

**SUPPLEMENTARY MATERIAL**

**Studies on a novel series of 3(2H)-pyridazinones: Synthesis, molecular modelling, antimicrobial activity**

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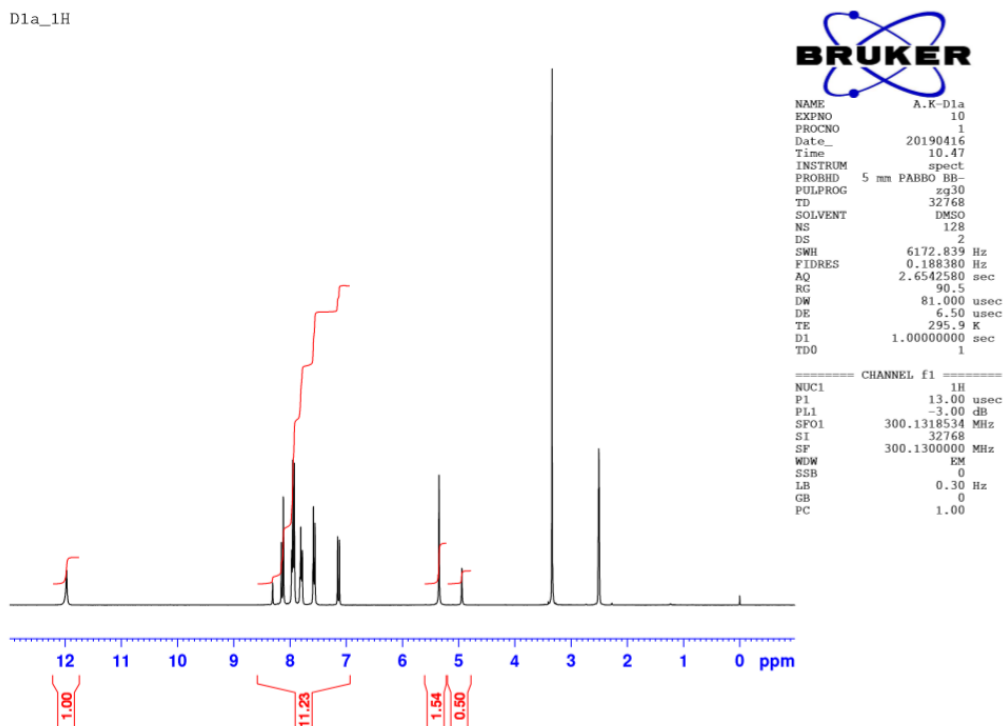
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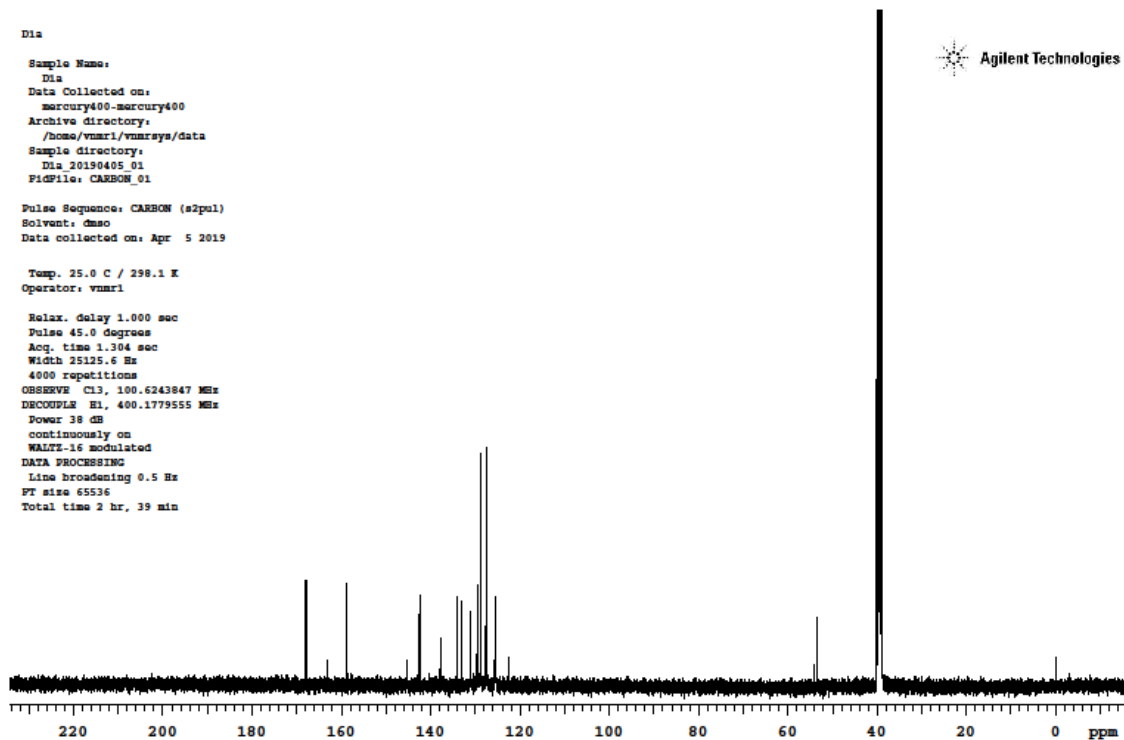
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## Data 1. <sup>1</sup>H-NMR spectrum of compound D1a

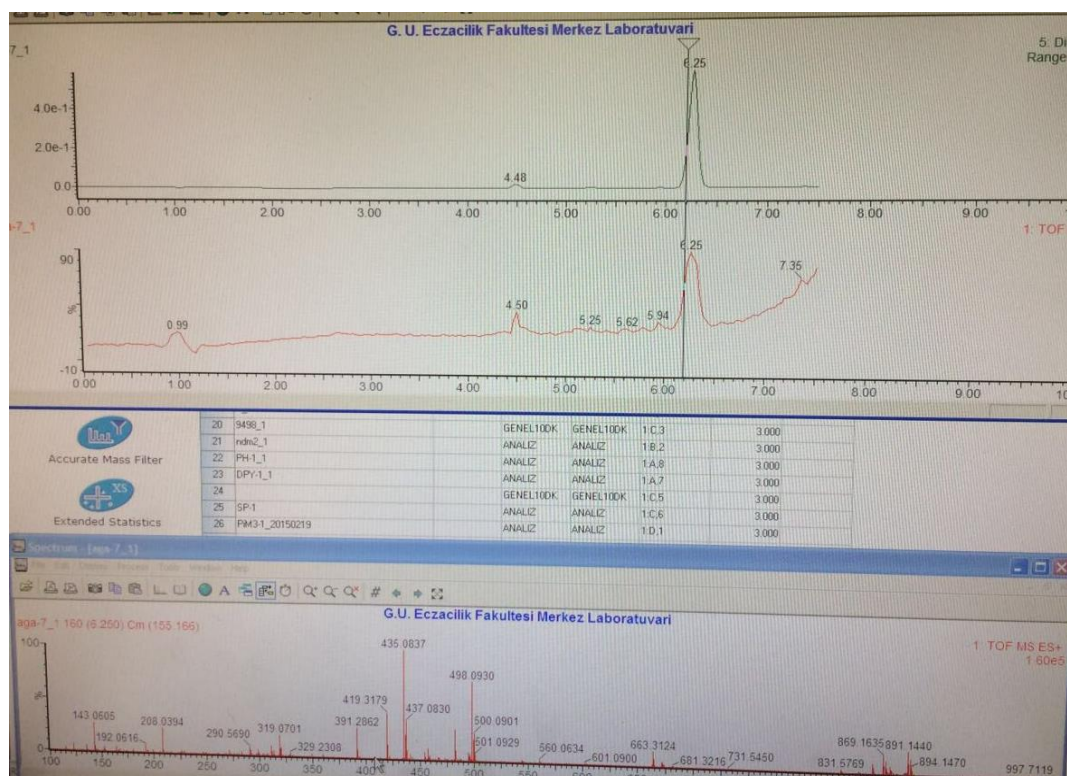
D1a\_1H



## Data 2. <sup>13</sup>C-NMR spectrum of compound D1a

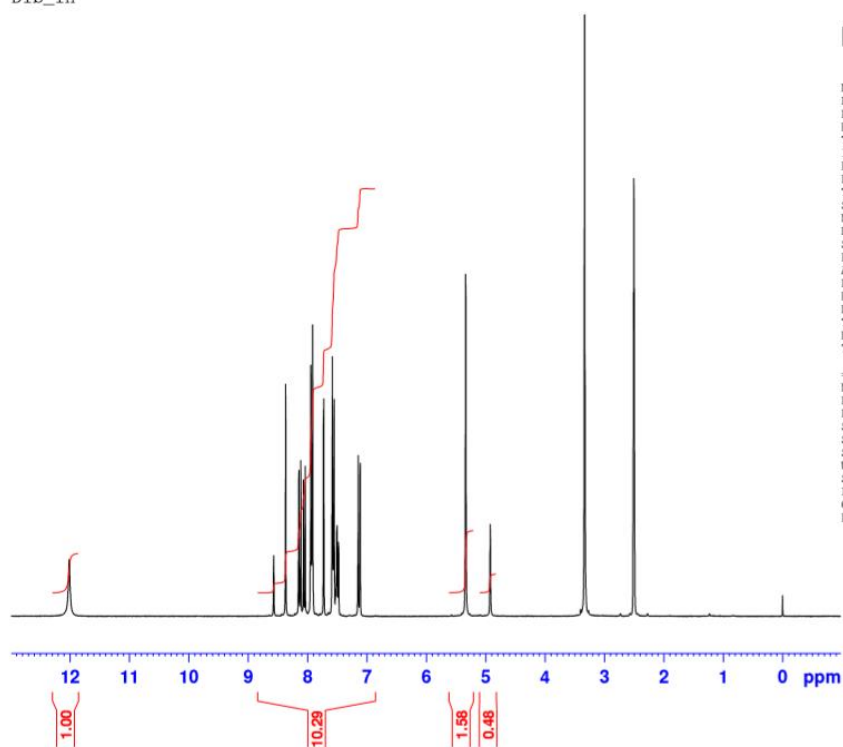


### Data 3. Mass spectrum of compound D1a



### Data 4. <sup>1</sup>H-NMR spectrum of compound D1b

D1b\_1H



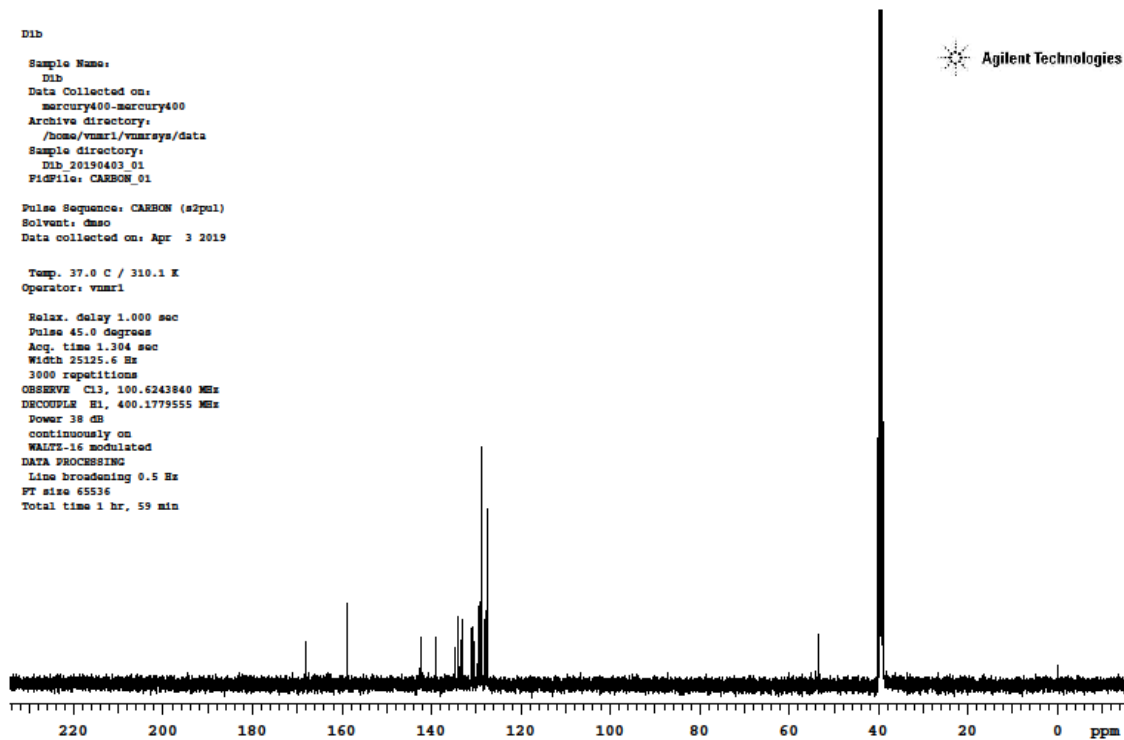
```

NAME      A.K-D1b
EXPNO     10
PROCNO    1
Date_     20190416
Time      10.36
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         32768
SOLVENT   DMSO
NS         79
DS         2
SWH        6172.839 Hz
FIDRES     0.188380 Hz
AQ         2.6542580 sec
RG         128
DW         81.000 usec
DE         6.50 usec
TE         295.9 K
D1         1.0000000 sec
TD0        1
    
```

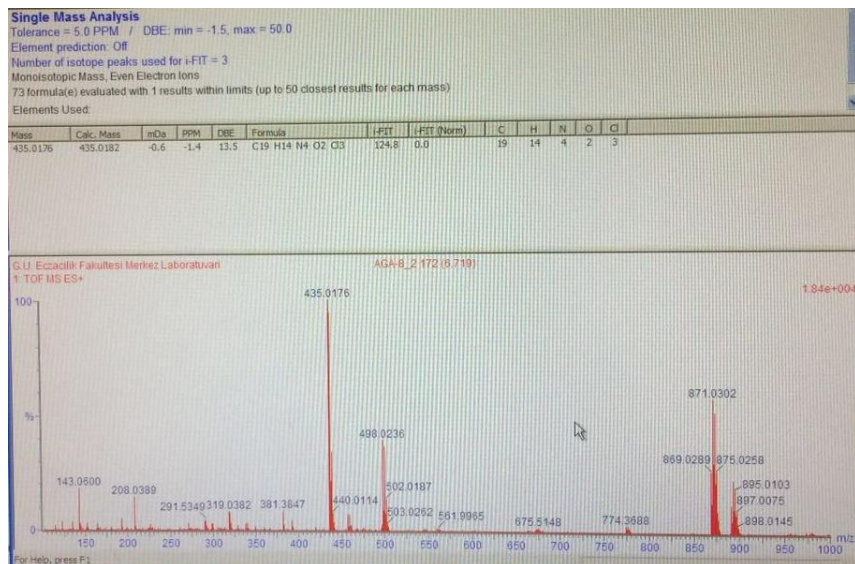
```

===== CHANNEL f1 =====
NUC1      1H
P1        13.00 usec
PL1       -3.00 dB
SFO1      300.1318534 MHz
SI        32768
SF        300.1300000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

## Data 5. <sup>13</sup>C-NMR spectrum of compound D1b

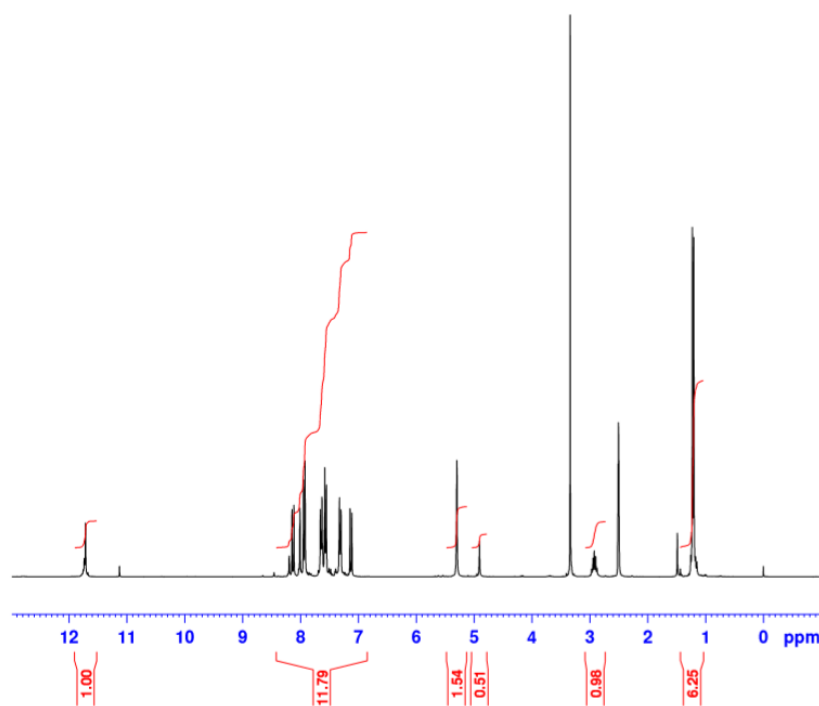


## Data 6. Mass spectrum of compound D1b



## Data 7. <sup>1</sup>H-NMR spectrum of compound D<sub>1c</sub>

D1c\_1H



```
NAME          A.K-D1c
EXPNO         10
PROCNO        1
Date_         20190416
Time          10.59
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            128
DS            2
SWH           6172.839 Hz
FIDRES        0.188380 Hz
AQ            2.6542580 sec
RG            71.8
DW            81.000 usec
DE            6.50 usec
TE            295.8 K
D1            1.00000000 sec
TD0           1
```

```
===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           -3.00 dB
SFO1          300.1318534 MHz
SI            32768
SF            300.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

## Data 8. <sup>13</sup>C-NMR spectrum of compound D<sub>1c</sub>

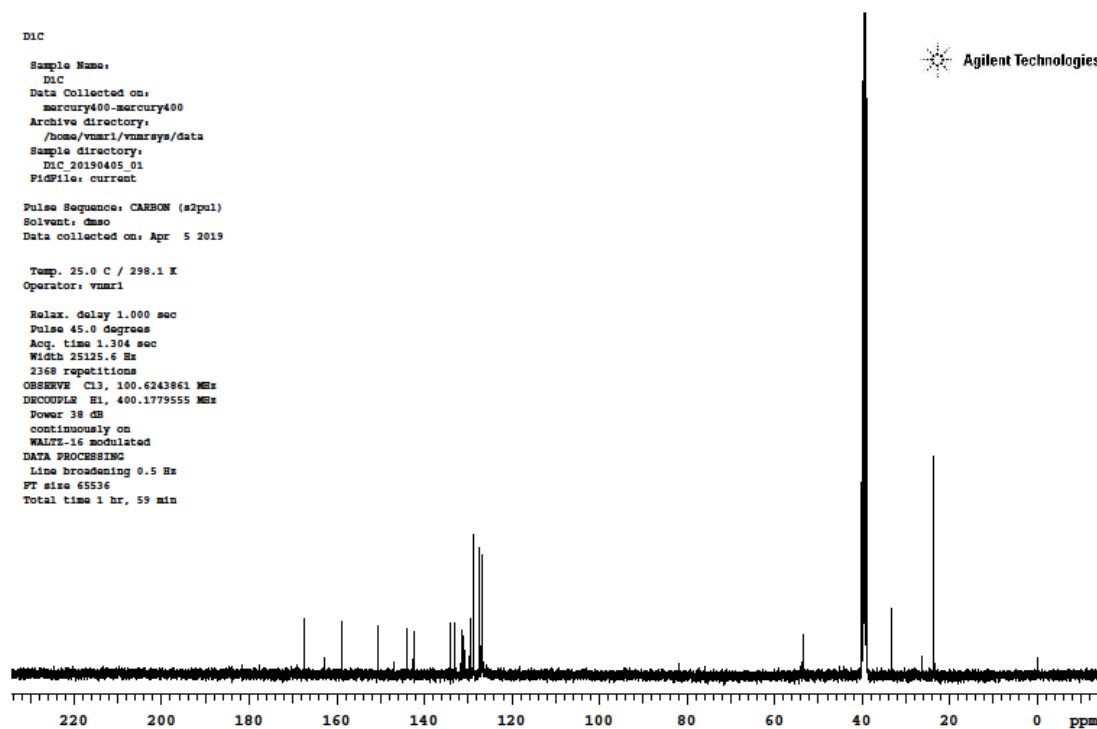
D1C

```
Sample Name:
D1C
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
D1C_20190405_01
FidFile: current

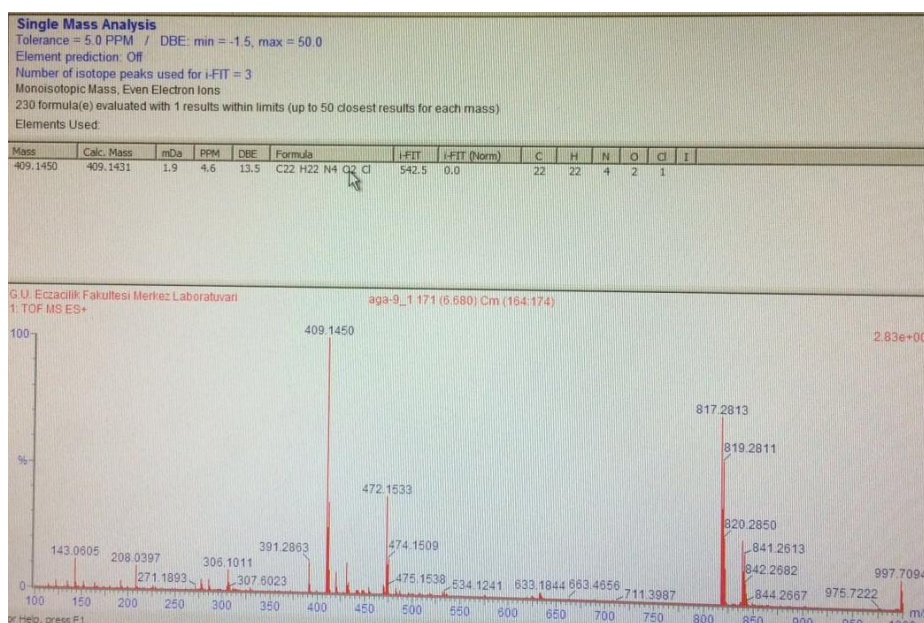
Pulse Sequence: CARBON (s2pul)
Solvent: dmsc
Data collected on: Apr 5 2019
```

```
Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
2368 repetitions
OBSERVE C13, 100.6243861 MHz
DECOUPLE H1, 400.1779555 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 59 min
```

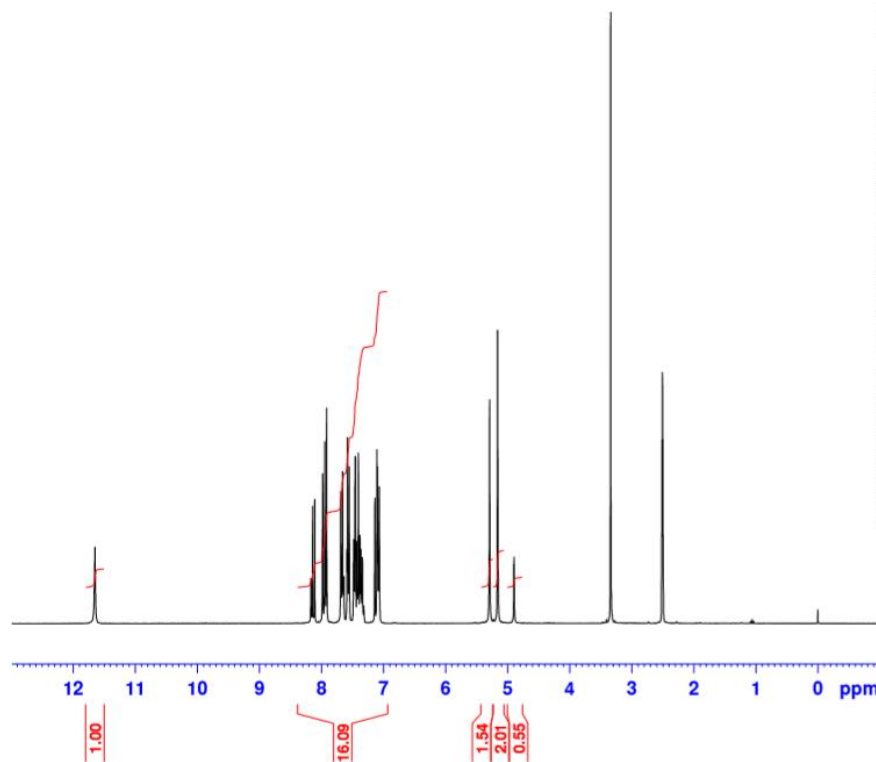


## Data 9. Mass spectrum of compound D1c



## Data 10. <sup>1</sup>H-NMR spectrum of compound D1d

D1d\_1H



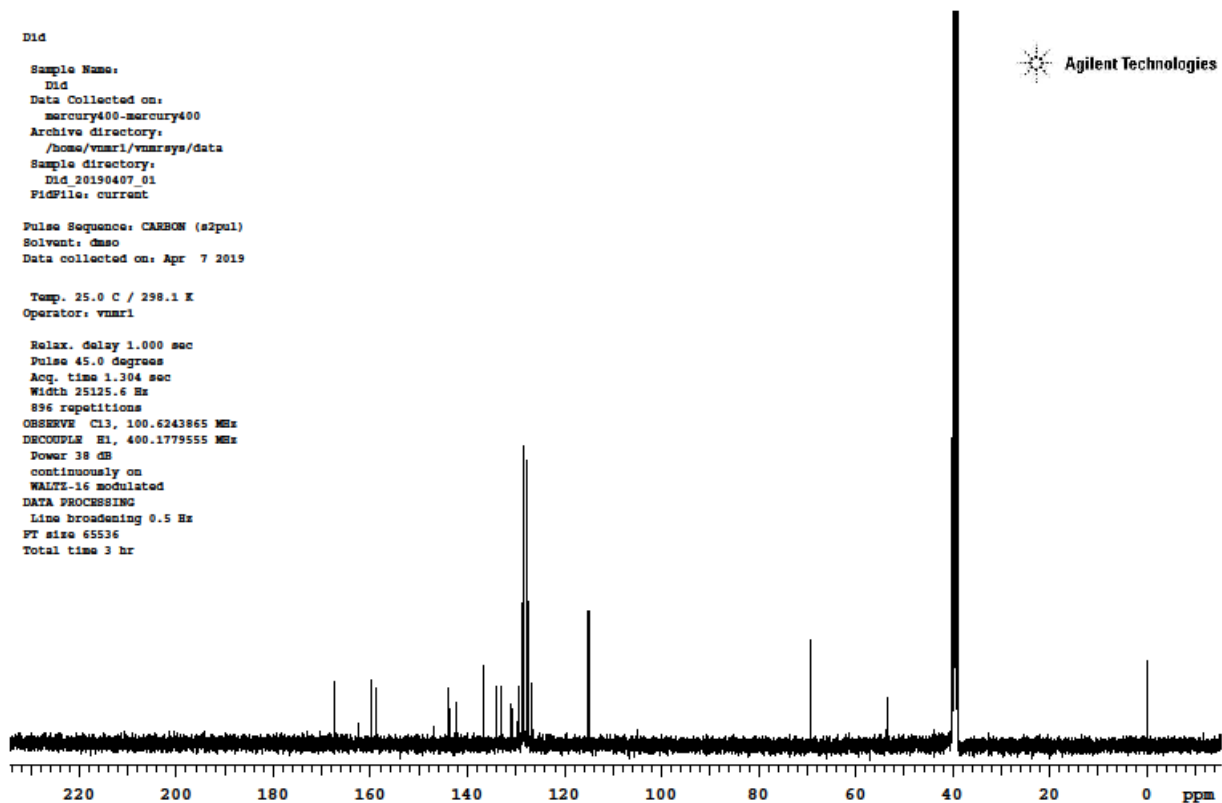
```

NAME          A.K-D1d
EXPNO         10
PROCNO        1
Date_         20190416
Time          11.56
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            128
DS            2
SWH           6172.839 Hz
FIDRES        0.188380 Hz
AQ            2.6542580 sec
RG            90.5
DW            81.000 usec
DE            6.50 usec
TE            295.7 K
D1            1.00000000 sec
TD0           1

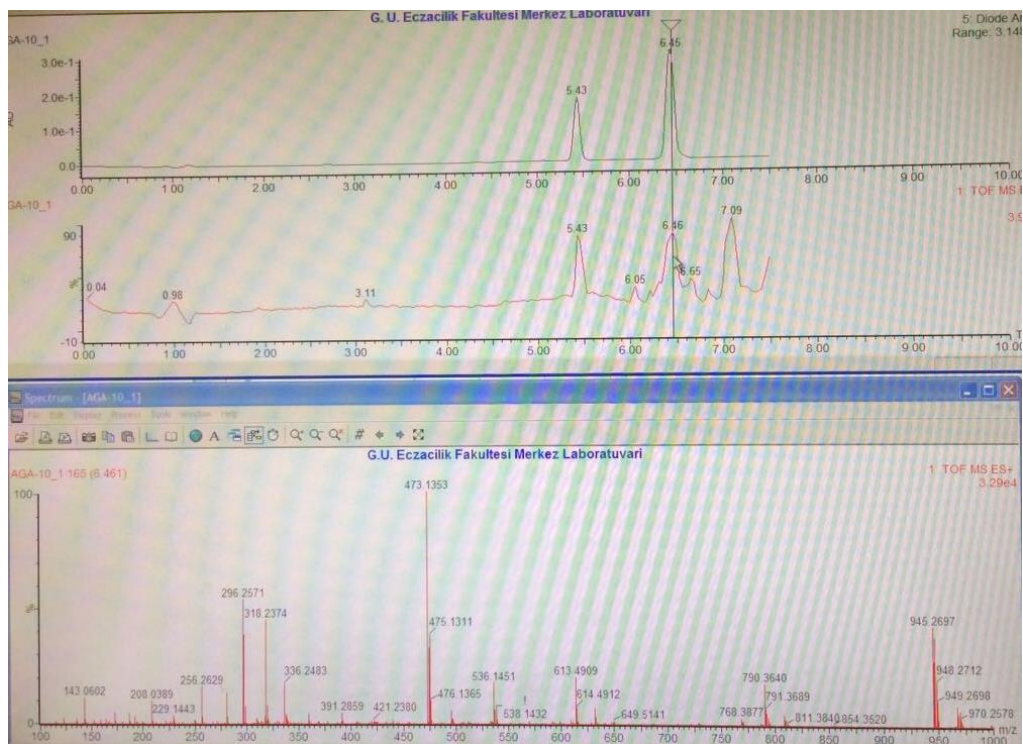
===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           -3.00 dB
SFO1         300.1318534 MHz
SI           32768
SF           300.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



## Data 11. $^{13}\text{C}$ -NMR spectrum of compound D1d

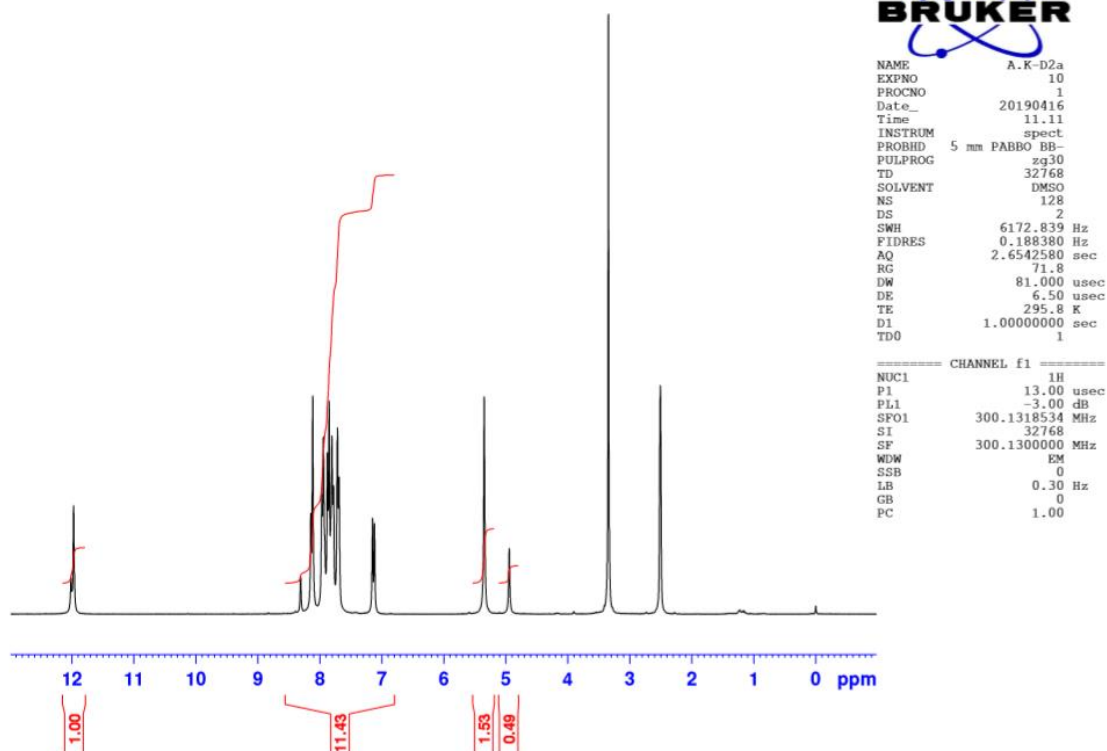


## Data 12. Mass spectrum of compound D1d

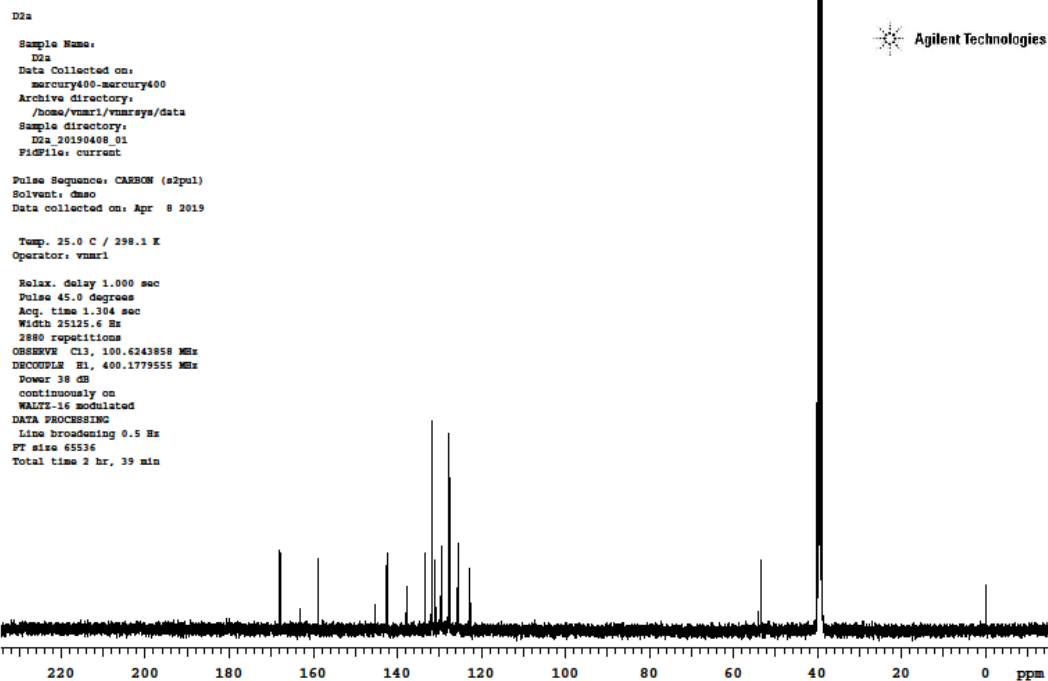


### Data 13. <sup>1</sup>H-NMR spectrum of compound D2a

D2a\_1H

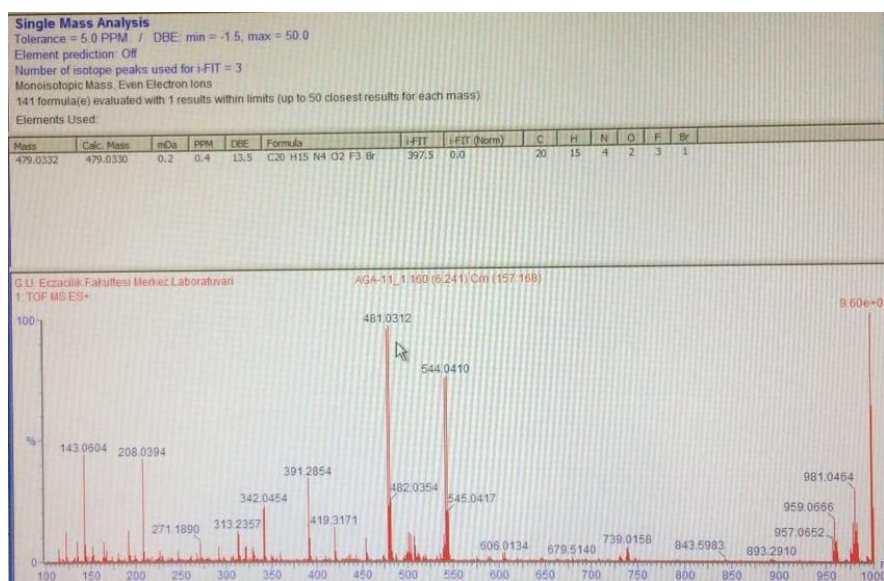


### Data 14. <sup>13</sup>C-NMR spectrum of compound D2a



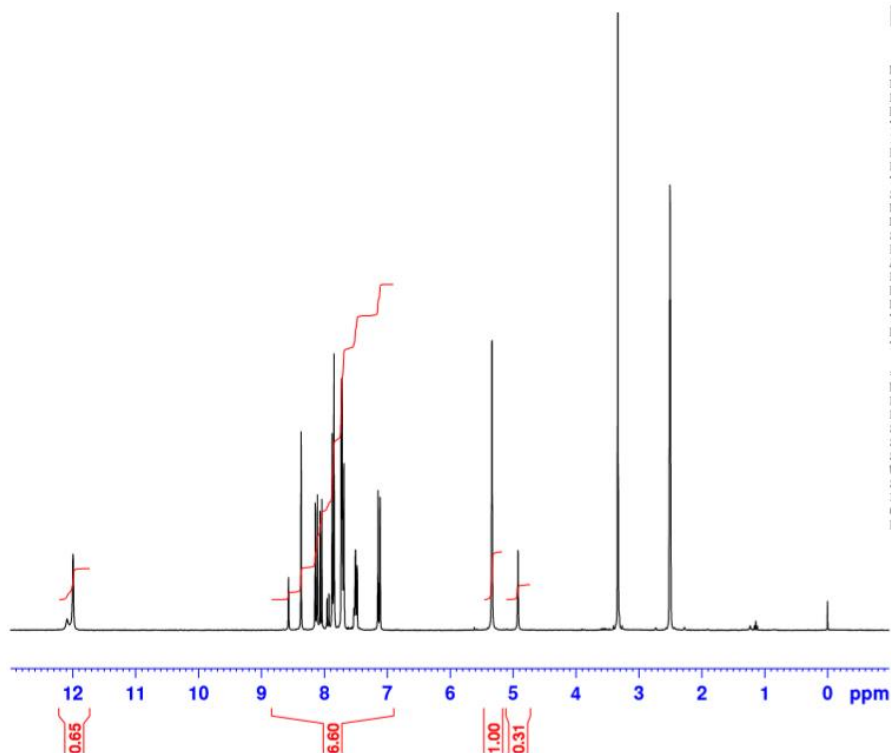


## Data 15. Mass spectrum of compound D2a



## Data 16. <sup>1</sup>H-NMR spectrum of compound D2b

D2b\_1H

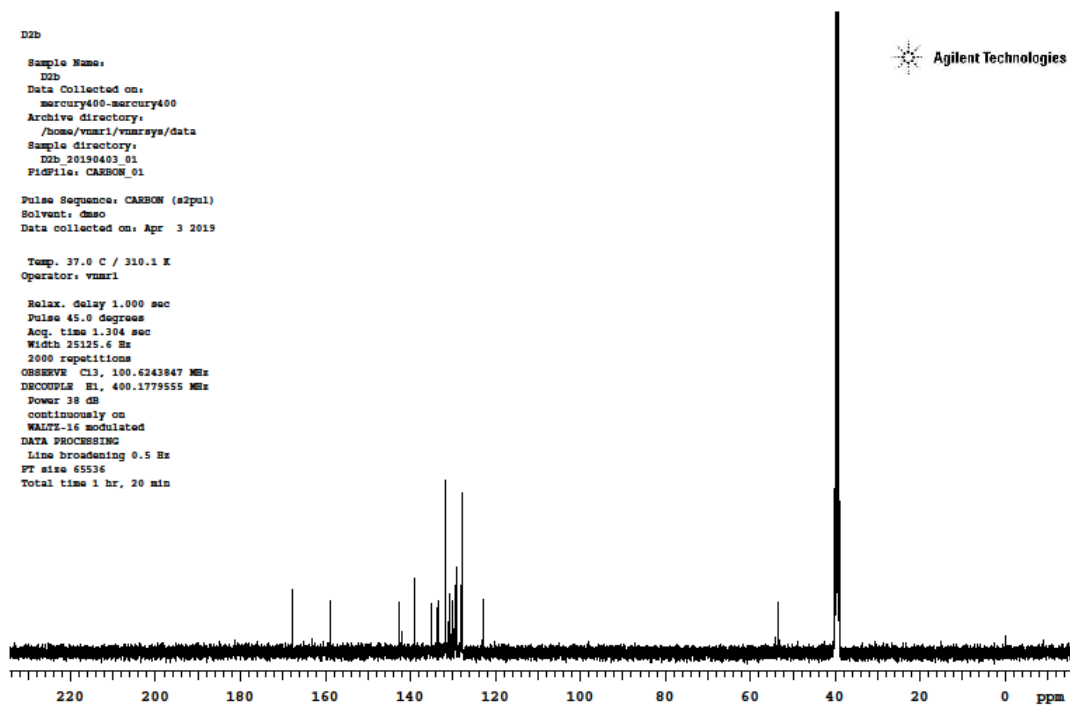


```

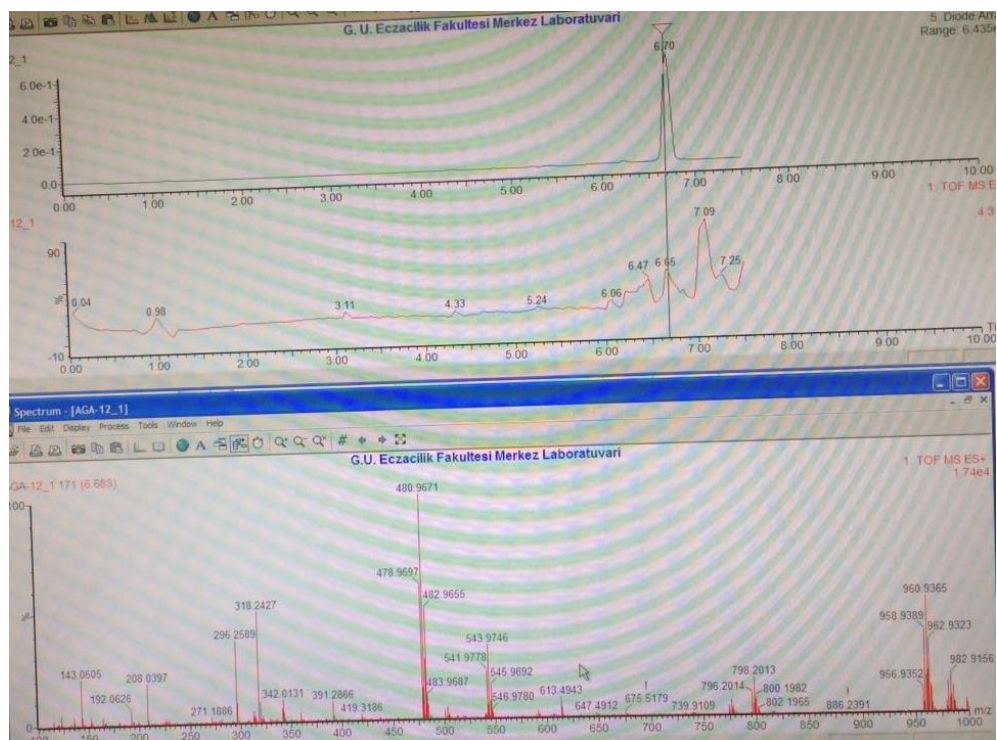
NAME          A.K-D2b
EXPNO         10
PROCNO        1
Date_         20190416
Time          11.45
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            128
DS            2
SWH           6172.839 Hz
FIDRES        0.188380 Hz
AQ            2.6542580 sec
RG            114
DW            81.000 usec
DE            6.50 usec
TE            295.9 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           -3.00 dB
SFO1          300.1318534 MHz
SI            32768
SF            300.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

## Data 17. $^{13}\text{C}$ -NMR spectrum of compound D2b

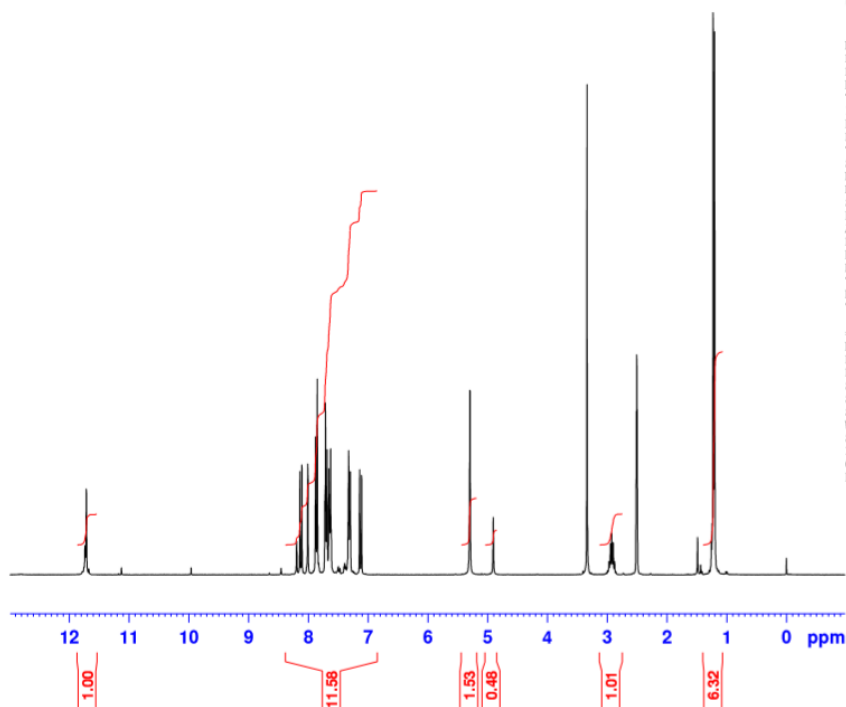


## Data 18. Mass spectrum of compound D2b



# Data 19. <sup>1</sup>H-NMR spectrum of compound D2c

D2c\_1H

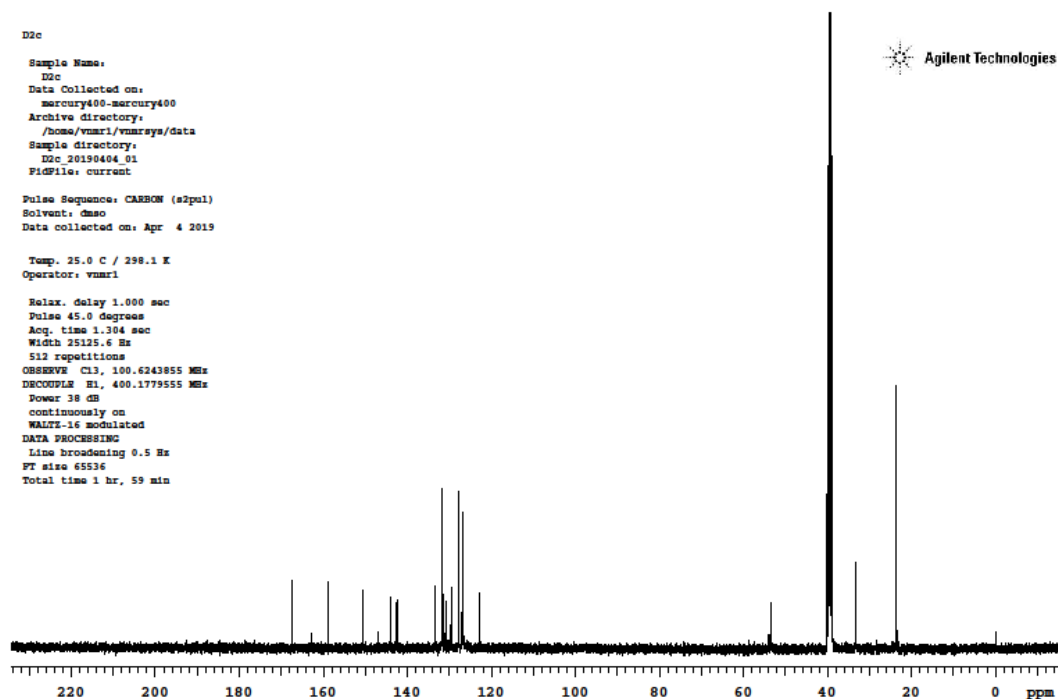


NAME A.K-D2c  
EXPNO 10  
PROCNO 1  
Date\_ 20190416  
Time 11.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 32768  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.188380 Hz  
AQ 2.6542580 sec  
RG 71.8  
DW 81.000 usec  
DE 6.50 usec  
TE 295.7 K  
D1 1.00000000 sec  
TD0 1

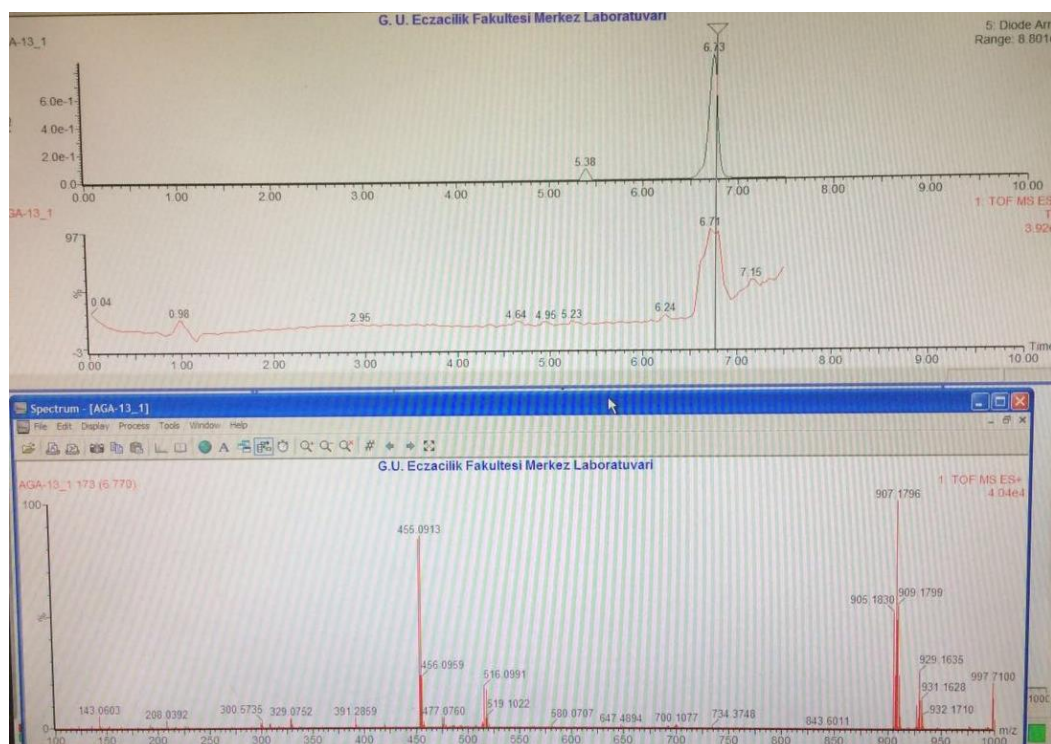
===== CHANNEL f1 =====  
NUC1 1H  
P1 13.00 usec  
PL1 -3.00 dB  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

# Data 20. <sup>13</sup>C-NMR spectrum of compound D2c

D2c  
Sample Name:  
D2c  
Data Collected on:  
mercury400-mercury400  
Archive directory:  
/home/vnmr1/vnmrswy/data  
Sample directory:  
D2c 20190404.01  
FidFile: current  
Pulse Sequence: CARBON (s2pul)  
Solvent: dmsd  
Data collected on: Apr 4 2019  
Temp. 25.0 C / 298.1 K  
Operator: vnmr1  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
Siz repetitions  
OBSERVE C13, 100.6243855 MHz  
DECOUPLE H1, 400.1779555 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 59 min

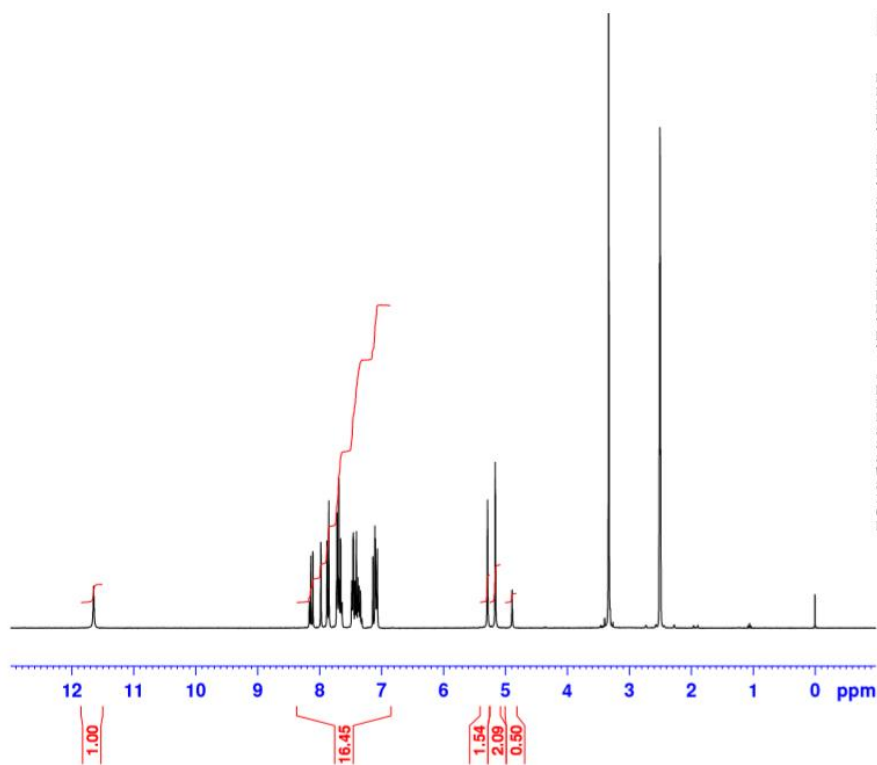


## Data 21. Mass spectrum of compound D2c



## Data 22. <sup>1</sup>H-NMR spectrum of compound D2a

D2d\_1H



```

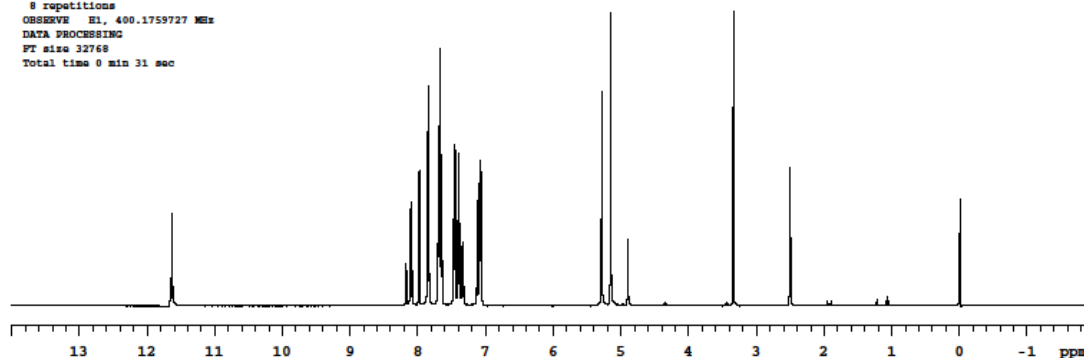
NAME          A.K-D2d
EXPNO         10
PROCNO        1
Date_         20190416
Time          11.34
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            128
DS            2
SWH           6172.839 Hz
FIDRES        0.188380 Hz
AQ            2.6542580 sec
RG            128
DW            81.000 usec
DE            6.50 usec
TE            295.9 K
D1            1.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1           -3.00 dB
SFO1         300.1318534 MHz
SI            32768
SF           300.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

## Data 23. <sup>13</sup>C-NMR spectrum of compound D2a

D2d  
Sample Name:  
D2d  
Data Collected on:  
mercury400-mercury400  
Archive directory:  
/home/vnmr1/vnmrsw/data  
Sample directory:  
D2d\_20190405\_01  
File: PROTON\_02  
Pulse Sequence: PROTON (s2pul)  
Solvent: dmsc  
Data collected on: Apr 5 2019  
Temp. 25.0 C / 298.1 K  
Operator: vnmr1  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.559 sec  
Width 6402.0 Hz  
8 repetitions  
OBSERVE H1, 400.1759727 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 31 sec



## Data 24. Mass spectrum of compound D2a

