sec
PR            0.000000 sec
PC2           0.000000 sec
D4            0.00277778 sec
=====
-50 MHz
P1            92.000000 sec
PR            0.000000 sec
PC2           0.000000 sec
D4            0.00277778 sec
=====
CQ          0.000000 sec
CQ2         0.000000 sec
CQ3         0.000000 sec
CQ4         0.000000 sec
CQ5         0.000000 sec
CQ6         0.000000 sec
CQ7         0.000000 sec
CQ8         0.000000 sec
=====
0 ----- CHANNEL F1 *****
PRCL        14
PC           11.50 usec
P2           23.20 usec
P3           1000.00 usec
F1           3.30 dB
F2           3.30 dB
F3           400.13 dB
=====
***** CHANNEL F2 *****
CPRPGM2      gprb
PC2           1.80
PR            0.00
PC3           11.52 usec
PC4           2.30 usec
PC5           150.00 usec
PC6           150.00 usec
F112         20.34 dB
F113         20.34 dB
F114         40.54 dB
F115         40.54 dB
=====
150 ----- GRABEND CHANNEL *****
GPRM1        GRABEND.100
GPRM2        GRABEND.100
GPRM3        GRABEND.100
GPRM4        GRABEND.100
=====
200 MHz
P1            92.000000 sec
PR            0.000000 sec
PC2           0.000000 sec
D4            0.00277778 sec
=====
PQ          0.000000 sec
PQ2         0.000000 sec
PQ3         0.000000 sec
PQ4          0.000000 sec
PQ5          0.000000 sec
PQ6          0.000000 sec
PQ7          0.000000 sec
PQ8          0.000000 sec
PQ9          0.000000 sec
PQ10         0.000000 sec
PQ11         0.000000 sec
PQ12         0.000000 sec
PQ13         0.000000 sec
PQ14         0.000000 sec
PQ15         0.000000 sec
PQ16         0.000000 sec
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PQ98         0.000000 sec
PQ99         0.000000 sec
PQ100        0.000000 sec
PQ101        0.000000 sec
PQ102        0.000000 sec
PQ103        0.000000 sec
PQ104        0.000000 sec
PQ105        0.000000 sec
PQ106        0.000000 sec
PQ107        0.000000 sec
PQ108        0.000000 sec
PQ109        0.000000 sec
PQ110        0.000000 sec
PQ111        0.000000 sec
PQ112        0.000000 sec
PQ113        0.000000 sec
PQ114        0.000000 sec
PQ115        0.000000 sec
PQ116        0.000000 sec
PQ117        0.000000 sec
PQ118        0.000000 sec
PQ119        0.000000 sec
PQ120        0.000000 sec
PQ121        0.000000 sec
PQ122        0.000000 sec
PQ123        0.000000 sec
PQ124        0.000000 sec
PQ125        0.000000 sec
PQ126        0.000000 sec
PQ127        0.000000 sec
PQ128        0.000000 sec
PQ129        0.000000 sec
PQ130        0.000000 sec
PQ131        0.000000 sec
PQ132        0.000000 sec
PQ133        0.000000 sec
PQ134        0.000000 sec
PQ135        0.000000 sec
PQ136        0.000000 sec
PQ137        0.000000 sec
PQ138        0.000000 sec
PQ139        0.000000 sec
PQ140        0.000000 sec
PQ141        0.000000 sec
PQ142        0.000000 sec
PQ143        0.000000 sec
PQ144        0.000000 sec
PQ145        0.000000 sec
PQ146        0.000000 sec
PQ147        0.000000 sec
PQ148        0.000000 sec
PQ149        0.000000 sec
PQ150        0.000000 sec
PQ151        0.000000 sec
PQ152        0.000000 sec
PQ153        0.000000 sec
PQ154        0.000000 sec
PQ155        0.000000 sec
PQ156        0.000000 sec
PQ157        0.000000 sec
PQ158        0.000000 sec
PQ159        0.000000 sec
PQ160        0.000000 sec
PQ161        0.000000 sec
PQ162        0.000000 sec
PQ163        0.000000 sec
PQ164        0.000000 sec
PQ165        0.000000 sec
PQ166        0.000000 sec
PQ167        0.000000 sec
PQ168        0.000000 sec
PQ169        0.000000 sec
PQ170        0.000000 sec
PQ171        0.000000 sec
PQ172        0.000000 sec
PQ173        0.000000 sec
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PQ183        0.000000 sec
PQ184        0.000000 sec
PQ185        0.000000 sec
PQ186        0.000000 sec
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PQ188        0.000000 sec
PQ189        0.000000 sec
PQ190        0.000000 sec
PQ191        0.000000 sec
PQ192        0.000000 sec
PQ193        0.000000 sec
PQ194        0.000000 sec
PQ195        0.000000 sec
PQ196        0.000000 sec
PQ197        0.000000 sec
PQ198        0.000000 sec
PQ199        0.000000 sec
PQ200        0.000000 sec
PQ201       
```

144.9  
152.0



```

NAME          SP03-0320-040
FXPRO        25
TIME         1
DATE         2020/09/04
TIME         14
INSTRUM      spect
FREQIDB      5 mhz PABED SB
FREQIDB      50000000 Hz
FREQIDB      4076
SOLVENT      DMS
PMS          16
SNI          5274.262 Hz
FIDRES      1.287662 Hz
RG          0.188500 sec
NG          26008
RG          0.000000 sec
RG          6.000000 sec
PE         25.5 K
CNST2       80.000000
CNST3       8.000000
CNST4       0.000000 sec
EI          1.50409903 sec
EI          0.000000 sec
EI          0.06250000 sec
D1          0.000000 sec
D2          0.000000 sec
D3          0.00002840 sec

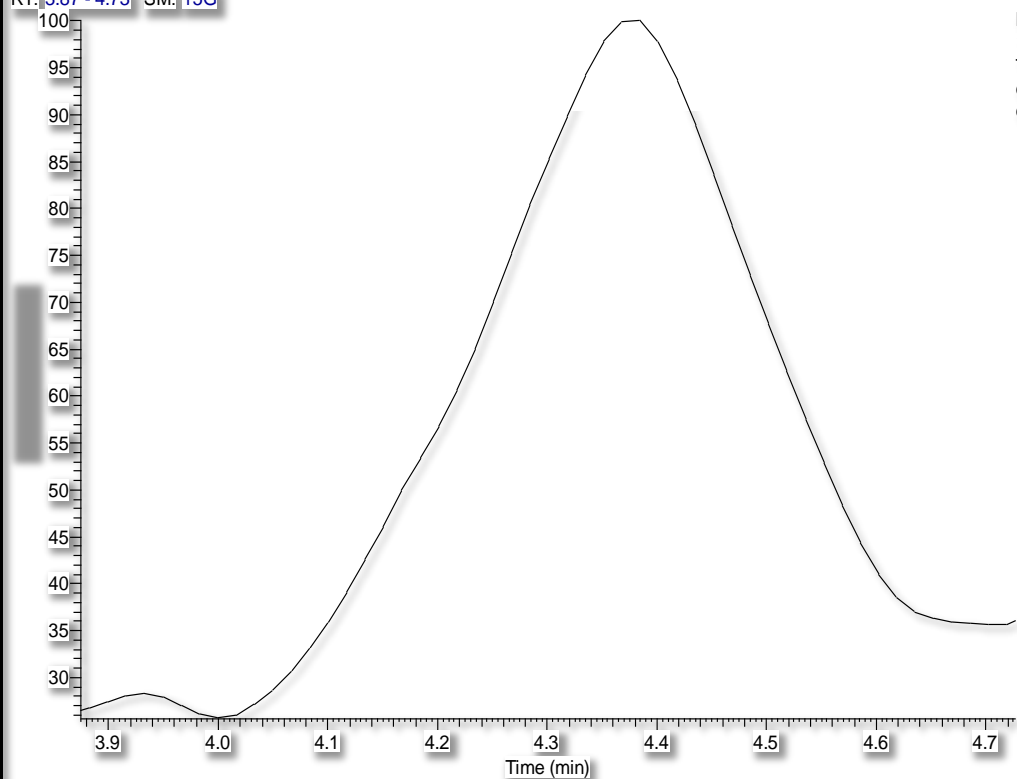
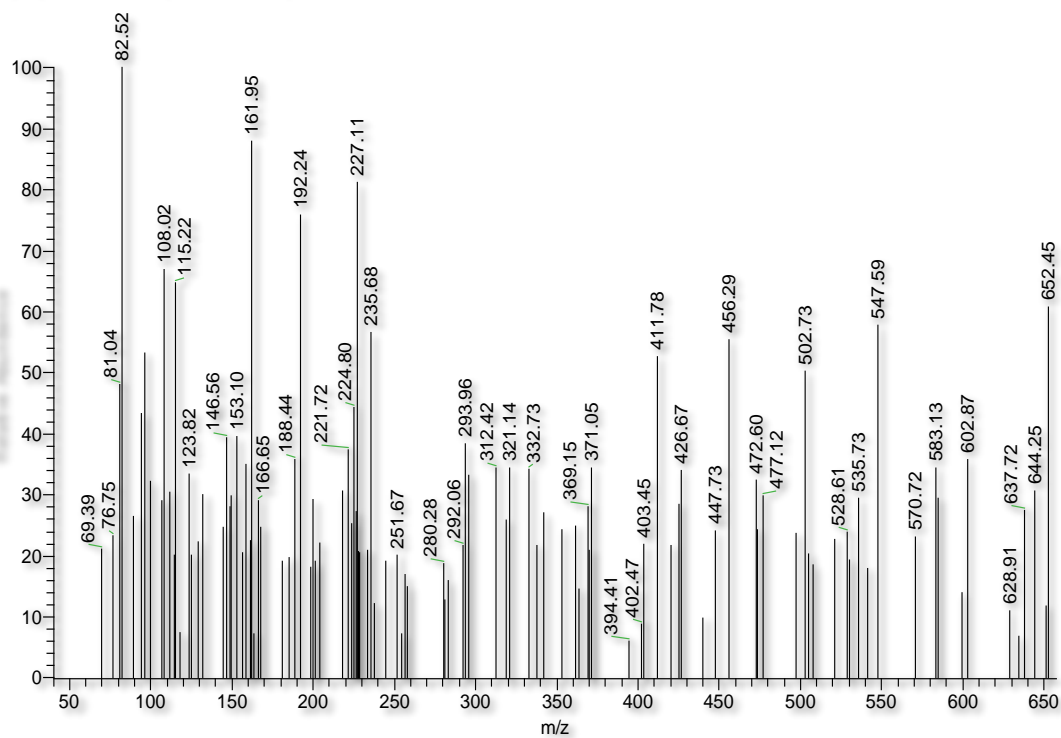
***** CHANNEL f1 *****
NUC1         13
P1           13.00 usec
P2           23.20 usec
P3           23.20 usec
SF01         400.135323 MHz

***** CHANNEL f2 *****
NUC2         15N
P1           13.50 usec
P2           4.00 usec
P3           4.00 usec
SF02         400.544620 MHz

150***** GRADIENT CHANNEL *****
GPGM02       15N
GPGM03       15N
GPGM04       15N
GPGM05       15N
GPG1         70.00 %
OPF0         70.00 %
OPF1         50.10 %
M1           100.0000 usec
P10          2
D2           512
SF03         400.544620 MHz
G1          43.58361 Hz
SM           550.000 ppm
FREQIDB      50
ST           3
SF           400.135323 MHz
D1           0.000000 sec
CN01         15N
CN02         15N
CN03         15N
CN04         15N
CN05         15N
CN06         15N
CN07         15N
CN08         15N
CN09         15N
CN10         15N
CN11         15N
CN12         15N
CN13         15N
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CN35         15N
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CN76         15N
CN77         15N
CN78         15N
CN79         15N
CN80         15N
CN81         15N

```

RT: 3.87 - 4.73 SM: 15G

NL:  
1.65E4  
TIC MS  
essmat-  
elshif-E18essmat-elshif-E18 #186 RT: 3.13 AV: 1 SB: 2 4.45, 4.45 NL: 4.45E2  
T: (0.0) + c EI Full ms [40.00-1000.00]

Spectrum data for Compound 8b

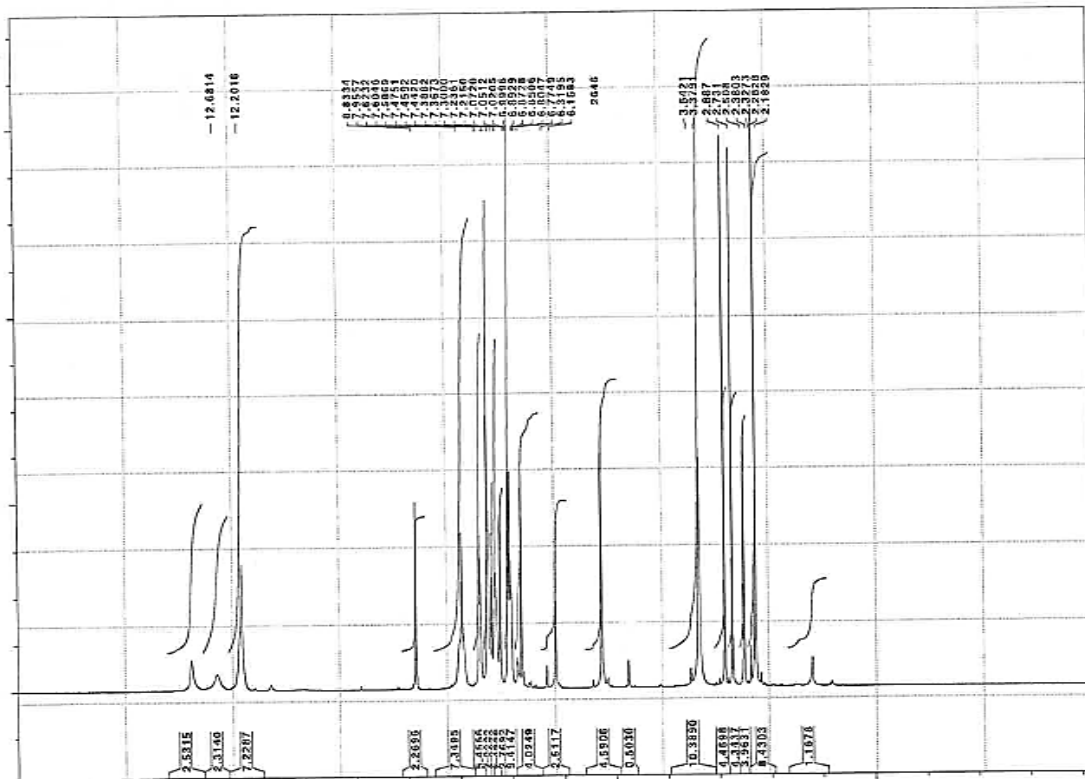


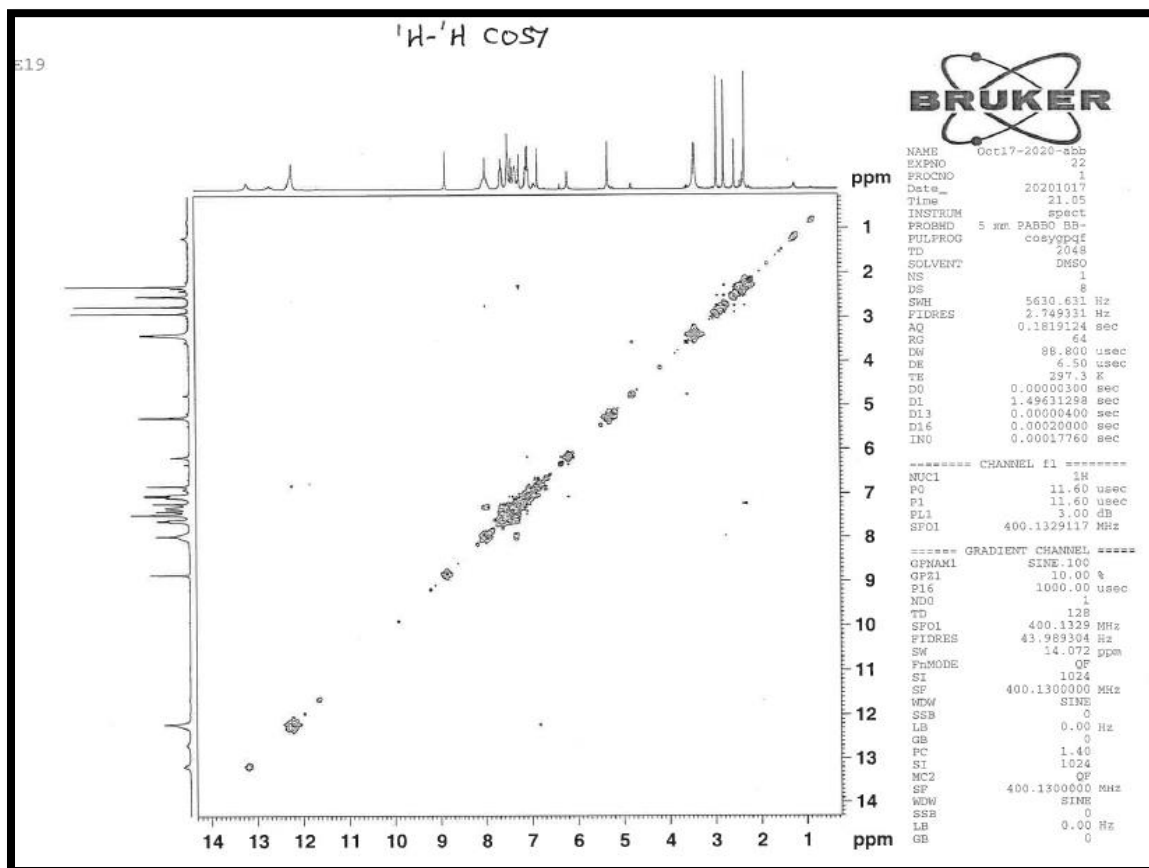
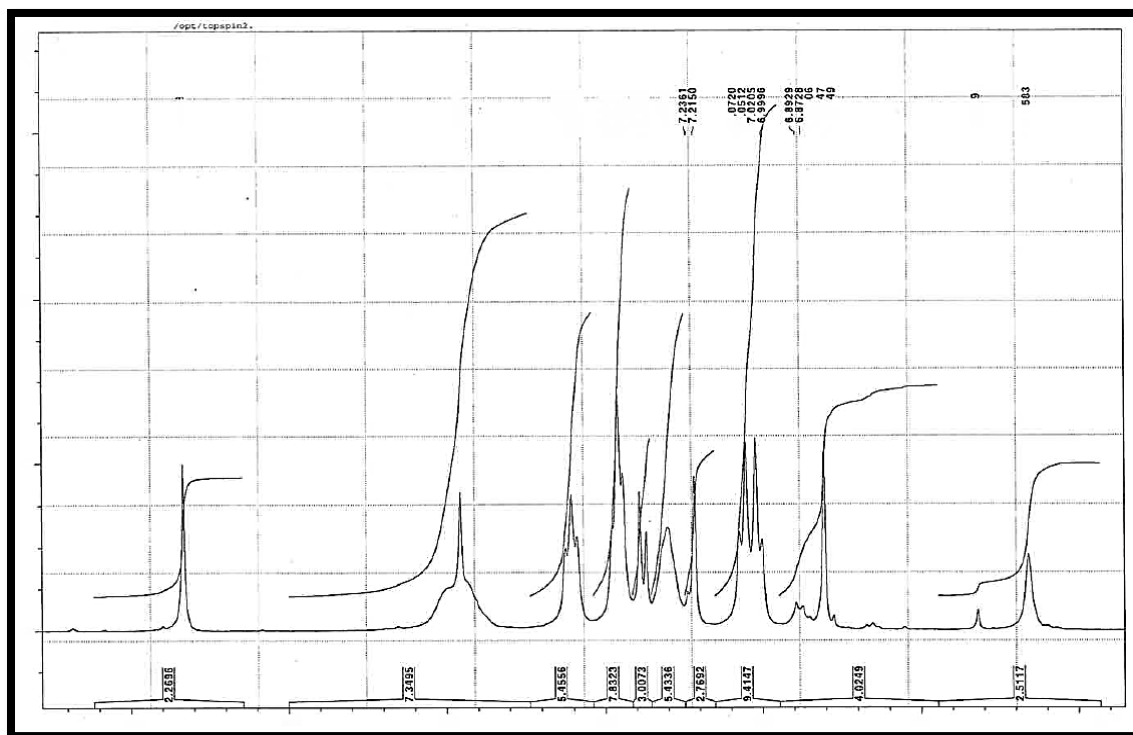
|         |                |
|---------|----------------|
| NAME    | Oct17-2020-abb |
| EXPNO   | 21             |
| PROCNO  | 1              |
| Date_   | 20201017       |
| Time    | 21.04          |
| INSTRUM | spect          |
| PROBHD  | 5 mm PABBO AB- |
| PULPROG | zgpg30         |
| TD      | 65536          |
| SOLVENT | DMSO           |
| NS      | 16             |
| DS      | 2              |
| SVH     | 8278.146 Hz    |
| FIDRES  | 0.126314 Hz    |
| AQ      | 3.9584243 sec  |
| RG      | 128            |
| EX      | 60.400 usec    |
| DE      | 6.50 usec      |
| TE      | 297.6 K        |
| TD0     | 1.0000000 sec  |
| TD0     | 1              |

```

===== CHANNEL f1 =====
NUC1                1H
PL                  11.60 usec
PL1                 3.00 dB
SFO1               400.1324710 MHz
SI                  32768
SF                 400.1300000 MHz
WDW                  EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00

```







E19

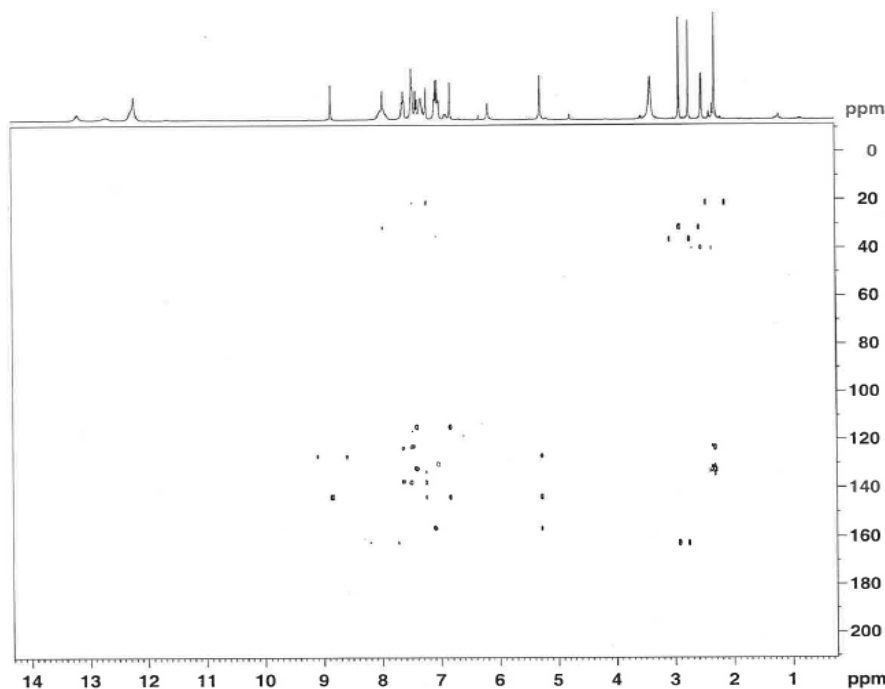
 $^1\text{H}$ - $^{13}\text{C}$  HMB C

NAME OC17-2020-abc  
EXPNO 24  
PROCNO 1  
Date\_ 20201015  
Time 9:17  
INSTRUM spect  
PROBHD 5 mm F400 BB-  
PULPROG zgpg30  
TD 4096  
SOLVENT DMF  
NS 32  
DS 16  
SWH 5630.631 Hz  
FIDRES 1.374566 Hz  
AQ 0.3637748 sec  
RG 26008  
DW 89.800 usec  
DE 6.50 usec  
TE 293.2 K  
CHST2 145.000000  
CHST13 10.000000  
DO 0.8000000 sec  
DI 1.5287198 sec  
D2 0.0044428 sec  
DE 0.0000000 sec  
D16 0.0000000 sec  
IN0 0.0002335 sec

----- CHANNEL f1 -----  
NUC1 1H  
P1 11.60 usec  
P2 23.20 usec  
PL1 3.00 dB  
SFO1 400.1329117 MHz

----- CHANNEL f2 -----  
NUC2 13C  
P3 9.15 usec  
P4 0.00 dB  
SFO2 100.628138 MHz

----- GRADIENT CHANNEL -----  
GPMAG1 SINE 100  
GPMAG2 SINE 100  
GPMAG3 SINE 100  
GPE1 50.00 %  
GPE2 50.00 %  
GPE3 50.00 %  
P16 1000.00 usec  
WDW 2  
SF01 100.628138 MHz  
FIDRES 174.592422 Hz  
SW 222.095 ppm  
FNUC2 13C  
SF 400.1300000 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40  
ST 1024  
MC2 QF  
SF 100.6127690 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0



E19

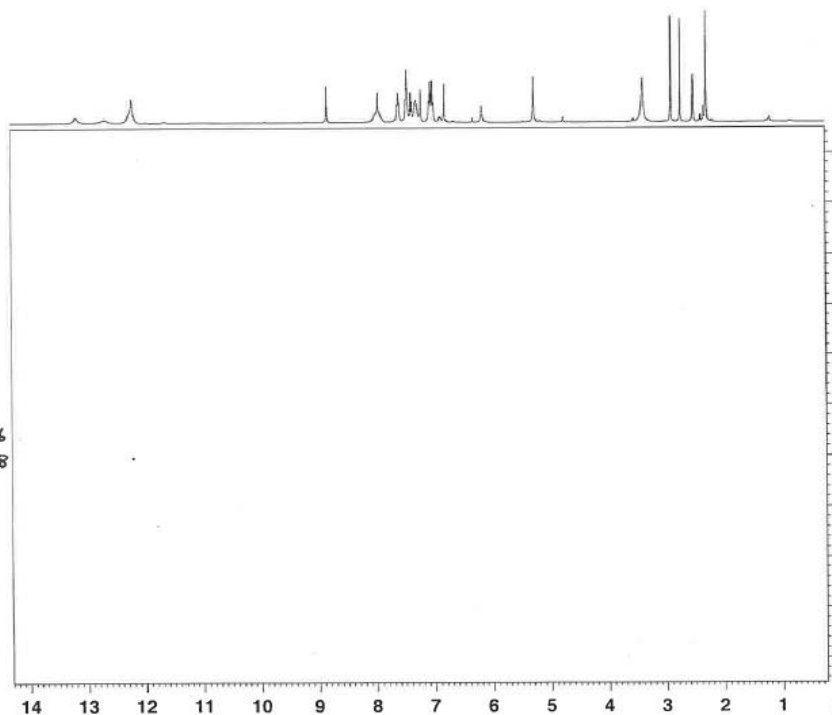
 $^1\text{H}$ - $^{15}\text{N}$  HSQC

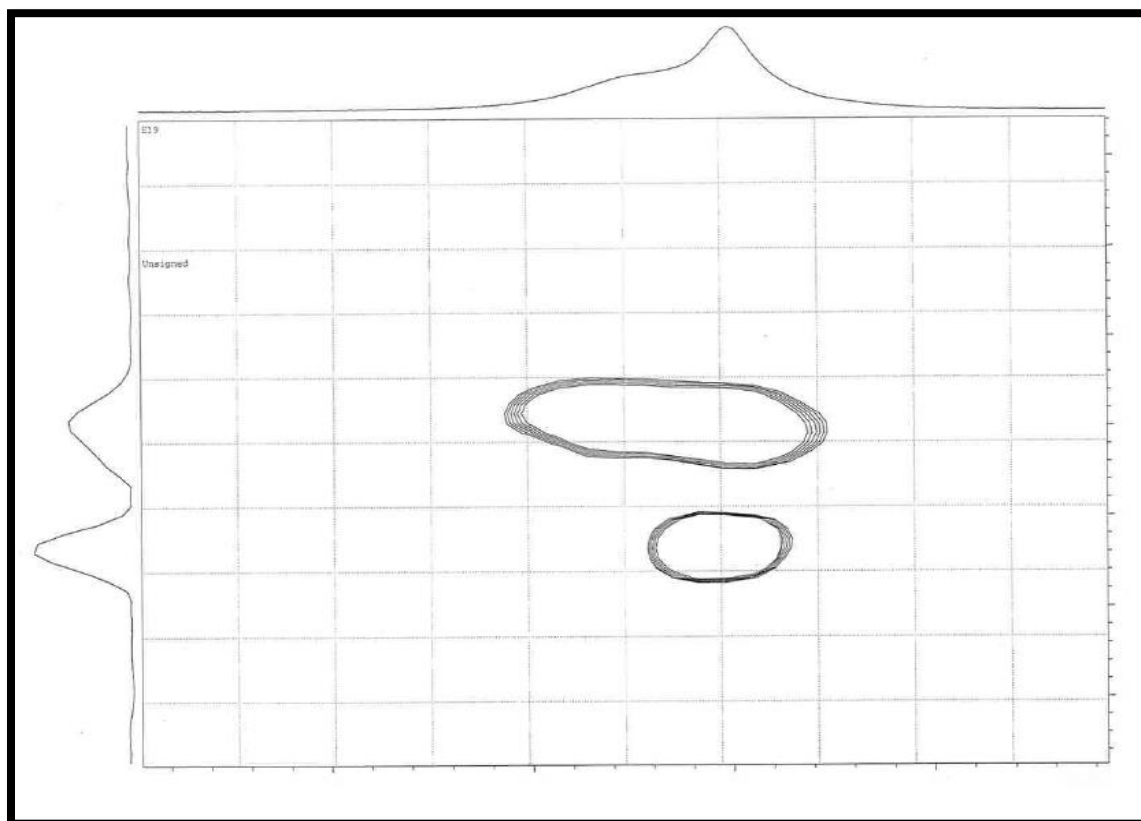
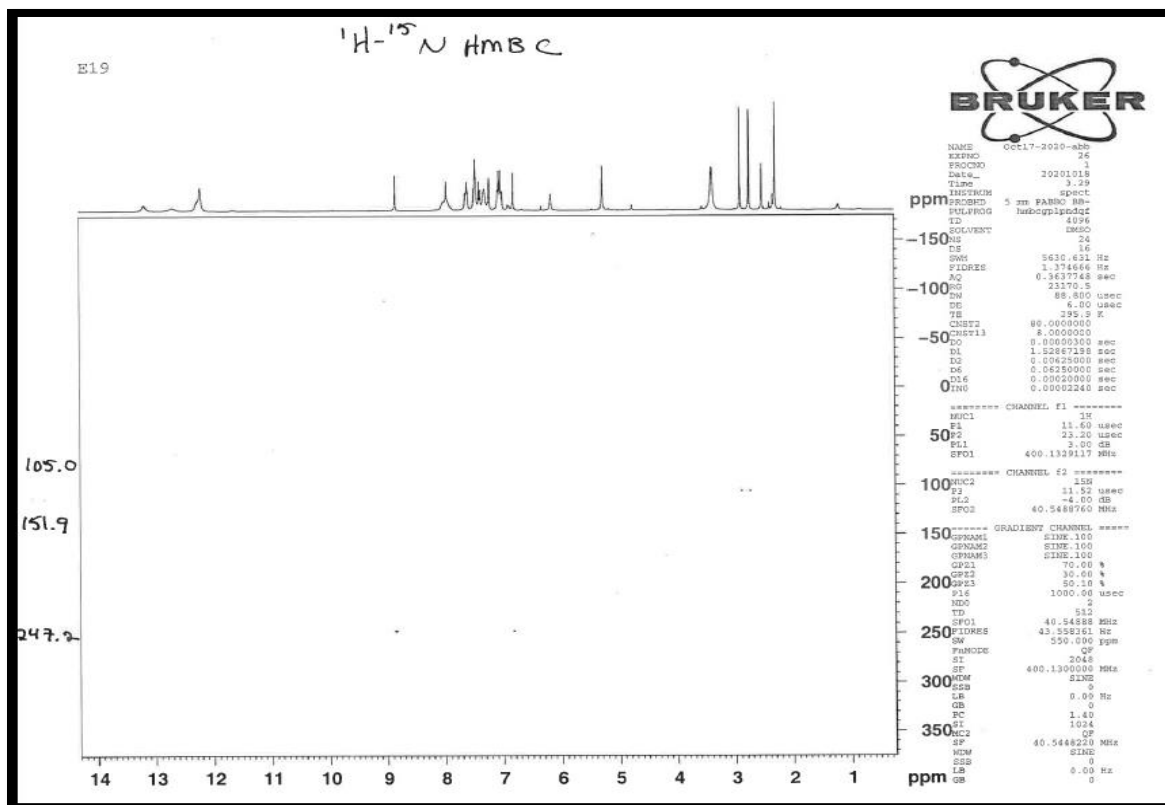
NAME OC17-2020-abc  
EXPNO 25  
PROCNO 1  
Date\_ 20201015  
Time 9:31  
INSTRUM spect  
PROBHD 5 mm F400 BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMF  
NS 32  
DS 16  
SWH 5630.631 Hz  
FIDRES 1.374566 Hz  
AQ 0.3637748 sec  
RG 26008  
DW 89.800 usec  
DE 6.50 usec  
TE 293.2 K  
CHST2 145.000000  
CHST13 10.000000  
DO 0.8000000 sec  
DI 1.5287198 sec  
D2 0.0044428 sec  
DE 0.0000000 sec  
D16 0.0000000 sec  
IN0 0.0002335 sec

----- CHANNEL f1 -----  
NUC1 1H  
P1 11.60 usec  
P2 23.20 usec  
PL1 3.00 dB  
SFO1 400.1329117 MHz

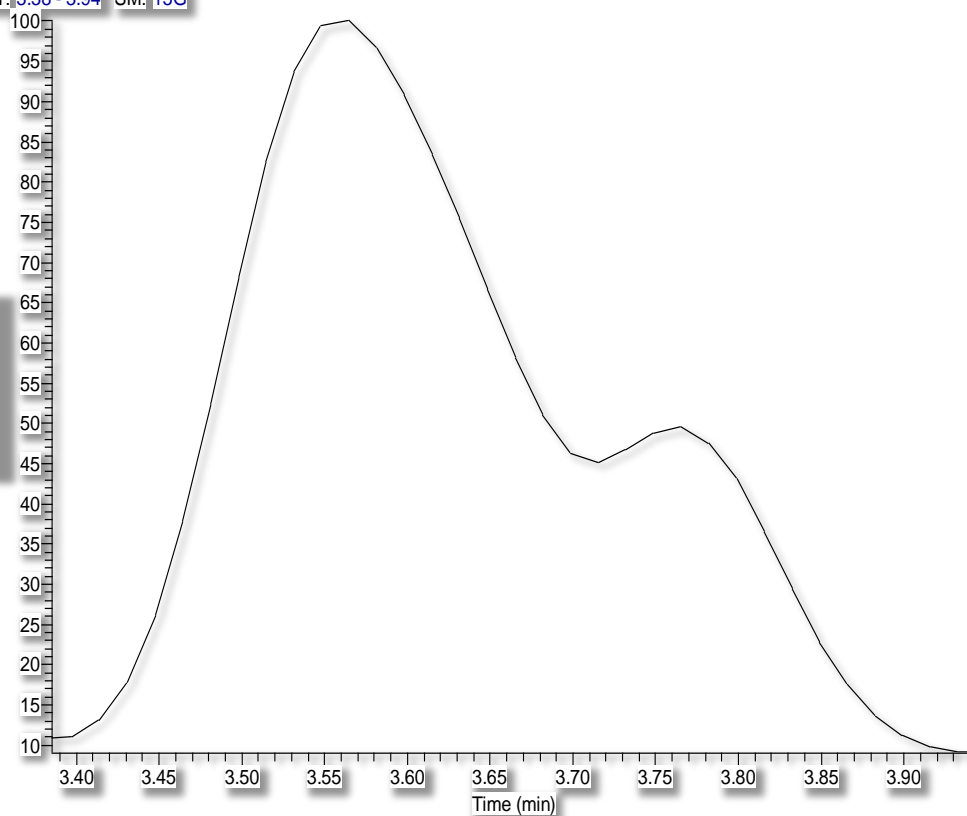
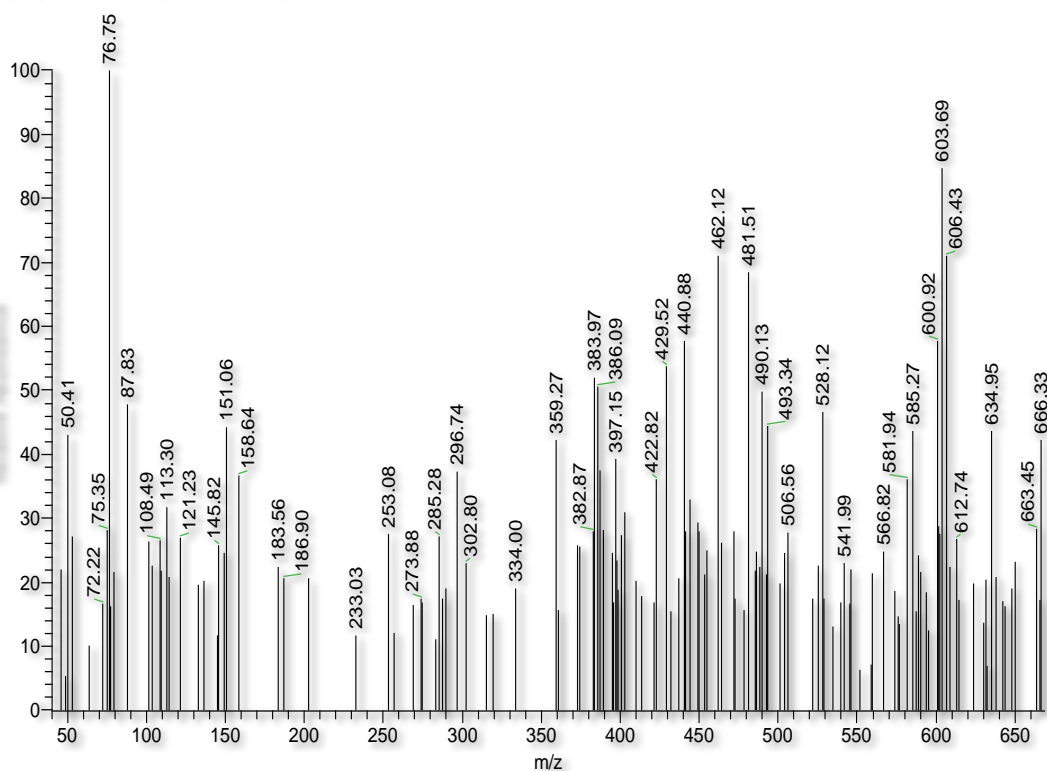
----- CHANNEL f2 -----  
CPDPRG2 gcp  
NUC2 15N  
P3 11.22 usec  
P4 23.20 usec  
P5 190.00 usec  
PL2 -4.00 dB  
PL3 20.14 dB  
SFO2 40.468755 MHz

----- GRADIENT CHANNEL -----  
GPMAG1 SINE 100  
GPMAG2 SINE 50  
GPMAG3 SINE 100  
GPMAG4 SINE 100  
GPE1 50.00 %  
GPE2 50.00 %  
GPE3 50.00 %  
GPE4 50.00 %  
P16 1000.00 usec  
WDW 2  
SF01 100.628138 MHz  
FIDRES 174.592422 Hz  
SW 222.095 ppm  
FNUC2 15N  
SF 400.1300000 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40  
ST 1024  
MC2 QF  
SF 100.6127690 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0

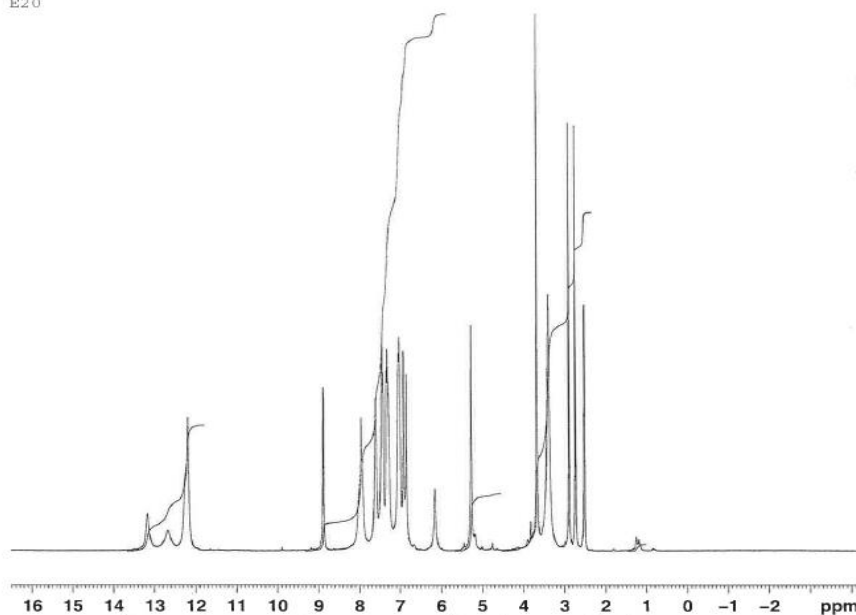
144.6  
151.8



RT: 3.38 - 3.94 SM: 15G

NL:  
2.22E4  
TIC MS  
essmat-  
elshif-E19essmat-elshif-E19 #170 RT: 2.86 AV: 1 SB: 2 4.45, 4.45 NL: 4.47E2  
T: (0,0) + c EI Full ms [40.00-1000.00]

<sup>1</sup>H NMR (400 mHz, DMSO-d<sub>6</sub>)

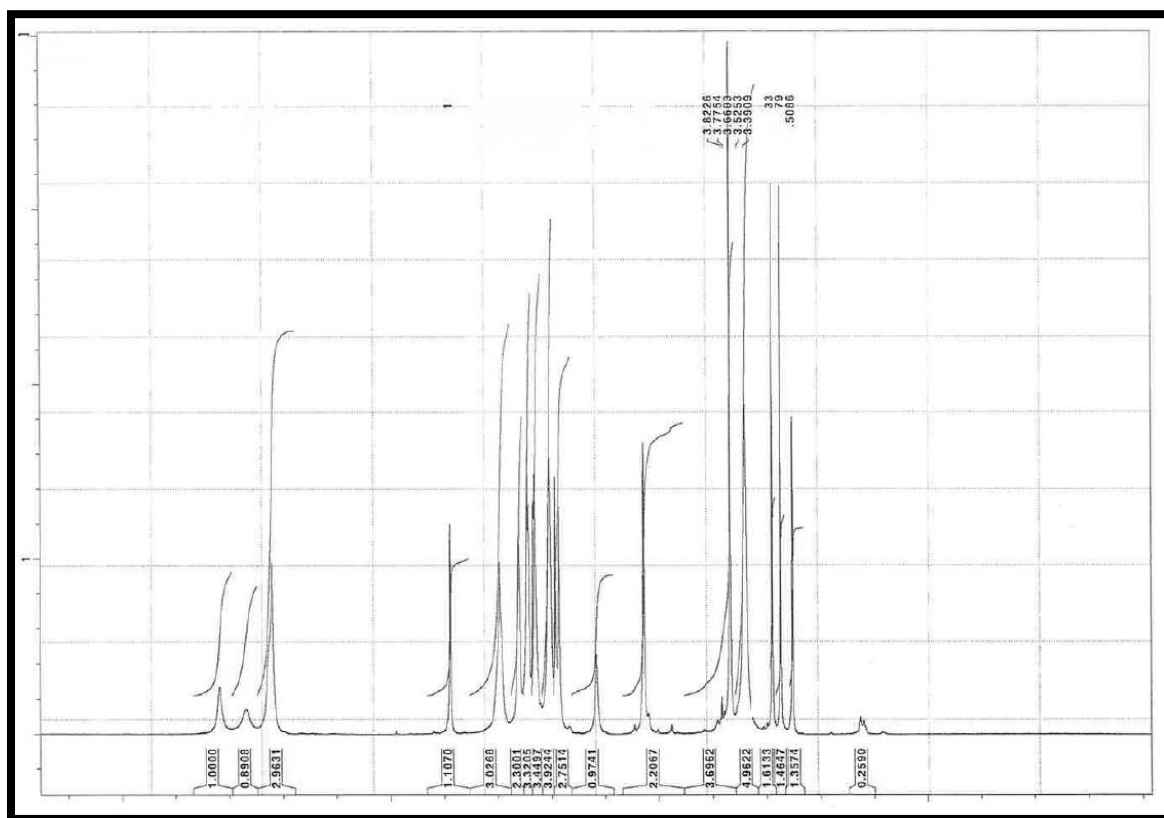


```
NAME      Nov19-2020-abb
EXPNO     11
PROCNO    1
Date_     20201119
Time      23.20
INSTRUM    spect
PROBHD     5 mm PABBO BB
PULPROG    zg30
TD         65536
SOLVENT    DMSC
NS         16
DS         2
SWH         8278.146 Hz
FIDRES     0.126314 Hz
AQ         3.9584243 sec
RG          314
RQ         60.400 usec
DE         6.50 usec
TE         296.9 K
D1         1.00000000 sec
TD0        1
```

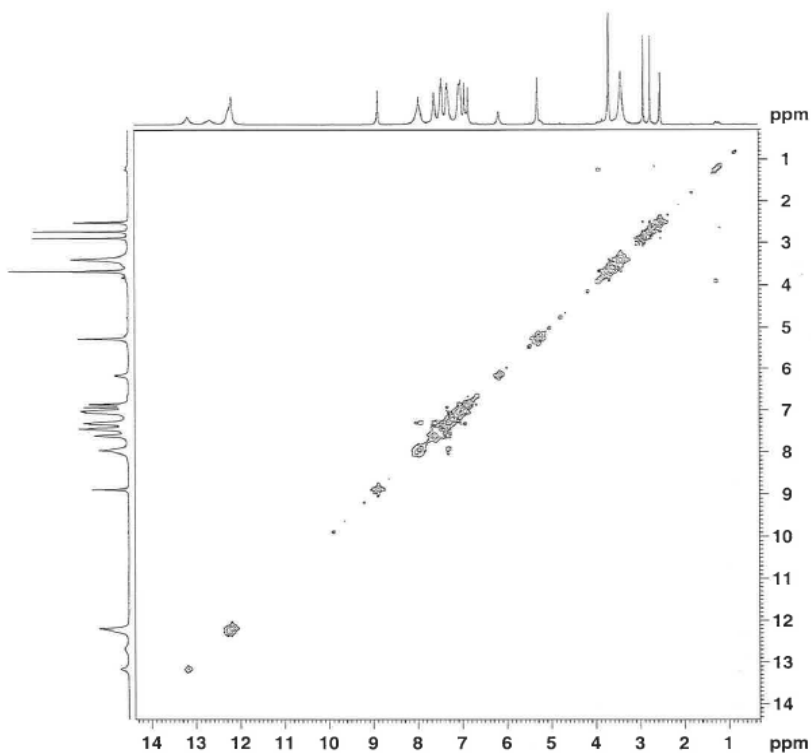
```

===== CHANNEL f1 =====
NUC1                      1H
P1                      11.60 usec
PL1                      3.00 dB
SF01                   400.1324710 MHz
SI                      32768
SF                   400.1300000 MHz
WDW                      EM
SSB                      0
LB                      0.30 Hz
GB                      0
PC                      1.00

```



E20

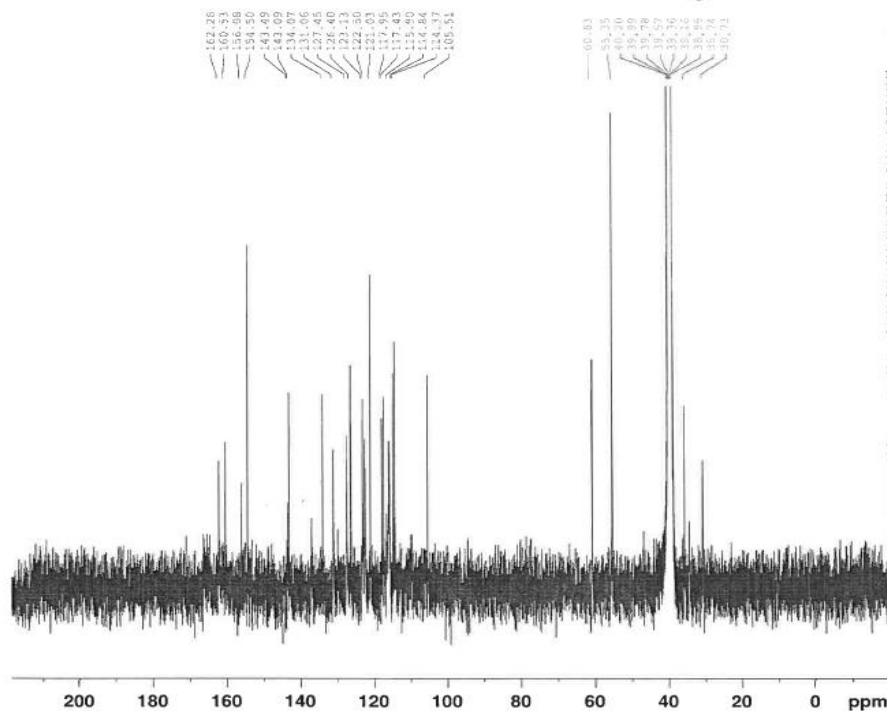
<sup>1</sup>H-<sup>1</sup>H COSY

NAME Nov19-2020-abb  
EXPNO 12  
PROCNO 1  
Date\_ 20201119  
Time 23.21  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG cosygpgf  
TD 2048  
SOLVENT DMSO  
NS 1  
DS 8  
SWH 5630.631 Hz  
FIDRES 2.749331 Hz  
AQ 0.1819124 sec  
RG 64  
DM 88.800 usec  
DE 6.50 usec  
TE 296.6 K  
DO 0.00000300 sec  
D1 1.49611298 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00017760 sec

===== CHANNEL f1 =====  
NUC1 1H  
P0 11.60 usec  
P1 11.60 usec  
PL1 3.00 dB  
SFO1 400.1329351 MHz

===== GRADIENT CHANNEL =====  
GPMAM1 SINE.100  
GP21 10.00 %  
P16 1000.00 usec  
ND0 1  
TD 128  
SFO1 400.1329 MHz  
FIDRES 43.989304 Hz  
SW 14.072 ppm  
FPMODE GF  
SI 1024  
SF 400.1300000 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40  
SI 1024  
MC2 GF  
SF 400.1300000 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0

E20

<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>)

NAME Nov19-2020-abb  
EXPNO 10  
PROCNO 1  
Date\_ 20201119  
Time 23.17  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 4096  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 32768  
DM 20.850 usec  
DE 6.50 usec  
TE 300.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 14.75 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 12.54 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6128193 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

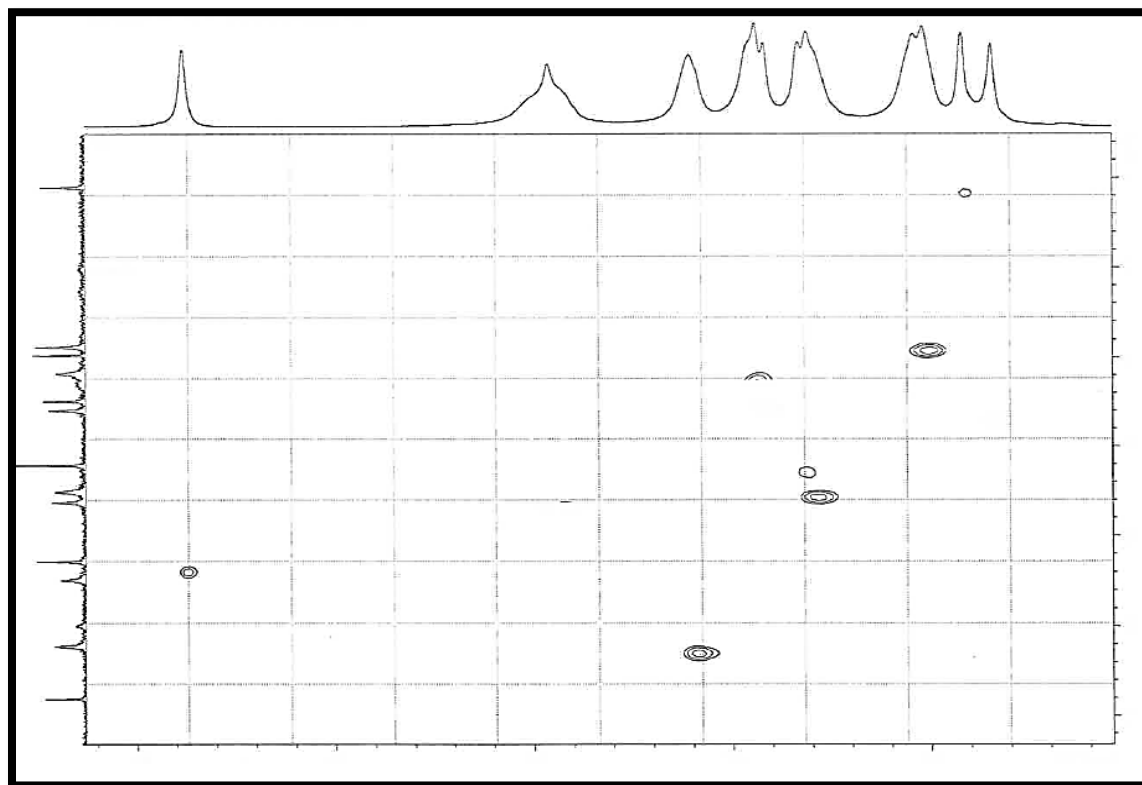
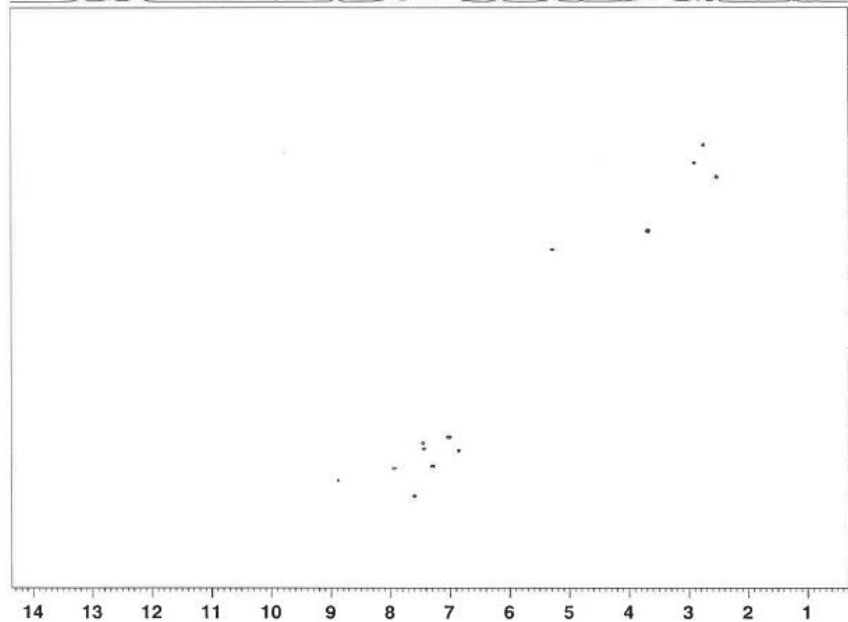
E20

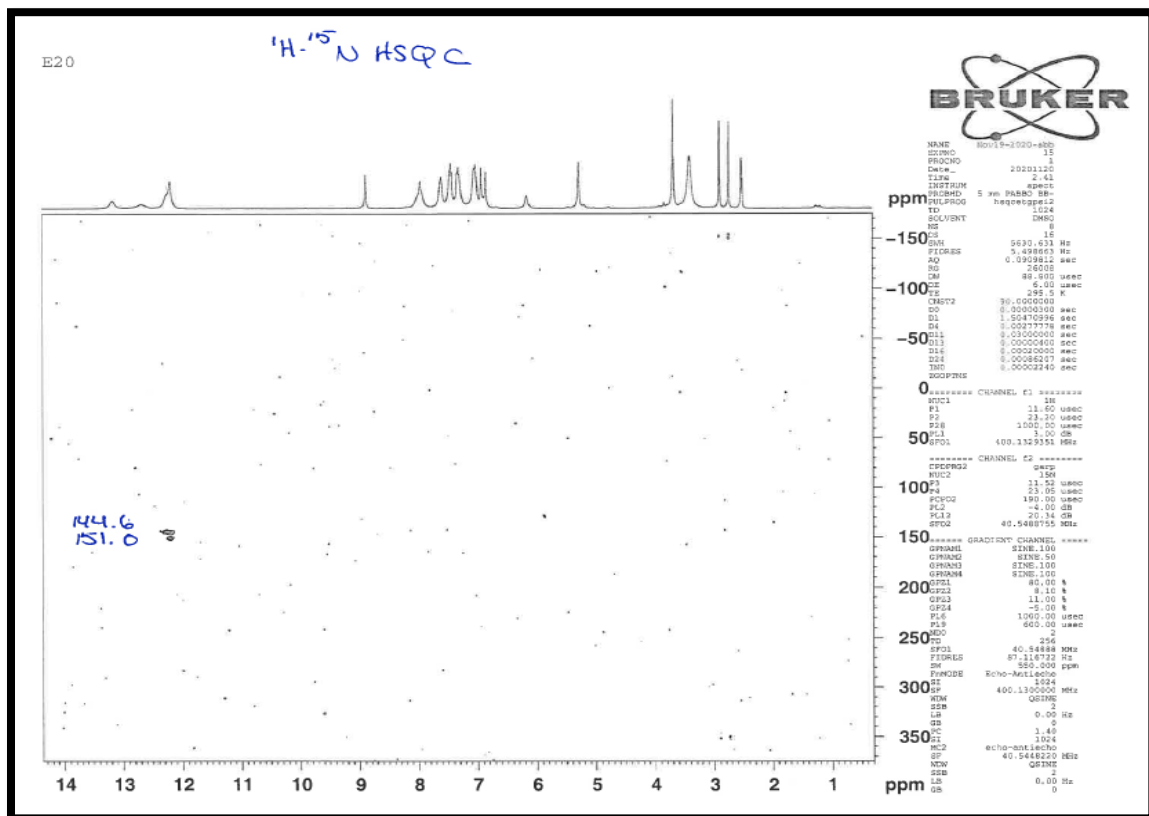
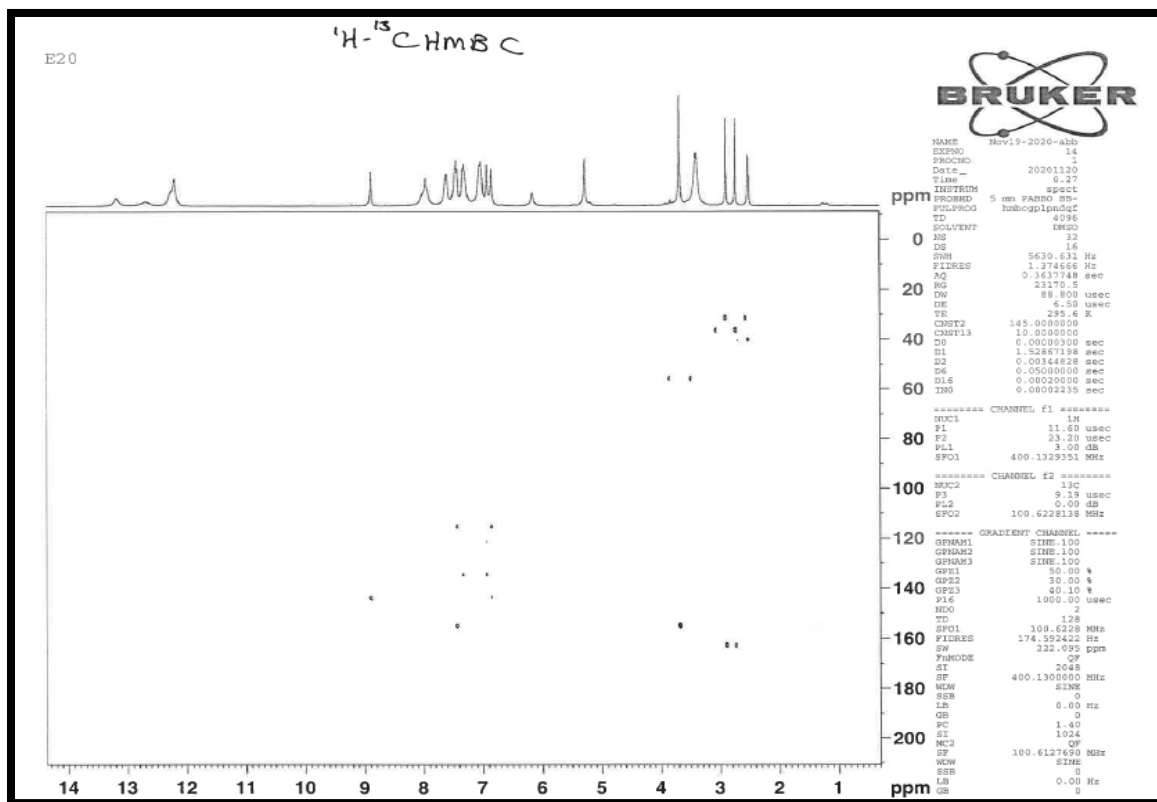
 $^1\text{H}-^{13}\text{C}$  HSQC

NAME: 80012-2010-000  
EXPNO: 1  
PROCNO: 1  
Date\_: 20011119  
Time: 11.32  
INSTRUM: spect  
PROBHD: 5 mm mmeo 5h-  
PULPROG: zgpg30  
TD: 65536  
SOLVENT: DMSO  
NS: 8  
DS: 16  
SWH: 5630.631 Hz  
FIDRES: 0.428664 Hz  
AQ: 0.0000812 sec  
RG: 327.5  
CQ: 18190.4  
DE: 88.800 usec  
TE: 300.2 K  
DVT2: 145.000000 sec  
DO: 0.0000000 sec  
DI: 1.50470896 sec  
D4: 0.00172414 sec  
C12: 0.01900000 sec  
C13: 0.00000000 sec  
S16: 0.00000000 sec  
S24: 0.00000000 sec  
S36: 0.00000000 sec  
DQCP7M5  
----- CHANNEL F1 -----  
NUC1: 1H  
P1: 11.40 usec  
P2: 27.20 usec  
P22: 1000.00 usec  
PL1: 0.00 dB  
PL2: 400.1329352 MHz  
----- CHANNEL F2 -----  
CPDPRG2: zgpg30  
NUC2: 13C  
P3: 9.10 usec  
P4: 14.38 usec  
PCTD3: 80.00 usec  
PL3: 0.00 dB  
PL12: 10.80 dB  
PLD2: 100.6203124 MHz  
----- GRADIENT CHANNEL -----  
GPMAX1: SENSE: 100  
GPMAX2: SENSE: 100  
GPMAX3: SENSE: 100  
GPMAX4: SENSE: 100  
GPD1: 80.00 %  
GPD2: 20.10 %  
GPD3: 11.00 %  
GPD4: -5.00 %  
P10: 100.000 usec  
P20: 80.00 usec  
RDC: 250  
TD: 65536  
SFO1: 100.6203124 MHz  
F2RES2: 0.108421 Hz  
SW: 160.450 ppm  
F2H2O: 80.00 MHz  
SI: 32768  
SF: 400.1300000 MHz  
UCM: 2  
SSB: 0.00 Hz  
LB: 0  
GB: 1.40  
SI: 1024  
MC3: wcho-anti-echo  
DF: 100.6121690 MHz  
VCM: QFHM  
SSB: 2  
GB: 0.00 Hz

ppm

ppm





E20

<sup>1</sup>H-<sup>15</sup>N HMBc

NAME Movip-2020-000  
EXPNO 16  
PROCNO 1  
DATE\_ 20201120  
TIME 3.39  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmbcpg1pddgc  
TD 4096  
SOLVENT DMSO  
DS 16  
SWH 5630.521 Hz  
FIDRES 1.374666 Hz  
AQ 0.3637748 sec  
RG 25193  
DW 88.800 usec  
DE 6.00 usec  
TE 295.5 K  
CHST2 80.0090000  
CHST3 8.0090000  
D0 0.0090000 sec  
D1 1.52867198 sec  
D2 0.00525000 sec  
D6 0.04250000 sec  
D16 0.00200000 sec  
D10 0.0002240 sec

\*\*\*\*\* CHANNEL F1 \*\*\*\*\*  
NUC1 <sup>1</sup>H  
P1 11.60 usec  
F2 23.20 usec  
P2 1.00 dB  
SFO1 400.1329351 MHz

\*\*\*\*\* CHANNEL F2 \*\*\*\*\*  
NUC2 <sup>15</sup>N  
P3 11.52 usec  
P4 4.00 dB  
SFO2 40.5468760 MHz

\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*  
GPMAN1 SINE.100  
GPMAN2 SINE.100  
GPMAN3 SINE.100  
GP21 70.00 %  
GP22 30.00 %  
GP23 50.10 %  
P16 1000.00 usec  
ND0 2  
S12 512  
SFO1 40.5468760 MHz  
FIDRES 43.958361 Hz  
SW 550.000 ppm  
P2MODE OF  
ST 2048  
SF 400.1300000 MHz  
SINE  
NDW 0  
LB 0.00 Hz  
GB 0  
PC 1.40  
ST 1024  
NUC1 <sup>15</sup>N  
SF 40.5468220 MHz  
SINE  
SGB 0  
LB 0.00 Hz  
GB 0

ppm

-150

-100

-50

0

50

100

150

200

250

300

350

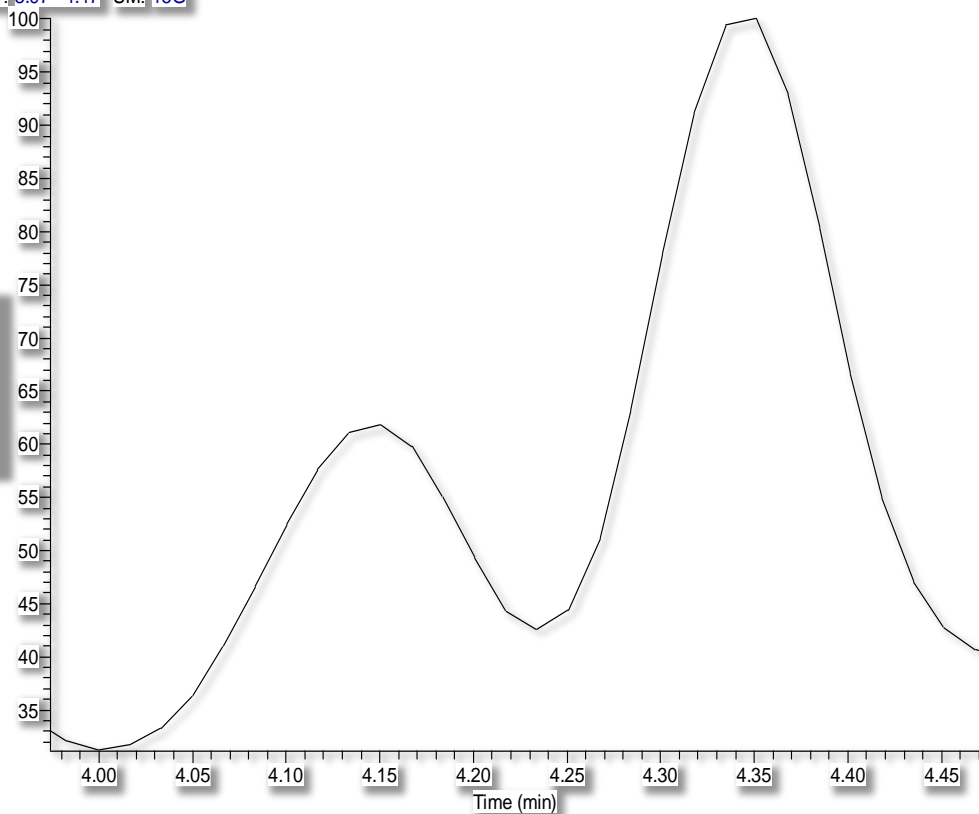
ppm

105.3

248.1

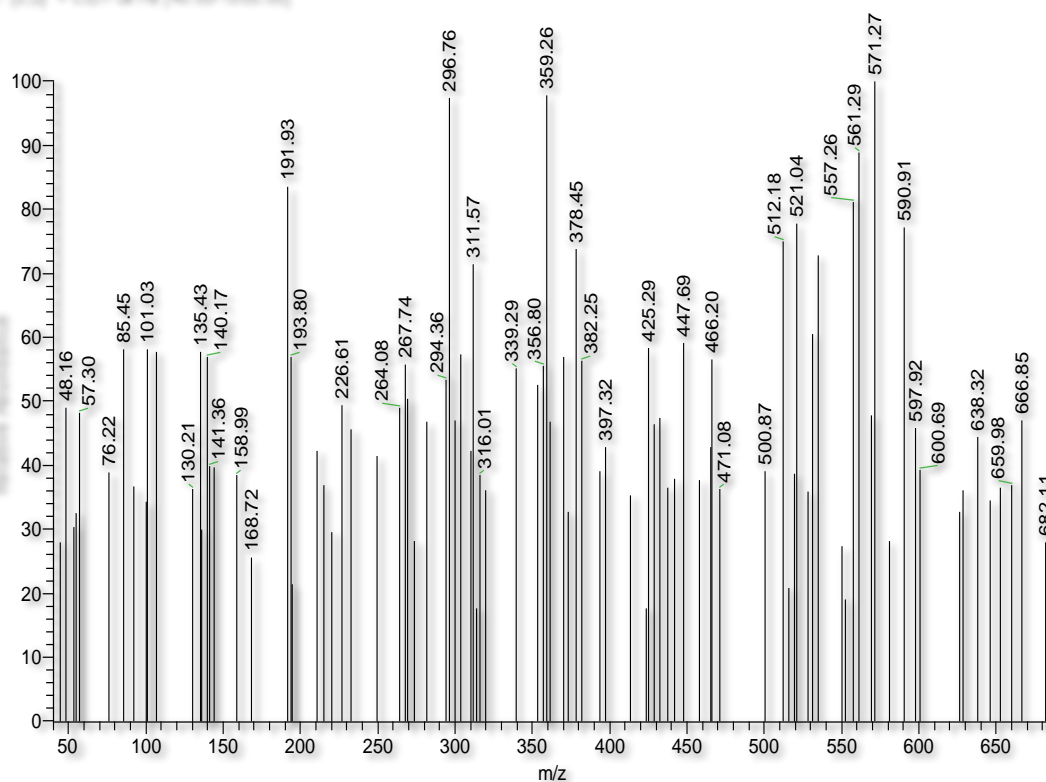
14 13 12 11 10 9 8 7 6 5 4 3 2 1

RT: 3.97 - 4.47 SM: 15G

NL:  
8.51E3  
TIC MS  
essmat-  
elshif-E20

essmat-elshif-E20 #226 RT: 3.80 AV: 1 SB: 2 4.45, 4.45 NL: 2.48E2

T: (0,0) + c EI Full ms [40.00-1000.00]



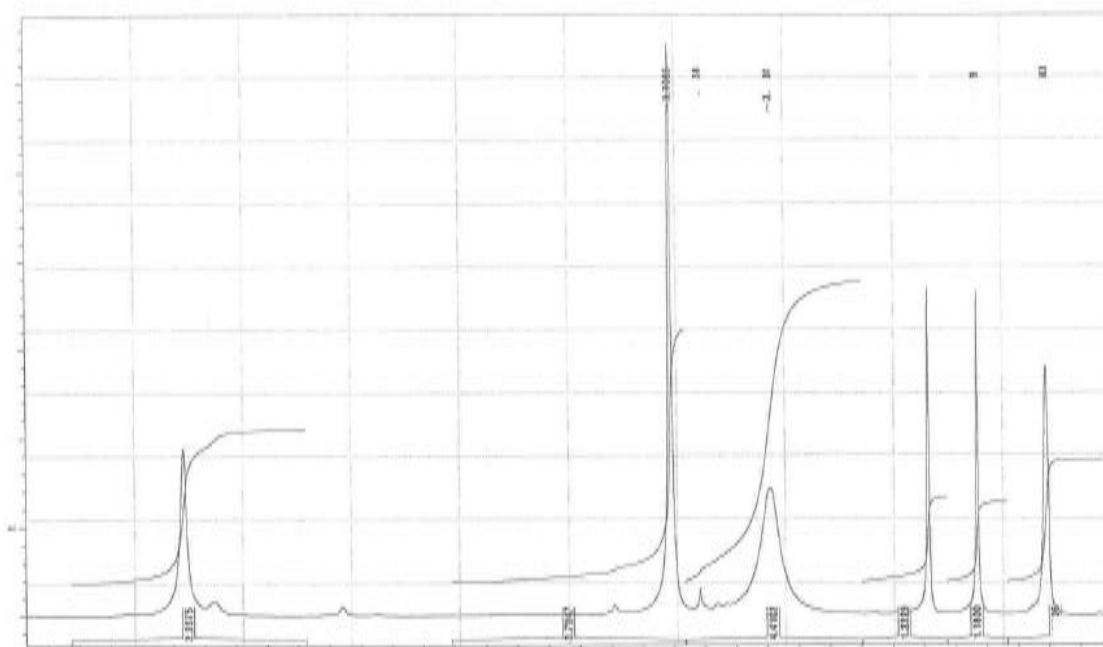
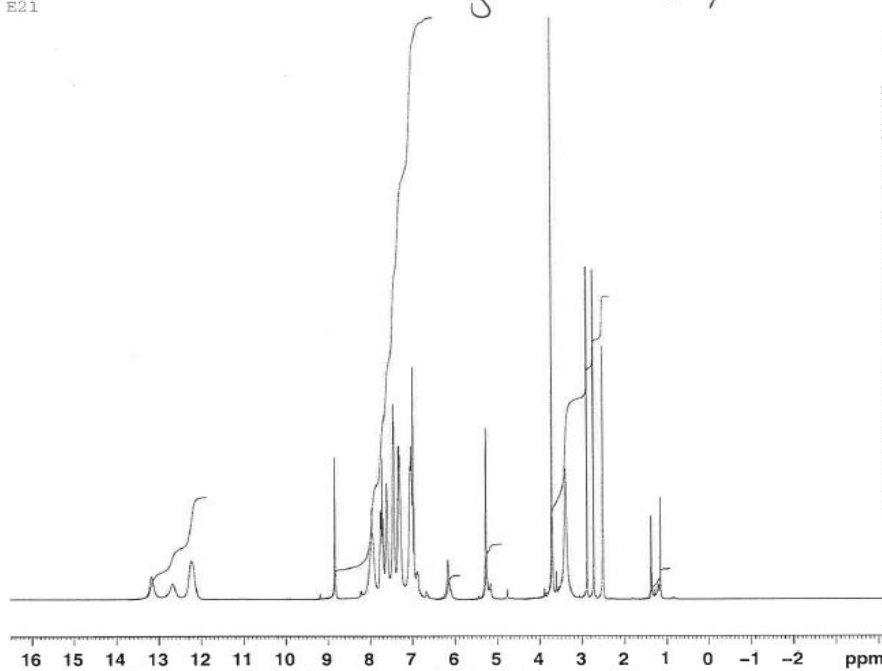
Spectrum data for Compound 8d

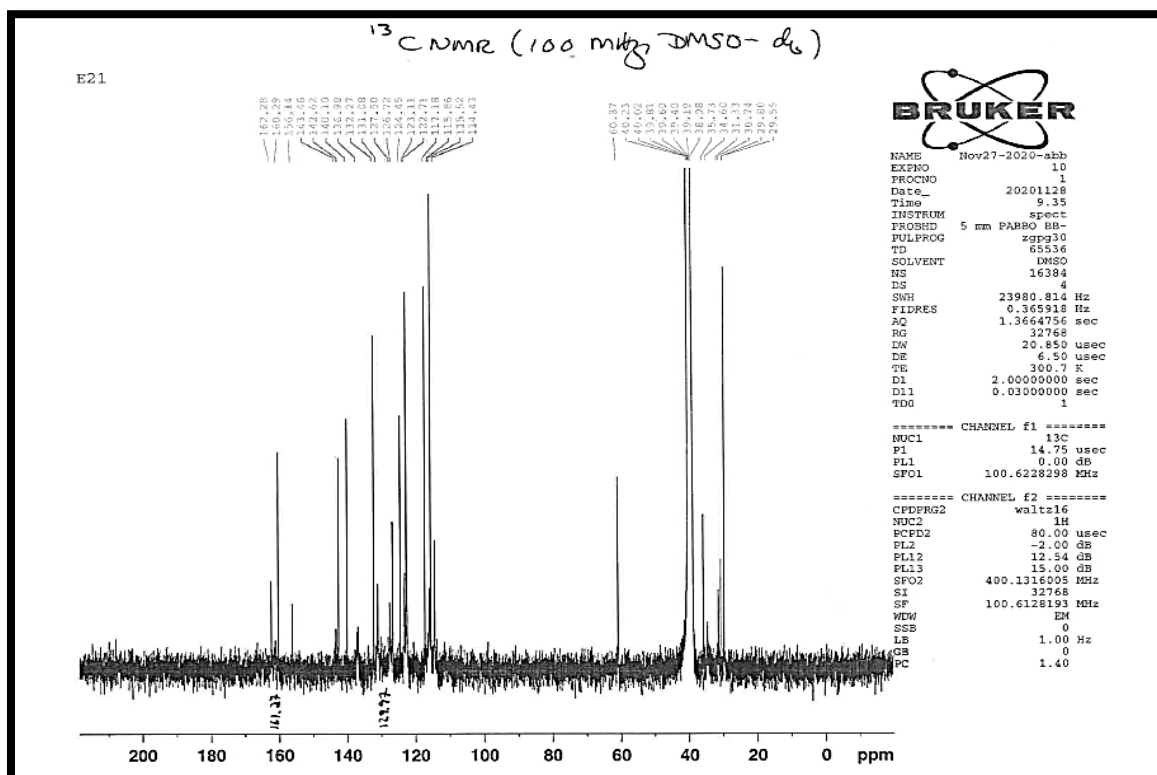
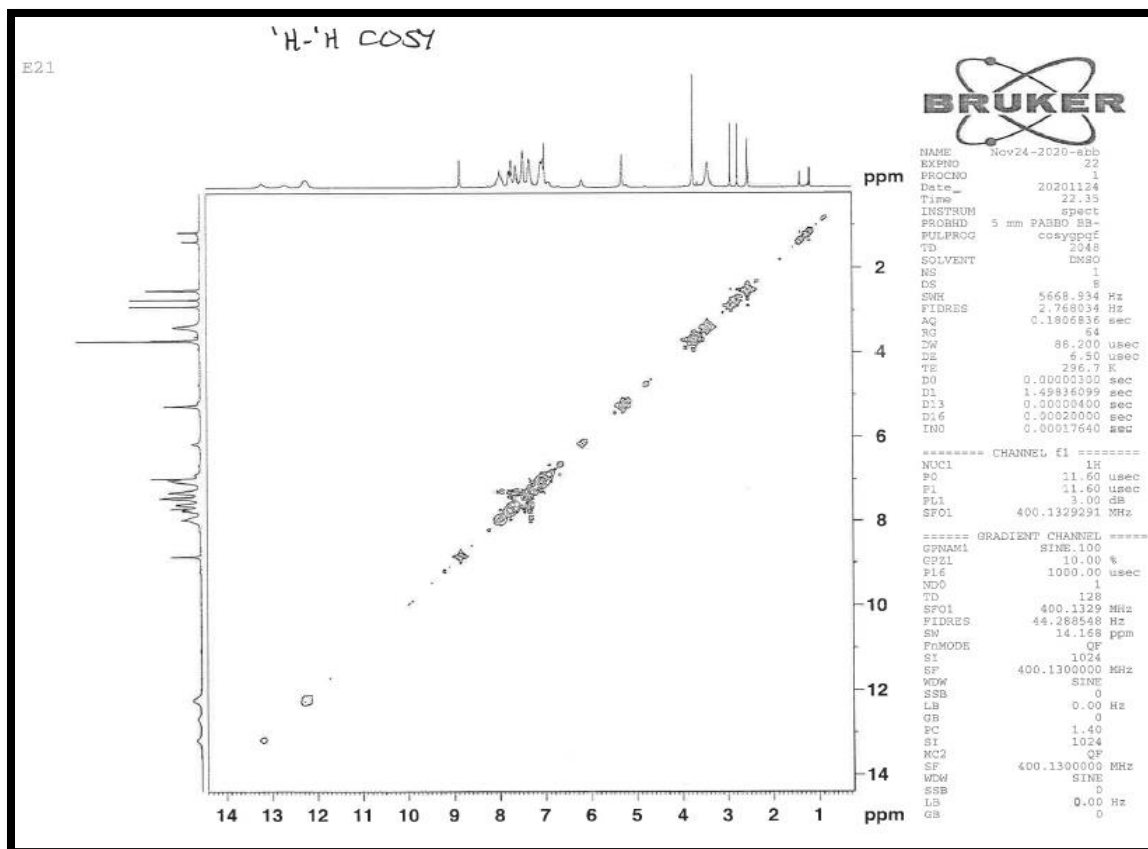
E21

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>)

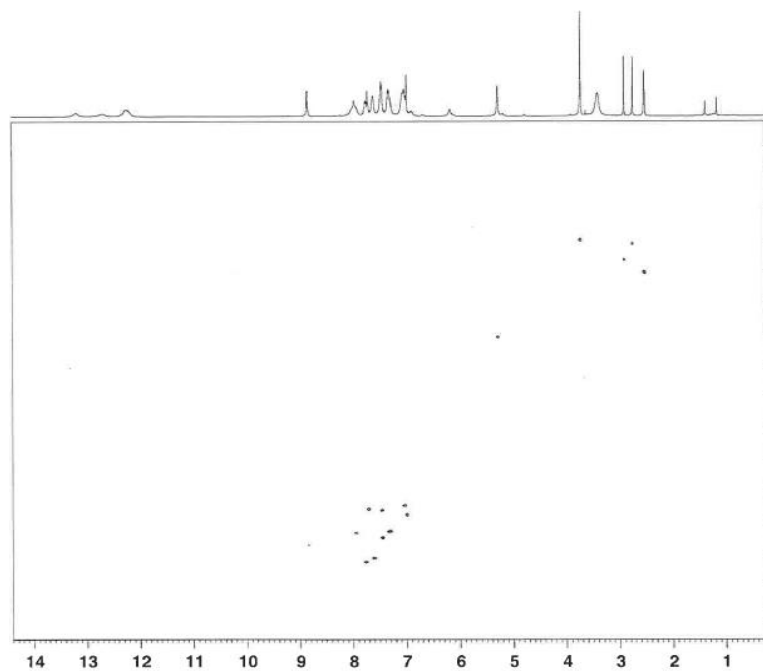
NAME Nov24-2020-abb  
EXPNO 21  
PROCNO 1  
Date\_ 20201124  
Time 22.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 128  
LW 60.400 usec  
DS 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 11.60 usec  
PL1 3.00 dB  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





E21

 $^1\text{H}$ - $^{13}\text{C}$  HSQC

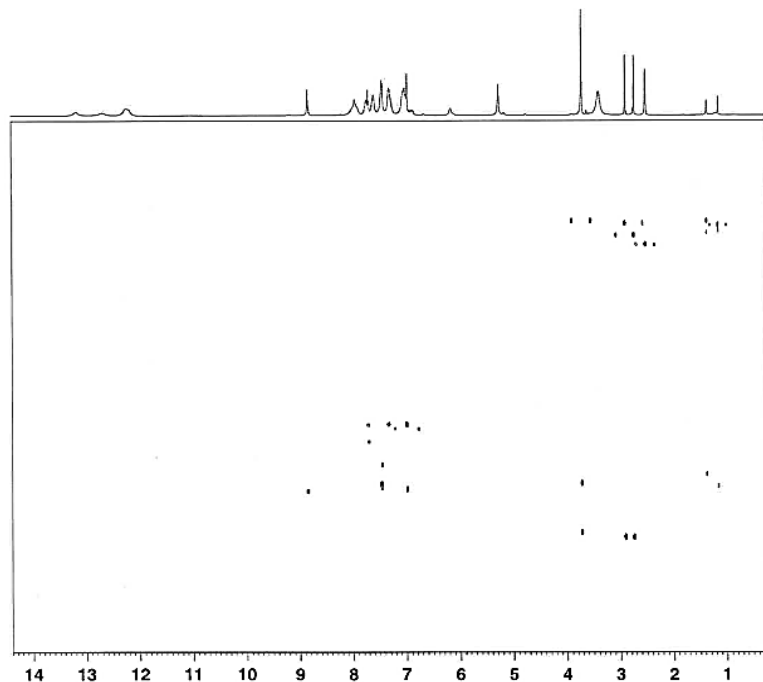
NAME Ruv24-2020-4b0  
EXPNO 24  
PROCNO 1  
DATE\_ 20201124  
TIME 22.41  
INSTRUM spect  
PROBHD 5 mm FARGO SB-  
PULPROG hmqcsgprh  
TD 4096  
SOLVENT DMSO  
NS 32  
DS 16  
SWH 5669.934 Hz  
FIDRES 1.384017 Hz  
AQ 0.3612172 sec  
RG 16384  
DK 88.200 usec  
DE 6.50 usec  
TE 295.7 K  
CNS2 145.000000 sec  
CNS23 10.000000 sec  
D1 0.0000180 sec  
D11 1.52176891 sec  
D2 0.00346828 sec  
D6 0.00000000 sec  
D16 0.00020000 sec  
D10 0.00022295 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 11.60 usec  
P2 23.20 usec  
PL1 9.00 dB  
SFO1 400.1326191 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
NUC2 13C  
P3 9.15 usec  
P2 6.00 dB  
SFO2 100.6228138 MHz

\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*  
GPM1 SINE 100  
GPM2 SINE 100  
GPM3 SINE 100  
OP1 30.00 %  
OP2 30.00 %  
OP3 40.10 %  
P16 1000.00 usec  
TD 128  
SFO1 100.6228138 MHz  
FIDRES 174.382822 Hz  
SW 223.095 ppm  
FNUC2 13C  
S1 2048  
S2 400.1300000 MHz  
WDM SINC  
LB 0.00 Hz  
GB 0  
PC 1.00  
SI 1024  
SC 0  
SFO 100.6127690 MHz  
WDW SINC  
SSB 0  
LB 0.00 Hz  
GB 0

E21

 $^1\text{H}$ - $^{13}\text{C}$  HMBSC

NAME Ruv24-2020-4b0  
EXPNO 24  
PROCNO 1  
DATE\_ 20201124  
TIME 23.39  
INSTRUM spect  
PROBHD 5 mm FARGO SB-  
PULPROG hmbzgprh  
TD 4096  
SOLVENT DMSO  
NS 32  
DS 16  
SWH 5669.934 Hz  
FIDRES 1.384017 Hz  
AQ 0.3612172 sec  
RG 16384  
DK 88.200 usec  
DE 6.50 usec  
TE 295.7 K  
CNS2 145.000000 sec  
CNS23 10.000000 sec  
D1 0.0000180 sec  
D11 1.52176891 sec  
D2 0.00346828 sec  
D6 0.00000000 sec  
D16 0.00020000 sec  
D10 0.00022295 sec

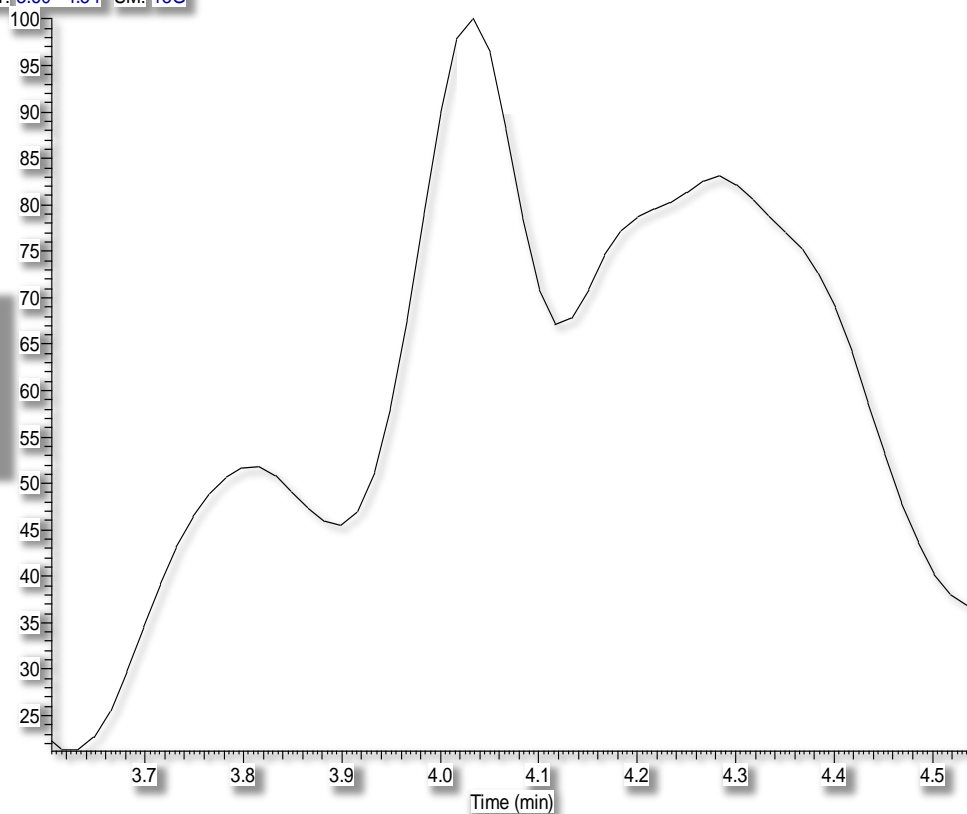
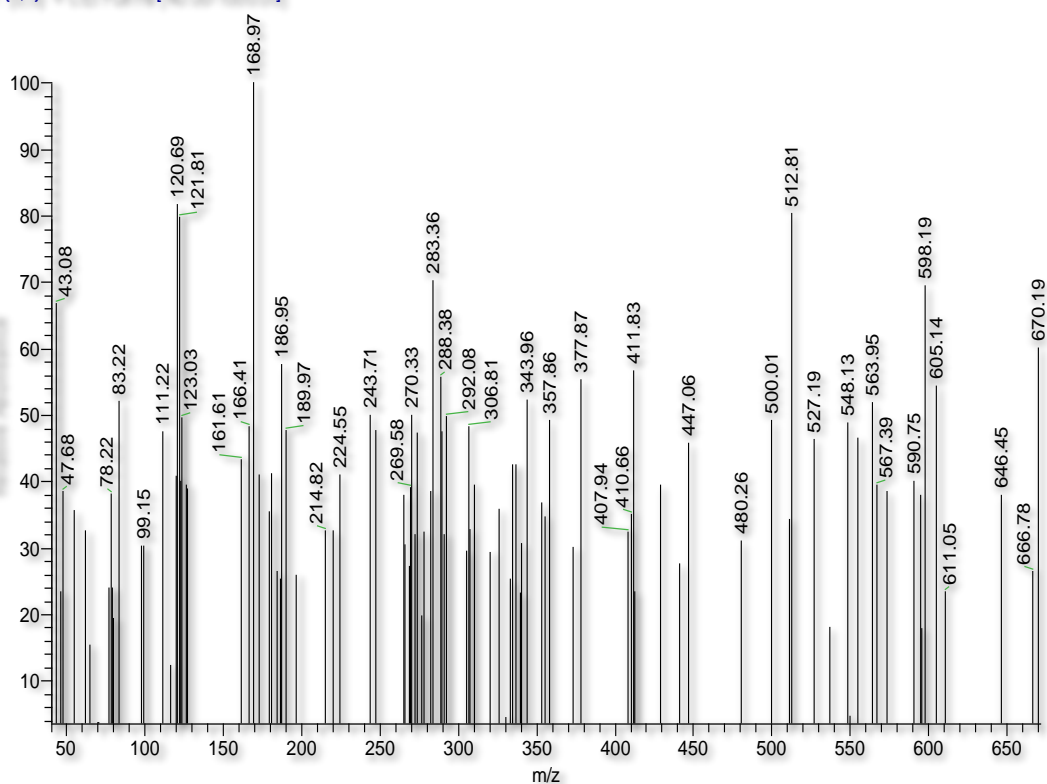
\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 11.60 usec  
P2 23.20 usec  
PL1 9.00 dB  
SFO1 400.1326191 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
NUC2 13C  
P3 9.15 usec  
P2 6.00 dB  
SFO2 100.6228138 MHz

\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*  
GPM1 SINE 100  
GPM2 SINE 100  
GPM3 SINE 100  
OP1 30.00 %  
OP2 30.00 %  
OP3 40.10 %  
P16 1000.00 usec  
TD 128  
SFO1 100.6228138 MHz  
FIDRES 174.382822 Hz  
SW 223.095 ppm  
FNUC2 13C  
S1 2048  
S2 400.1300000 MHz  
WDM SINC  
LB 0.00 Hz  
GB 0  
PC 1.00  
SI 1024  
SC 0  
SFO 100.6127690 MHz  
WDW SINC  
SSB 0  
LB 0.00 Hz  
GB 0



RT: 3.60 - 4.54 SM: 15G

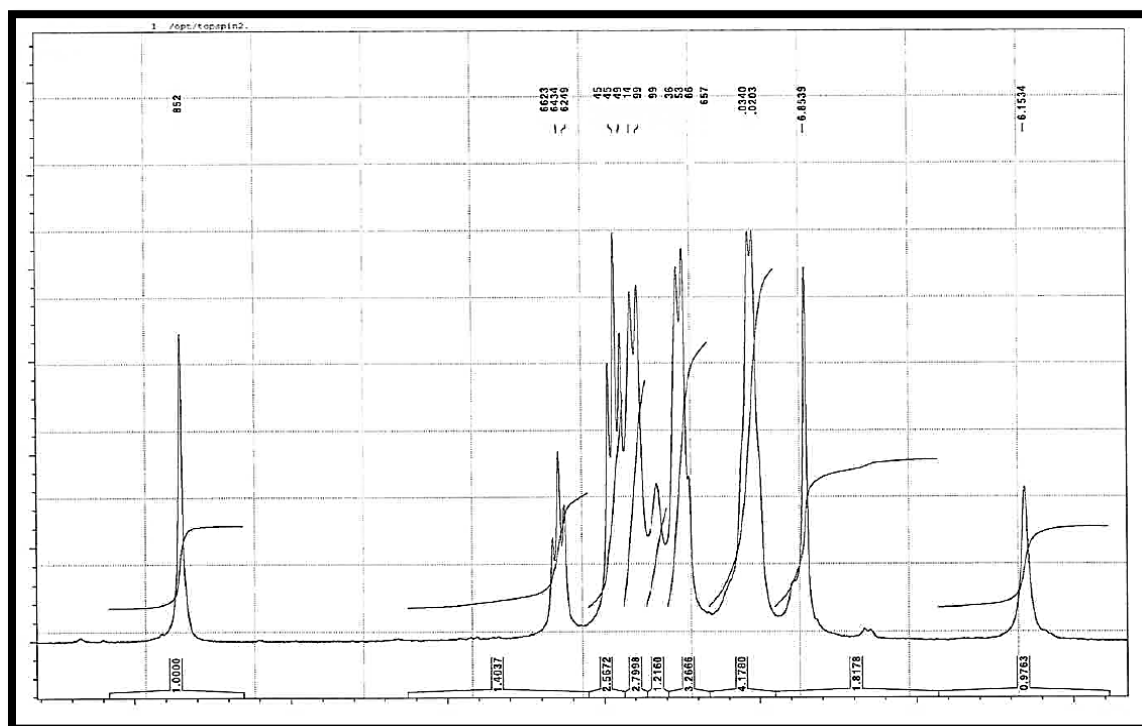
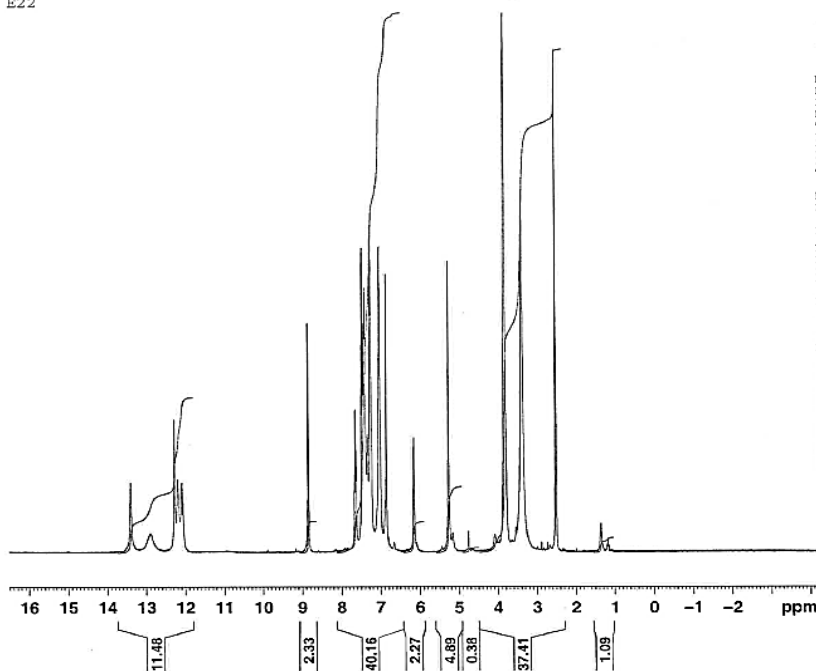
NL:  
1.85E4  
TIC MS  
essmat-  
elshif-E21essmat-elshif-E21 #256 RT: 4.30 AV: 1 SB: 2 4.45, 4.45 NL: 2.63E2  
T: (0,0) + c EI Full ms [40.00-1000.00]

E22

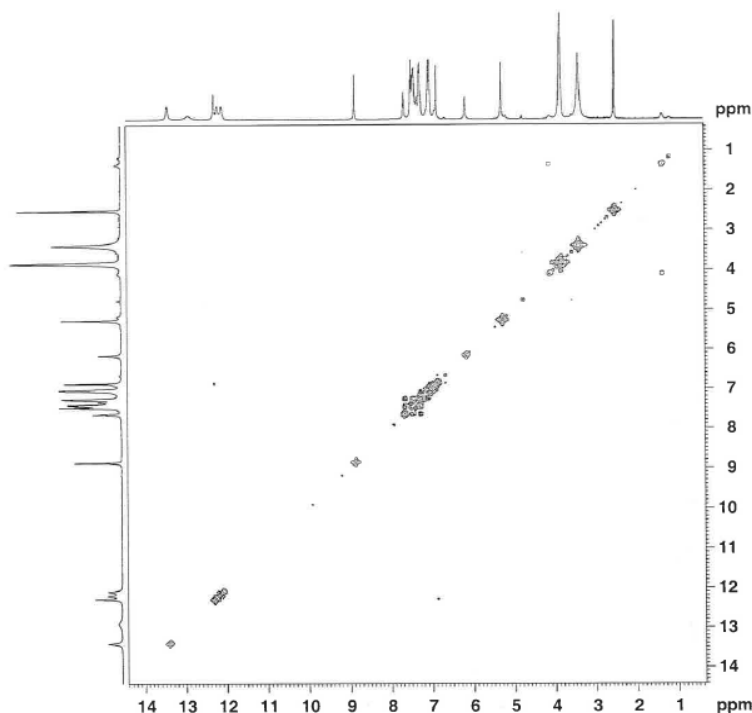
<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>)

NAME Nov03-2020-abb  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20201103  
 Time 21.20  
 INSTRUM spect  
 PROBRD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 181  
 DW 60.400 usec  
 DE 6.50 usec  
 TE 297.1 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.60 usec  
 PL1 3.00 dB  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300000 MHz  
 WNW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



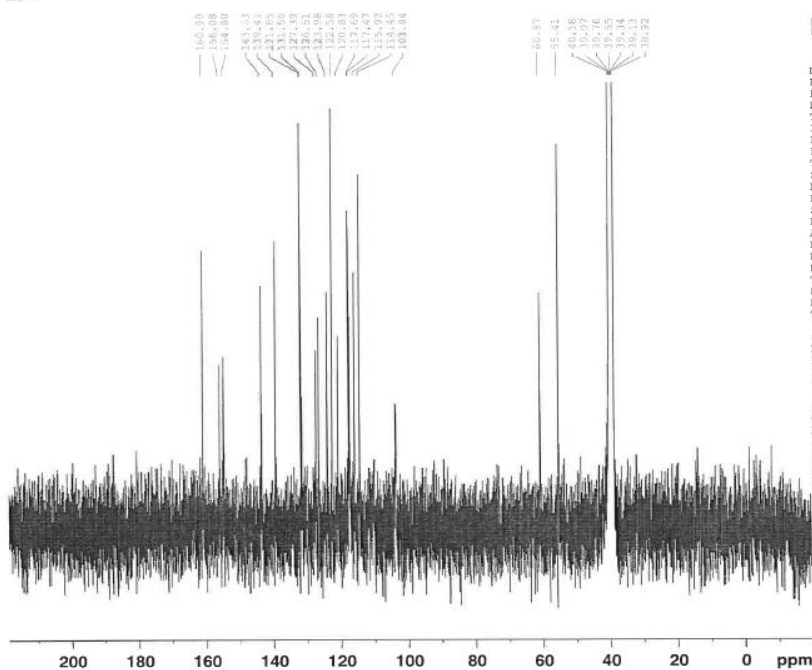
E22

<sup>1</sup>H-<sup>1</sup>H COSY

NAME Nov03-2020-abb  
 EXPNO 12  
 PROCNO 1  
 Date\_ 20201103  
 Time 21.22  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosygpcpf  
 TD 2048  
 SOLVENT DMSO  
 NS 1  
 DS 8  
 SWH 5630.631 Hz  
 FIDRES 2.749331 Hz  
 AQ 0.1819124 sec  
 RG 64  
 DW 86.800 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D0 0.00000308 sec  
 D1 1.49631298 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 IN0 0.00017760 sec


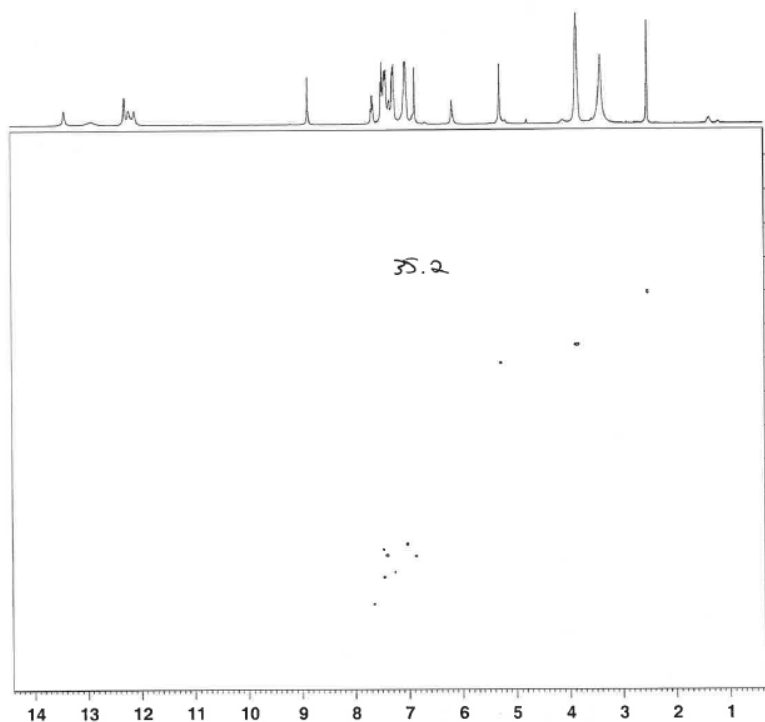
===== CHANNEL f1 =====  
 NUC1 1H  
 P0 11.60 usec  
 P1 11.60 usec  
 PL1 3.00 dB  
 SFO1 400.1329535 MHz  
 ===== GRADIENT CHANNEL =====  
 GPM1 SINE 100  
 GP1 10.00 %  
 P16 1000.00 usec  
 ND0 1  
 TD 128  
 SFO1 400.133 MHz  
 FIDRES 43.989304 Hz  
 SW 14.072 ppm  
 FMODE QF  
 SI 1024  
 SF 400.1300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40  
 SI 1024  
 MC2 QF  
 SF 400.1300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

E22

<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>)

NAME Nov03-2020-abb  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20201103  
 Time 21.17  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 4096  
 DS 4  
 SWH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664756 sec  
 RG 52768  
 DW 20.850 usec  
 DE 6.50 usec  
 TE 300.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 14.75 usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz  
 ===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -2.00 dB  
 PL12 12.54 dB  
 PL13 15.00 dB  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6128193 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

${}^1\text{H}-{}^{13}\text{C}$  HSQC

```

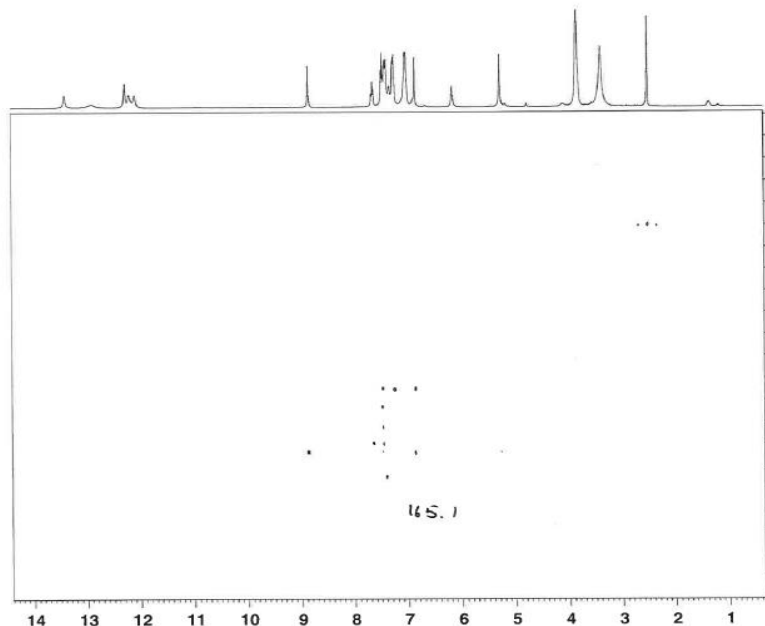
NAME      HWY12-2020-abb
EXPNO     13
PROCNO    1
Date_     20101101
Time      21:23
INSTRUM    spect
PROBHD     5 mm PABBO
PULPROG    zgpg30
PHASPROG   hsqcpg30f1
F2         124
SOLVENT    H2O
NS          2
DS          16
AQ          5.539 s      Hz
RG          5.496665 Hz
NUC1        0.039899 Hz
RG          18359.4
NUC2        88.650000 usec
RG          6.50 usec
NUC3        2
DS          16
AQ          5.539000 Hz
RG          145.000000 Hz
NUC1        0.000000 usec
RG          1.804709 usec
NUC2        0.0017144 usec
RG          0.0100000 usec
NUC3        0.00020490 usec
RG          0.00020100 usec
NUC4        0.00082027 usec
RG          0.00030000 usec

===== CHANNEL f1 =====
NUC1      P1
P2         11.60 usec
RG          21.20 usec
P3         1800.15 usec
RG          10.00 usec
RF01      120.139355 MHz

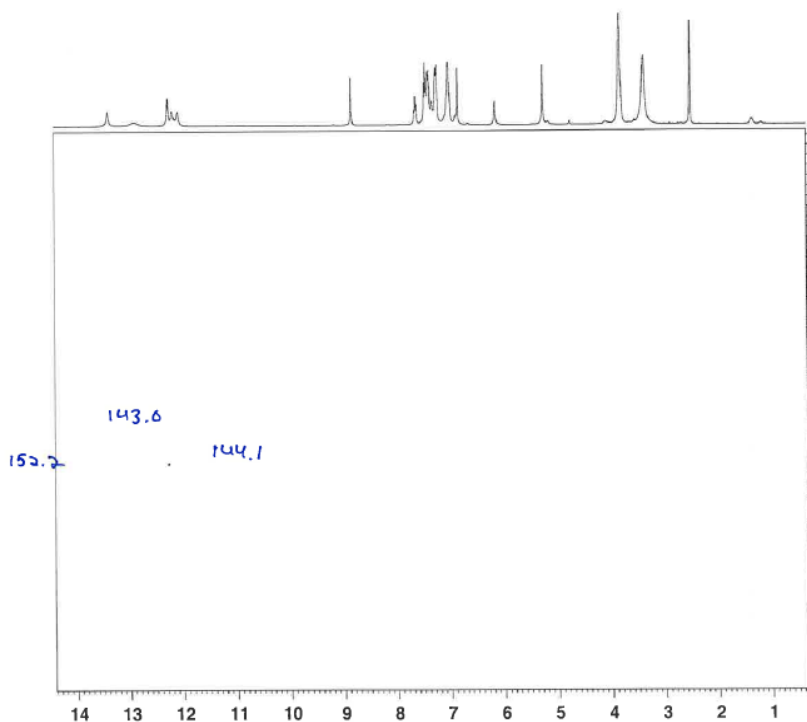
===== CHANNEL f2 =====
NUC1      P1
P2         11.60 usec
RG          21.20 usec
P3         1800.15 usec
RG          10.00 usec
RF02      120.139355 MHz

===== GRADIENT CHIRP =====
GPRPM1    STNK-100
GPRPM2    STNK-100
GPRPM3    STNK-100
GPRPM4    STNK-100
GPR1       80.00 %
GPR2       11.00 %
GPR3       1.00 %
GPR4       0.00 %
P16        1000.00 usec
P17        600.00 usec
RF01        120.139355 MHz
RF02        120.139355 MHz
RF03        100.618000 MHz
RF04        106.284621 Hz
RF05        148.198000 MHz
PRGNAME    Echo-Antiecho
NUC1        400.1300000 MHz
CPDPRG1    CPMAS
SF          600.130000 MHz
SSB         0.000 Hz
PC          0.000 Hz
PC2         0.000 Hz
RG          0.1024
RG2          0.1024
RG3          0.1024
RG4          100.618000 MHz
RG5          0.1024
RG6          0.000 Hz
RG7          0.000 Hz

```

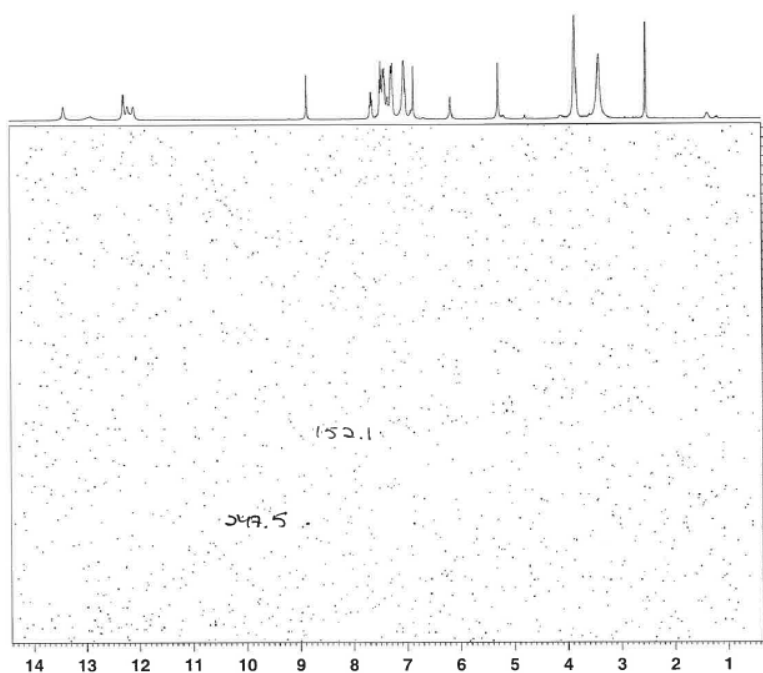
 $^1\text{H}-^{13}\text{C}$  HmB C[illegible]

E22

 $^1\text{H}$ - $^{15}\text{N}$  HSQC

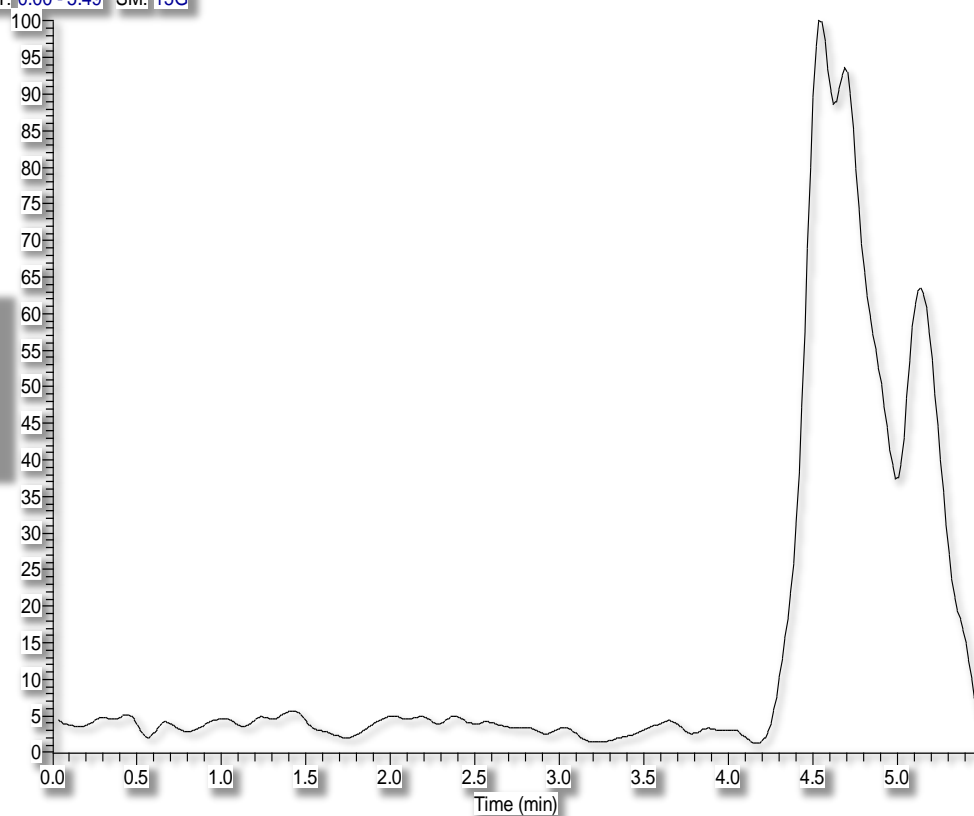
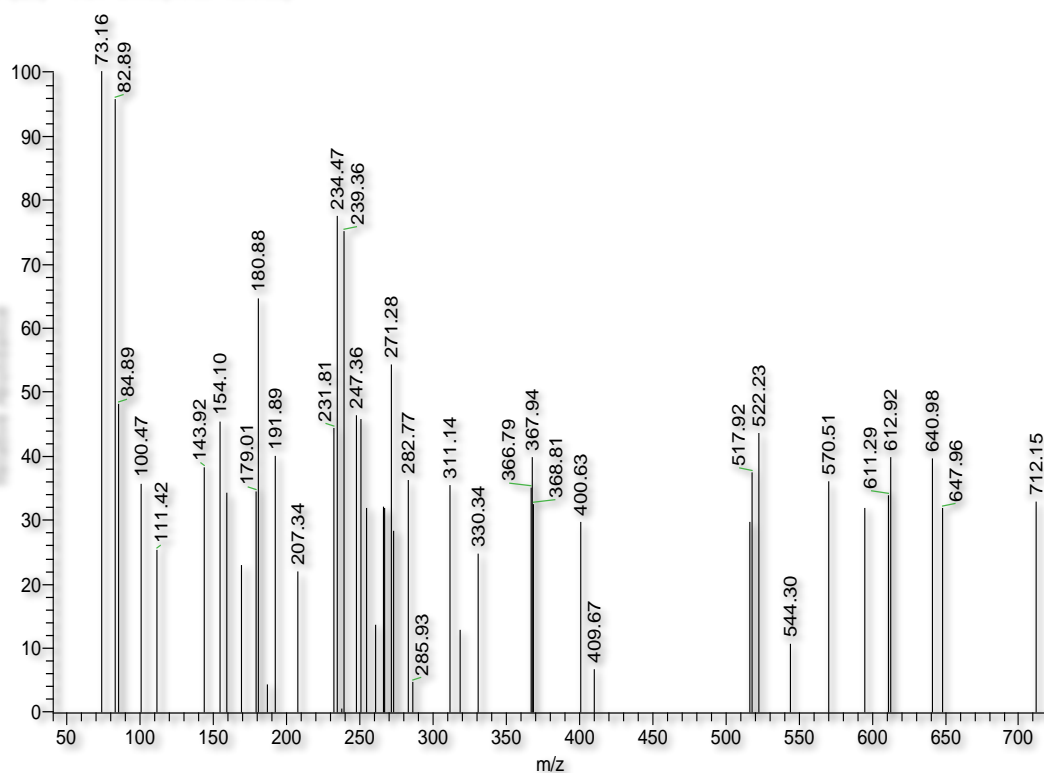
NAME: hmv03-2020-abc  
EXPNO: 1  
PROCNO: 1  
Date\_: 20201104  
Time: 9.41  
INSTRUM: spect  
PROBHD: 5 mm PABBO BB-  
PULPROG: hmqcwgpp12  
TD: 1024  
SOLVENT: DMSO  
DS: 4  
SS: 16  
SWH: 5630.631 Hz  
FIDRES: 0.496681 Hz  
AQ: 0.0909812 sec  
RG: 21370.5  
DQ: 88.800 usec  
DE: 6.00 usec  
TE: 295.6 K  
CHST2: 80.000000  
DQ: 0.0000000 sec  
D1: 1.5047984 sec  
D2: 0.0277778 sec  
D3: 0.0300000 sec  
D4: 0.0300000 sec  
D5: 0.0300000 sec  
D6: 0.0086207 sec  
D7: 0.0092240 sec  
SCOPFMS  
===== CHANNEL f1 =====  
NUC1: 15N  
P1: 13.60 usec  
P2: 23.20 usec  
P22: 1000.00 usec  
PL1: 1.00 dB  
PL2: 436.1329335 MHz  
===== CHANNEL f2 =====  
CPDPRG2: gddp  
NUC2: 1H  
P1: 11.52 usec  
P2: 23.15 usec  
P22: 190.00 usec  
PL1: -4.00 dB  
PL2: 20.34 dB  
PL3: 40.5488755 MHz  
===== GRADIENT CHANNEL =====  
GPRAM1: SINE.100  
GPRAM2: SINE.50  
GPRAM3: SINE.100  
GPRAM4: SINE.100  
GR1: 40.00 %  
GR2: 8.10 %  
GR3: 11.00 %  
GR4: -5.00 %  
P16: 1000.00 usec  
P19: 600.00 usec  
NUC3: 2  
TD: 256  
FIDRES: 40.54888 MHz  
FIDRES2: 87.116722 Hz  
SW: 550.000 ppr  
F2FREQ: Echo-AntiEcho  
SFO1: 400.1360000 MHz  
SFO2: 400.1360000 MHz  
SFB: 0.00 Hz  
LB: 0  
GB: 0  
PC: 1.40  
FC: 1024  
SC: 0  
SF: 40.5488220 MHz  
WDW: SINE  
SSB: 0  
LB: 0.00 Hz  
GB: 0

E22

 $^1\text{H}$ - $^{15}\text{N}$  HMQC

NAME: hmv03-2020-abc  
EXPNO: 16  
PROCNO: 1  
Date\_: 20201104  
Time: 1.18  
INSTRUM: spect  
PROBHD: 5 mm PABBO BB-  
PULPROG: hmqcwgpp12  
TD: 4096  
SOLVENT: DMSO  
DS: 16  
SS: 16  
SWH: 5630.631 Hz  
FIDRES: 1.374664 Hz  
AQ: 0.3627748 sec  
RG: 20000  
DQ: 88.800 usec  
DE: 6.00 usec  
TE: 295.6 K  
CHST2: 80.000000  
CHST13: 8.0000000  
D1: 0.0000000 sec  
D2: 1.5047984 sec  
D3: 0.0025000 sec  
D4: 0.0425000 sec  
D5: 0.0025000 sec  
D6: 0.0000000 sec  
D7: 0.0000000 sec  
===== CHANNEL f1 =====  
NUC1: 15N  
P1: 13.60 usec  
P2: 23.20 usec  
PL1: 3.00 dB  
PL2: 400.1329335 MHz  
===== CHANNEL f2 =====  
NUC2: 1H  
P1: 11.52 usec  
P2: 23.15 usec  
PL1: -4.00 dB  
PL2: 40.5488760 MHz  
===== GRADIENT CHANNEL =====  
GPRAM1: SINE.100  
GPRAM2: SINE.100  
GPRAM3: SINE.100  
GR1: 40.00 %  
GR2: 8.10 %  
GR3: 11.00 %  
GR4: -5.00 %  
P16: 1000.00 usec  
P19: 600.00 usec  
NUC3: 2  
TD: 256  
FIDRES: 40.54888 MHz  
FIDRES2: 43.558361 Hz  
SW: 550.000 ppr  
F2FREQ: Echo-AntiEcho  
SFO1: 400.1360000 MHz  
SFO2: 400.1360000 MHz  
SFB: 0.00 Hz  
LB: 0  
GB: 0  
PC: 1.40  
FC: 1024  
SC: 0  
SF: 40.5488220 MHz  
WDW: SINE  
SSB: 0  
LB: 0.00 Hz  
GB: 0

RT: 0.00 - 5.49 SM: 15G

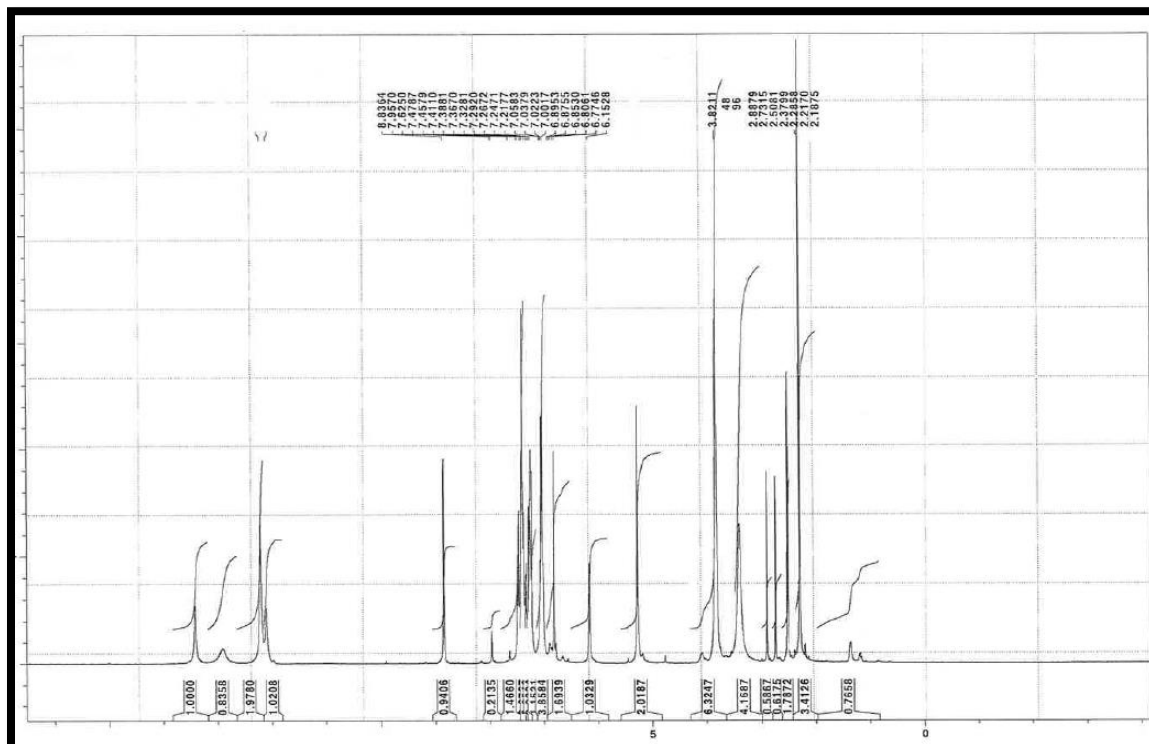
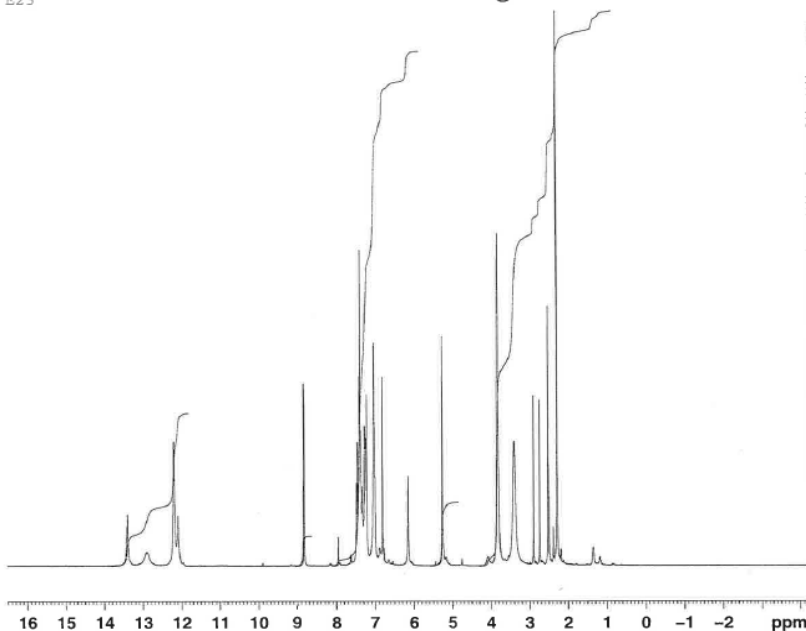
NL:  
5.03E5  
TIC MS  
essmat-  
elshif-E22essmat-elshif-E22 #103 RT: 1.74 AV: 1 SB: 2 4.45, 4.45 NL: 3.03E2  
T: (0.0) + c EI Full ms [40.00-1000.00]

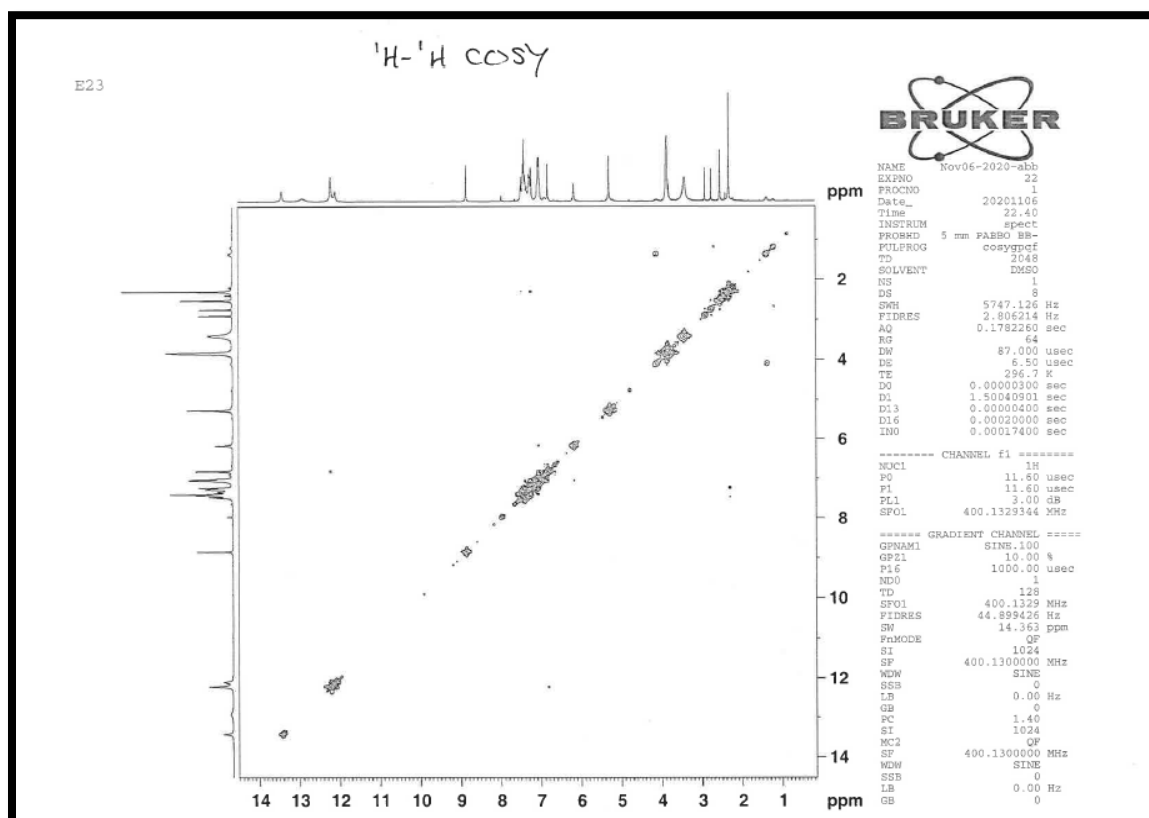
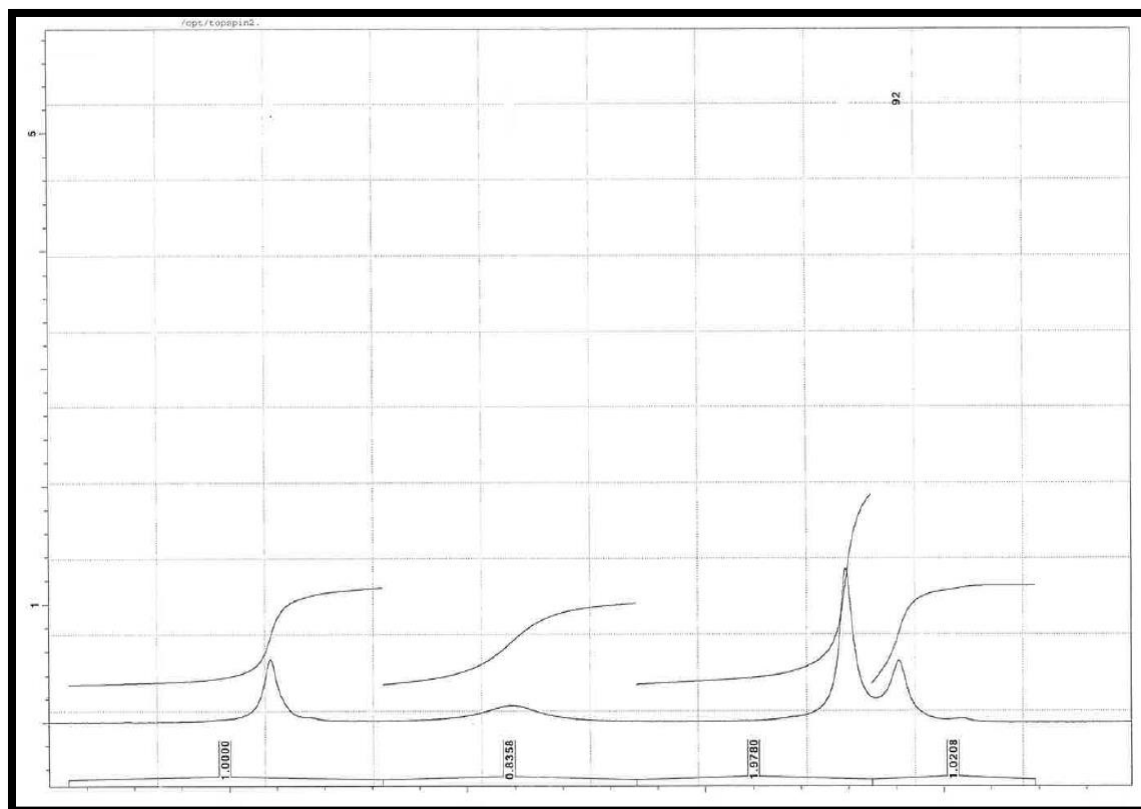
E23

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>)

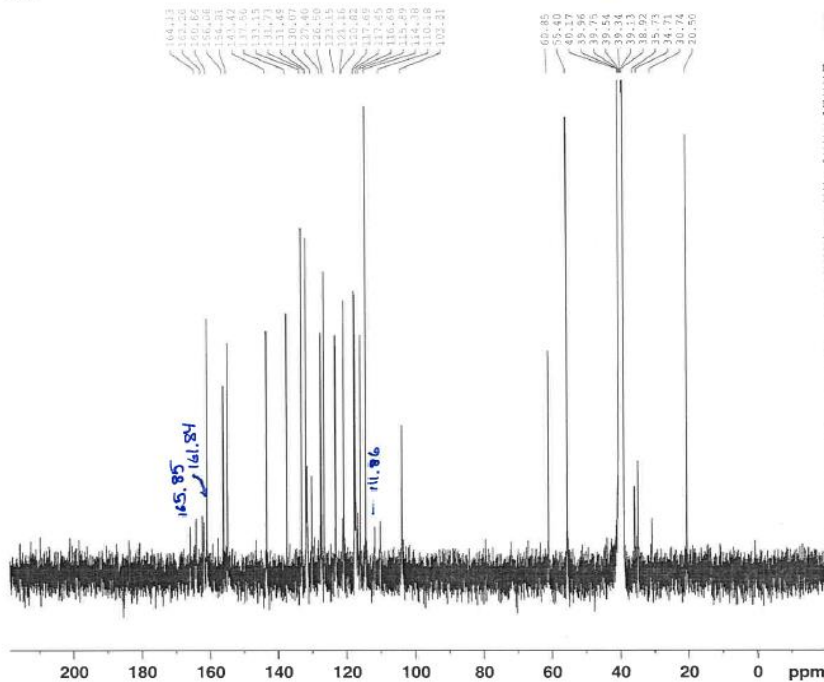
NAME Nov06-2020-abb  
EXPNO 21  
PROCNO 1  
Date\_ 20201106  
Time 22.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 128  
IN 60.400 usec  
DE 6.50 usec  
TE 297.0 K  
DL 1.0000000 sec  
TD0 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 11.60 usec  
PL1 3.00 dB  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





E23

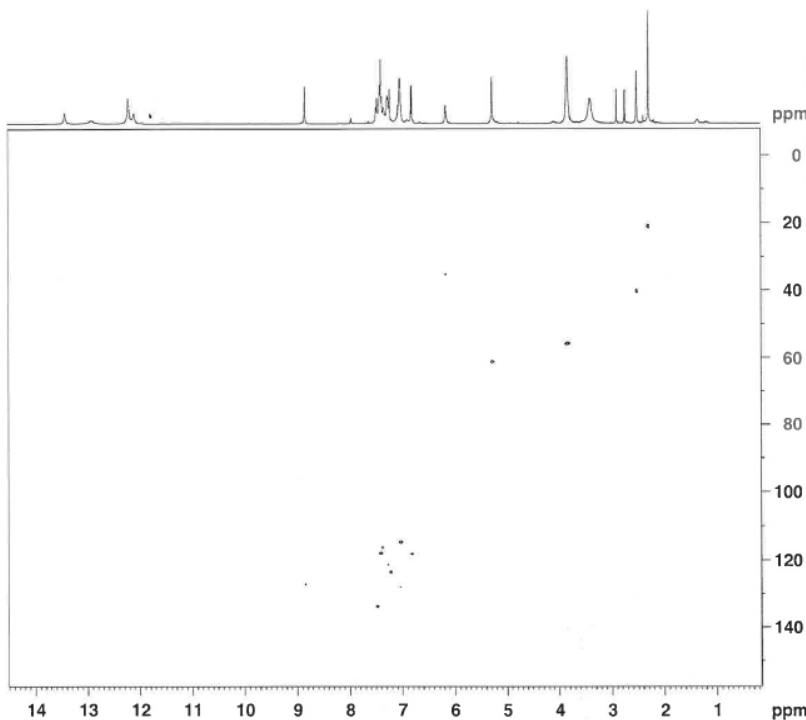
 $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )

NAME Nov06-2020-abb  
EXPNO 27  
PROCNO 1  
Date\_ 20201108  
Time\_ 5.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 16384  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 32768  
DW 20.850 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1  $^{13}\text{C}$   
P1 14.75 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2  $^1\text{H}$   
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 12.54 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6128193 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

E23

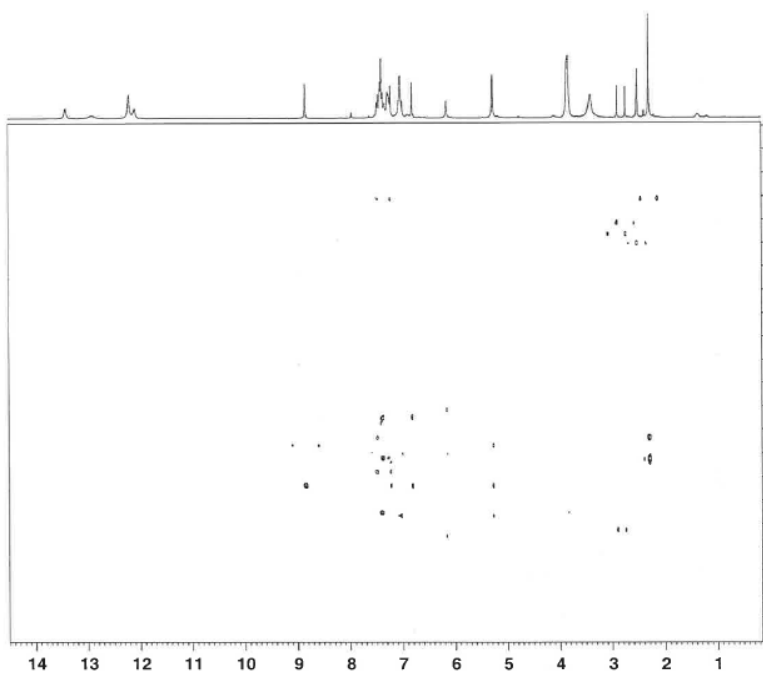
 $^1\text{H}$ - $^{13}\text{C}$  HSQC

NAME Nov06-2020-abb  
EXPNO 27  
PROCNO 1  
Date\_ 20201108  
Time\_ 5.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 16384  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 32768  
DW 20.850 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1  $^{13}\text{C}$   
P1 14.75 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

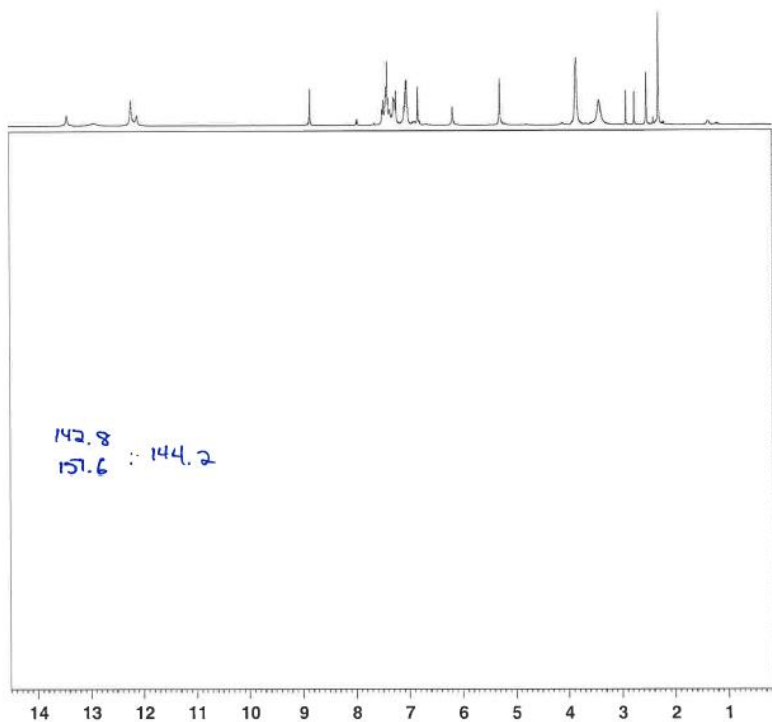
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2  $^1\text{H}$   
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 12.54 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6128193 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

E23

 $^1\text{H}-^{13}\text{C}$  HmBC

NAME Nov06-2020-02b  
 EXPNO 24  
 PROCNO 1  
 Date\_ 20201104  
 Time 22.44  
 INSTRUM spect  
 PULPROG 5 nm F2BBO BB-  
 SOLVENT DMSO  
 NS 32  
 DS 16  
 SMS 5747.124 Hz  
 FIDRES 1.403107 Hz  
 AQ 0.3564021 sec  
 RG 26008  
 DW 87.000 usec  
 DE 4.50 usec  
 TE 295.7 K  
 CMT2 145.000000 sec  
 CNST1 10.0000000  
 D0 0.0000000 sec  
 D1 2.53664604 sec  
 D2 0.0034828 sec  
 D6 0.0000000 sec  
 D16 0.0002000 sec  
 INO 0.0002235 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.60 usec  
 P2 21.20 usec  
 PC1 1.00 dB  
 SFO1 400.1329344 MHz  
 ===== CHANNEL f2 =====  
 NUC2 13C  
 P3 9.19 usec  
 PC2 0.00 dB  
 SFO2 100.6228138 MHz  
 ===== GRADIENT CHANNEL =====  
 GPMAX1 SINE 100  
 GPMAX2 SINE 100  
 GPMAX3 SINE 100  
 GPC1 50.00 %  
 GPC2 10.00 %  
 GPC3 40.10 %  
 P16 1000.00 usec  
 MD0 2  
 TD 128  
 SFO1 100.6228138 MHz  
 FIDRES 174.592422 Hz  
 SM 222.090 ppm  
 FWHM02 0  
 SI 2048  
 SF 400.1300000 MHz  
 MDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40  
 ST 1024  
 MC1 0  
 SF 100.6127450 MHz  
 MDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

E23

 $^1\text{H}-^{15}\text{N}$  HsQC

NAME Nov06-2020-02b  
 EXPNO 24  
 PROCNO 1  
 Date\_ 20201104  
 Time 22.54  
 INSTRUM spect  
 PULPROG 5 nm F2BBO BB-  
 SOLVENT DMSO  
 NS 32  
 DS 16  
 SMS 5747.124 Hz  
 FIDRES 1.403107 Hz  
 AQ 0.3564021 sec  
 RG 26008  
 DW 87.000 usec  
 DE 4.50 usec  
 TE 295.7 K  
 CMT2 90.000000 sec  
 D0 0.0000000 sec  
 D1 1.50675797 sec  
 D4 0.0037777 sec  
 D11 0.0000000 sec  
 D12 0.0000000 sec  
 D16 0.0002000 sec  
 INO 0.0002240 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.60 usec  
 P2 21.20 usec  
 PC1 1.00 dB  
 SFO1 400.1329344 MHz  
 ===== CHANNEL f2 =====  
 NUC2 15N  
 P3 11.53 usec  
 PC2 21.00 usec  
 PC3 190.00 usec  
 PC4 -4.00 dB  
 SFO2 100.6228138 MHz  
 ===== GRADIENT CHANNEL =====  
 GPMAX1 SINE 100  
 GPMAX2 SINE 100  
 GPMAX3 SINE 100  
 GPC1 50.00 %  
 GPC2 10.00 %  
 GPC3 40.10 %  
 P16 1000.00 usec  
 MD0 2  
 TD 128  
 SFO1 100.6228138 MHz  
 FIDRES 174.592422 Hz  
 SM 222.090 ppm  
 FWHM02 0  
 SI 2048  
 SF 400.1300000 MHz  
 MDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40  
 ST 1024  
 MC1 0  
 SF 100.6127450 MHz  
 MDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

E23

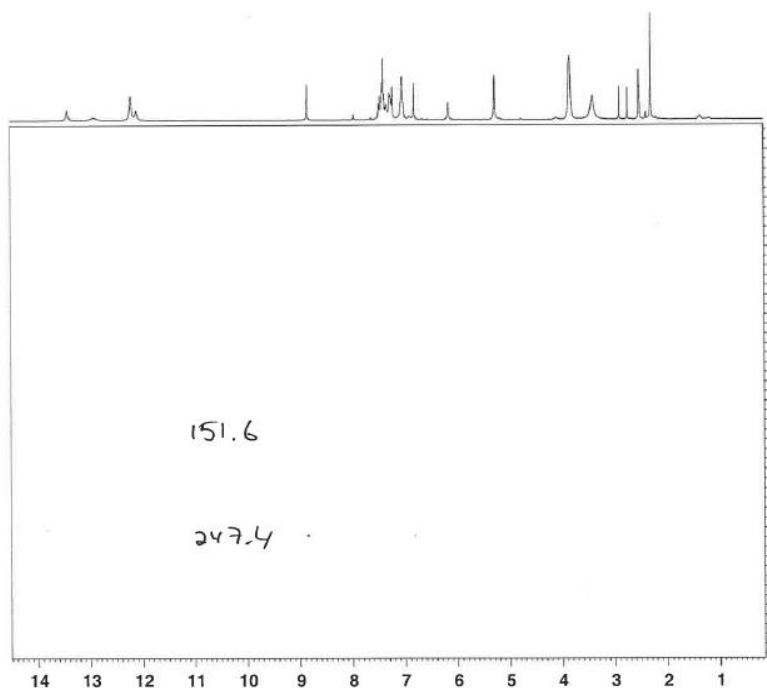
 $^1\text{H}-^{15}\text{N}$  HMBC

NAME Nov06-2020-abc  
 EXPNO 36  
 PROCNO 1  
 DATE\_ 20201107  
 TIME 2.55  
 INSTRUM spect  
 F2PROG 5 mm PANKO SR-  
 PULPROG hmcgpg1gndat  
 TD 4096  
 SOLVENT DMSO  
 NS 16  
 DS 16  
 SWH 5747.156 Hz  
 FIDRES 1.483107 Hz  
 AQ 0.3564820 sec  
 RG 36008  
 DW 87.600 usec  
 DE 6.00 usec  
 TE 295.5 K  
 CQZT2 88.000000  
 CQZT3 8.000000  
 D0 0.0000000 sec  
 D1 1.53656404 sec  
 D2 0.0025000 sec  
 D3 0.0025000 sec  
 D16 0.0025000 sec  
 D10 0.0002240 sec

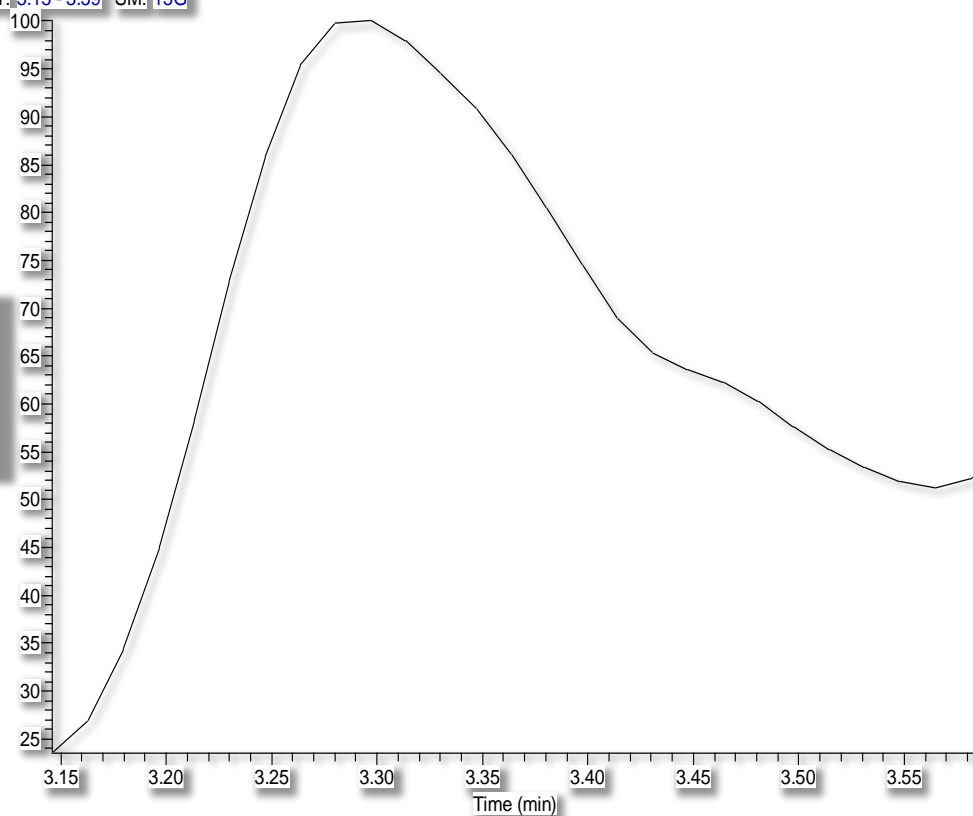
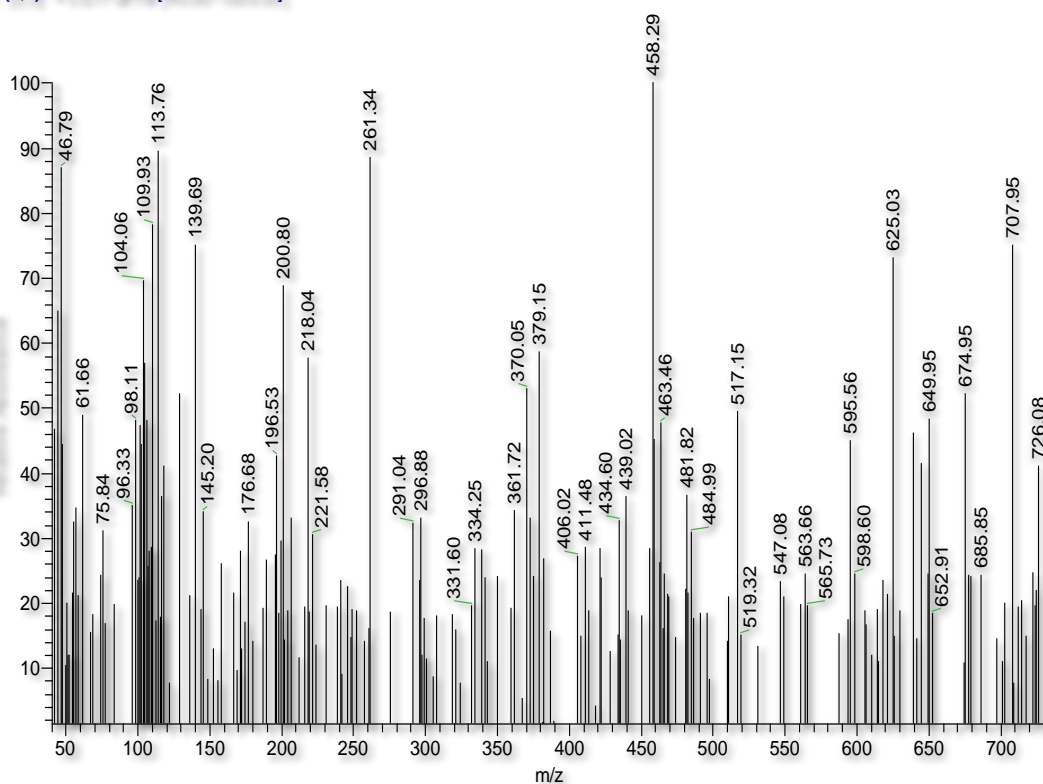
----- CHANNEL f1 -----  
 NUCL 1H  
 P1 11.60 usec  
 P2 23.20 usec  
 PL1 3.00 dB  
 SFO1 400.1329344 MHz

----- CHANNEL f2 -----  
 NUCL 15N  
 P1 11.52 usec  
 P2 4.00 dB  
 SFO2 40.548760 MHz

----- GRADIENT CHANNEL -----  
 GPHAM1 SINE.100  
 GPHAM2 SINE.100  
 GPHAM3 SINE.100  
 GPC1 70.00 %  
 GPC2 30.00 %  
 GPC3 50.10 %  
 P16 1000.00 usec  
 NDO 2  
 TD 512  
 SFO1 40.54888 MHz  
 SFO2 40.54888 MHz  
 SW 550.060 ppm  
 FWHM 2048  
 SF 400.1300000 MHz  
 SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 2.40  
 TC 1024  
 SC 0  
 SF 40.5488225 MHz  
 SSB 0  
 LB 0.00 Hz  
 GB 0



RT: 3.15 - 3.59 SM: 15G

NL:  
1.89E4  
TIC MS  
essmat-  
elshif-E23essmat-elshif-E23 #178 RT: 3.00 AV: 1 SB: 2 4.45, 4.45 NL: 5.00E2  
T: (0,0) + c EI Full ms [40.00-1000.00]

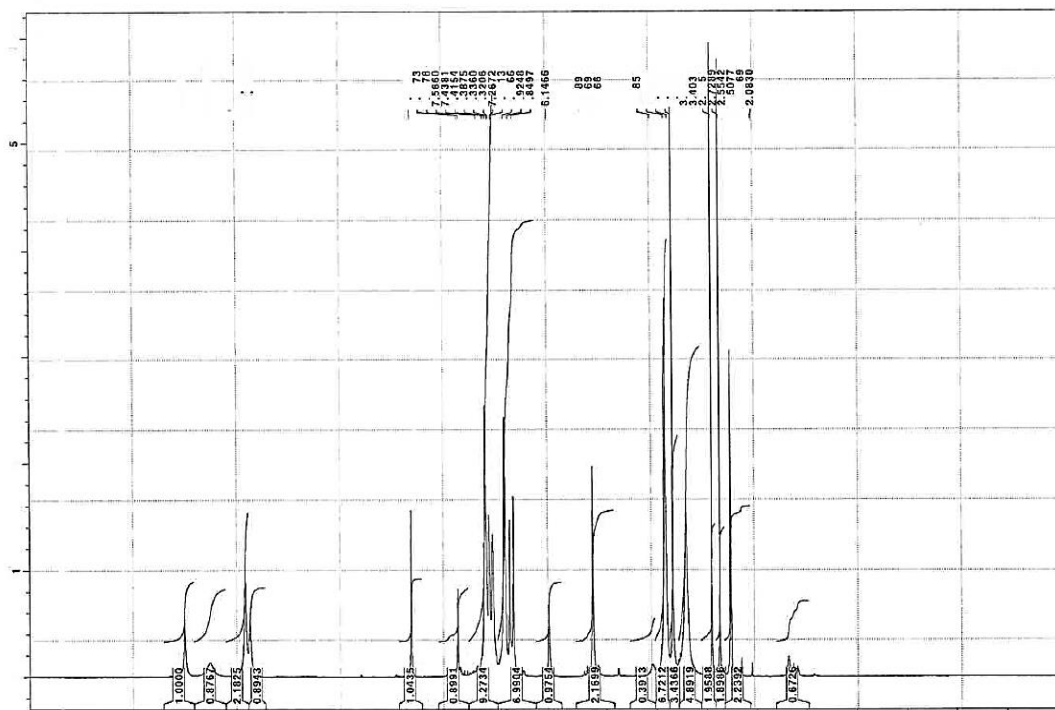
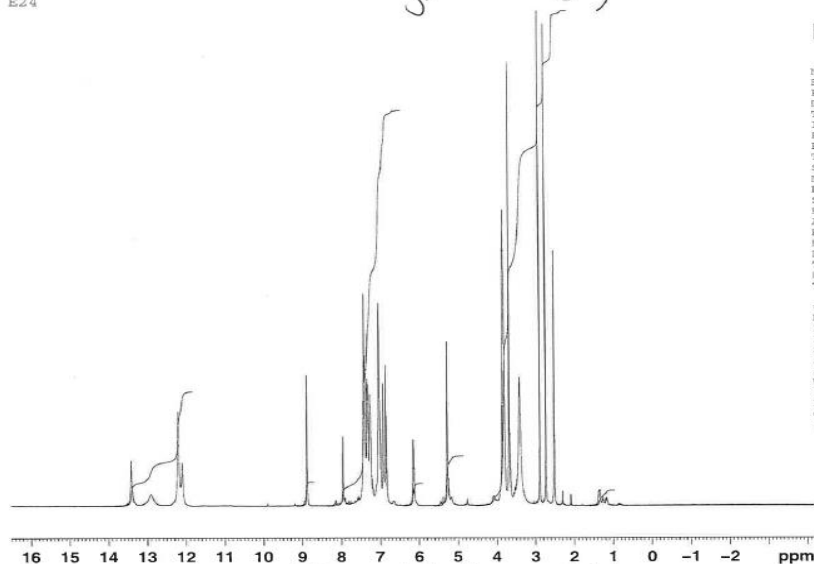
Spectrum data for Compound 8g

E24

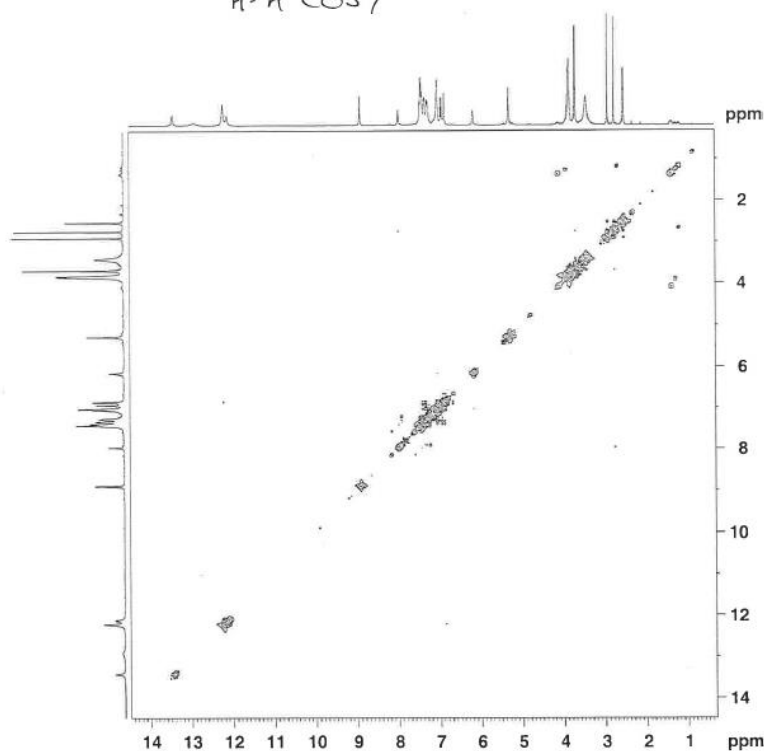
<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>)

NAME Dec05-2020-abb  
EXPNO 20  
PROCNO 1  
Date\_ 20201205  
Time 19.02  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 128  
DW 60.400 usec  
DE 6.50 usec  
TE 294.5 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 11.60 usec  
PL1 3.00 dB  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



E24

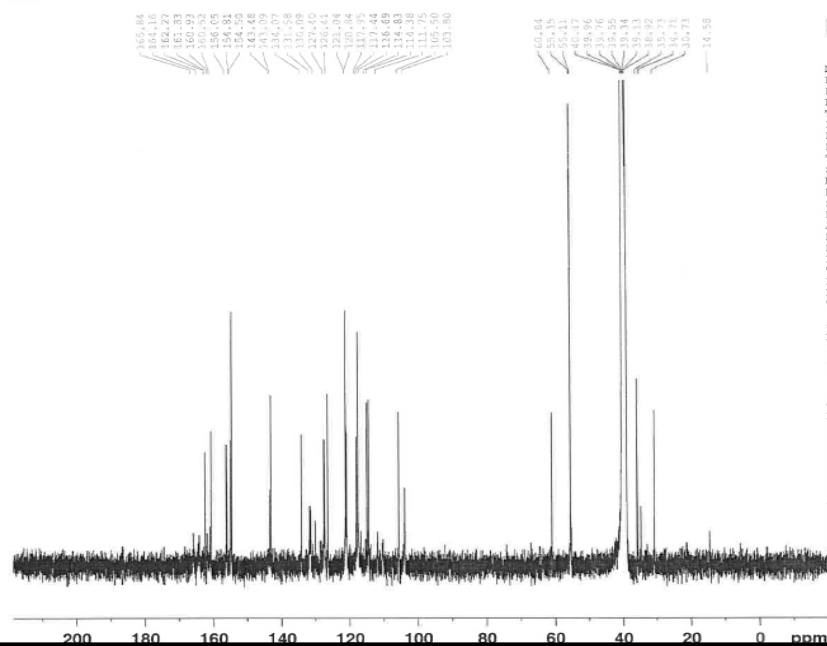
<sup>1</sup>H-<sup>1</sup>H COSY

NAME Dec05-2020-abb  
EXPNO 21  
PROCNO 1  
Date\_ 20201205  
Time 15.04  
INSTRUM spect  
PROBHD 5 mm F4BBO BB-  
PULPROG cosygpgp  
TD 2048  
SOLVENT DMSO  
NS 1  
DS 8  
SWH 5668.934 Hz  
FIDRES 2.768034 Hz  
AQ 0.1806816 sec  
RG 64  
DN 88.200 usec  
DE 6.50 usec  
TE 294.4 K  
D0 0.00000300 sec  
D1 1.49836039 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
INU 0.00017640 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P0 11.60 usec  
P1 11.60 usec  
PL1 3.00 dB  
SFO1 400.1329617 MHz

\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*  
GPM1 SINE.100  
GPI1 10.00 usec  
PI6 1000.00 usec  
ND0 1  
TD 128  
SFO1 400.133 MHz  
FIDRES 44.288548 Hz  
SW 14.168 ppm  
P0MODE QF  
SI 1024  
SF 400.1300000 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40  
SI 1024  
MC2 QF  
SF 400.1300000 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0

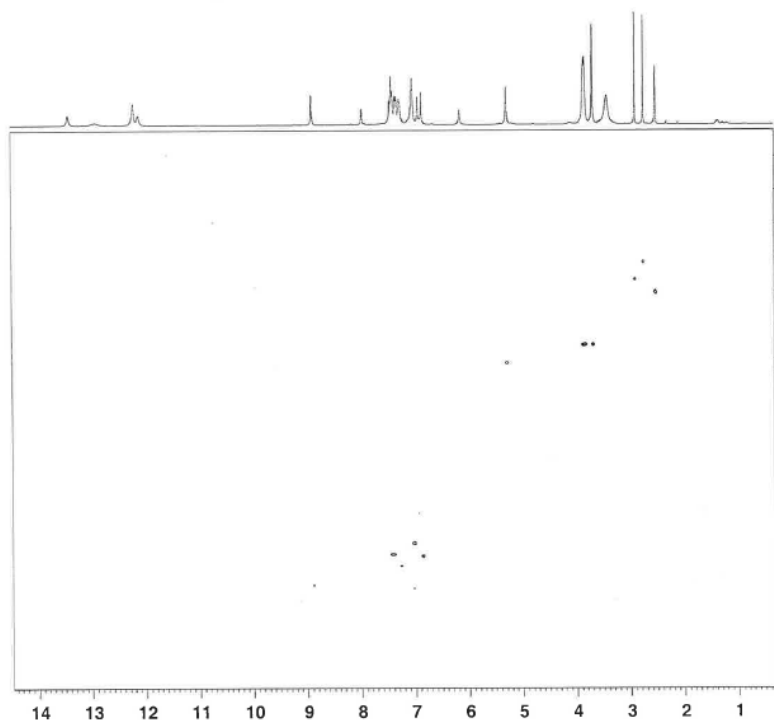
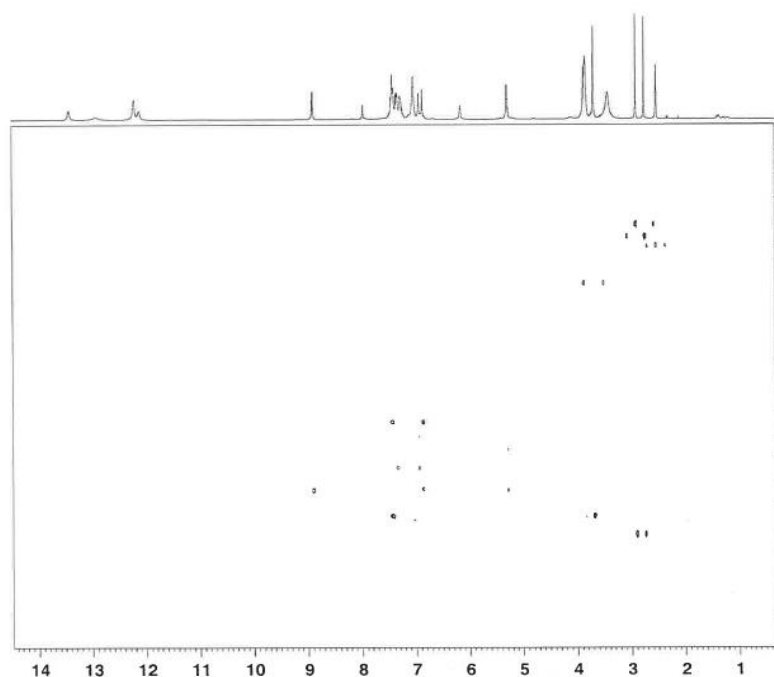
E24

<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>)

NAME Dec04-2020-abb  
EXPNO 20  
PROCNO 1  
Date\_ 20201205  
Time 11.19  
INSTRUM spect  
PROBHD 5 mm F4BBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 16384  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 32768  
DN 20.850 usec  
DE 6.50 usec  
TE 299.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

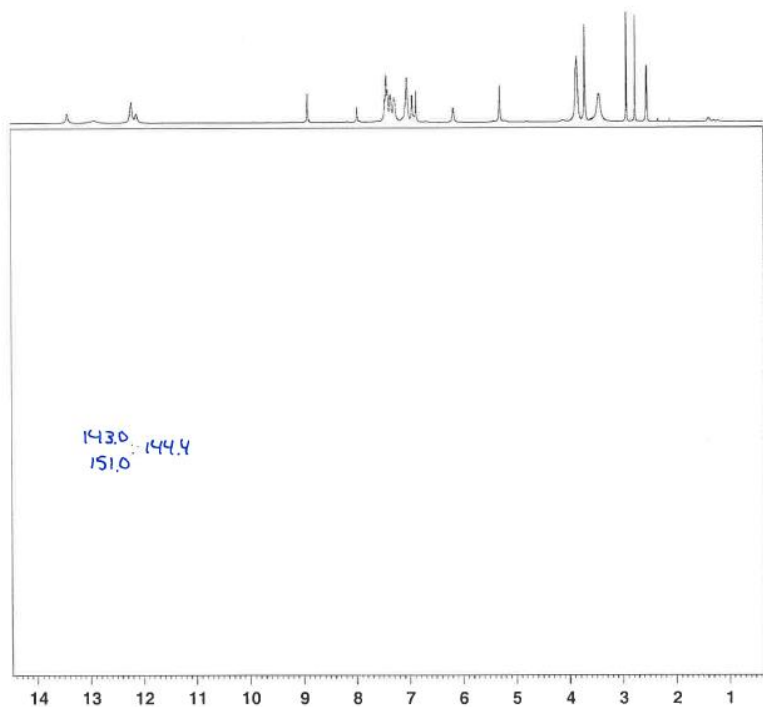
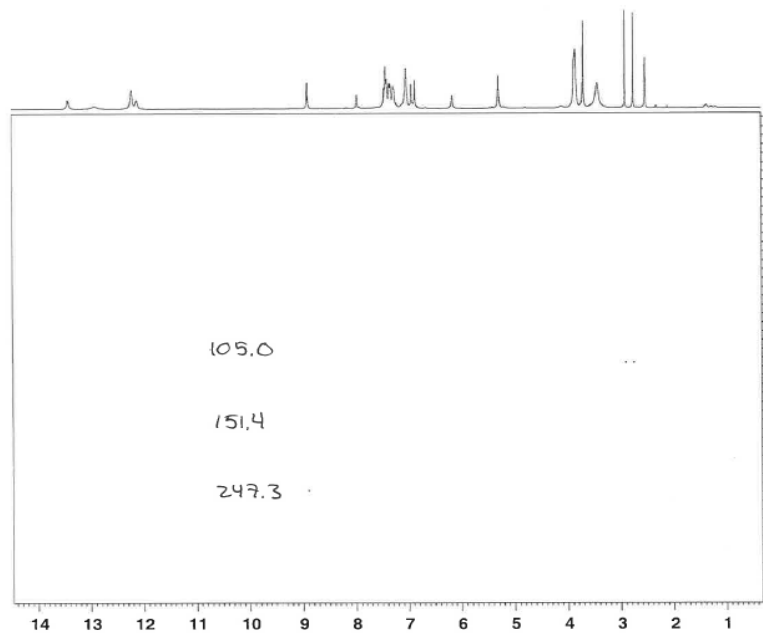
\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 13C  
P1 14.75 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 12.54 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6128193 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

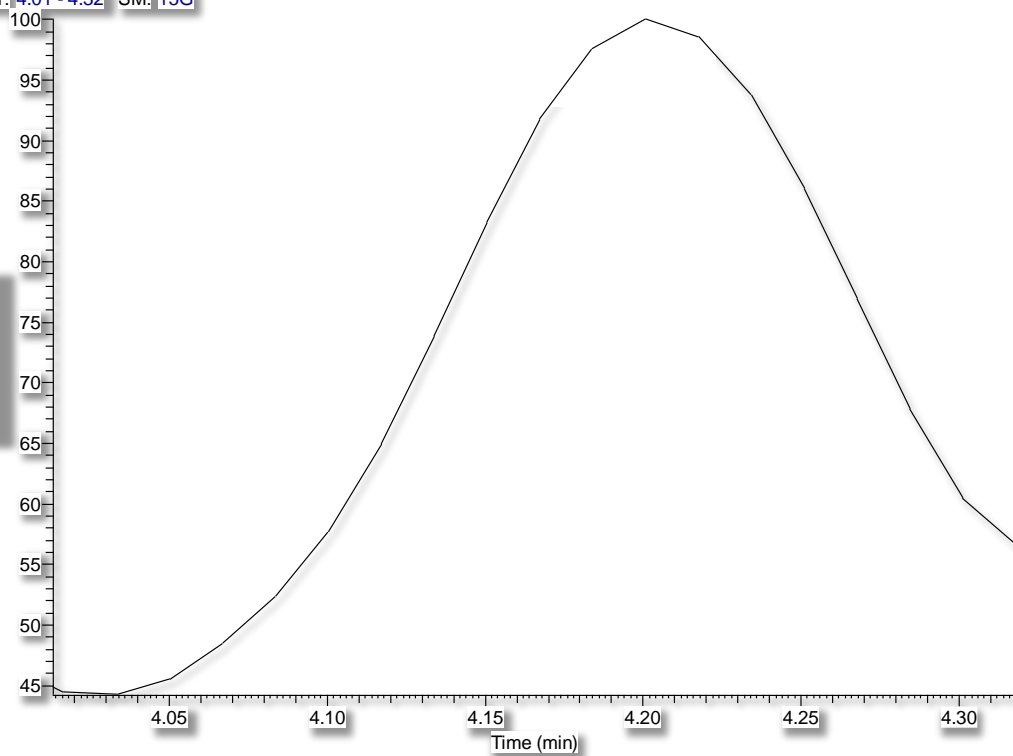
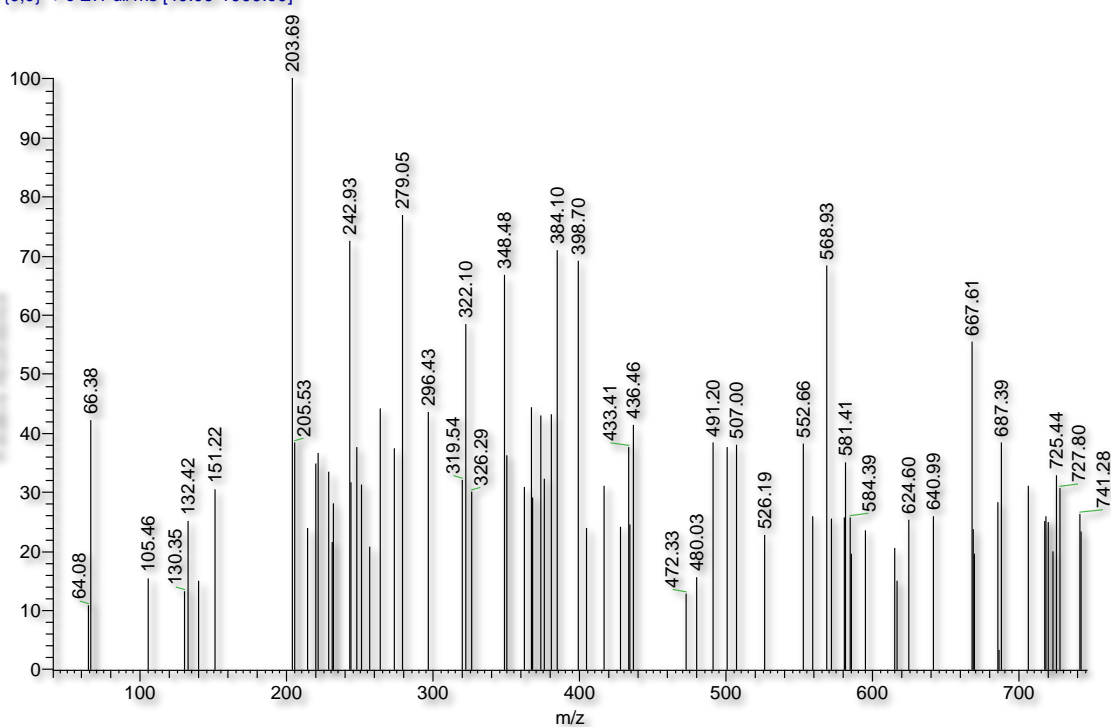
$${}^1\text{H} - {}^{13}\text{C} \text{ HSQC}$$
[illegible] $^1\text{H}-^{13}\text{C}$  HMBB

**BRUKER**

[illegible]

$^1\text{H}-^{15}\text{N HSQC}$ [illegible] ${}^1\text{H}-{}^{15}\text{N}$  HmBC[illegible]

RT: 4.01 - 4.32 SM: 15G

NL:  
7.95E3  
TIC MS  
esmat-  
elsherif-e-  
24esmat-elsherif-e-24 #270 RT: 4.54 AV: 1 SB: 2 4.45, 4.45 NL: 3.57E2  
T: {0,0} + c EI Full ms [40.00-1000.00]

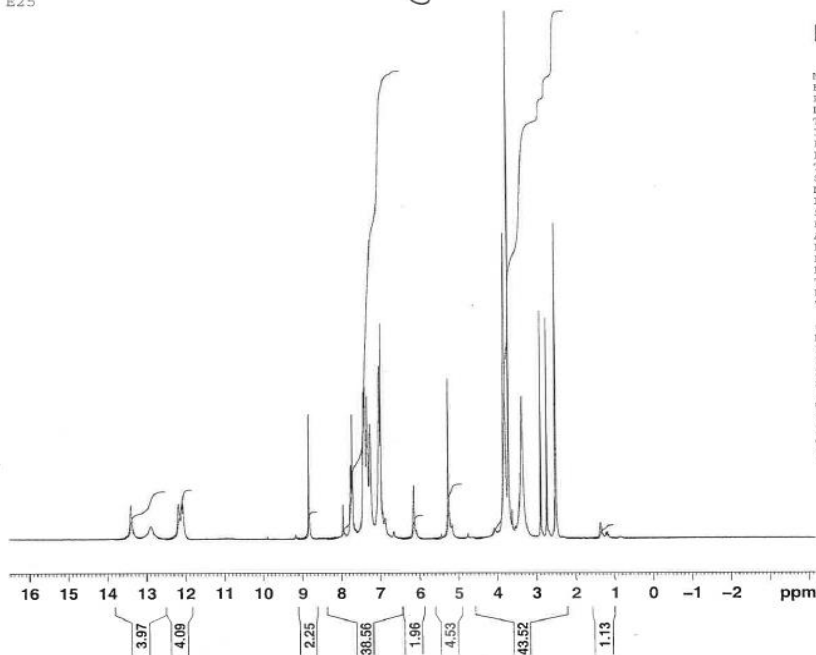
Spectrum data for Compound 8h

E25

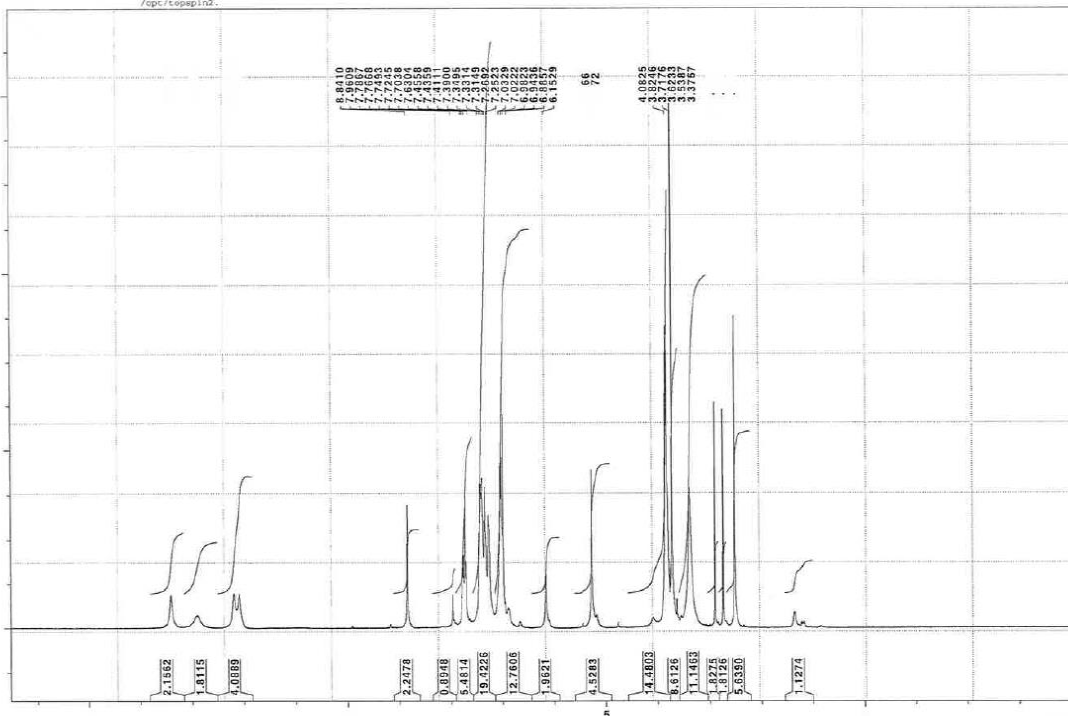
<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>)

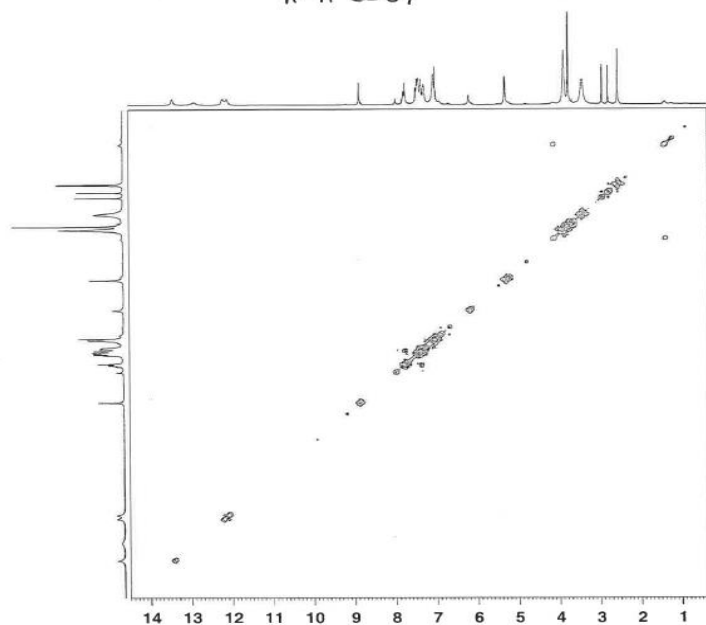
NAME Oct29-2020-abb  
EXPNO 21  
PROCNO 1  
Date\_ 20201029  
Time 21.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 181  
DW 60.400 usec  
DE 6.50 usec  
TE 297.8 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 11.60 usec  
PL1 3.00 dB  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



/opt/ropepin2.





```
NAME          Oct-29-2020-abb
EXPNO         2
PROCNO        1
Date_         20201029
Time          23.32
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       cysyprdg
TD            2048
SOLVENT       DMSO
NS            1
DS            8
AQ            5668.334 Hz
FIDRES        2.768034 Hz
RG            0.1806836 sec
NO            64
DWT           88.200 usec
DE            6.50 usec
TE            297.5 K
D1            0.00000300 sec
D2            1.49836099 sec
D3            0.00000400 sec
D4            0.00020000 sec
INQ           0.00017640 sec
```

```
===== CHANNEL f1 =====  
NUC1                1H  
P0                  11.60 usec  
P1                  11.60 usec  
PL1                 3.00 dB  
SFO1               400.1329675 MHz
```

```
***** GRADIENT CHANNEL *****
GPNAM1      SINE.100
GPZ1        10.00 %
P16         1000.00 usoc
```

|       |              |
|-------|--------------|
| NDQ   | 1            |
| TD    | 128          |
| SFO1  | 400.133 MHz  |
| PDRES | 44.288548 Hz |
| SW    | 14.168 ppm   |

```

PnMODE      QF
SI           1024
SF           400.1300000 MHz
WDW          SINE

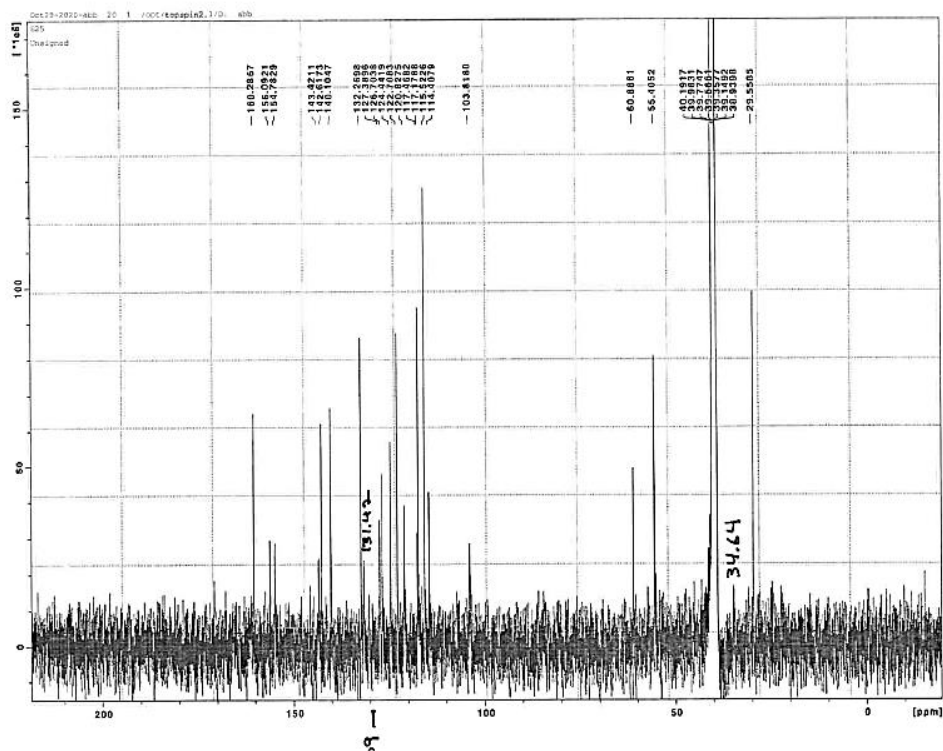
```

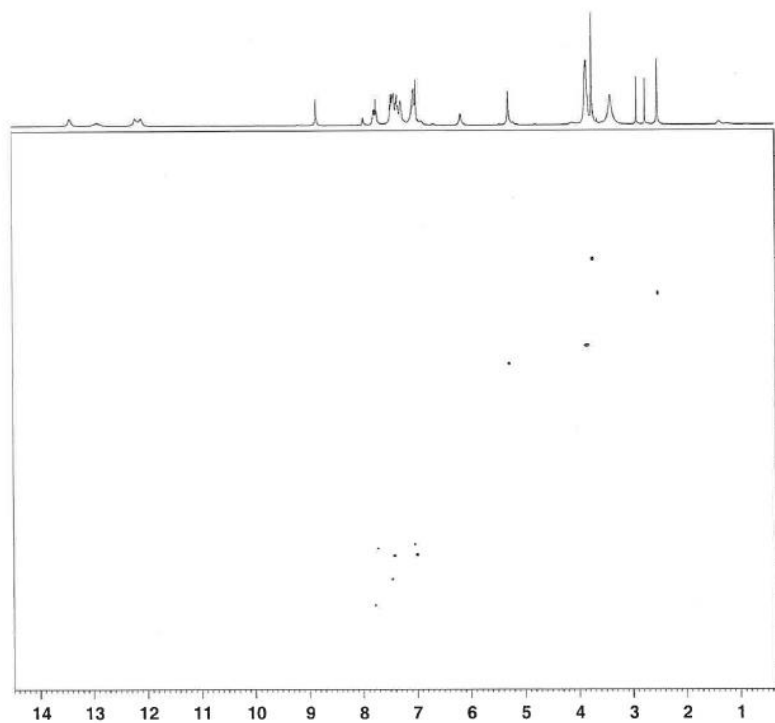
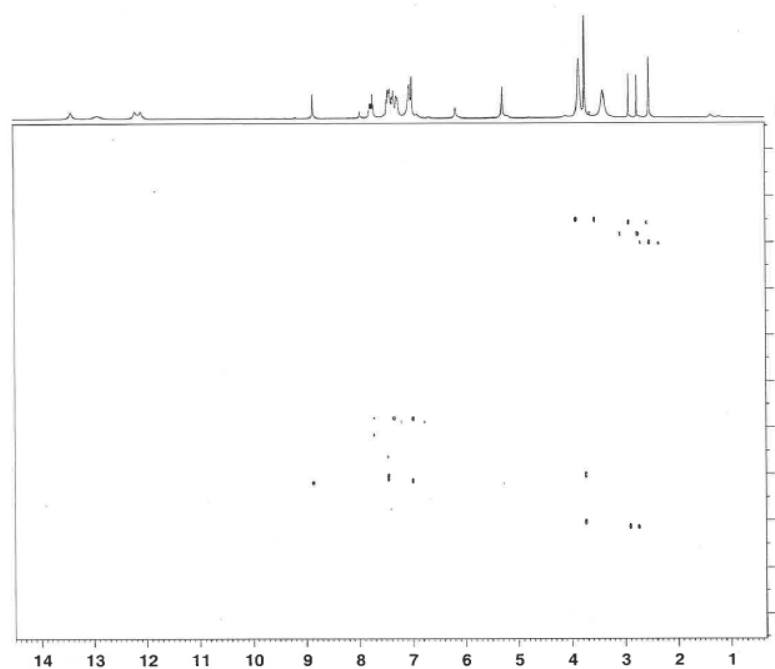
|     |         |
|-----|---------|
| SSB | 0       |
| LB  | 0.00 Hz |
| GB  | 0       |
| PC  | 1.40    |
| SI  | 1024    |

```

MC2          QF
SF          400.1300000 MHz
WDW          SINE
SSB          0
LB          0.00 Hz

```



$^1\text{H}-^{13}\text{C}$  HSQC[illegible] $^1\text{H}-^{13}\text{C}$  HMB C

```

NAME          CH19-2020-ABC
EXPNO         1          24
PROCNO        1          1
Date_         20020130
TIME          0.36
INSTRUM       5 mm PABBO
PROBHD        mmcpcplcp4d4
PULPROG       zgpg30
PRG2          msmtcpl
SOLVENT       H2O
NS            12
DS            12
FIDRES       0.0001394 Hz
AQ            0.16121732 sec
RG            327.5
AQ            88.200 usec
RG            327.5
TS            296.2 K
CHET23        145.000000 sec
CHET24        10.000000 sec
D1            0.00000000 sec
D2            0.00000000 sec
D3            0.00044828 sec
D4            0.00000000 sec
D16           0.00028000 sec
D17           0.00000000 sec
----- CHANNEL f1 -----
NUC1          131
P1            1.10 usec
PL1           2.30 dB
PL1           4.00 dB
PL1           490.133775 MHz
----- CHANNEL f2 -----
NUC2          13C
P2            1.30 usec
PL2           1.90 dB
PL2           100.622280 MHz
SP02          100.622280 MHz
----- GRADIENT CHANNEL -----
G03H01        EPR1 10%
G03H02        SINK 10%
G03H03        SINK 10%
G021          50.06 %
G022          50.00 %
G023          49.10 %
G024          49.10 % usec
ND0           2
TD0           32
STO1          100.62228 MHz
FLKRES       174.592423 Hz
PRG2          20.23 sec
PRGNAME       zgpg30
RG            400.000000 MHz
SOLVENT       H2O
CB            0
GB            0.00 Hz
SB            0
SCB           1.40
TC2           10.24 sec
PC2           0.00
FIDRES       100.6127690 MHz
WDW           SINC
GB            0
LB            0.00 Hz
ppm

```

${}^1\text{H}-{}^{15}\text{N}$  HSQC

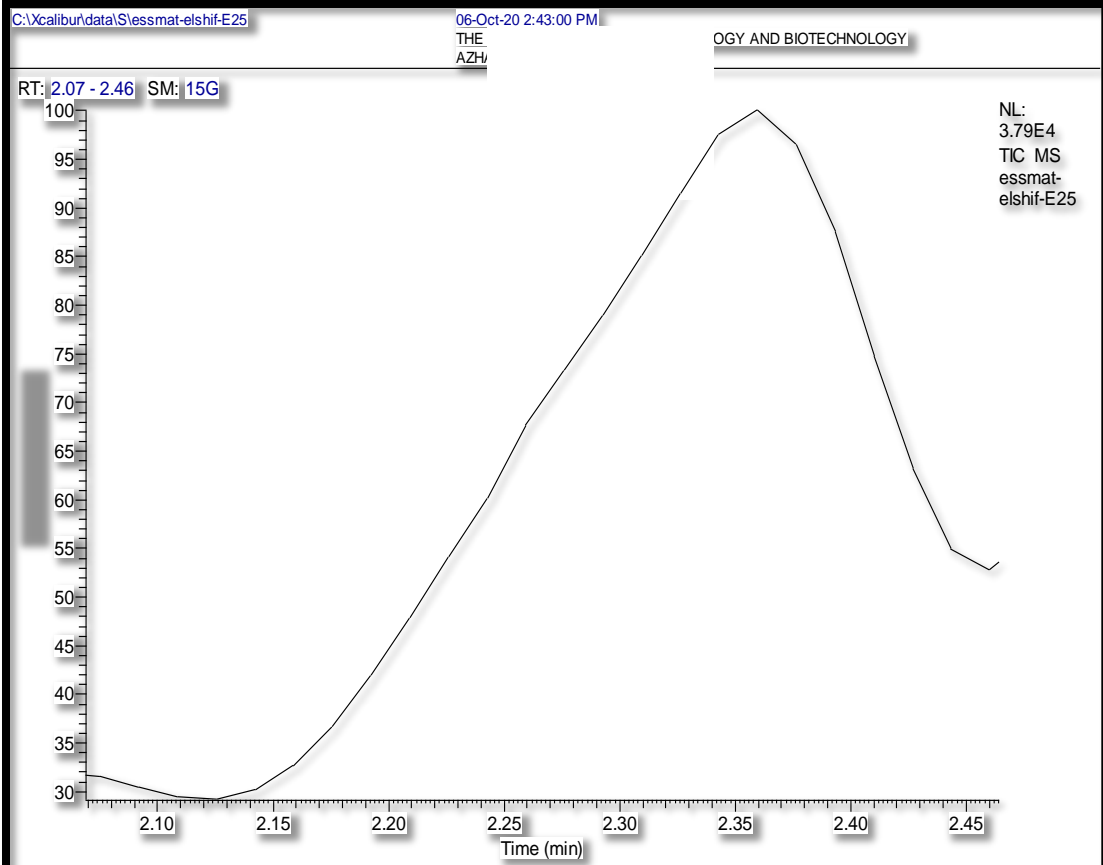
144.2

 $^1\text{H}-^{15}\text{N}$  HMB C

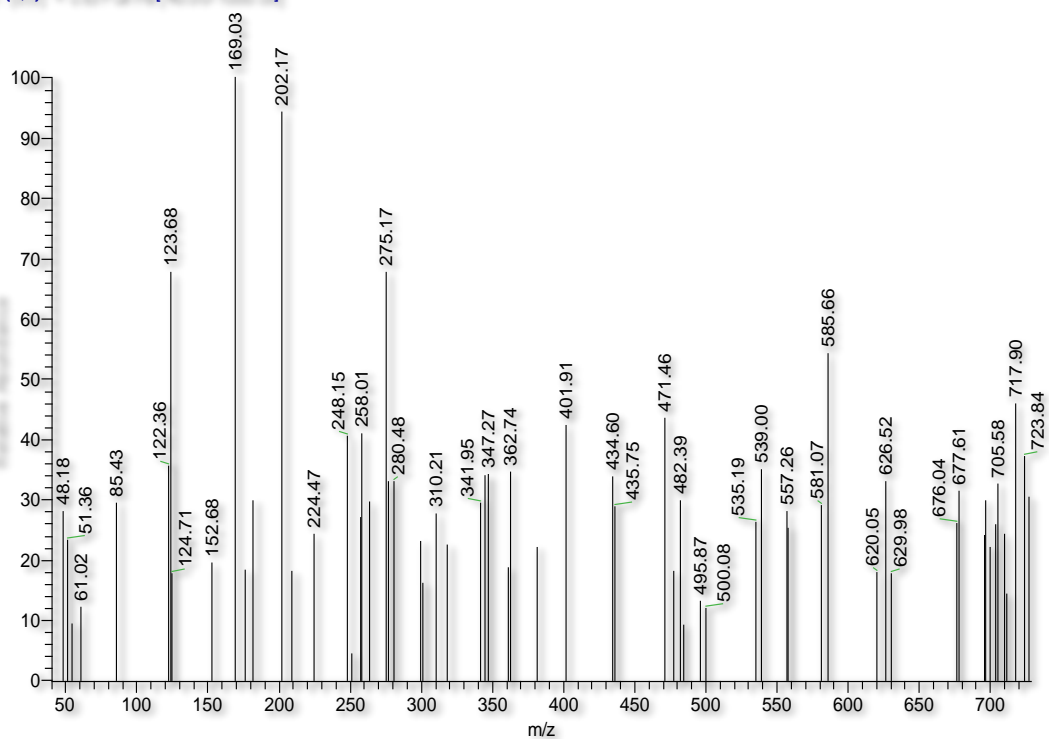
105.3

147.1

246.5



essmat-elshif-E25 #50 RT: 0.85 AV: 1 SB: 2 2.66, 2.66 NL: 4.16E2  
T: (0,0) + c EI Full ms [40.00-1000.00]



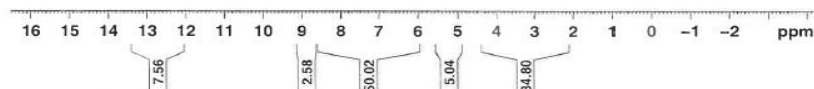
Spectrum data for Compound 8i

E28

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>)

NAME Dec16-2020-abb  
 EXPNO 21  
 PROCNO 1  
 Date\_ 20201217  
 Time 1.05  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 181  
 DW 60.400 usec  
 DE 6.50 usec  
 TE 296.4 K  
 D1 1.00000000 sec  
 D11  
 TDO 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 11.60 usec  
 PL1 3.00 dB  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300000 MHz  
 WDW EX  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



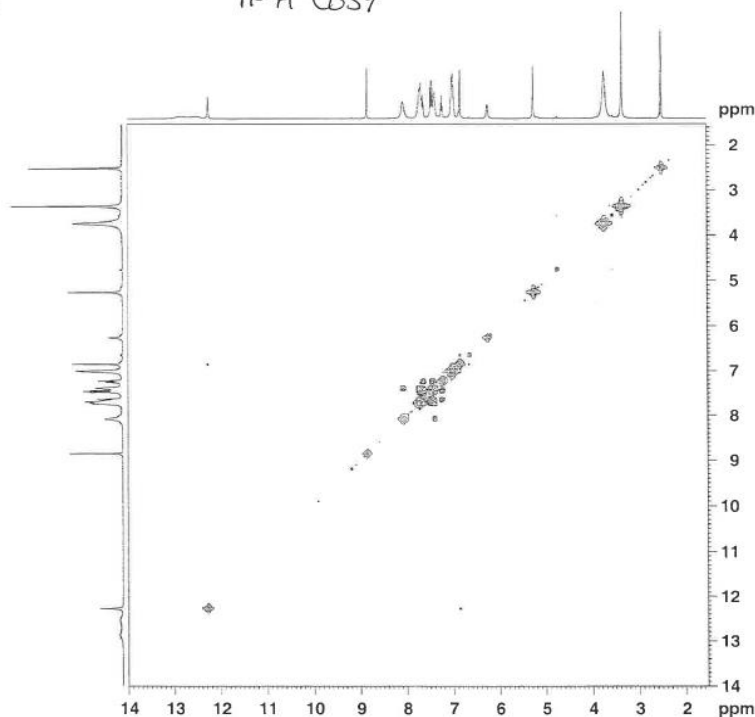
E28

<sup>1</sup>H-<sup>1</sup>H COSY

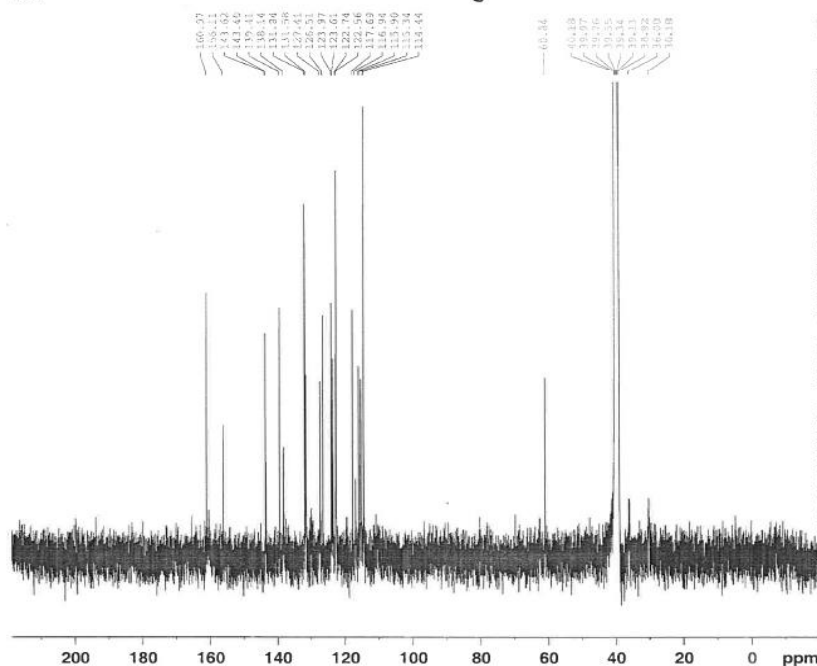
NAME Dec16-2020-abb  
 EXPNO 22  
 PROCNO 1  
 Date\_ 20201217  
 Time 1.06  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosygprf  
 TD 2048  
 SOLVENT DMSO  
 NS 1  
 DS 6  
 SWH 4990.020 Hz  
 FIDRES 2.436533 Hz  
 AQ 0.2052596 sec  
 RG 64  
 DW 100.200 usec  
 DE 6.50 usec  
 TE 296.2 K  
 D0 0.00000300 sec  
 D1 1.47378504 sec  
 D11 0.00000400 sec  
 D16 0.00020000 sec  
 INO 0.00020040 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 11.60 usec  
 PL1 3.00 dB  
 SFO1 400.1331069 MHz

\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*  
 GRNAM1 SINE.100  
 GP1 10.00 %  
 P16 1000.00 usec  
 MDO 1  
 TD 128  
 SFO1 400.1331 MHz  
 FIDRES 38.984531 Hz  
 SW 12.471 ppm  
 FRMCOE QF  
 SI 1024  
 SF 400.1300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40  
 SI 1024  
 MC2 QF  
 SF 400.1300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0



E28

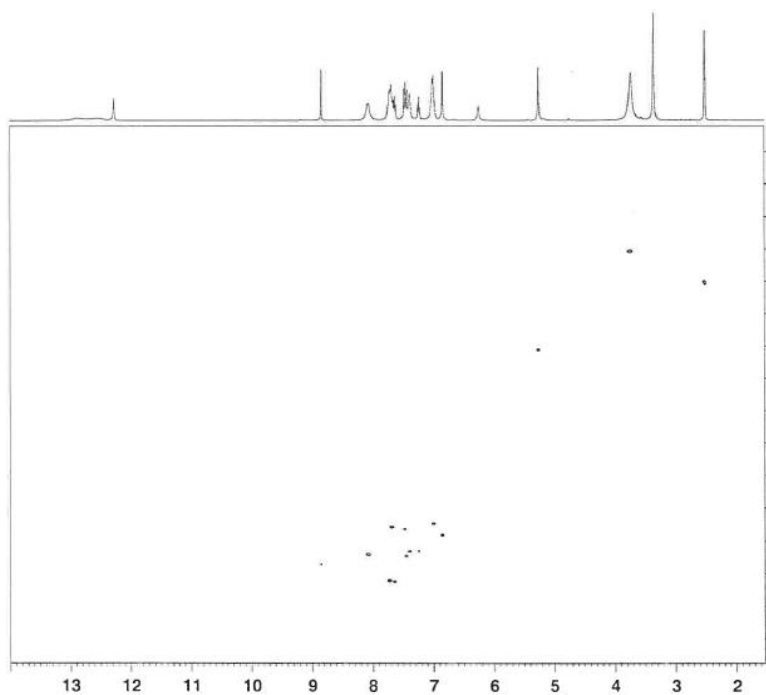
 $^{13}\text{C}$  NMR (100 MHz DMSO- $d_6$ )

BRUKER

NAME Dec16-2020-abb  
EXPNO 20  
PROCNO 1  
Date\_ 20201217  
Time 1.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
RS 8192  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 32768  
ZG 20.850 usec  
DE 6.50 usec  
TE 299.6 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

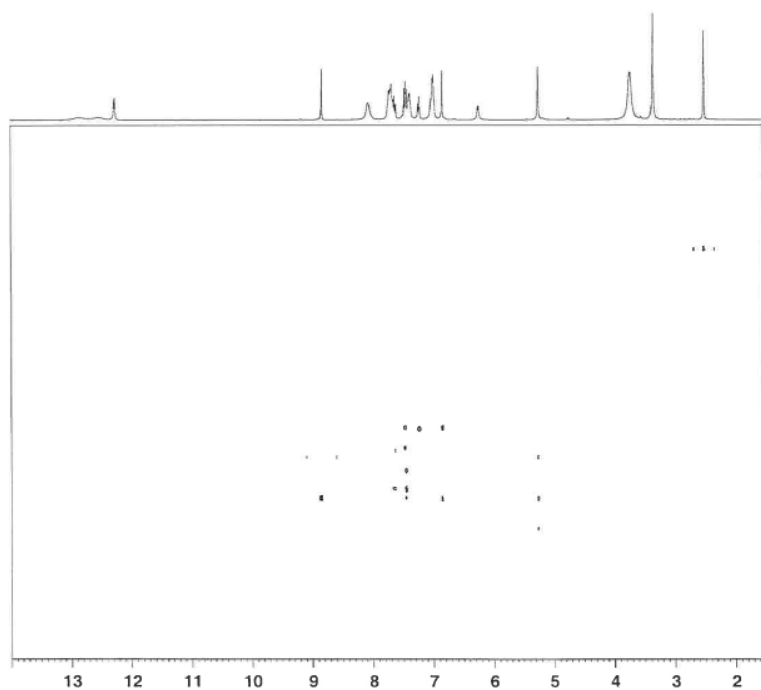
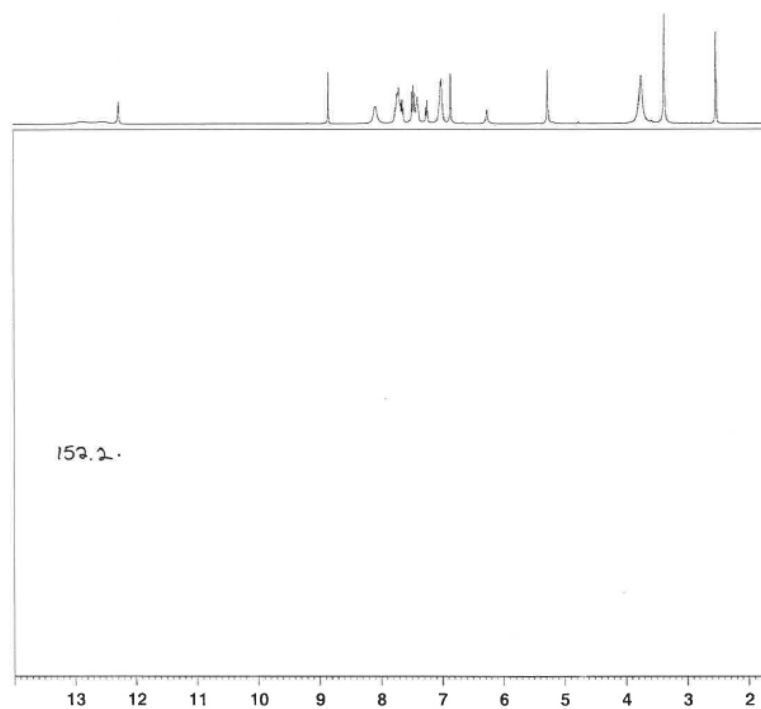
===== CHANNEL f1 =====  
NUC1  $^{13}\text{C}$   
P1 14.75 usec  
PL1 0.00 dB  
SFO1 100.6228298 MHz  
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2  $^1\text{H}$   
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 12.54 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6126193 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

E28

 $^1\text{H}$ - $^{13}\text{C}$  Hsqc

BRUKER

NAME Dec16-2020-abb  
EXPNO 20  
PROCNO 1  
Date\_ 20201217  
Time 1.12  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
RS 8192  
DS 4  
SWH 4993.830 Hz  
FIDRES 4.971884 Hz  
AQ 0.1026248 sec  
RG 32768  
ZG 20.850 usec  
DE 6.50 usec  
TE 299.6 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
D12 0.0000000 sec  
D13 0.0000000 sec  
D14 0.0000000 sec  
D15 0.0000000 sec  
D16 0.0000000 sec  
D17 0.0000000 sec  
D18 0.0000000 sec  
D19 0.0000000 sec  
D20 0.0000000 sec  
D21 0.0000000 sec  
D22 0.0000000 sec  
D23 0.0000000 sec  
D24 0.0000000 sec  
D25 0.0000000 sec  
D26 0.0000000 sec  
D27 0.0000000 sec  
D28 0.0000000 sec  
D29 0.0000000 sec  
D30 0.0000000 sec  
D31 0.0000000 sec  
D32 0.0000000 sec  
D33 0.0000000 sec  
D34 0.0000000 sec  
D35 0.0000000 sec  
D36 0.0000000 sec  
D37 0.0000000 sec  
D38 0.0000000 sec  
D39 0.0000000 sec  
D40 0.0000000 sec  
D41 0.0000000 sec  
D42 0.0000000 sec  
D43 0.0000000 sec  
D44 0.0000000 sec  
D45 0.0000000 sec  
D46 0.0000000 sec  
D47 0.0000000 sec  
D48 0.0000000 sec  
D49 0.0000000 sec  
D50 0.0000000 sec  
D51 0.0000000 sec  
D52 0.0000000 sec  
D53 0.0000000 sec  
D54 0.0000000 sec  
D55 0.0000000 sec  
D56 0.0000000 sec  
D57 0.0000000 sec  
D58 0.0000000 sec  
D59 0.0000000 sec  
D60 0.0000000 sec  
D61 0.0000000 sec  
D62 0.0000000 sec  
D63 0.0000000 sec  
D64 0.0000000 sec  
D65 0.0000000 sec  
D66 0.0000000 sec  
D67 0.0000000 sec  
D68 0.0000000 sec  
D69 0.0000000 sec  
D70 0.0000000 sec  
D71 0.0000000 sec  
D72 0.0000000 sec  
D73 0.0000000 sec  
D74 0.0000000 sec  
D75 0.0000000 sec  
D76 0.0000000 sec  
D77 0.0000000 sec  
D78 0.0000000 sec  
D79 0.0000000 sec  
D80 0.0000000 sec  
D81 0.0000000 sec  
D82 0.0000000 sec  
D83 0.0000000 sec  
D84 0.0000000 sec  
D85 0.0000000 sec  
D86 0.0000000 sec  
D87 0.0000000 sec  
D88 0.0000000 sec  
D89 0.0000000 sec  
D90 0.0000000 sec  
D91 0.0000000 sec  
D92 0.0000000 sec  
D93 0.0000000 sec  
D94 0.0000000 sec  
D95 0.0000000 sec  
D96 0.0000000 sec  
D97 0.0000000 sec  
D98 0.0000000 sec  
D99 0.0000000 sec  
D100 0.0000000 sec

[illegible][illegible]

C:\Xcalibur\data\Slessmat-elshif-E28

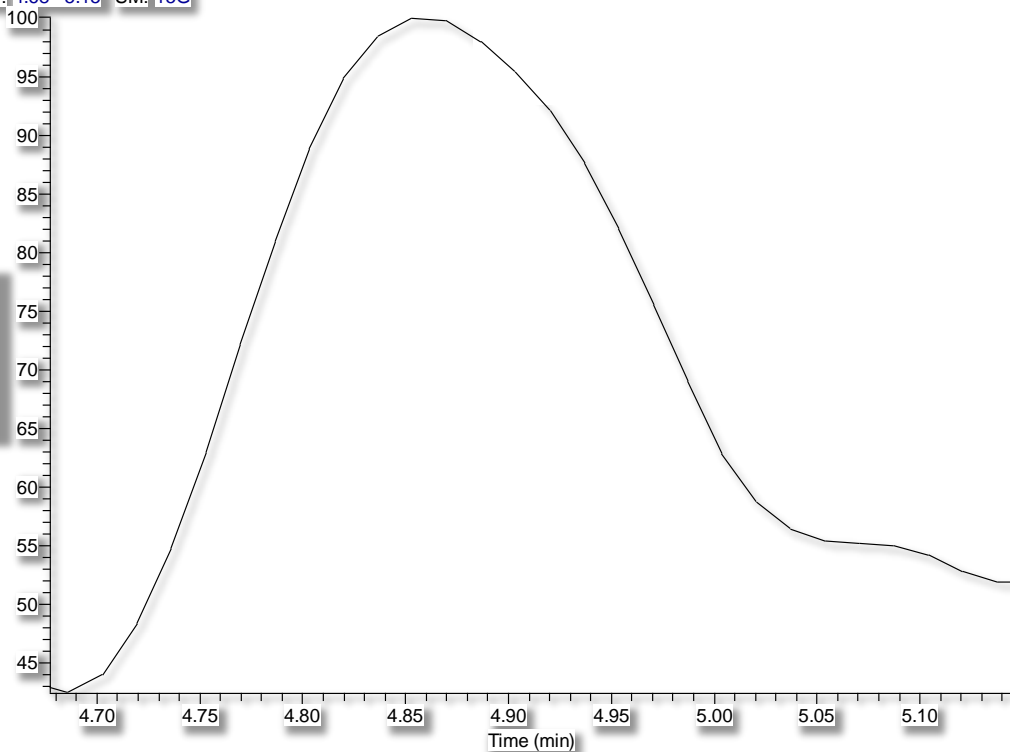
06-Oct-20 4:42:43 PM

THE  
AZH

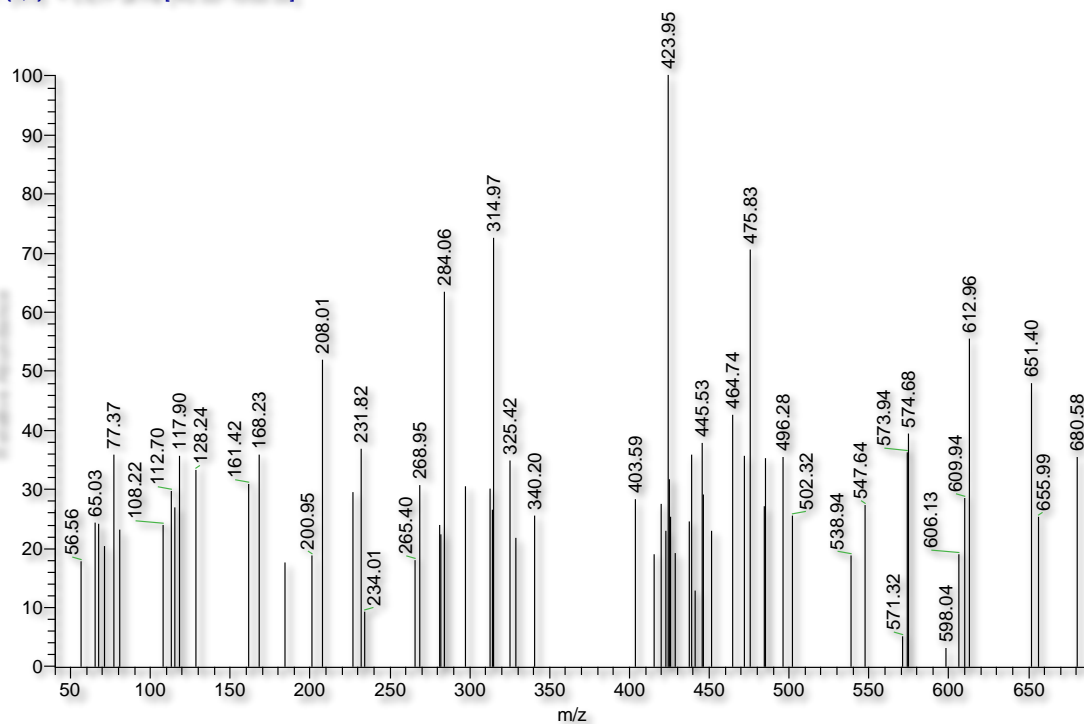
OGY AND BIOTECHNOLOGY

RT: 4.68 - 5.15 SM: 15G

NL:  
3.09E4  
TIC MS  
essmat-  
elshif-E28



essmat-elshif-E28 #278 RT: 4.67 AV: 1 SB: 2 4.45, 4.45 NL: 3.80E2  
T: {0,0} + c EI Full ms [40.00-1000.00]



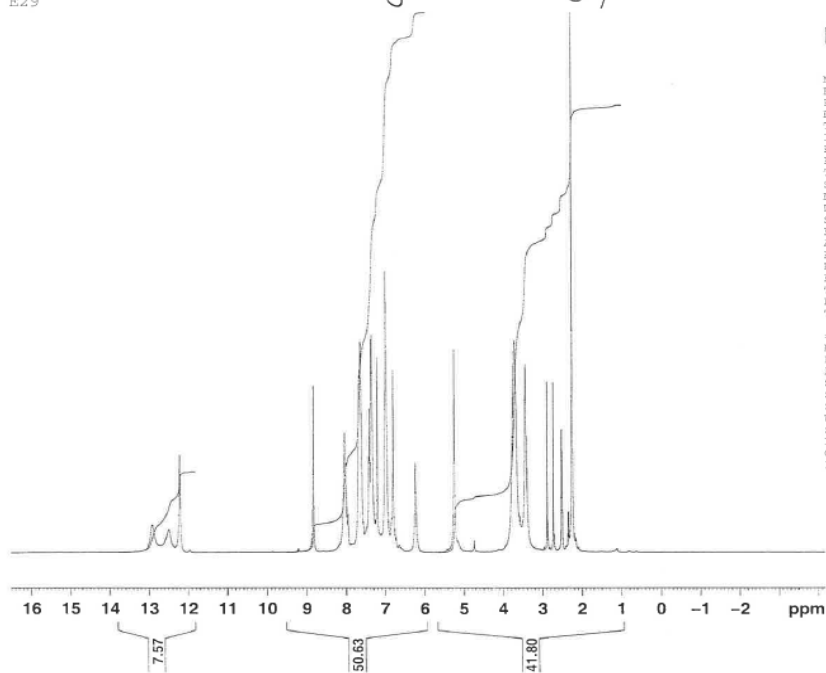
Spectrum data for Compound 8j

E29

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>)

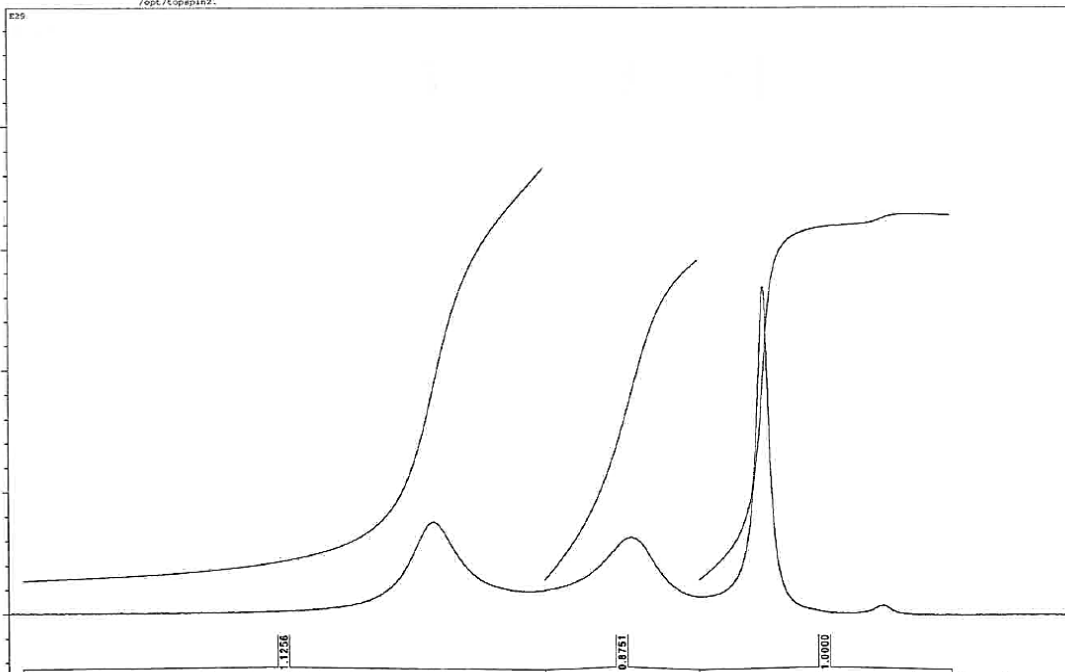
NAME Dec24-2020-ahh  
EXPNO 21  
PROCNO 1  
Date\_ 20201225  
Time 16.19  
INSTRUM spect  
PROBHD 5 mm FABS0 BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584242 sec  
RG 64  
DN 60.400 usec  
DE 6.50 usec  
TE 294.0 K  
D1 1.0000000 sec  
TDO 1

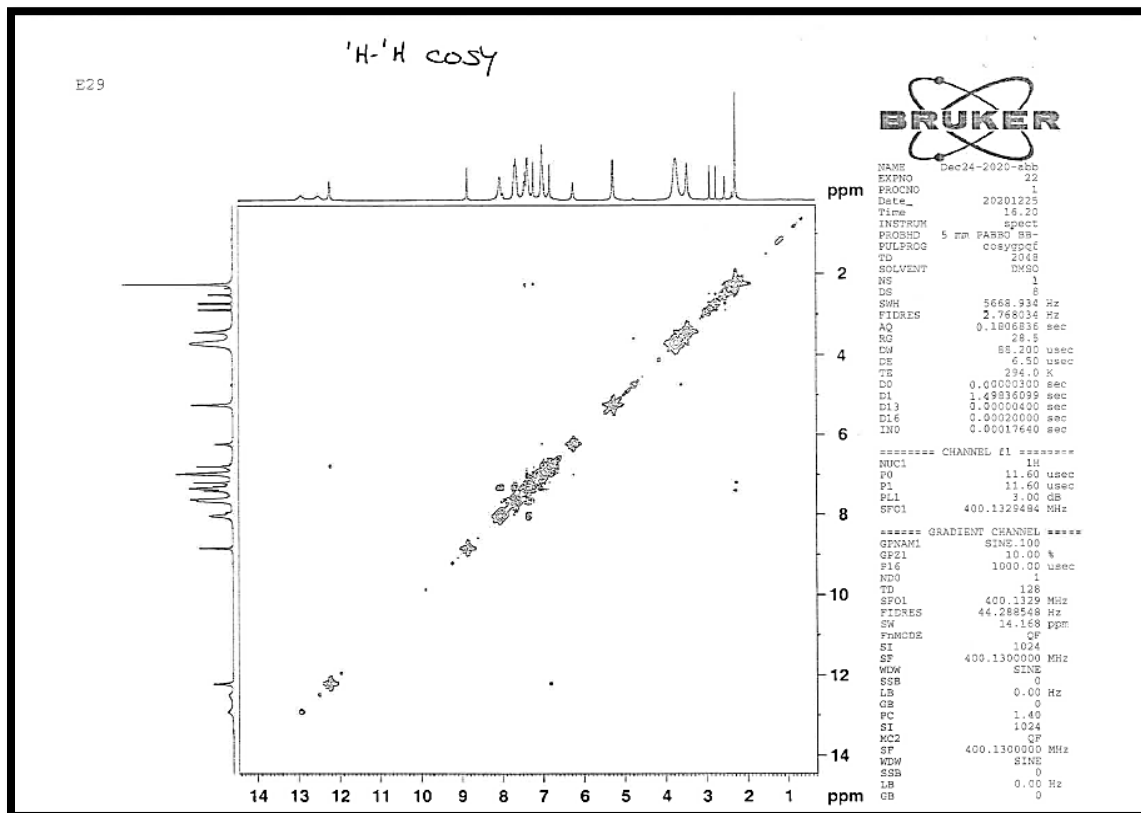
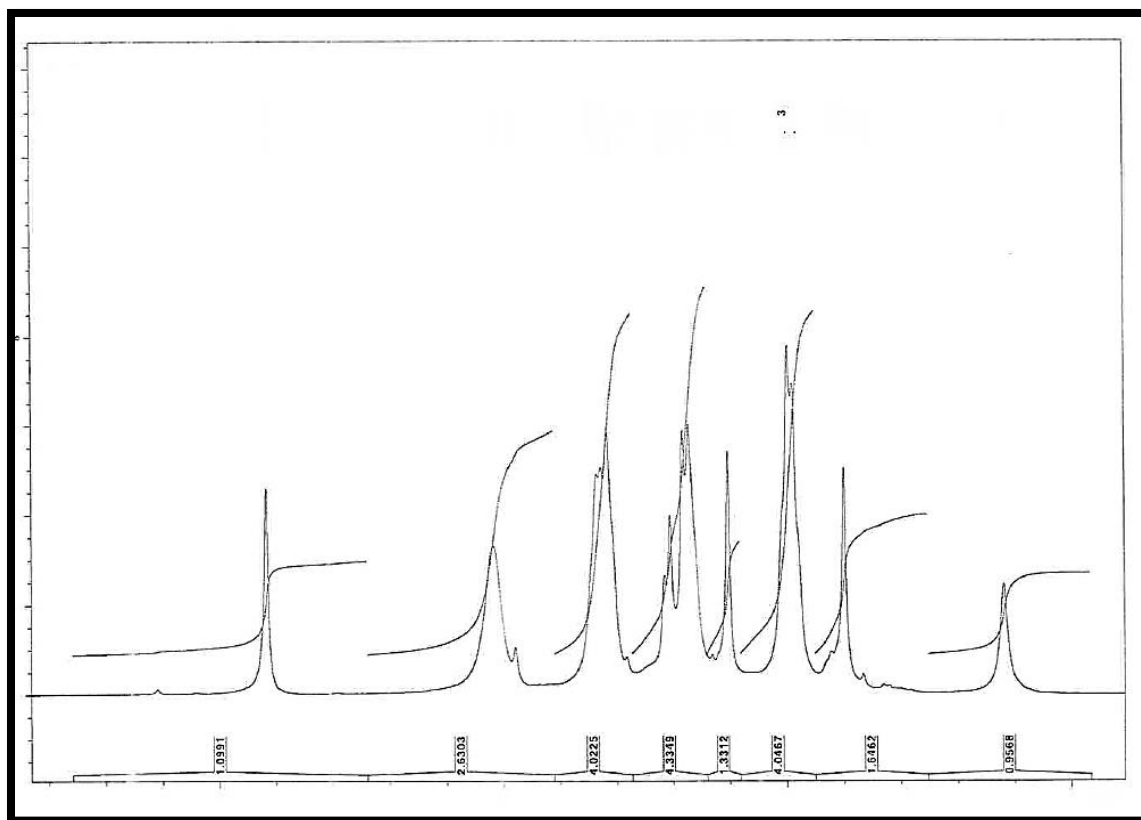
\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 11.60 usec  
PL1 3.00 dB  
SFO1 400.1324710 MHz  
ST 32768  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



E29

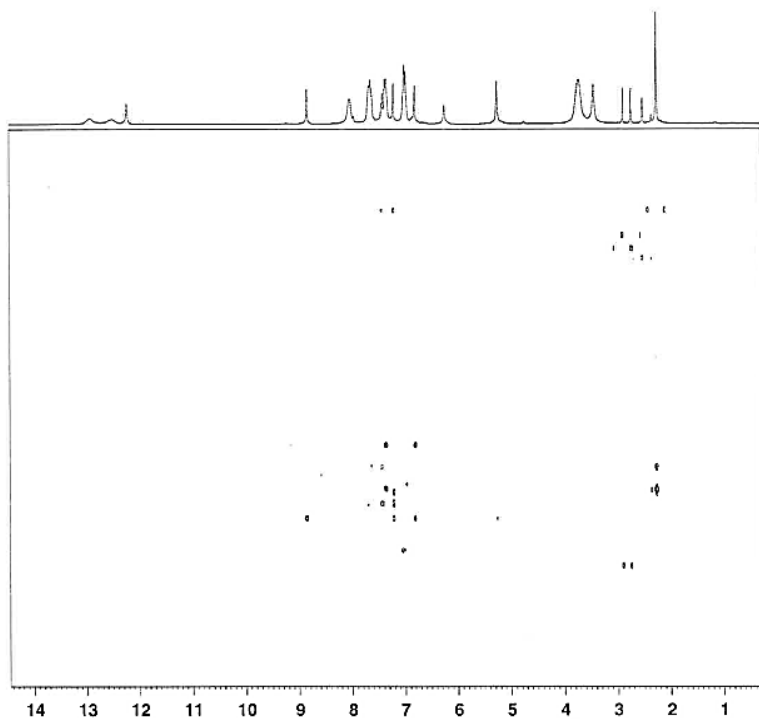
/opt/lopepin2.







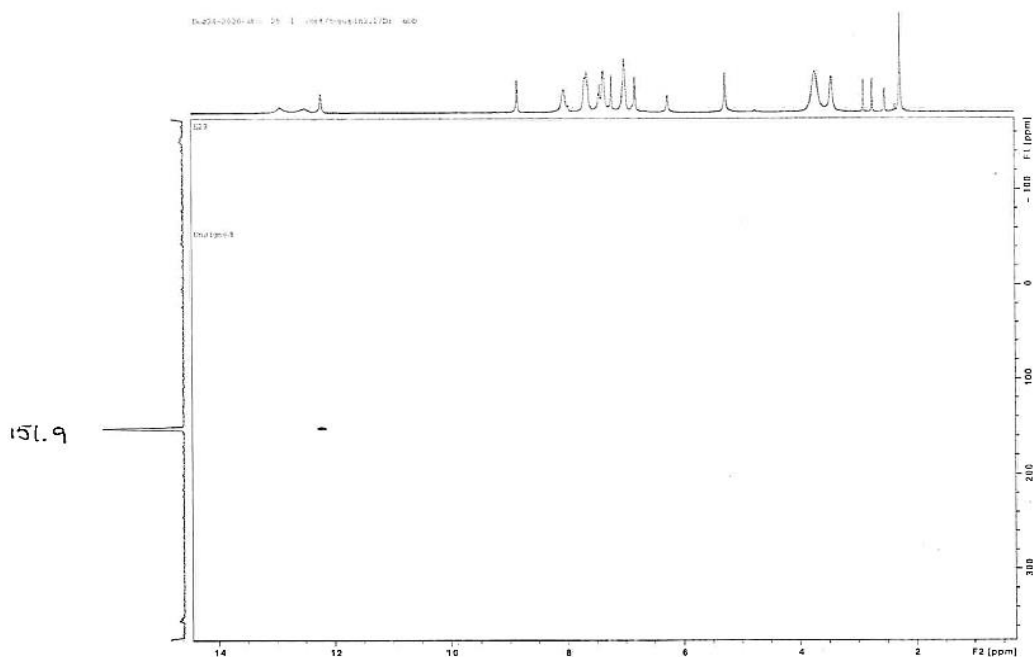
E29

 $^1\text{H}$ - $^{13}\text{C}$  HMB C

NAME Da24-2020-020  
EXPNO 24  
PROCNO 1  
Date\_ 20201225  
Time 17.24  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmcgcp1pmdgc  
TD 4096  
SOLVENT DMSO  
NS 2  
DS 2  
SWH 5668.916 Hz  
FIDRES 1.384017 Hz  
AQ 0.1613172 sec  
RG 16384  
DW 88.200 usec  
DE 6.50 usec  
TE 294.2 K  
CHST2 165.000000  
CHNU13 10.000000  
DO 8.0000000 sec  
D1 1.53276801 sec  
D2 0.03344828 sec  
D6 0.00000000 sec  
D16 0.00000000 sec  
IHU 0.00000000 sec  
\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1  $^1\text{H}$   
P1 11.60 usec  
PL1 23.20 usec  
PL1 0.00 dB  
SFO1 400.1329454 MHz  
\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
NUC2  $^{13}\text{C}$   
P2 9.19 usec  
PL2 0.00 dB  
SFO2 100.6228118 MHz  
\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*  
GPHAM1 SINE 100  
GPHAM2 SINE 100  
GPHAM3 SINE 100  
GFE1 50.00 %  
GFE2 50.00 %  
GFE3 40.10 %  
T16 1000.00 usec  
TD 2  
FID 128  
SFO1 100.6228 MHz  
FIDRES 174.592422 Hz  
SW 222.089 ppm  
FWMODE QF  
SF 400.1300000 MHz  
MDM SINE  
SGB 0  
LB 0.00 Hz  
EC 0  
SI 1024  
WC2 QF  
SF 100.6127690 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0

 $^1\text{H}$ - $^{15}\text{N}$  HSQC

Da24-2020-020 25 1 1000000000.000 usec



829



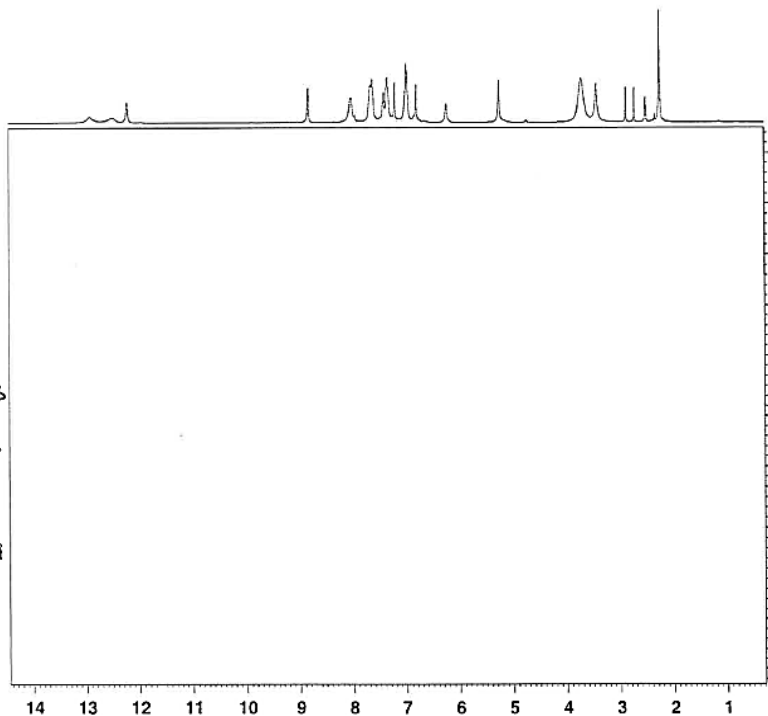
NAME Dec24-2020-880  
 EXPRNO 26  
 PROCNO 1  
 Date\_ 20201125  
 Time 20.36  
 INSTRUM spect  
 PROBRD 5 mm PABBO BB-  
 PULPROG hmcgcp1p00g1  
 TD 4096  
 SOLVENT DMSO  
 DS 16  
 SFO1 568.934 Hz  
 FIDRES 0.3613172 sec  
 AQ 23170.5  
 RM 88.280 usec  
 DE 6.00 usec  
 TE 294.2 K  
 CHSY2 80.0000000  
 CHSY13 8.0000000  
 DP 0.0000000 sec  
 D1 1.53276801 sec  
 D2 0.80625000 sec  
 D6 0.05230000 sec  
 D16 0.00020000 sec  
 D33 0.0002248 sec

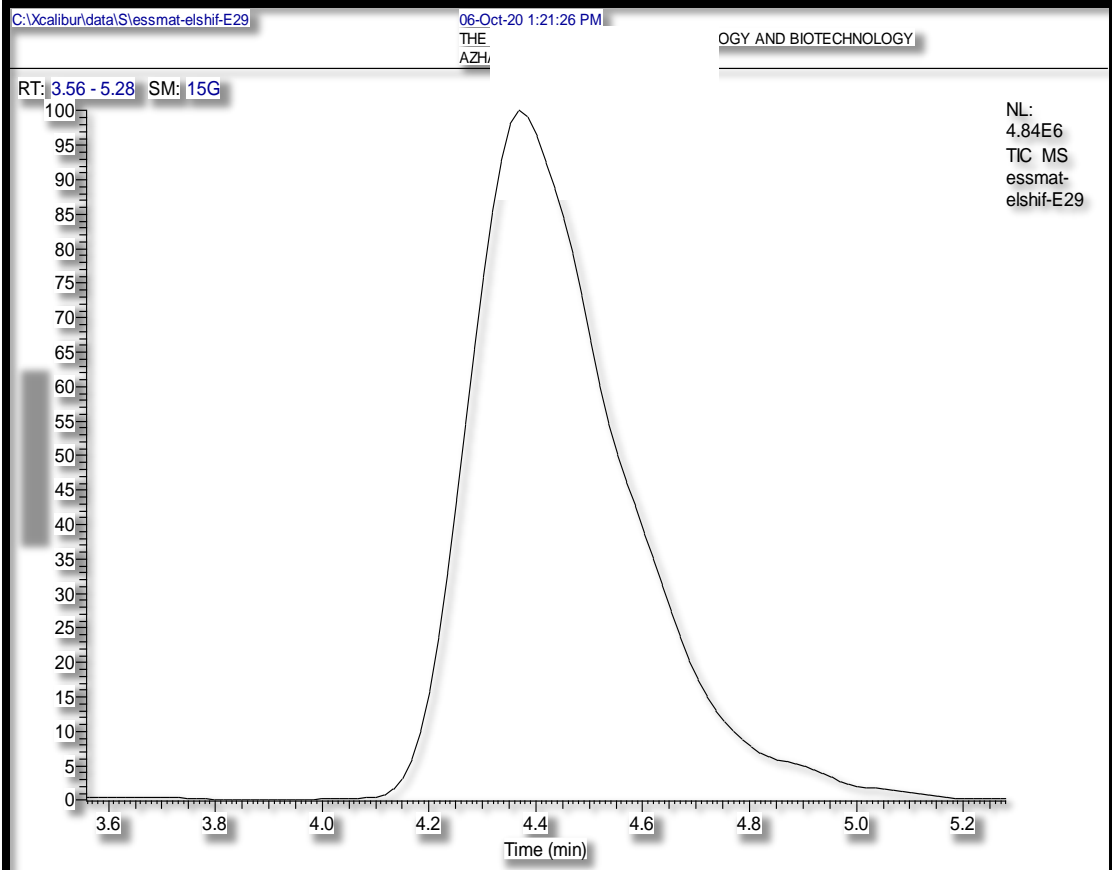
----- CHANNEL F1 -----  
 NUC1 1H  
 P1 11.60 usec  
 P2 23.20 usec  
 PCL 3.00 dB  
 SFO1 400.1129484 MHz

----- CHANNEL F2 -----  
 NUC2 15N  
 P2 11.22 usec  
 PCL 4.00 dB  
 SFO2 40.5488760 MHz

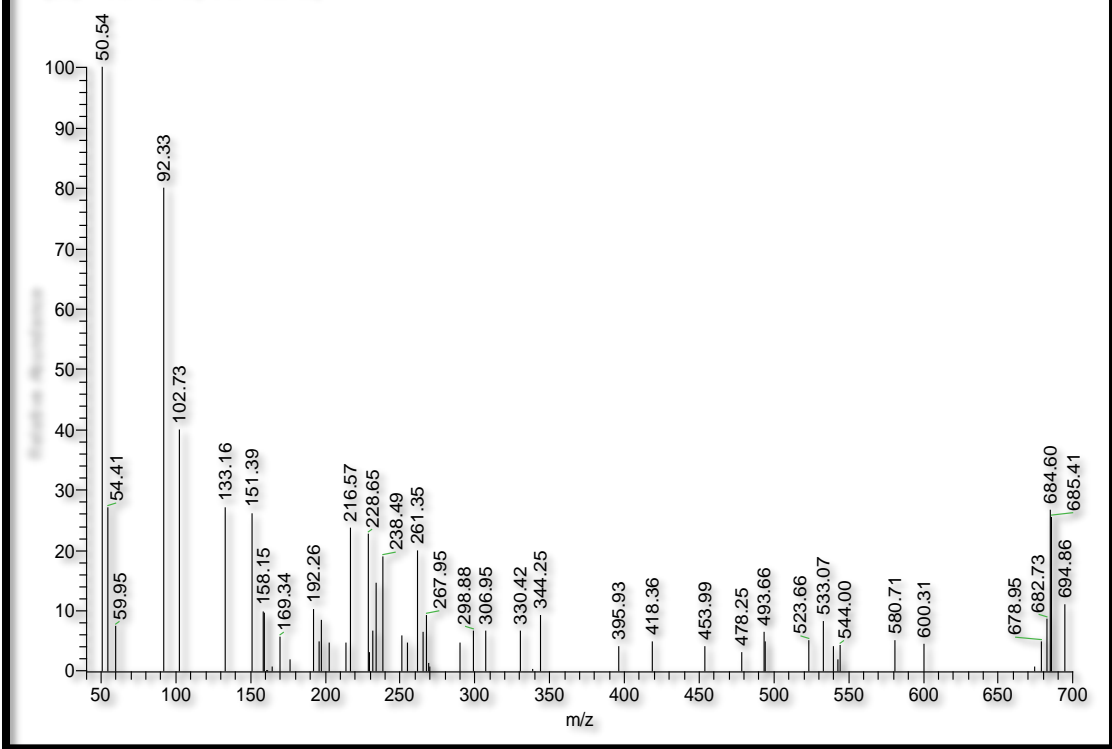
----- GRADIENT CHANNEL -----  
 GPRAM1 SINE.100  
 GPRAM2 SINE.100  
 GPRAM3 SINE.100  
 OP21 70.00 %  
 OP22 30.00 %  
 OP23 50.10 %  
 P16 1000.00 usec  
 MD 2  
 TD 632  
 SFO1 40.54888 MHz  
 FIDRES 43.58361 Hz  
 SFO 500.000 ppm  
 P16MODE QF  
 SI 2645  
 SF 400.1100000 MHz  
 SFO2 SINE  
 LB 0.00 Hz  
 CB 0  
 PC 1.40  
 PI 1024  
 SF 40.5448270 MHz  
 NCU SINE  
 SSB 0  
 GB 0.00 Hz  
 CB 0

ppm  
 -150  
 -100  
 -50  
 0  
 50  
 100  
 150  
 200  
 250  
 300  
 350  
 ppm



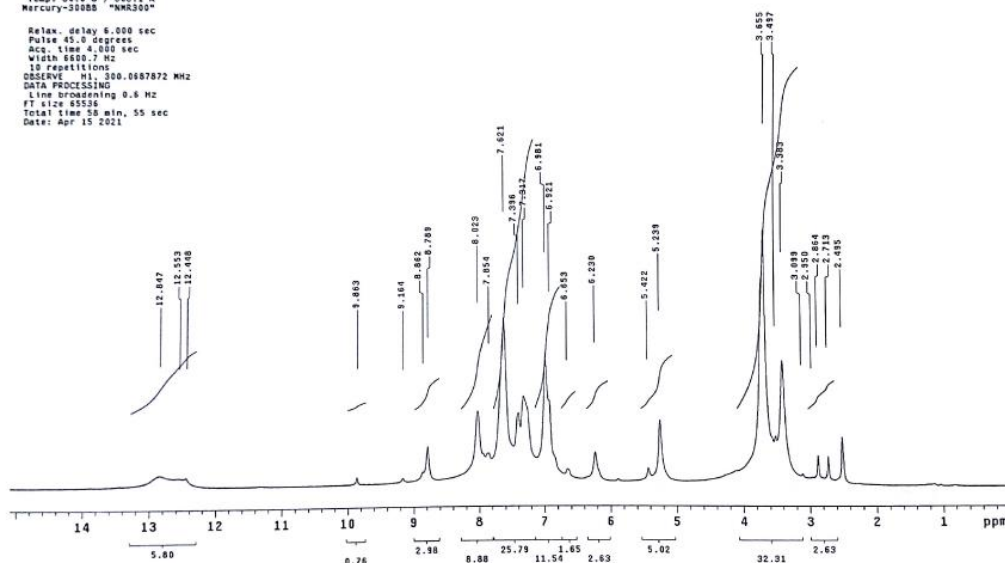


essmat-elshif-E29 #288 RT: 4.84 AV: 1 SB: 2 4.45, 4.45 NL: 1.74E3  
T: (0,0) + c EI Full ms [40.00-1000.00]

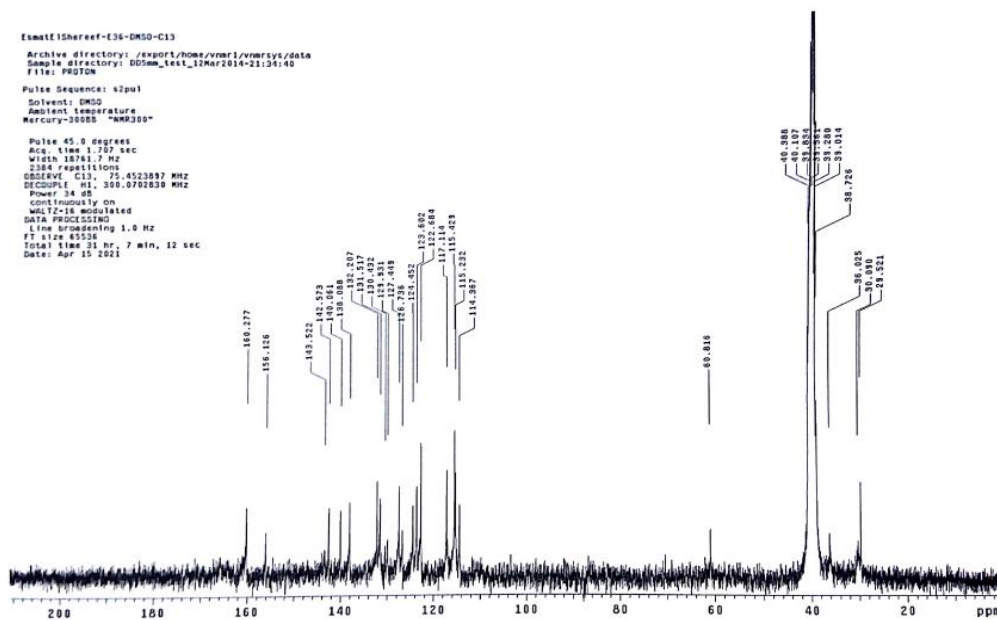


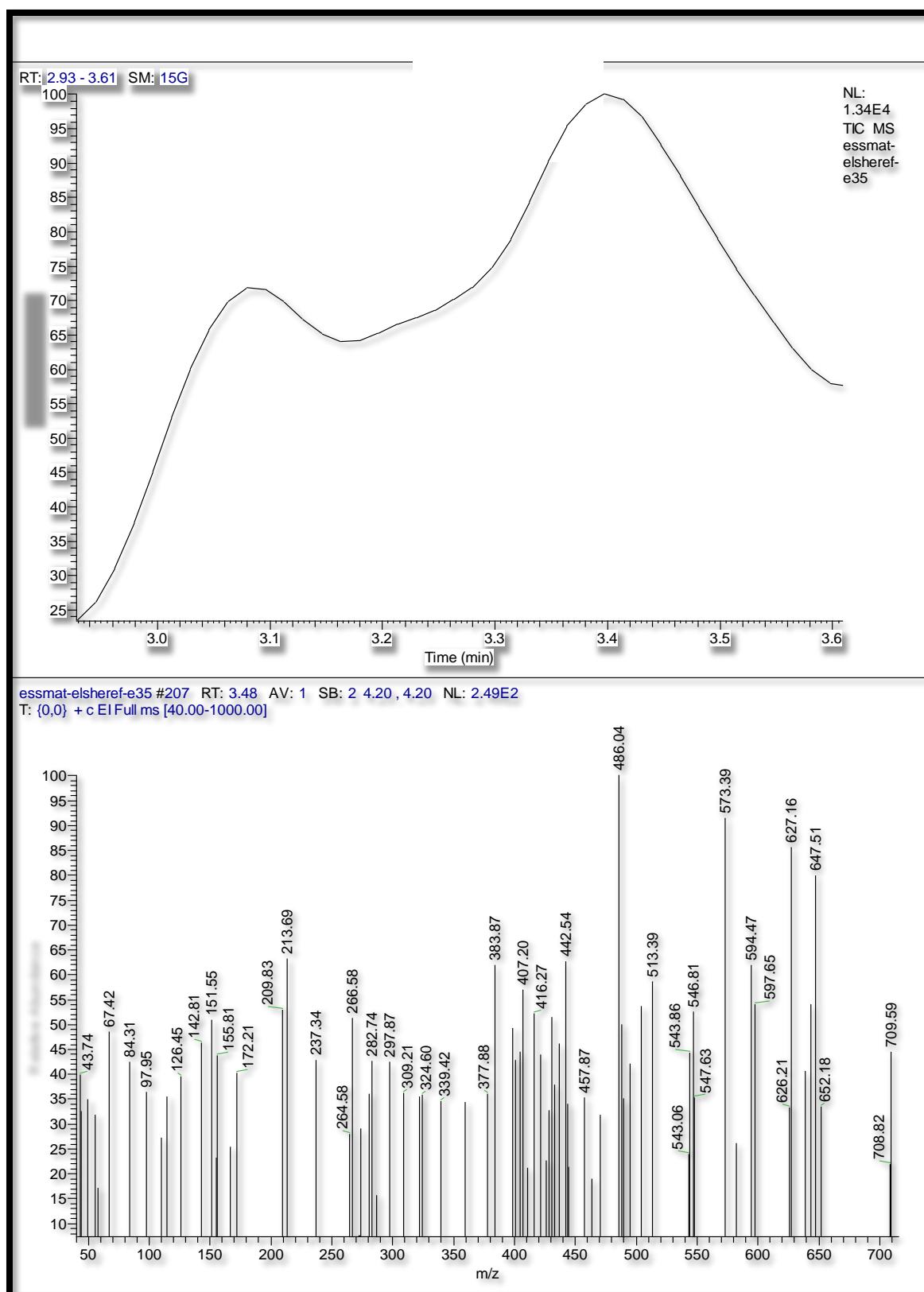
Spectrum data for Compound 8k

Esma115herref-E36-DMSO-H1  
 Archive directory: /export/home/vnmr1/vnmrsys/data  
 Sample directory: D05mm\_test\_12Mar2014-21:34:40  
 File: PR010N  
 Pulse Sequence: s2pul  
 Solvent: DMSO  
 Temp: 30.0 C / 303.1 K  
 Mercury-300MS "NMR300"  
 Relax. delay 6.000 sec  
 Pulse 45.0 degrees  
 Acq. time 4.000 sec  
 Width 6550.7 Hz  
 10 repetitions  
 OBSERVE M1: 300.0687872 MHz  
 DATA PROCESSING  
 Line broadening 0.6 Hz  
 FT size 65536  
 Total time 58 min, 55 sec  
 Date: Apr 15 2021



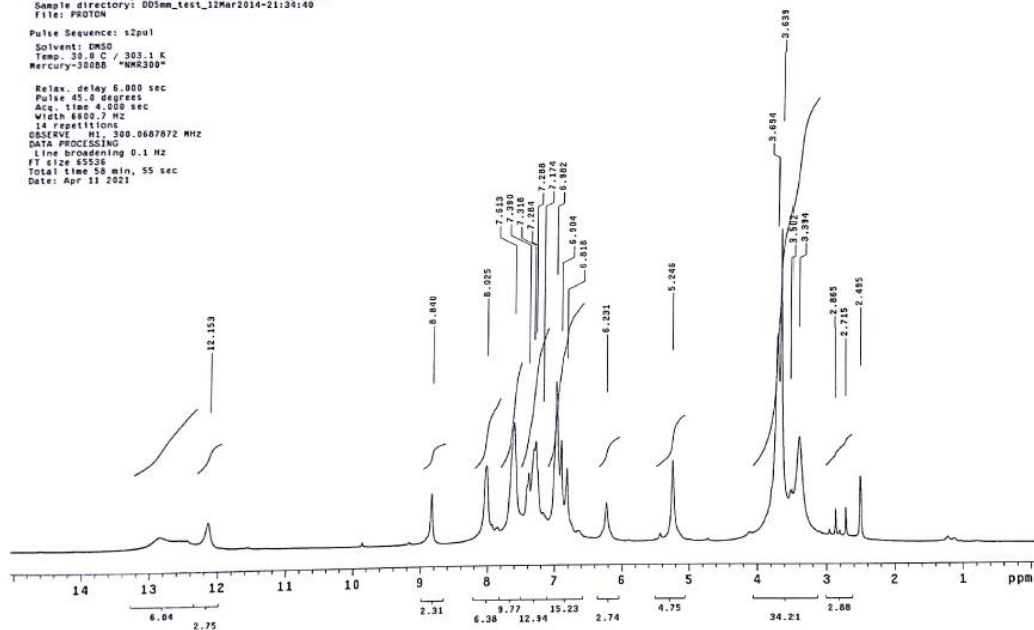
Esma115herref-E36-DMSO-C13  
 Archive directory: /export/home/vnmr1/vnmrsys/data  
 Sample directory: D05mm\_test\_12Mar2014-21:34:40  
 File: PR010N  
 Pulse Sequence: s2pul  
 Solvent: DMSO  
 Ambient temperature  
 Mercury-300MS "NMR300"  
 Pulse 45.0 degrees  
 Acq. time 1.707 sec  
 Width 18761.7 Hz  
 2384 repetitions  
 OBSERVE C13: 75.4523897 MHz  
 DECOUPLE M1: 300.0702830 MHz  
 Power 34.00  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 1.0 Hz  
 FT size 65536  
 Total time 31 hr, 7 min, 12 sec  
 Date: Apr 15 2021



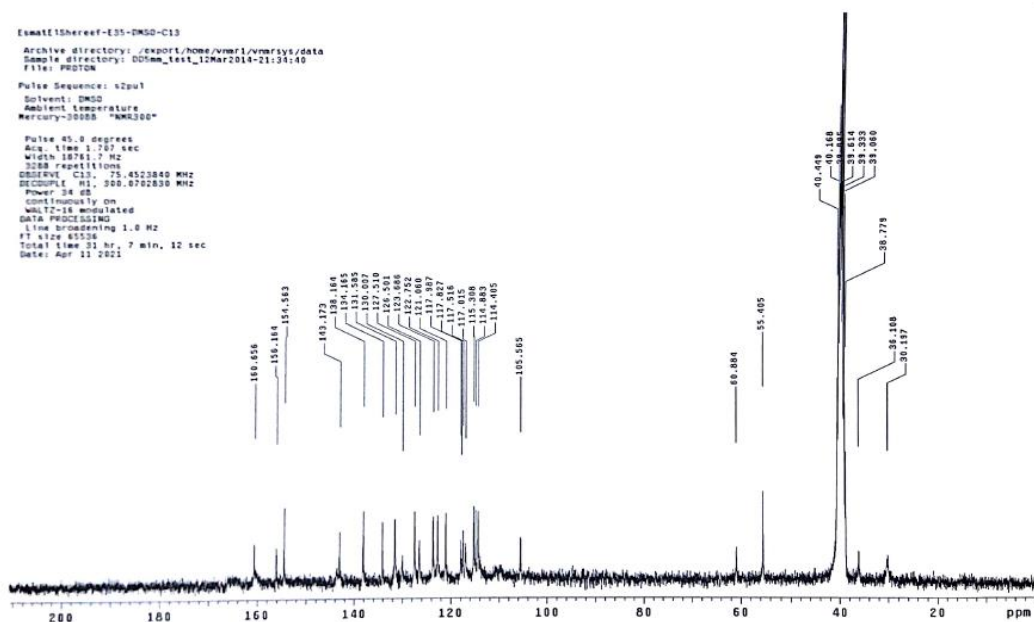


Spectrum data for Compound 8I

Esma11Shereef-E35-DMSO-H1  
 Archive directory: /export/home/vmr1/vmrsys/data  
 Sample directory: D05mm\_tst\_12Mar2014-21:34:40  
 File: PROTON  
 Pulse Sequence: s2pul  
 Solvent: DMSO  
 Temp: 30.0 C / 303.1 K  
 Mercury-3000B "NMR300"  
 Relax. delay 6.000 sec  
 Pulse 45.0 degrees  
 Acq. time 4.000 sec  
 Width 6600.7 Hz  
 14 repetitions  
 OBSERVE M1, 500.0607872 MHz  
 DATA PROCESSING  
 Line broadening 0.1 Hz  
 FT size 65536  
 Total time 58 min, 55 sec  
 Date: Apr 11 2021

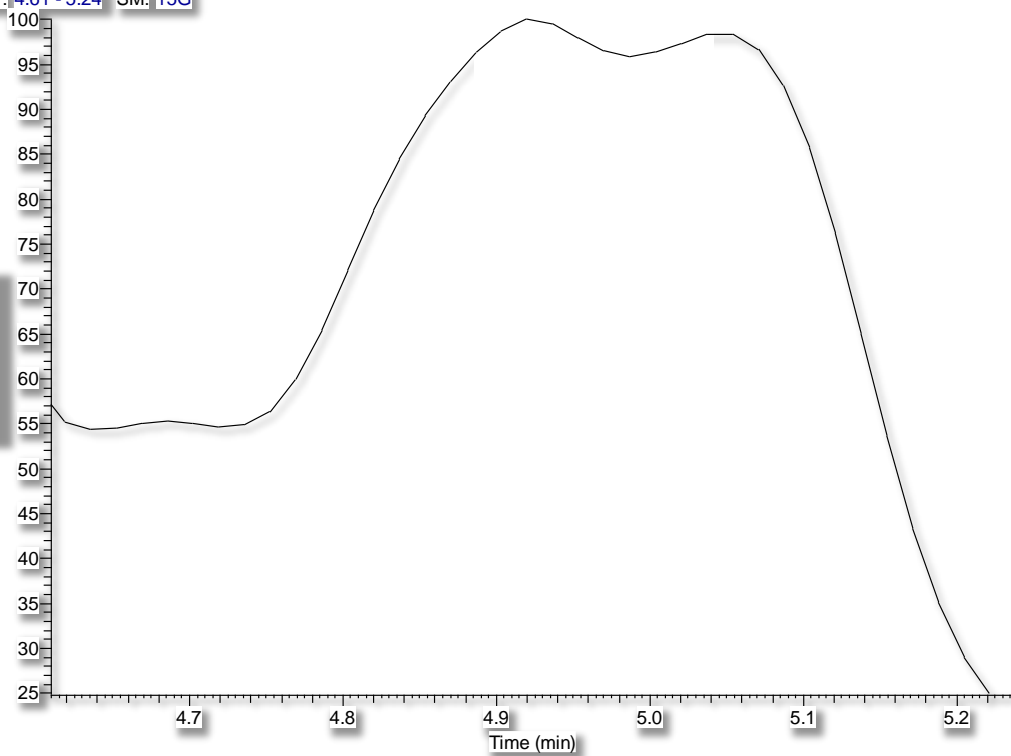


Esma11Shereef-E35-DMSO-C13  
 Archive directory: /export/home/vmr1/vmrsys/data  
 Sample directory: D05mm\_tst\_12Mar2014-21:34:40  
 File: PROTON  
 Pulse Sequence: s2pul  
 Solvent: DMSO  
 Ambient Temperature  
 Mercury-3000B "NMR300"  
 Pulse 45.0 degrees  
 Acq. time 1.787 sec  
 Width 18761.7 Hz  
 3200 repetitions  
 OBSERVE C13, 75.4523840 MHz  
 DECOUPLE M1, 500.0762830 MHz  
 Power 38 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 1.0 Hz  
 FT size 65536  
 Total time 31 hr, 7 min, 12 sec  
 Date: Apr 11 2021



RT: 4.61 - 5.24 SM: 15G

NL:  
1.18E4  
TIC MS  
essmat-  
elsheref-  
e36



essmat-elsheref-e36 #226 RT: 3.80 AV: 1 SB: 2 4.45, 4.45 NL: 6.70E2  
T: {0,0} + c EI Full ms [40.00-1000.00]

