SUPPORTING INFORMATION

Development of benzofuran derived sulfamates as dual aromatase-steroid sulfatase inhibitors (DASIs): Design, synthesis and biological evaluation

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Figure S1. Comparison between the ^{1}H NMR spectra of the sulfamate (**10a**) and carbamate (**10b**) products indicating the difference in the amino group signals.	S2
^{1}H, ^{13}C, ^{19}F NMR and HPLC of final compounds	S3-S29

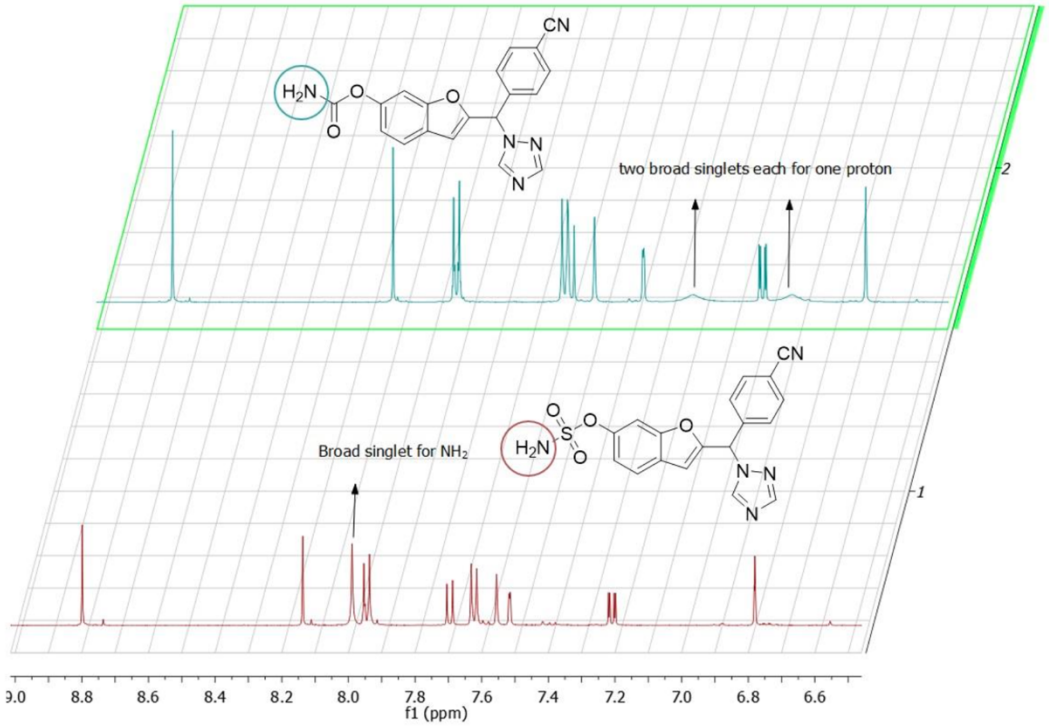
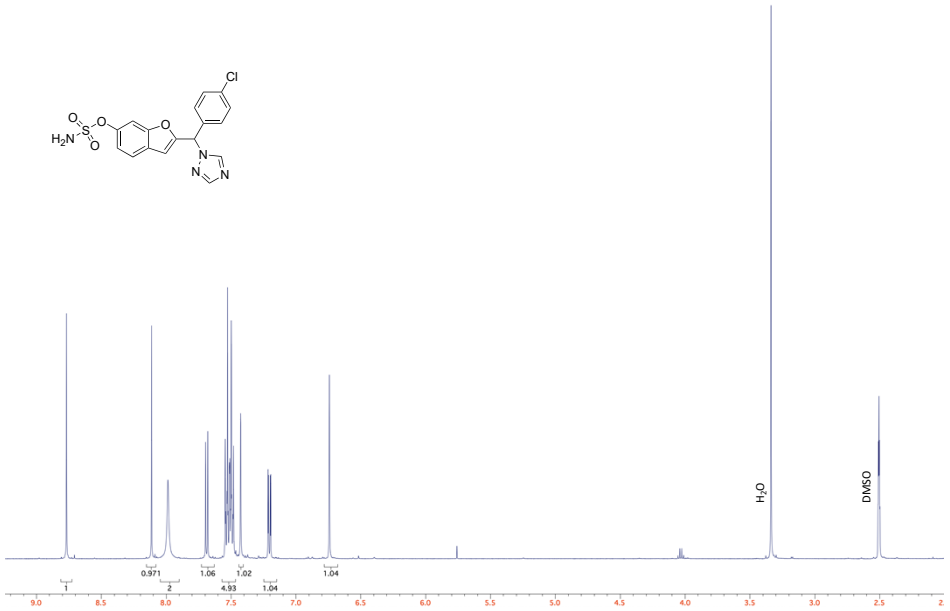


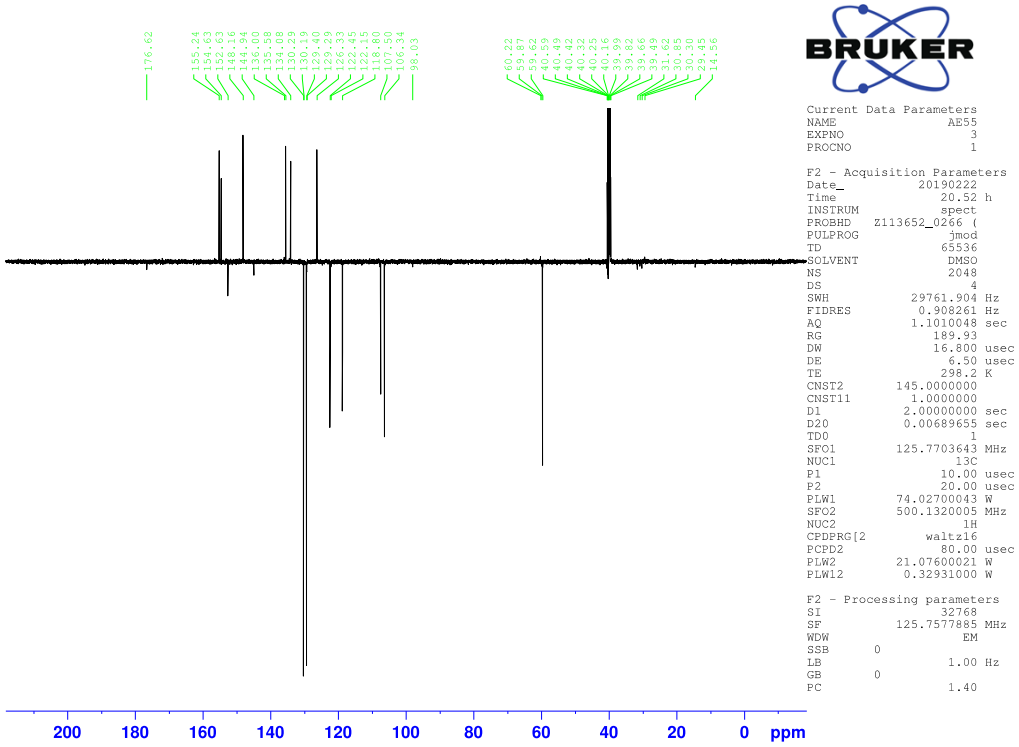
Figure S1. Comparison between the ^{1}H NMR spectra of the sulfamate (**10a**) and carbamate (**10b**) products indicating the difference in the amino group signals.

Compound **6**

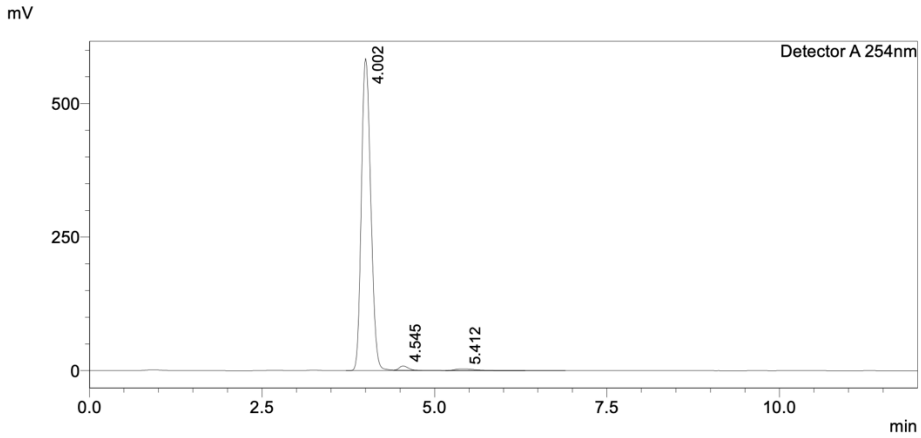
^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



HPLC



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
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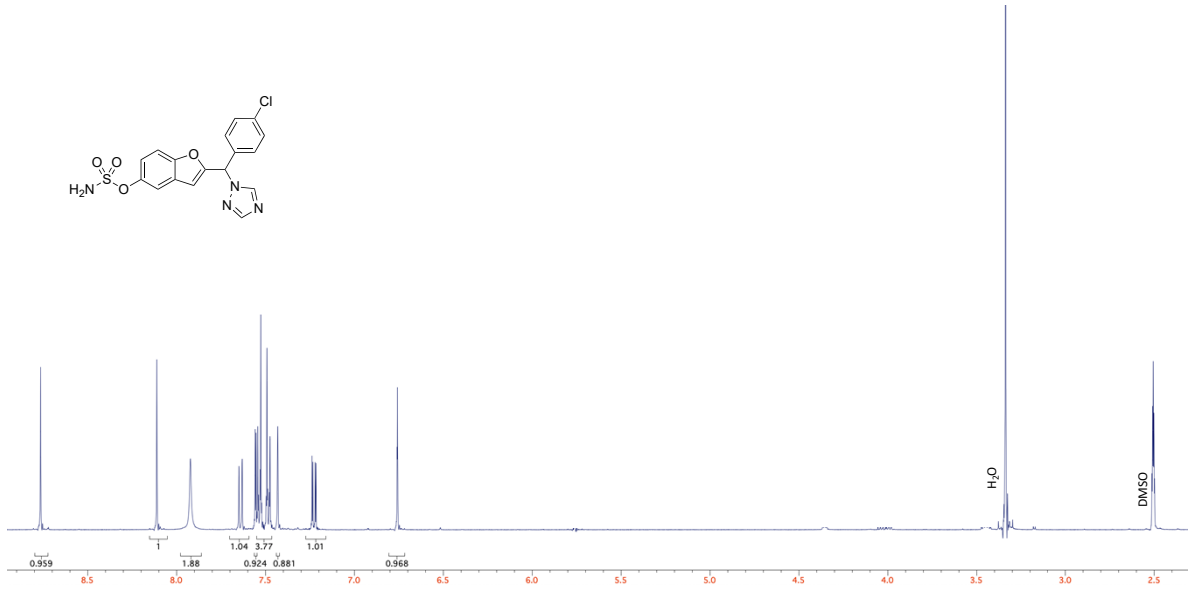
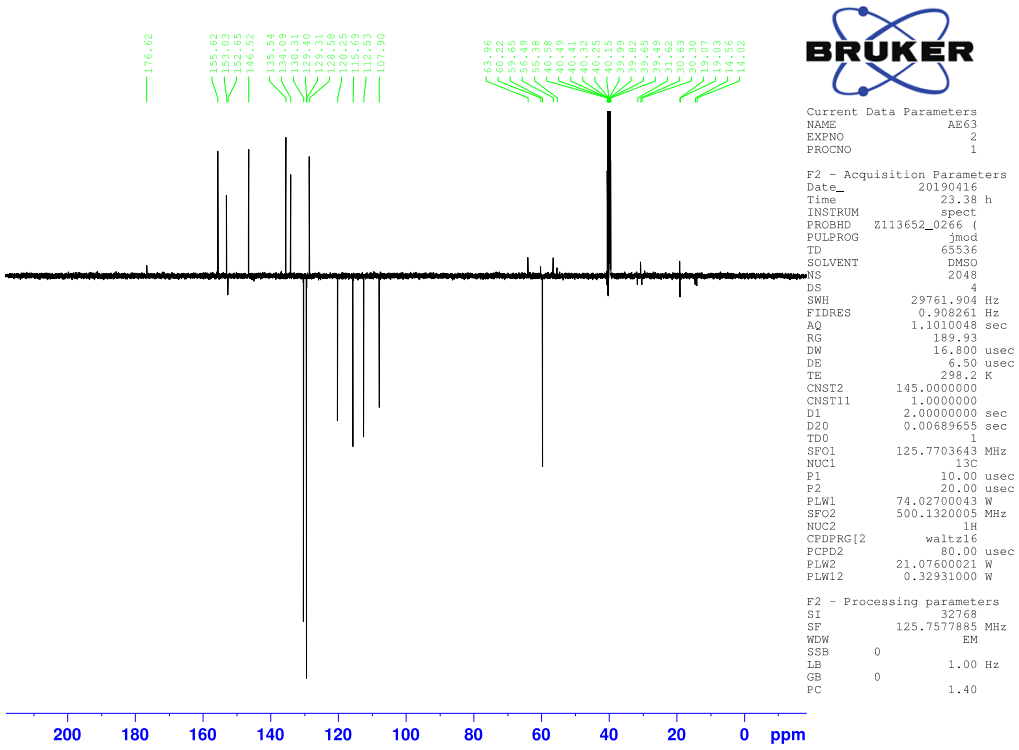
2	4.545	68644	7868	1.194	1.194
3	5.412	63752	2997	1.109	1.109
Total		5749295	594791		100.000

Compound **7**

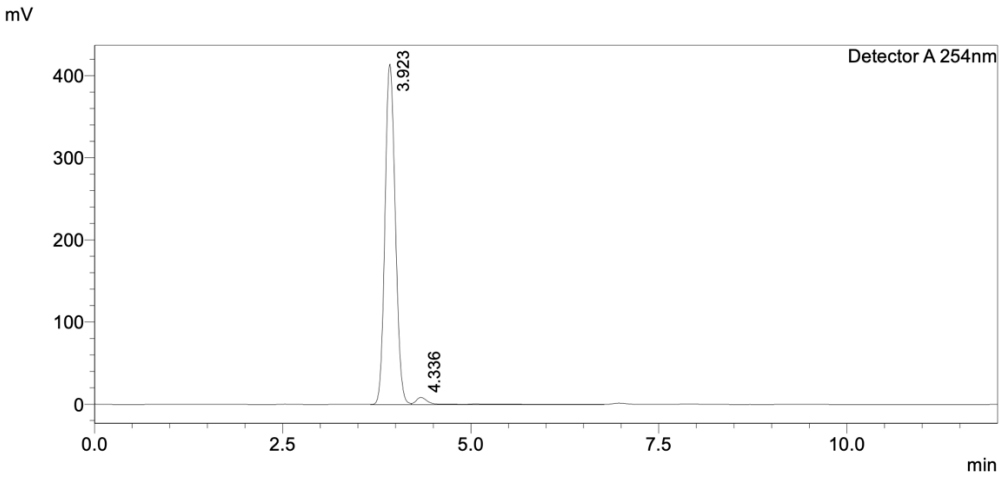
^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



HPLC data



<Peak Table>

Detector A 254nm

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2	4.336	102705	8574	2.519	2.519
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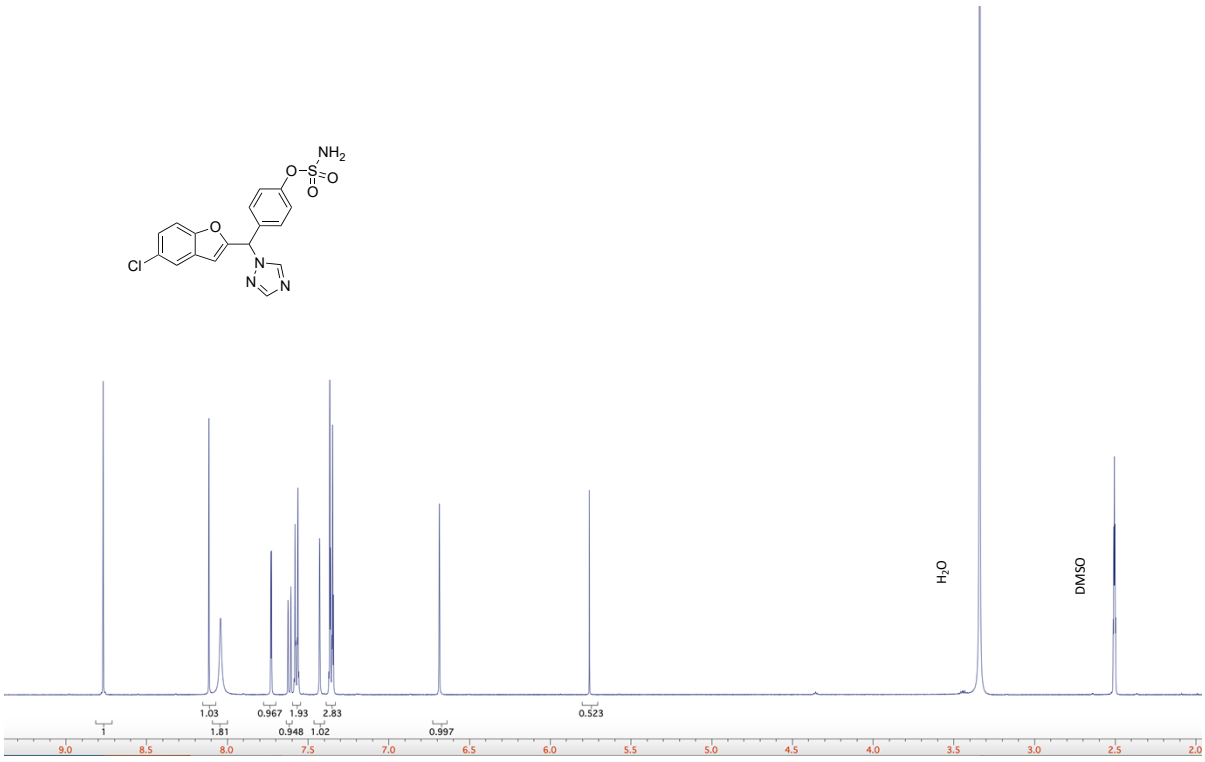
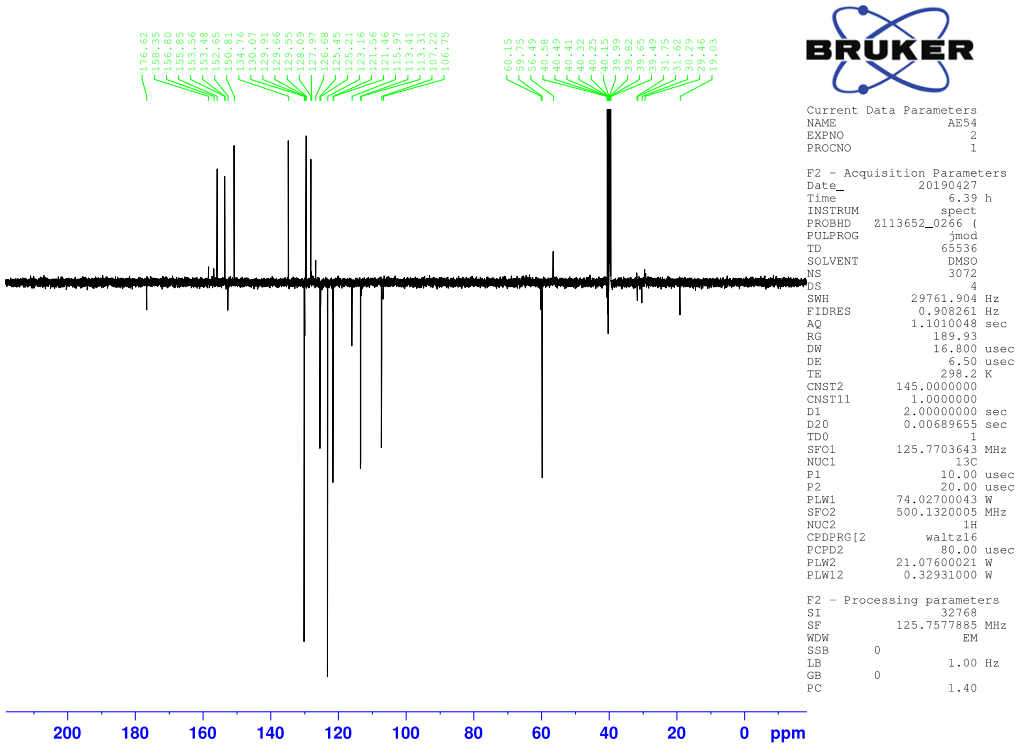
Compound **8a**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)

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PROCNO                   1

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TD                  65536
SOLVENT               DMSO
NS                    3072
DS                       4
SWH             29761.904 Hz
FIDRES          0.908261 Hz
AQ              1.1010048 sec
RG                 189.93
DW                16.800 usec
DE                 6.50 usec
TE                298.2 K
CNST2          145.0000000
CNST11           1.0000000
D1               2.00000000 sec
D20              0.00689655 sec
TD0                      1
SFO1           125.7703643 MHz
NUC1                   13C
P1                10.00 usec
P2                20.00 usec
PLW1           74.02700043 W
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2             80.00 usec
PLW2           21.07600021 W
PLW12           0.32931000 W

F2 - Processing parameters
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WDW                     EM
SSB          0
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PC                1.40
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HPLC

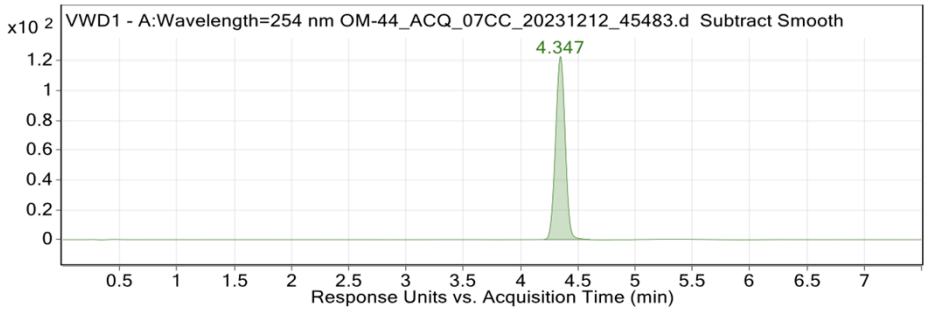


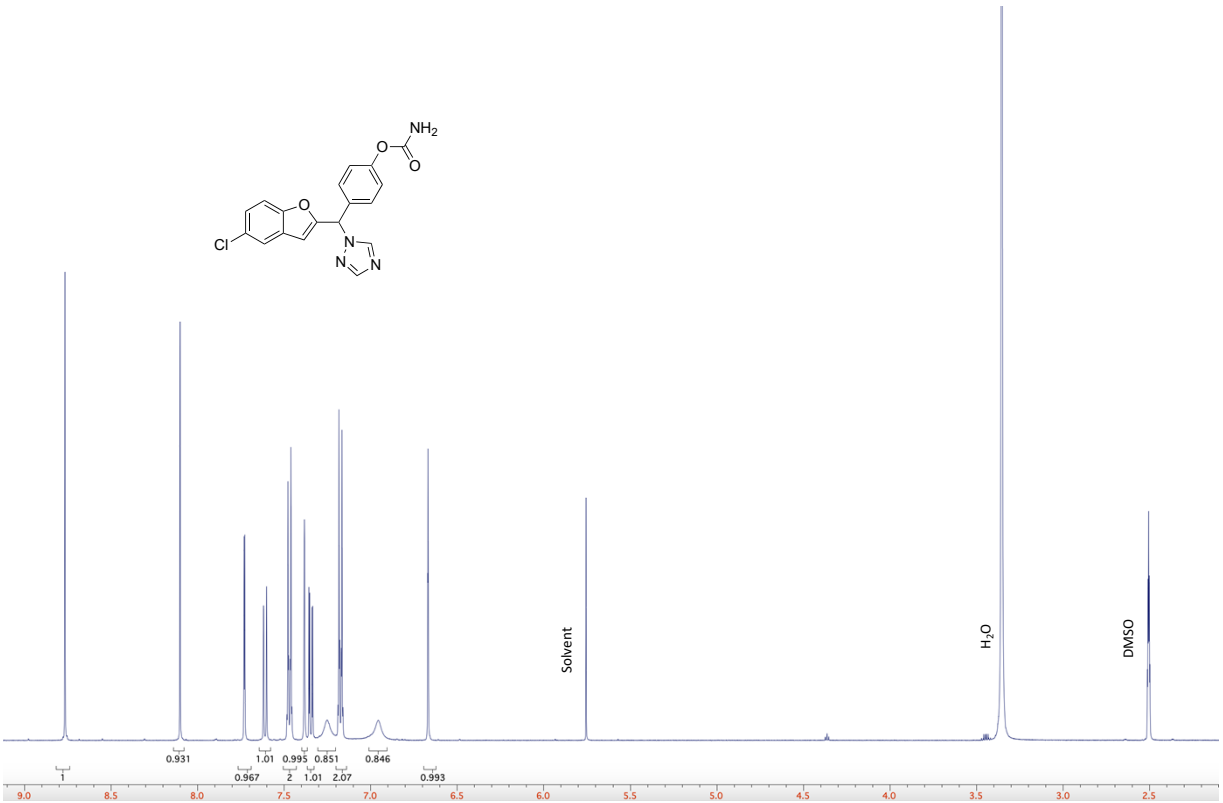
Figure: Base peak or HPLC chromatogram (indicated in left hand corner)

User Chromatogram Peak List

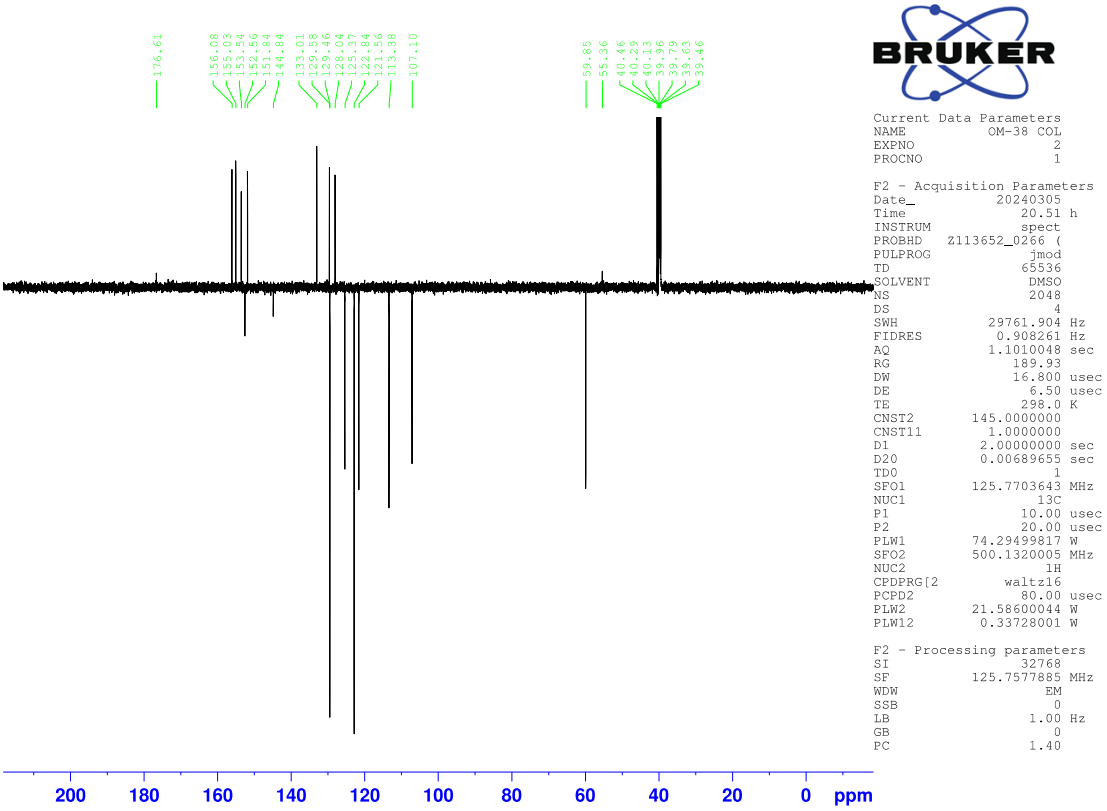
RT (min)	Area	Area %	Area Sum (%)	Symmetry	Width (min)
4.35	722.42	100.00	100.00	1.03	0.402

Compound **8b**

^{1}H NMR (DMSO-d_6)



^{13}C NMR ($CDCl_3$)



HPLC

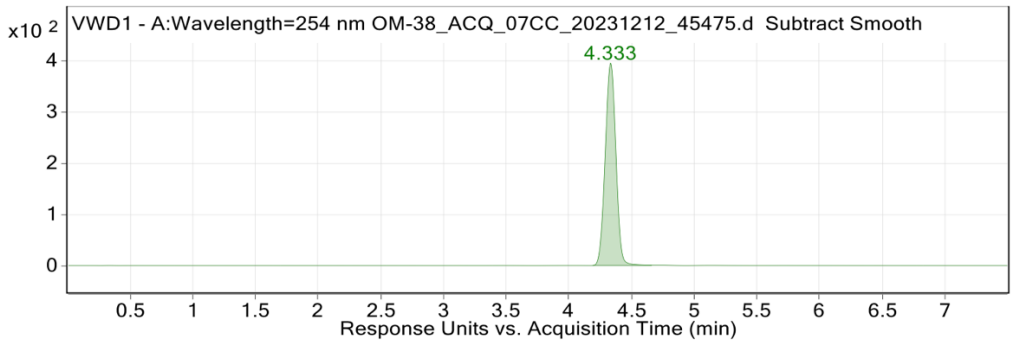


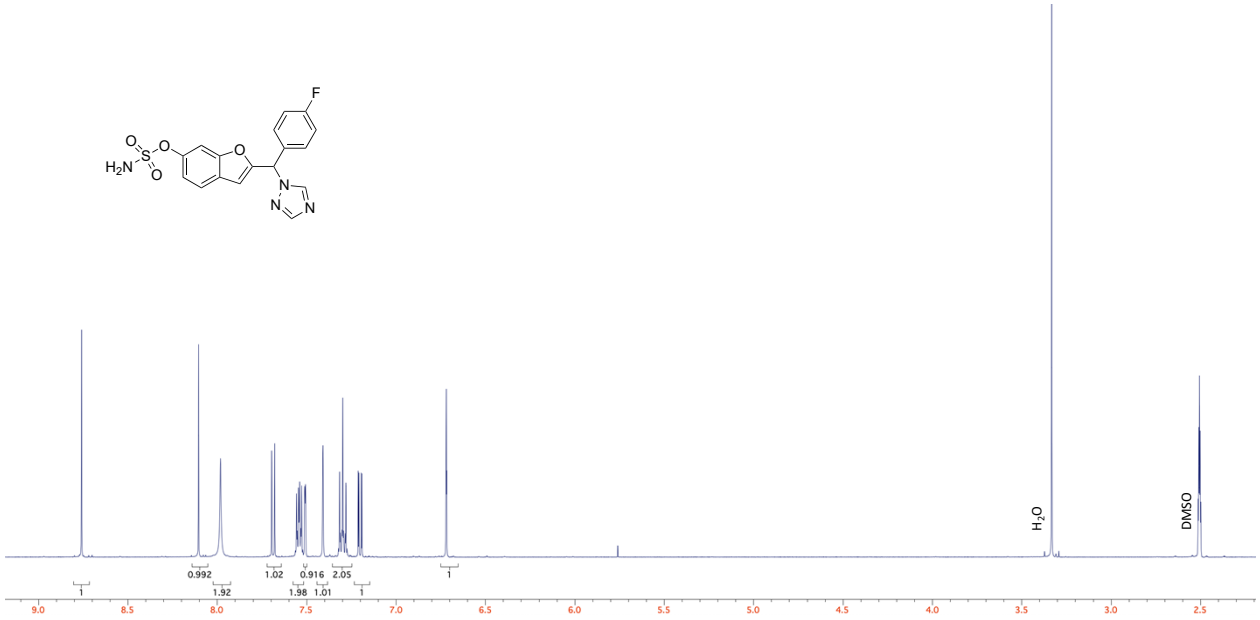
Figure: Base peak or HPLC chromatogram (indicated in left hand corner)

User Chromatogram Peak List

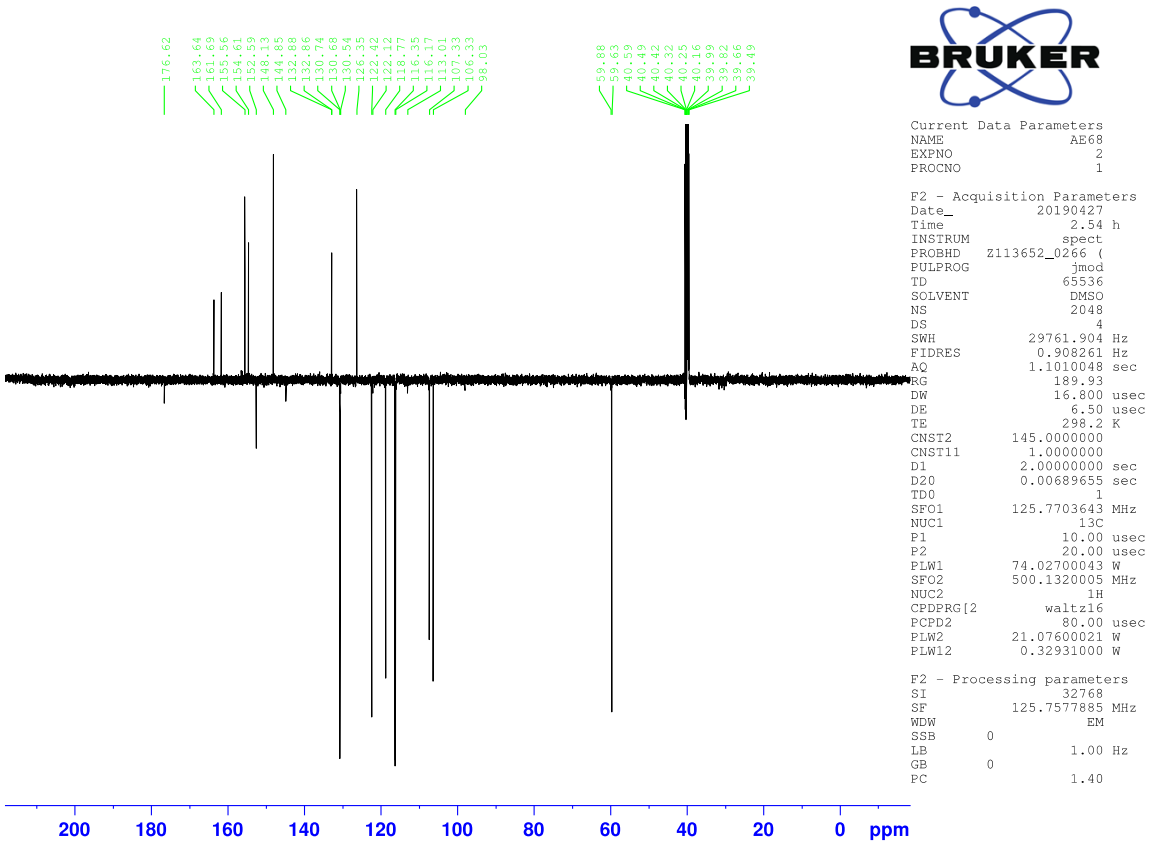
RT (min)	Area	Area %	Area Sum (%)	Symmetry	Width (min)
4.33	2354.83	100.00	100.00	1.02	0.467

Compound **9**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



BRUKER

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EXPNO                    2
PROCNO                   1

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SOLVENT             DMSO
NS                  2048
DS                     4
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FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                189.93
DW                16.800 usec
DE                 6.50 usec
TE                298.2 K
CNST2         145.0000000
CNST11          1.0000000
D1            2.00000000 sec
D20           0.00689655 sec
TD0                    1
SFO1          125.7703643 MHz
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1          74.02700043 W
SFO2          500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2          21.07600021 W
PLW12          0.32931000 W

F2 - Processing parameters
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WDW                    EM
SSB       0
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GB        0
PC                 1.40
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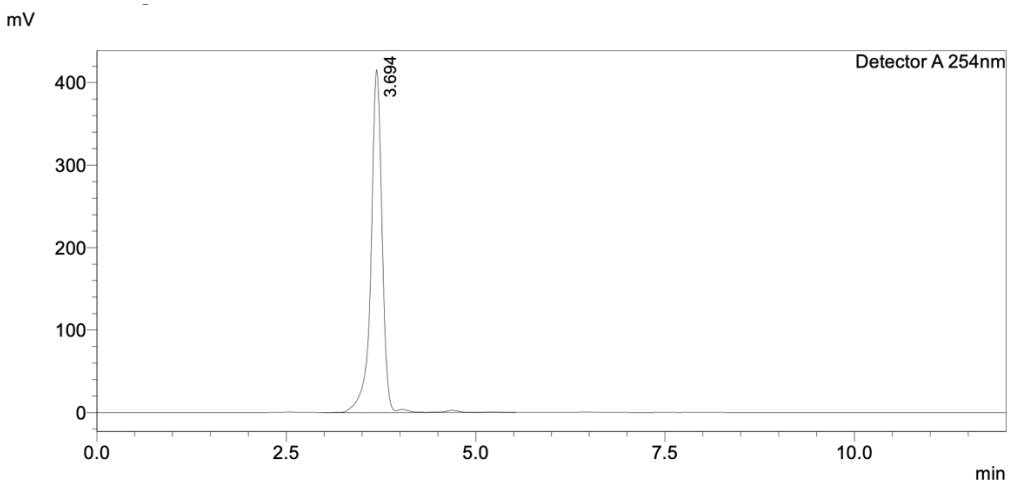
HPLC



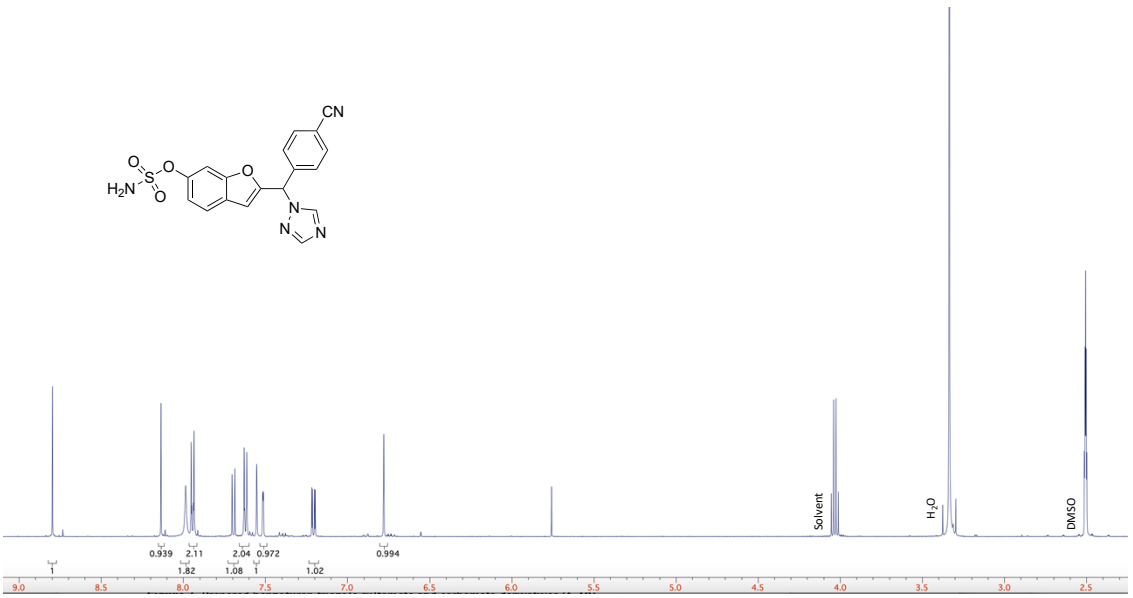
<Peak Table>

Detector A 254nm

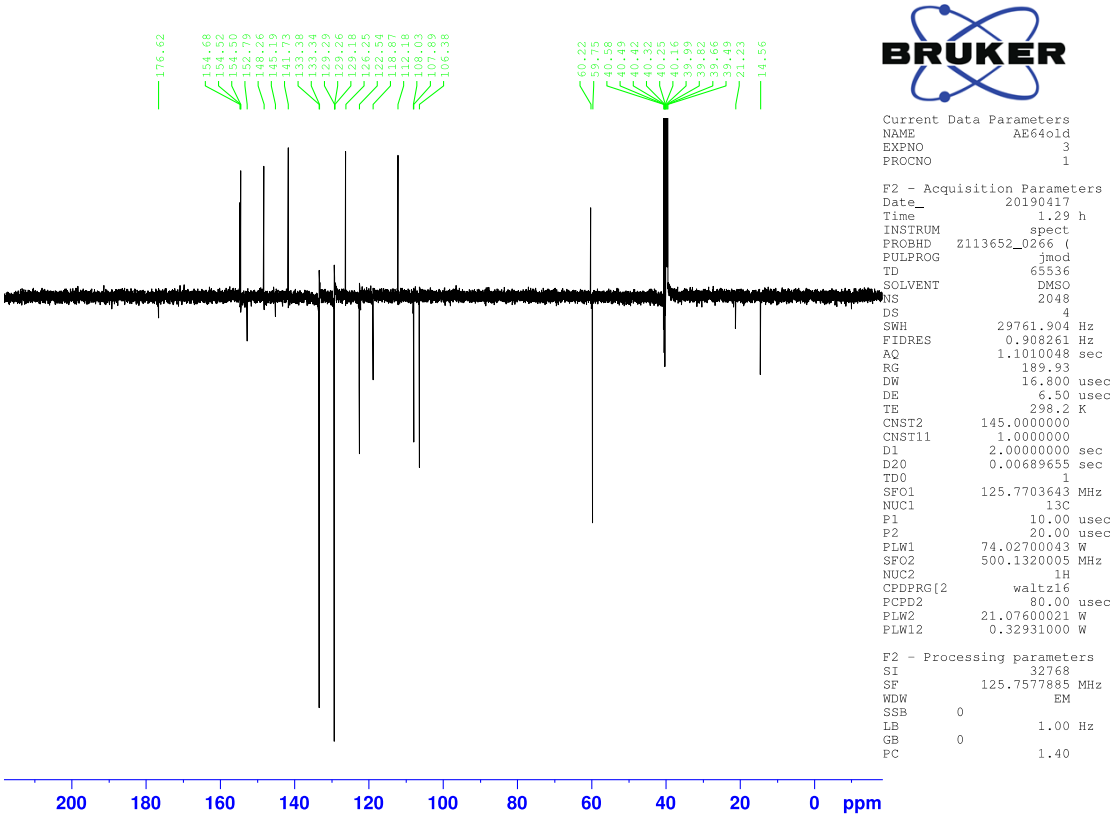
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	3.694	4250048	415523	100.000	100.000
Total		4250048	415523		100.000

Compound **10a**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



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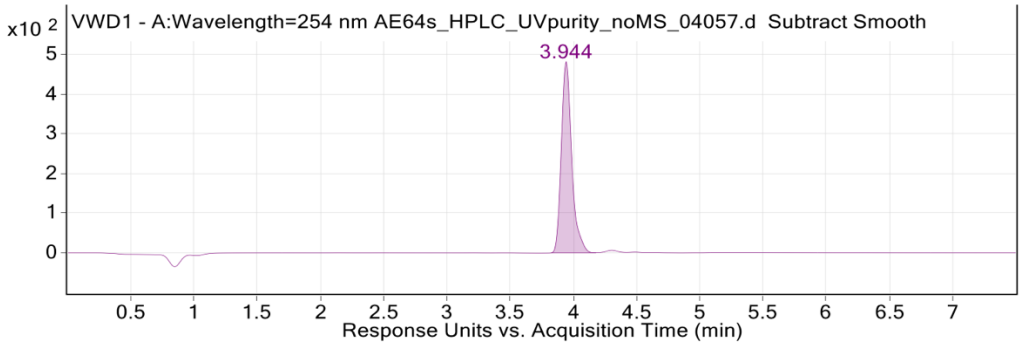


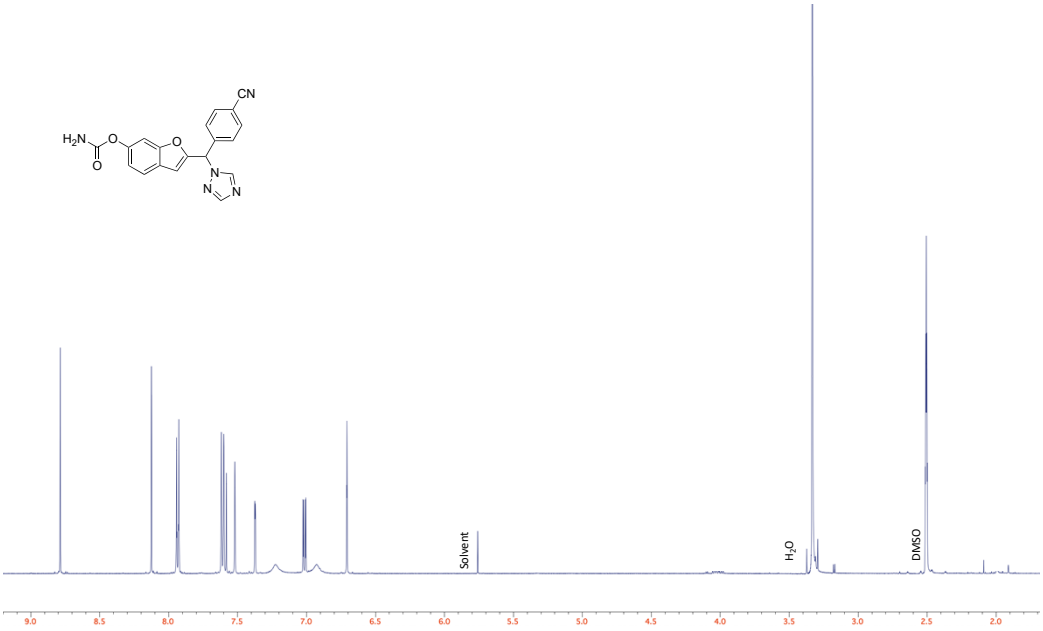
Figure: Base peak or HPLC chromatogram (indicated in left hand corner)

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Symmetry	Width (min)
3.94	2777.07	100.00	100.00	1.43	0.352

Compound **10b**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)

HPLC

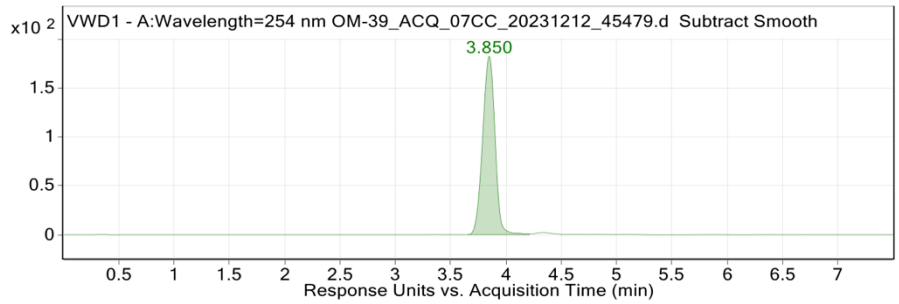


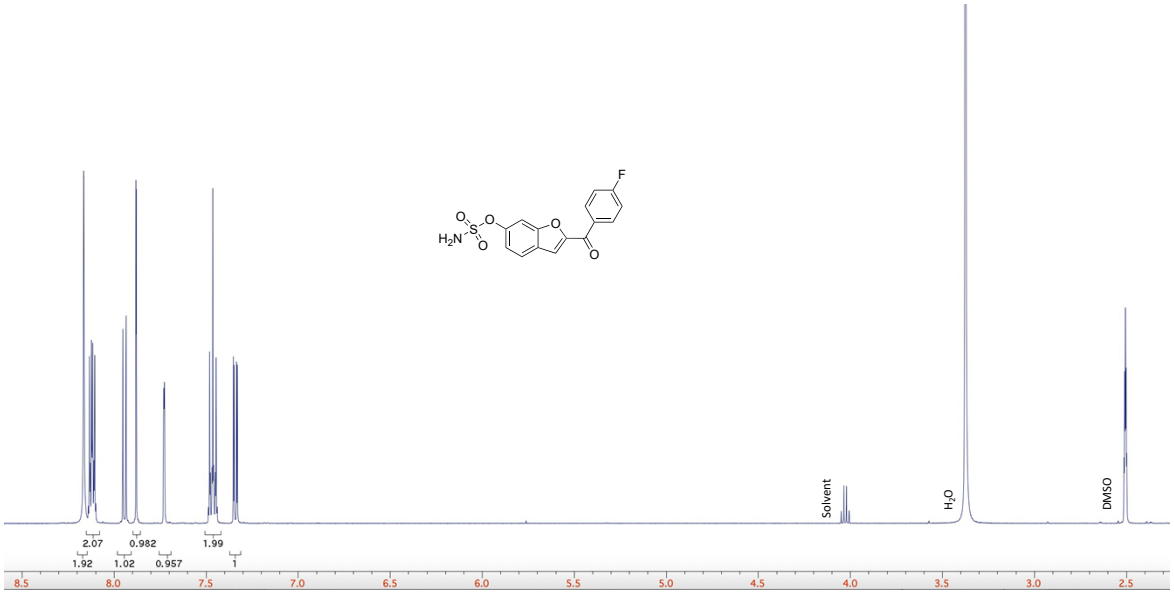
Figure: Base peak or HPLC chromatogram (indicated in left hand corner)

User Chromatogram Peak List

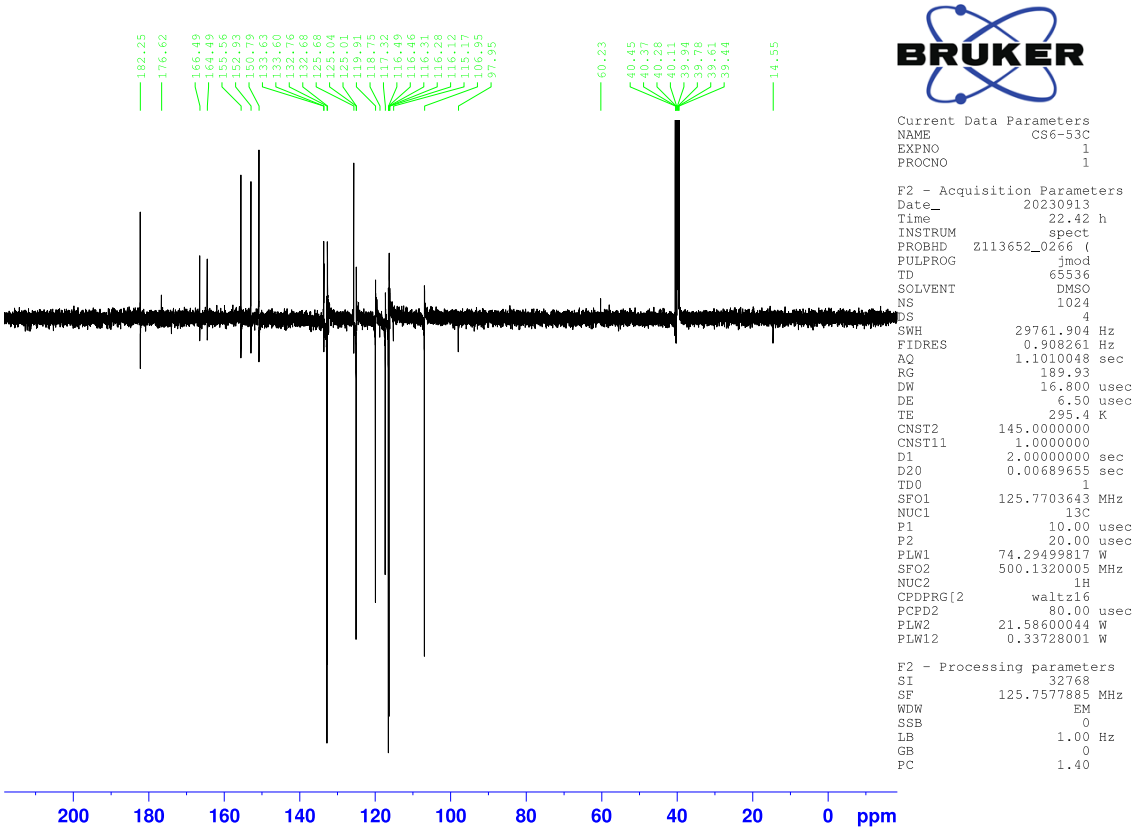
RT (min)	Area	Area %	Area Sum (%)	Symmetry	Width (min)
3.85	1427.25	100.00	100.00	0.85	0.553

Compound **18a**

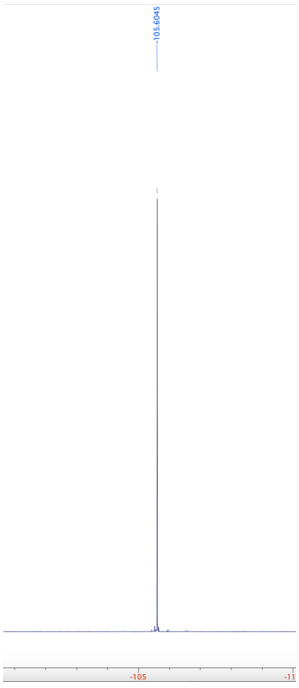
^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)

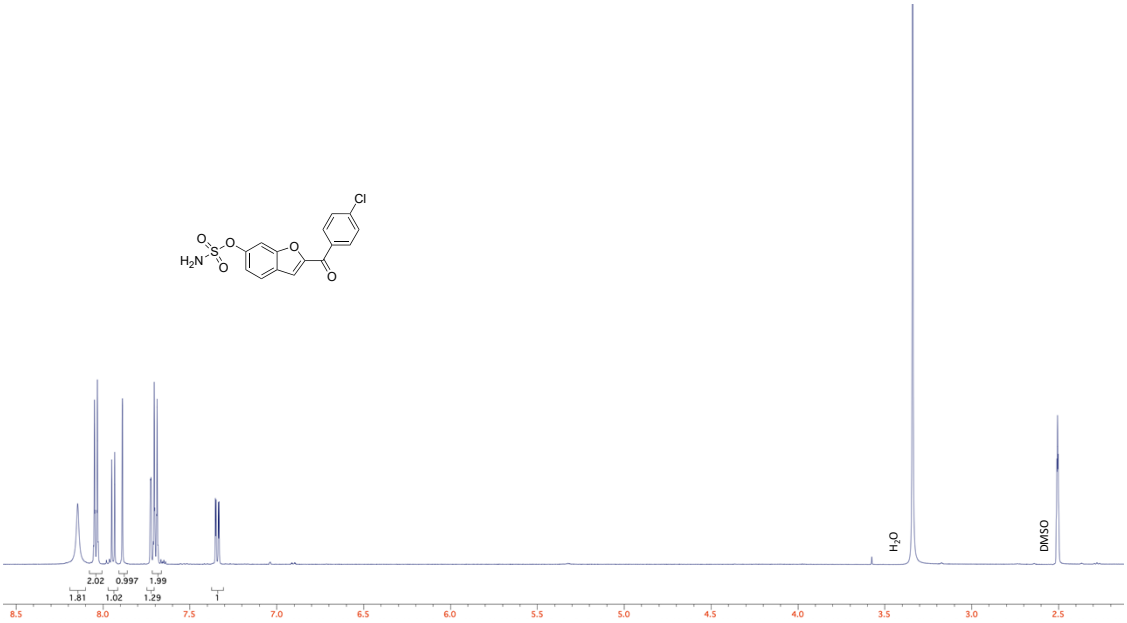


^{19}F NMR

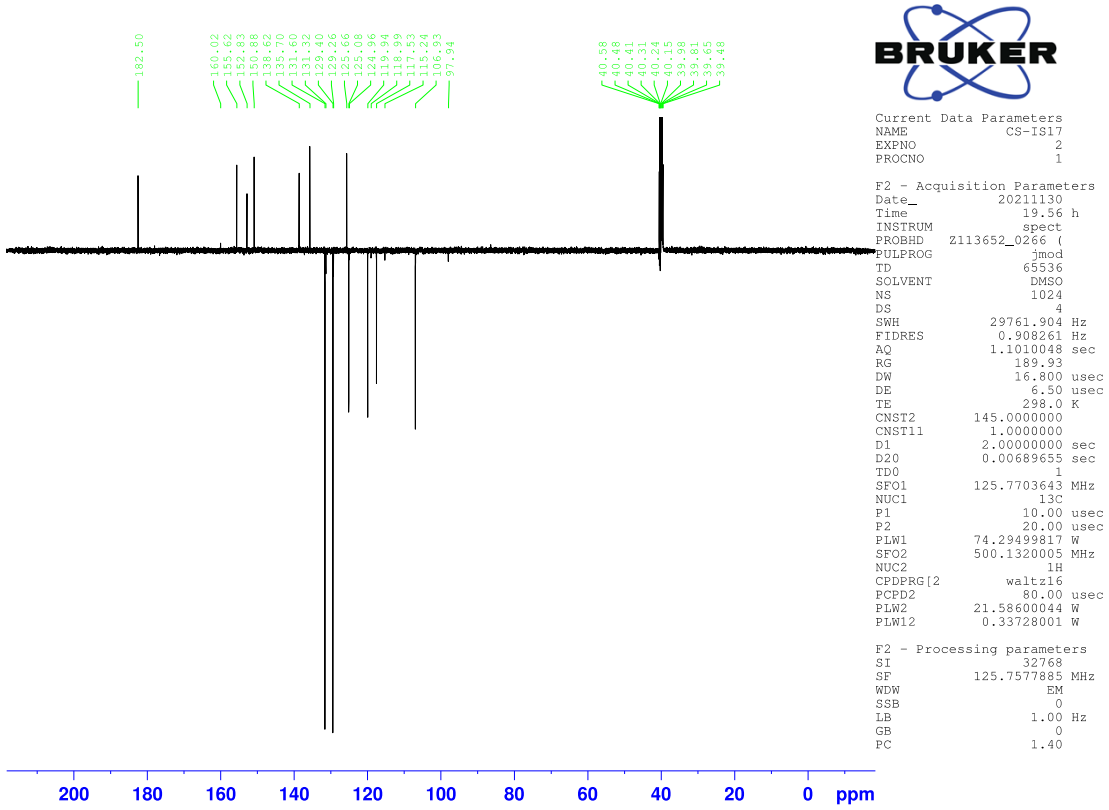


Compound **18b**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



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FIDRES            0.908261 Hz
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DW                  16.800 usec
DE                   6.50 usec
TE                  298.0 K
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CNST11            1.0000000
D1              2.00000000 sec
D20             0.00689655 sec
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NUC1                    13C
P1                  10.00 usec
P2                  20.00 usec
PLW1           74.29499817 W
SFO2           500.1320005 MHz
NUC2                    1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2           21.58600044 W
PLW12           0.33728001 W

F2 - Processing parameters
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WDW                      EM
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LB                     1.00 Hz
GB                        0
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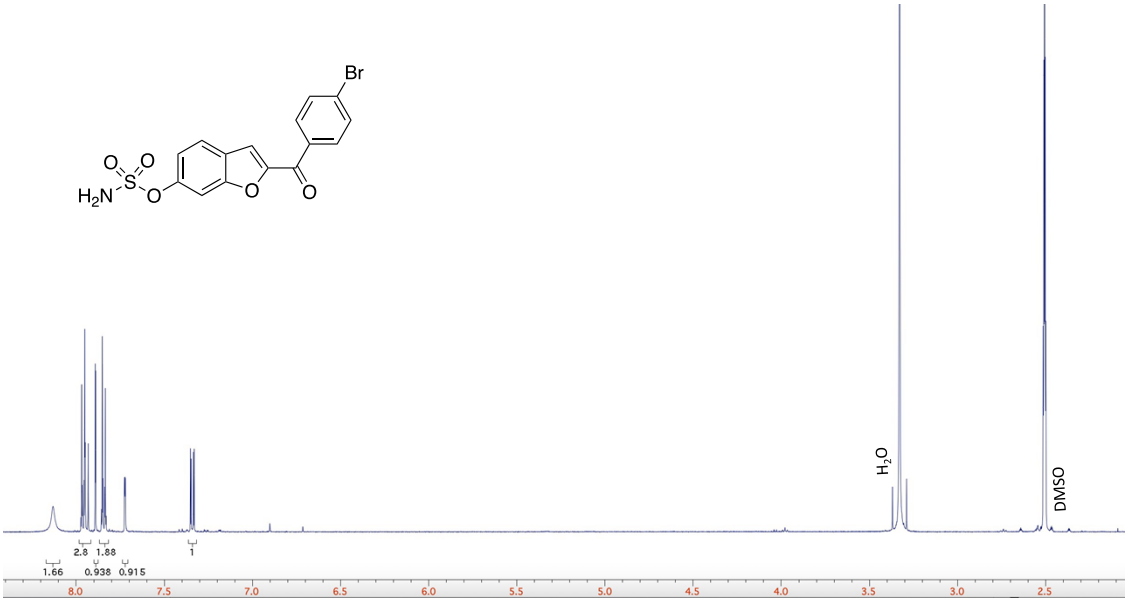
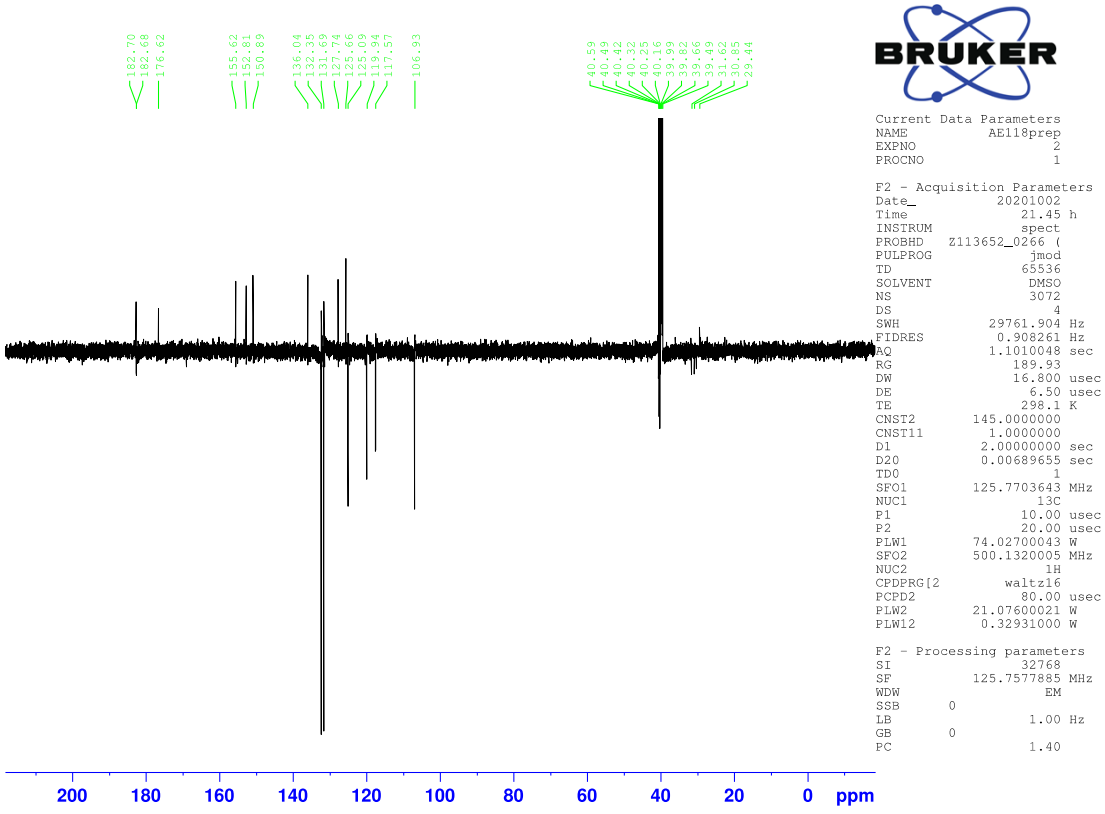
Compound **18c**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



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SOLVENT                     DMSO
NS                           3072
DS                              4
SWH                   29761.904 Hz
FIDRES                 0.908261 Hz
AQ                    1.1010048 sec
RG                       189.93
DW                       16.800 usec
DE                        6.50 usec
TE                       298.1 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                            1
SFO1                 125.7703643 MHz
NUC1                         13C
P1                        10.00 usec
P2                        20.00 usec
PLW1                 74.02700043 W
SFO2                 500.1320005 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2                 21.07600021 W
PLW12                 0.32931000 W

F2 - Processing parameters
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HPLC

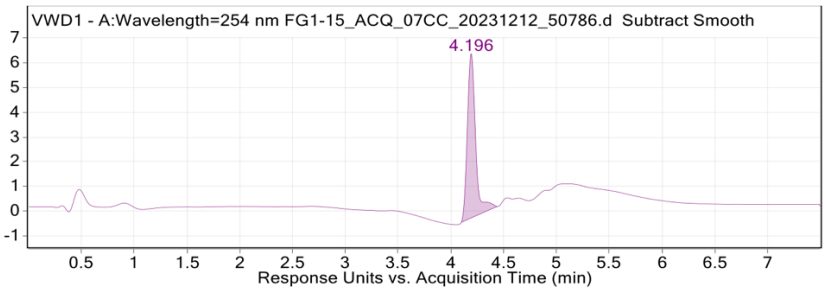


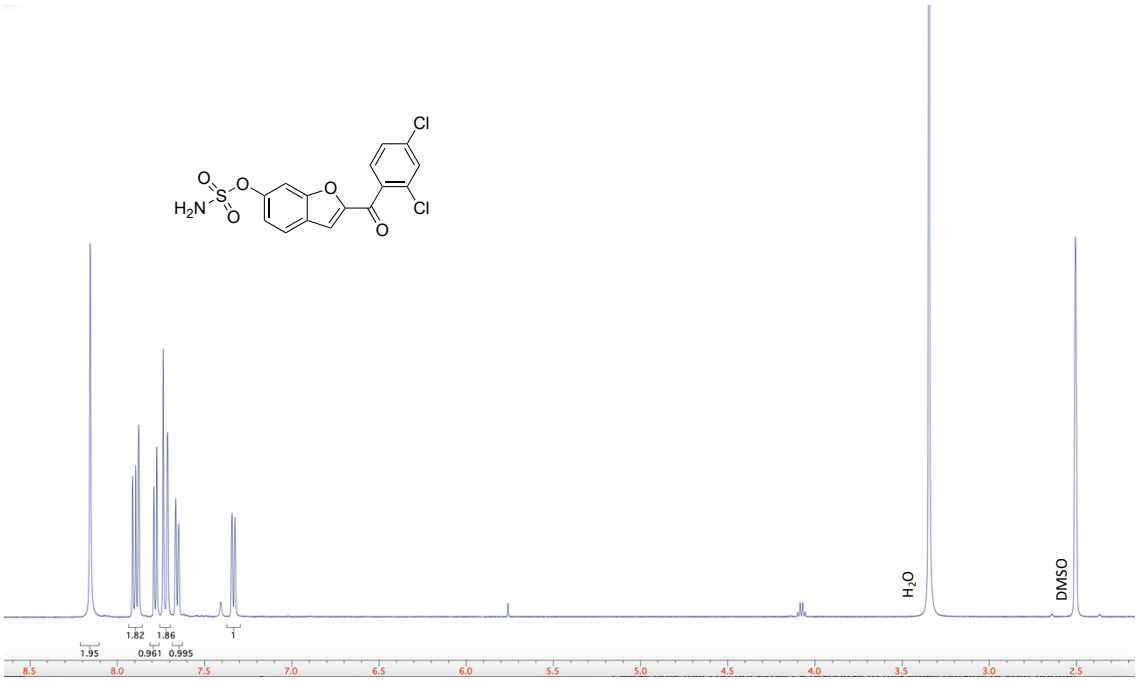
Figure: Base peak or HPLC chromatogram (indicated in left hand corner)

User Chromatogram Peak List

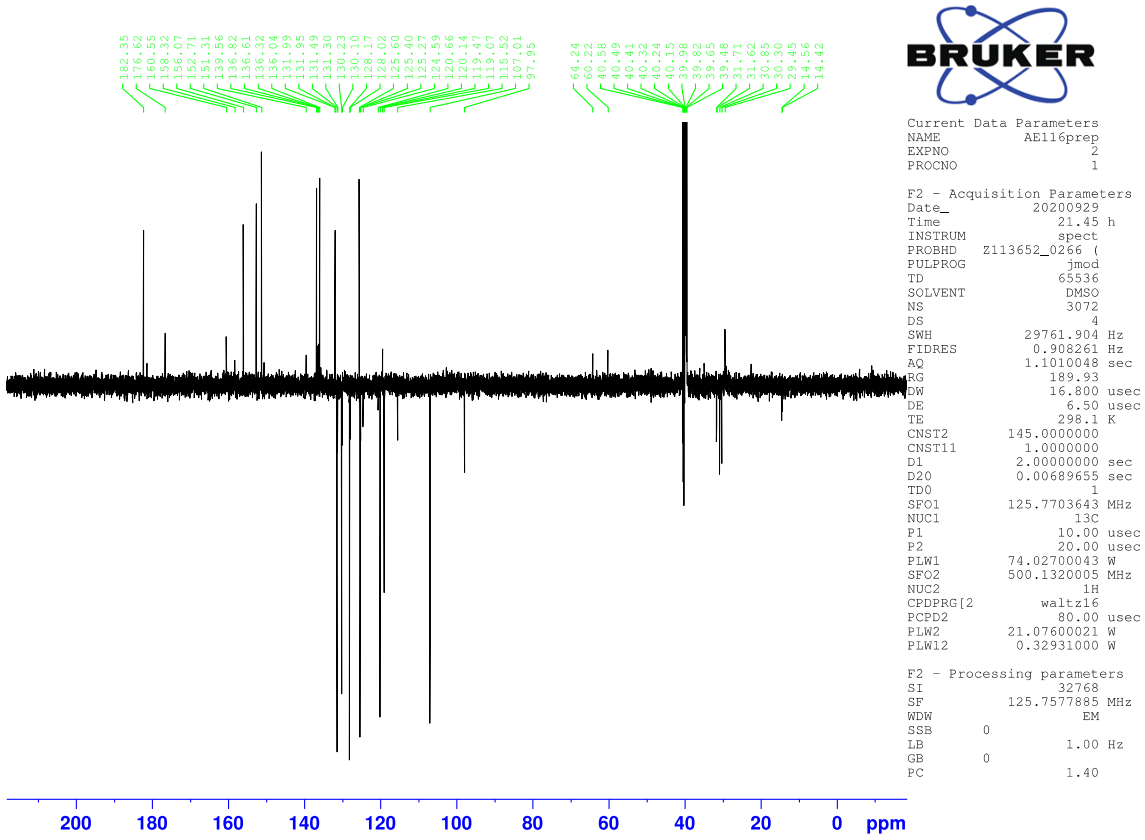
RT (min)	Area	Area %	Area Sum (%)	Symmetry	Width (min)
4.20	36.13	100.00	100.00	1.35	0.338

Compound **18d**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



BRUKER

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PROCNO                  1

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TD                    65536
SOLVENT                DMSO
NS                     3072
DS                        4
SWH               29761.904 Hz
FIDRES             0.908261 Hz
AQ                1.1010048 sec
RG                   189.93
DW                   16.800 usec
DE                    6.50 usec
TE                  298.1 K
CNST2           145.0000000
CNST11            1.0000000
D1                2.00000000 sec
D20               0.00689655 sec
TD0                       1
SFO1           125.7703643 MHz
NUC1                    13C
P1                   10.00 usec
P2                   20.00 usec
PLW1           74.02700043 W
SFO2           500.1320005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                80.00 usec
PLW2           21.07600021 W
PLW12           0.32931000 W

F2 - Processing parameters
SI                    32768
SF             125.7577885 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
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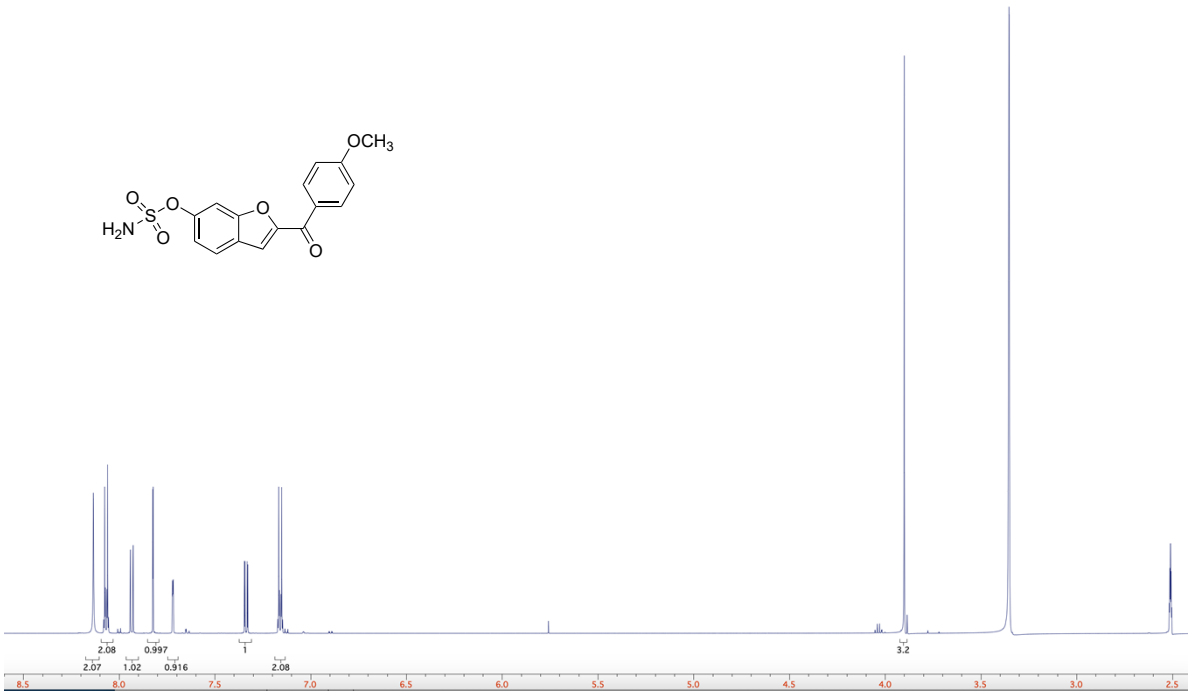
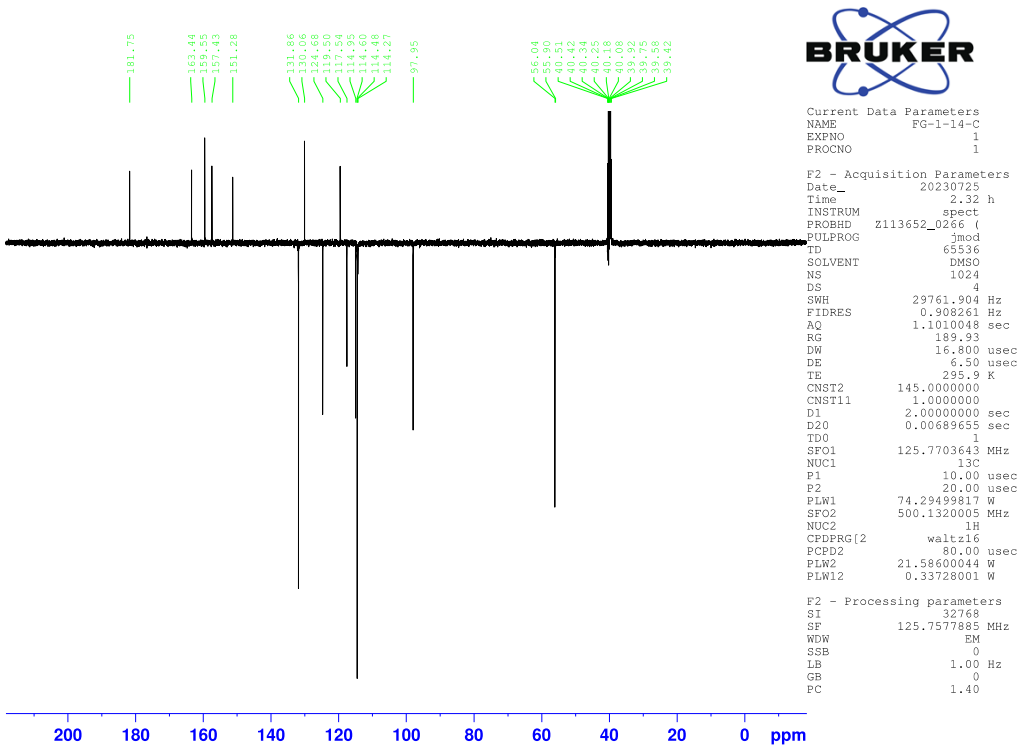
Compound **18e**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



HPLC

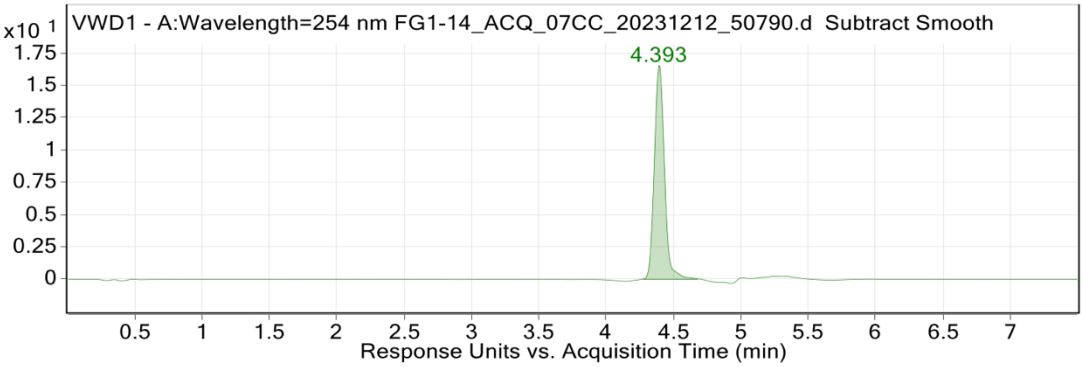


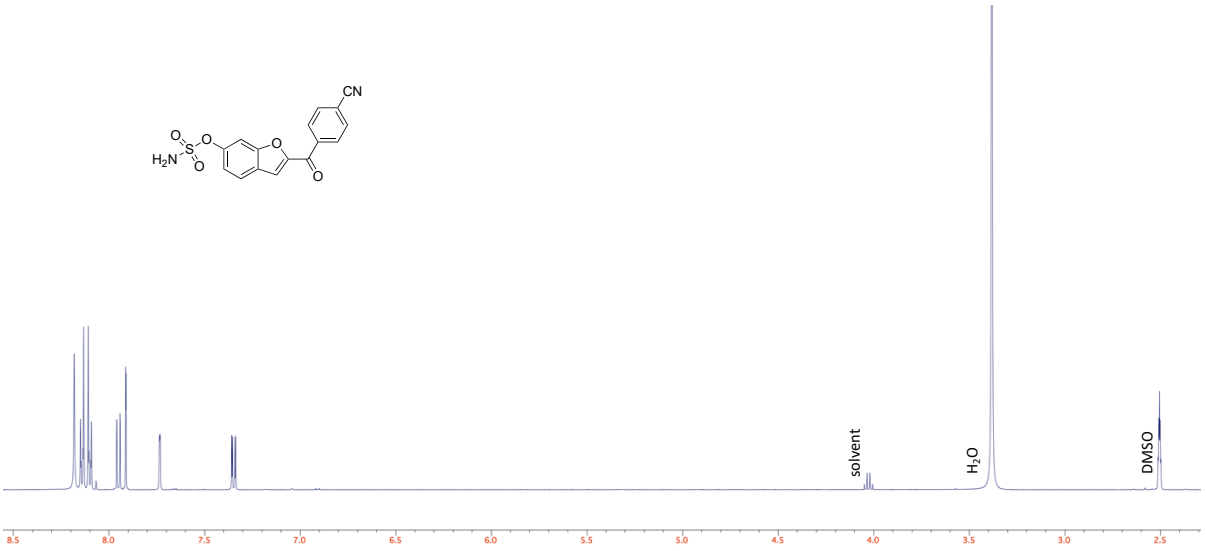
Figure: Base peak or HPLC chromatogram (indicated in left hand corner)

User Chromatogram Peak List

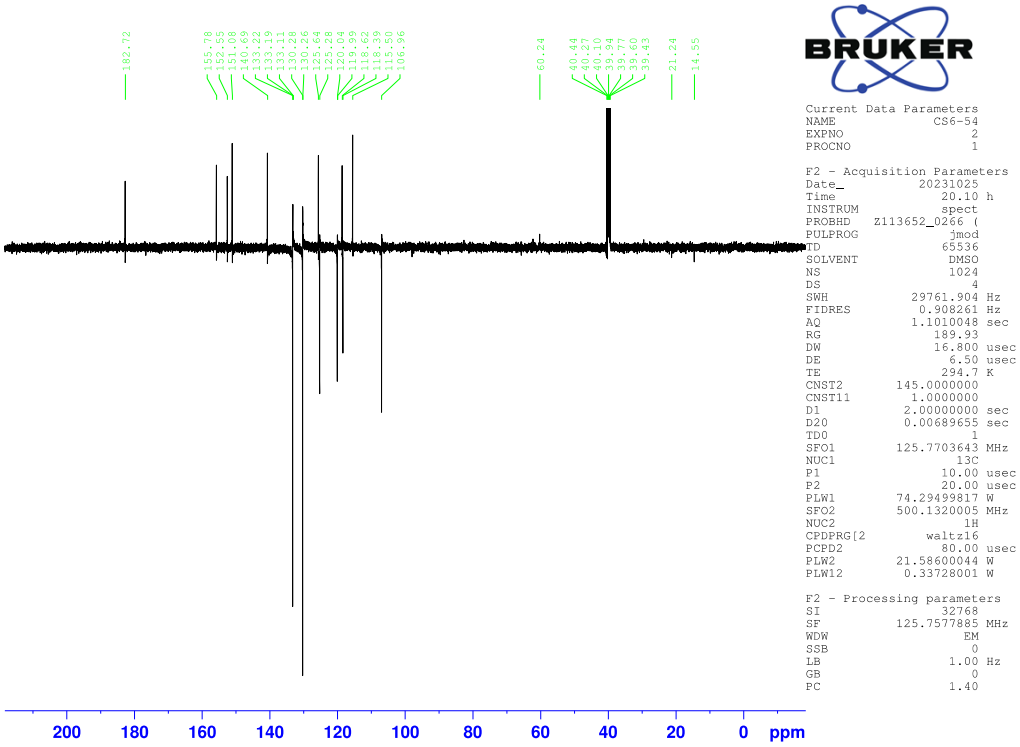
RT (min)	Area	Area %	Area Sum (%)	Symmetry	Width (min)
4.39	87.25	100.00	100.00	1.18	0.400

Compound **18f**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



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PROCNO                     1

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PULPROG               jmod
TD                   65536
SOLVENT               DMSO
NS                    1024
DS                       4
SWH              29761.904 Hz
FIDRES           0.908261 Hz
AQ               1.1010048 sec
RG                  189.93
DW                  16.800 usec
DE                   6.50 usec
TE                  294.7 K
CNST2           145.0000000
CNST11            1.0000000
D1                2.00000000 sec
D20               0.00689655 sec
TD0                       1
SFO1            125.7703643 MHz
NUC1                    13C
P1                  10.00 usec
P2                  20.00 usec
PLW1            74.29499817 W
SFO2            500.1320005 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2               80.00 usec
PLW2            21.58600044 W
PLW12            0.33728001 W

F2 - Processing parameters
SI                    32768
SF              125.7577885 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

HPLC

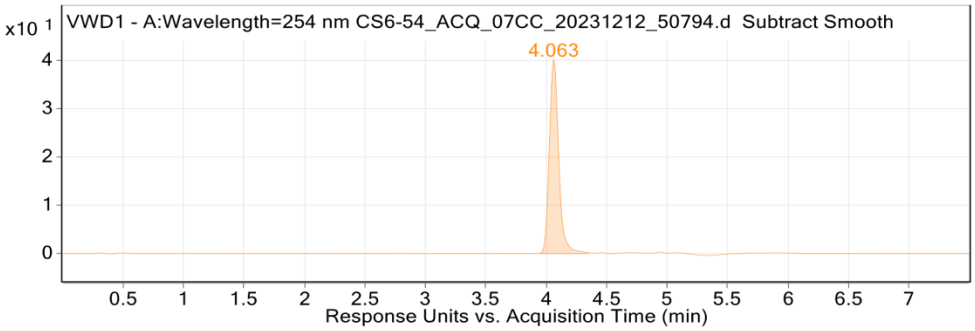


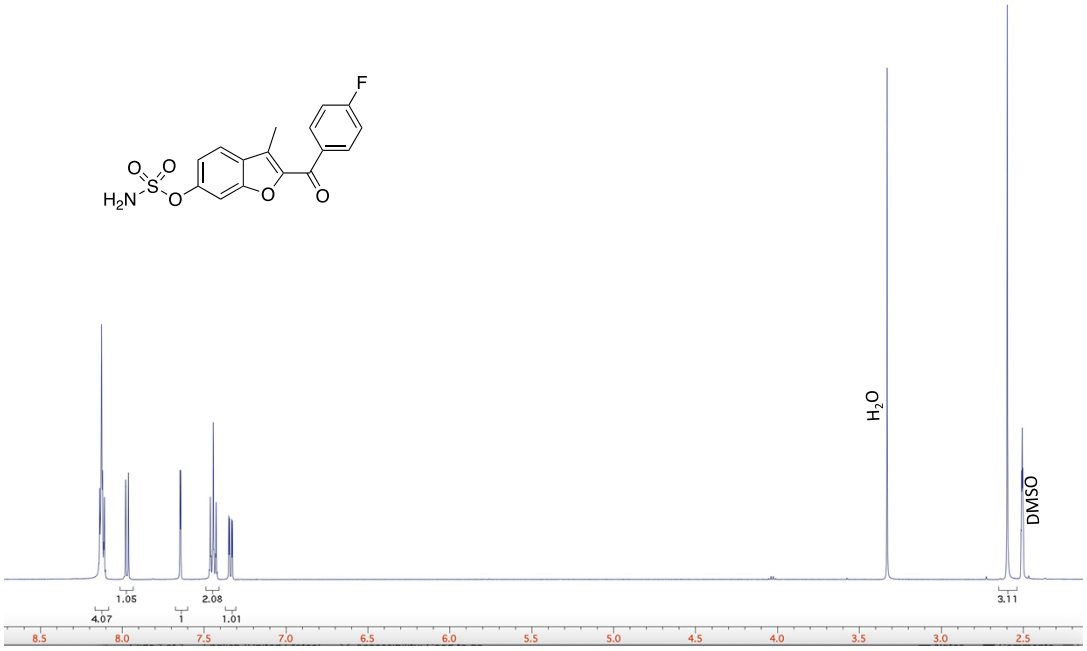
Figure: Base peak or HPLC chromatogram (indicated in left hand corner)

User Chromatogram Peak List

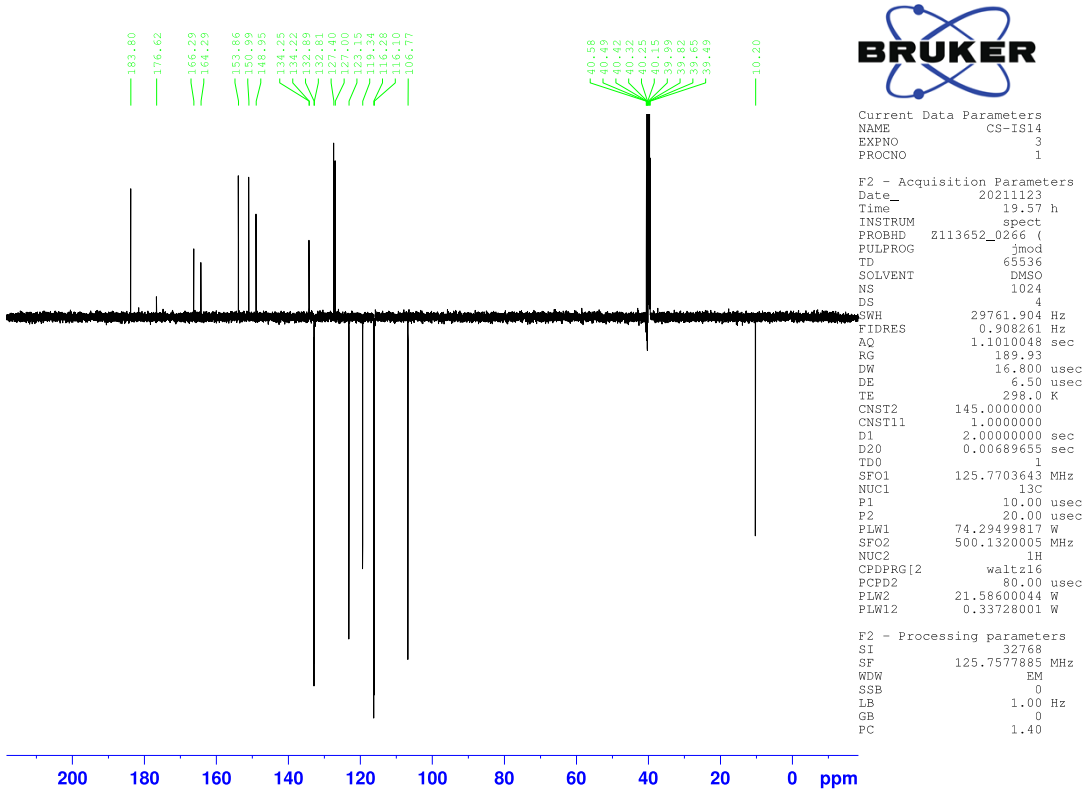
RT (min)	Area	Area %	Area Sum (%)	Symmetry	Width (min)
4.06	217.89	100.00	100.00	1.23	0.407

Compound **19a**

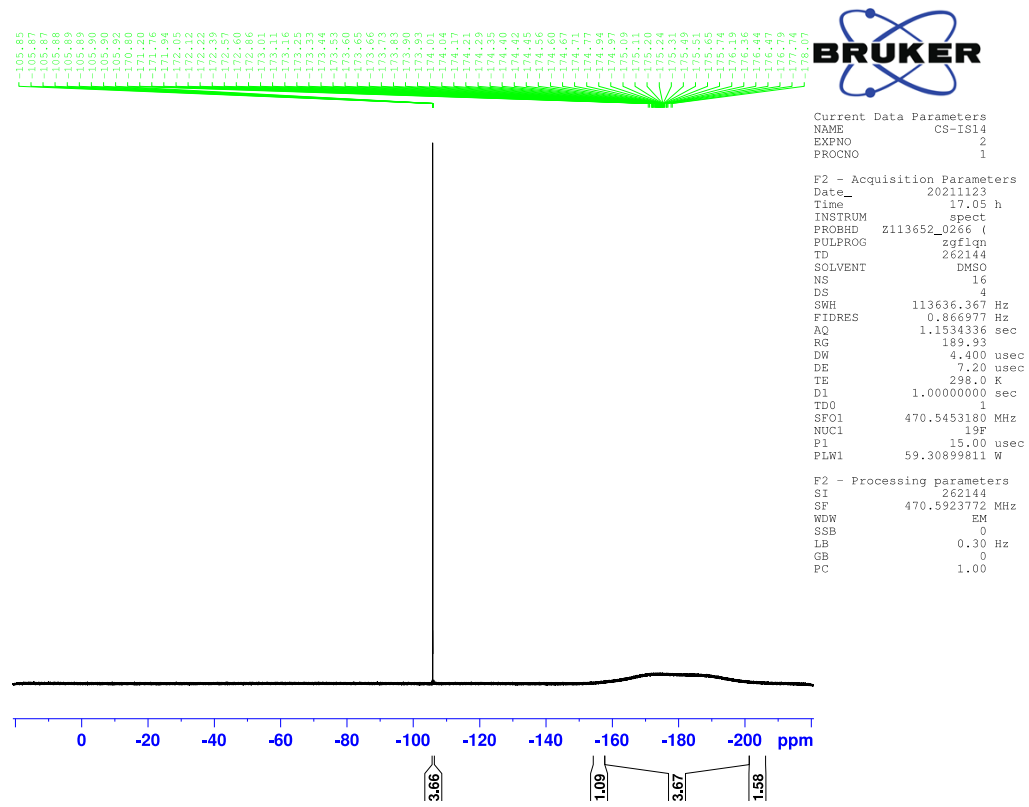
^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)

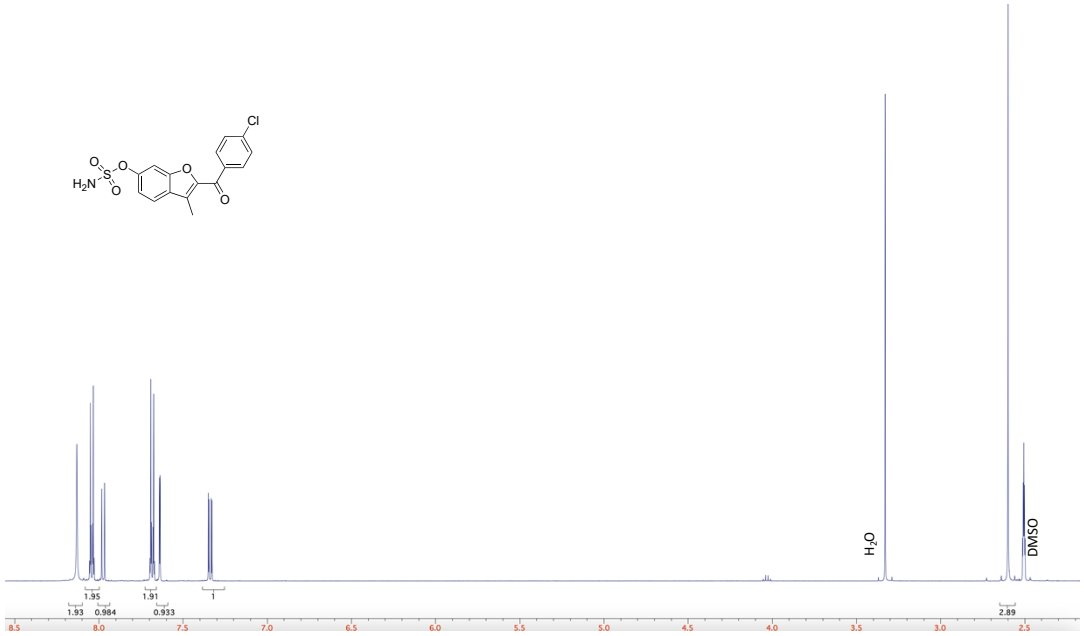


^{19}F NMR (DMSO-d_6)

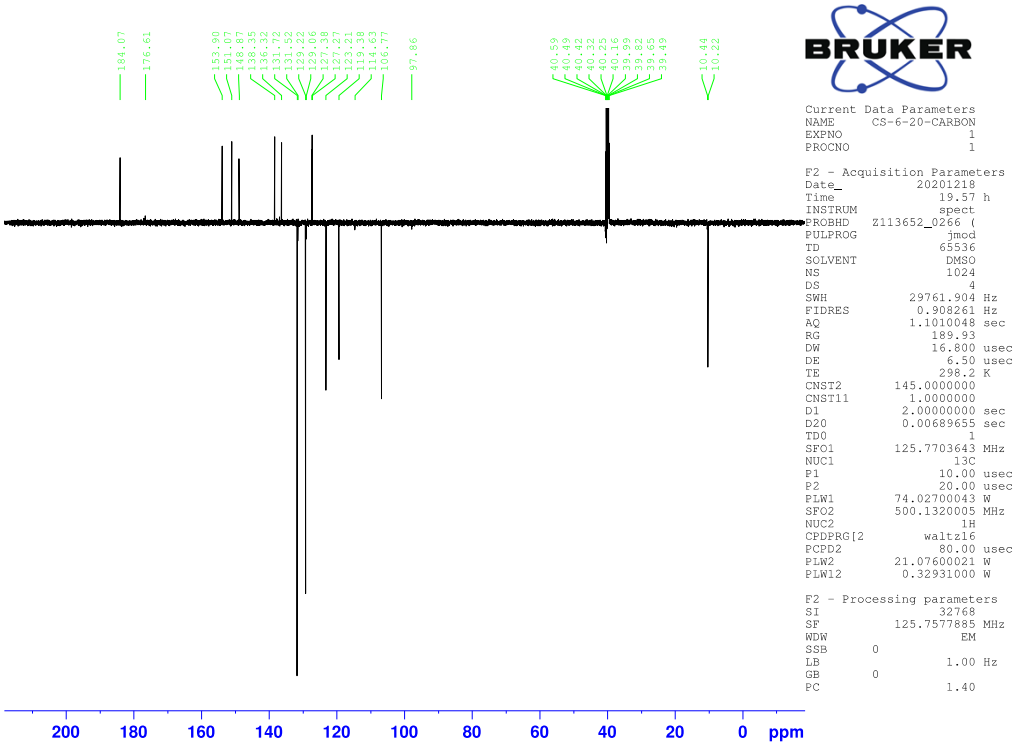


Compound **19b**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)

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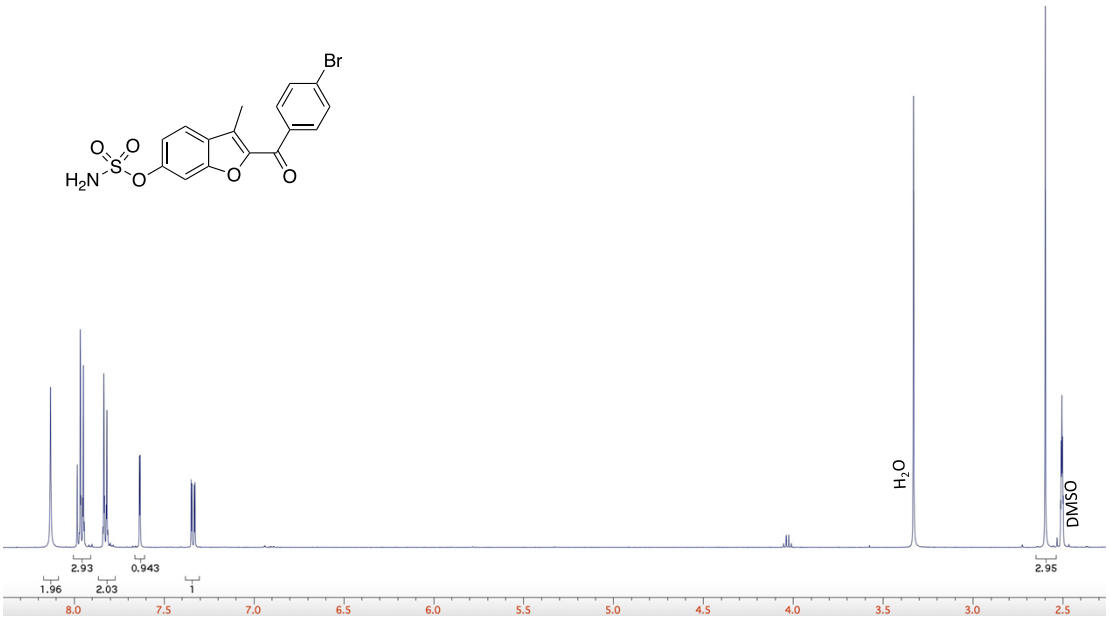
Current Data Parameters
NAME      CS-6-20-CARBON
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201218
Time              19.57 h
INSTRUM             spect
PROBHD   Z113652_0266 (
PULPROG             jmod
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                189.93
DW                16.800 usec
DE                 6.50 usec
TE                298.2 K
CNST2        145.0000000
CNST11         1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         74.02700043 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         21.07600021 W
PLW12         0.32931000 W

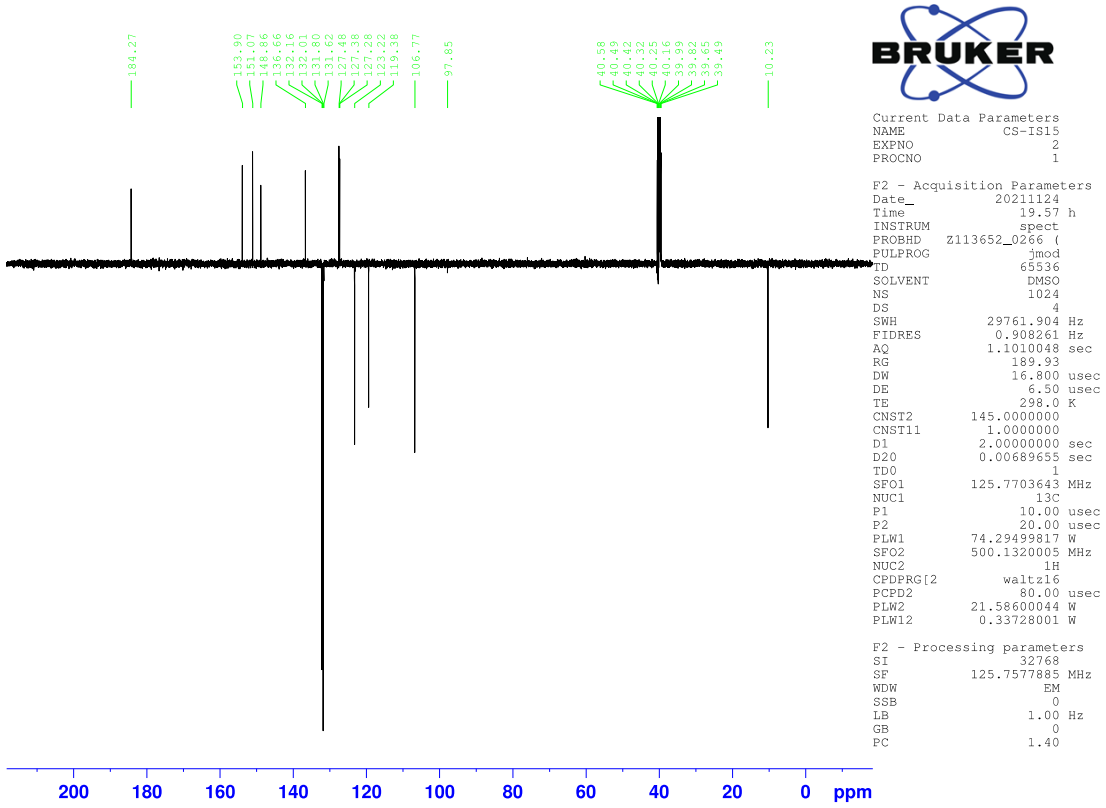
F2 - Processing parameters
SI                 32768
SF           125.7577885 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Compound **19c**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



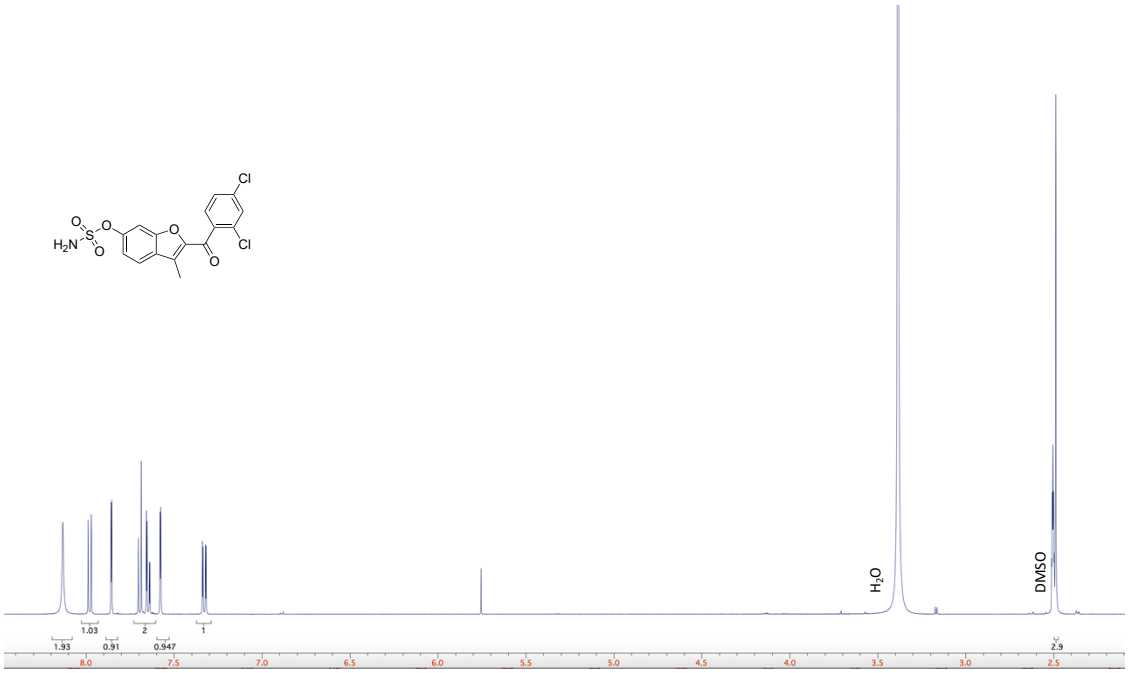

```
Current Data Parameters
NAME                  CS-IS15
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20211124
Time                   19.57 h
INSTRUM                spect
PROBHD    Z113652_0266 (
PULPROG                 jmod
TD                     65536
SOLVENT                 DMSO
NS                      1024
DS                         4
SWH                29761.904 Hz
FIDRES             0.908261 Hz
AQ                 1.1010048 sec
RG                    189.93
DW                    16.800 usec
DE                     6.50 usec
TE                    298.0 K
CNST2             145.0000000
CNST11              1.0000000
D1                  2.00000000 sec
D20                 0.00689655 sec
TD0                         1
SFO1              125.7703643 MHz
NUC1                      13C
P1                    10.00 usec
P2                    20.00 usec
PLW1              74.29499817 W
SFO2              500.1320005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 80.00 usec
PLW2              21.58600044 W
PLW12              0.33728001 W

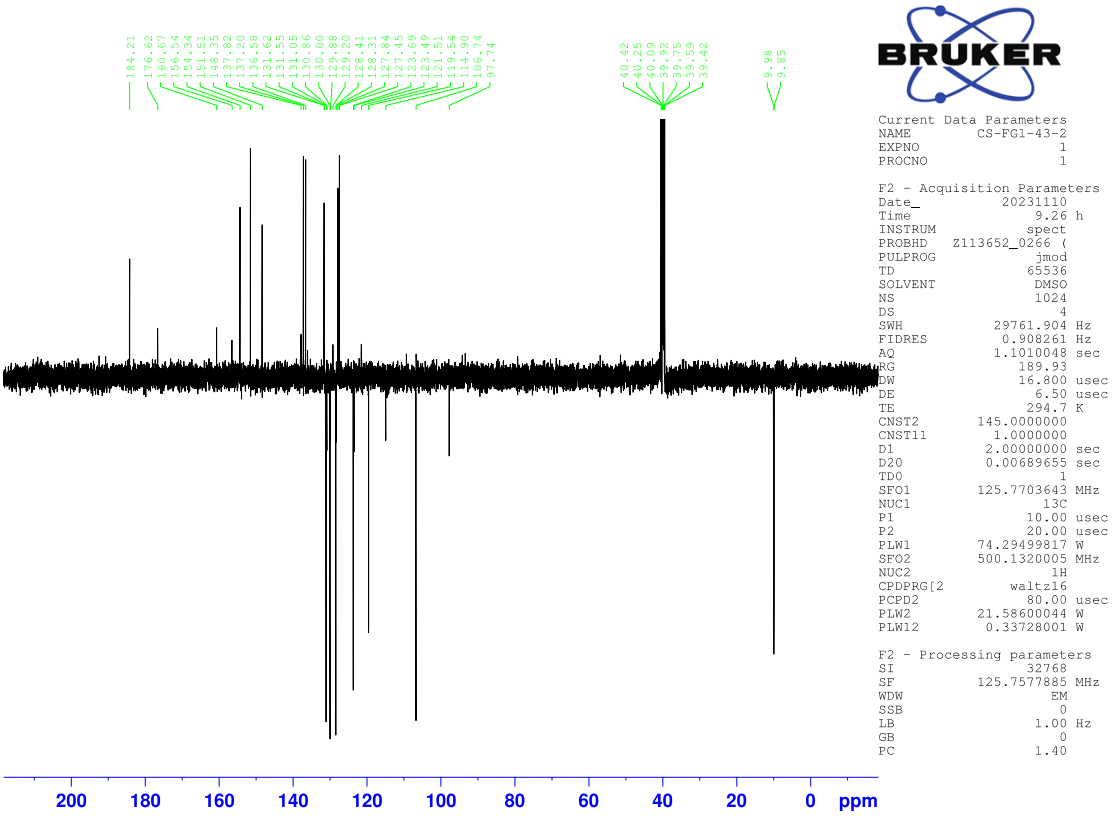
F2 - Processing parameters
SI                        32768
SF                125.7577885 MHz
WDW                        EM
SSB                         0
LB                     1.00 Hz
GB                          0
PC                     1.40
```

Compound **19d**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



BRUKER

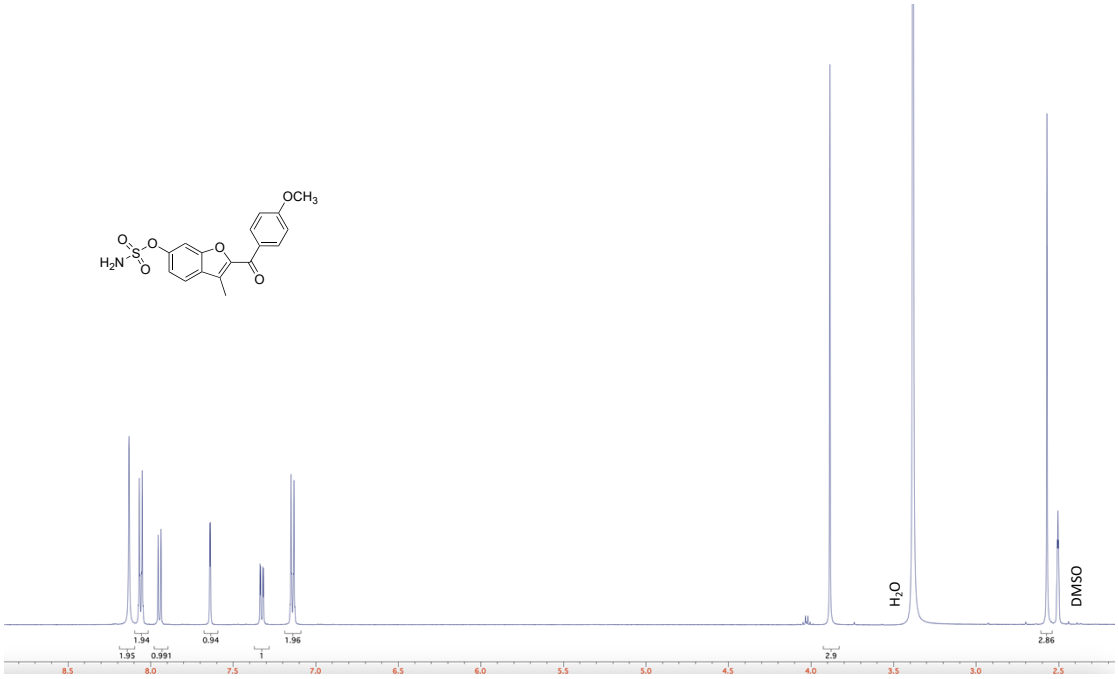
```
Current Data Parameters
NAME         CS-FG1-43-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231110
Time                9.26 h
INSTRUM            spect
PROBHD   Z113652_0266 (
PULPROG             jmod
TD                 65536
SOLVENT              DMSO
NS                   1024
DS                      4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                189.93
DW                16.800 usec
DE                 6.50 usec
TE                294.7 K
CNST2          145.0000000
CNST11           1.0000000
D1               2.00000000 sec
D20              0.00689655 sec
TD0                    1
SFO1           125.7703643 MHz
NUC1                  13C
P1                 10.00 usec
P2                 20.00 usec
PLW1           74.29499817 W
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2           21.58600044 W
PLW12           0.33728001 W

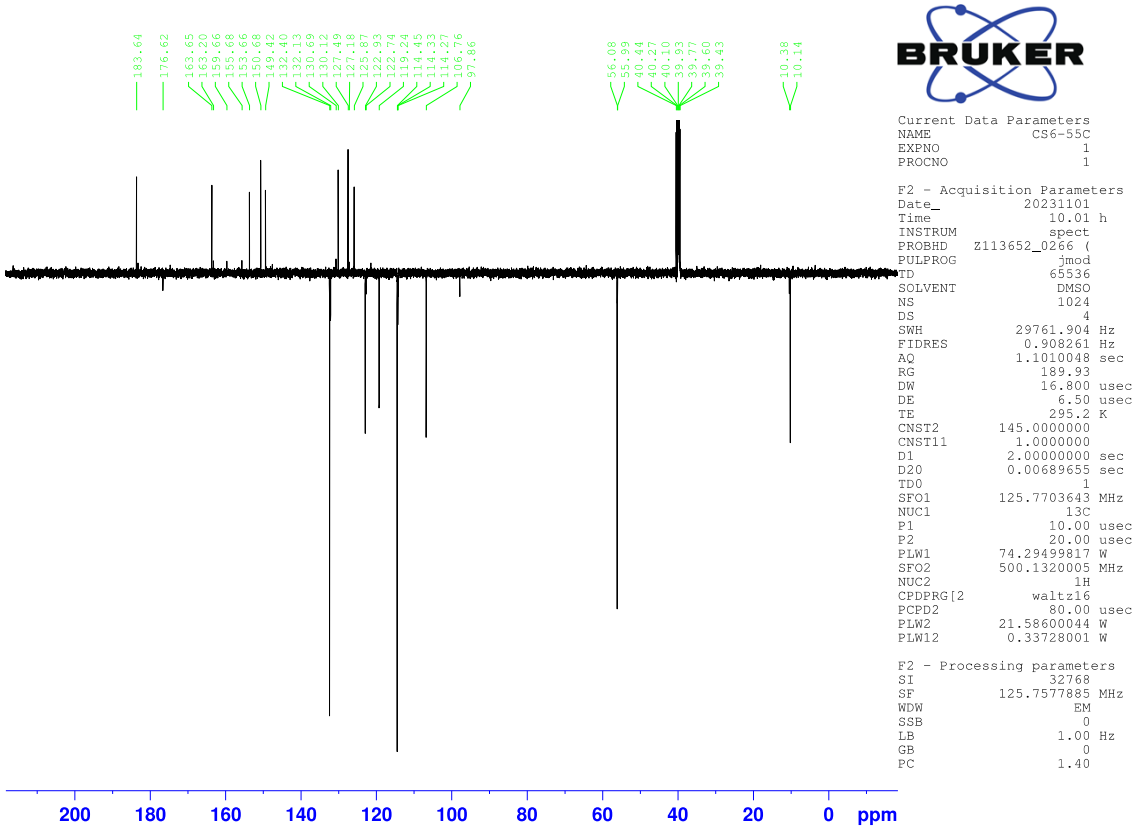
F2 - Processing parameters
SI                 32768
SF            125.7577885 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound **19e**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



BRUKER

```
Current Data Parameters
NAME                  CS6-55C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20231101
Time                 10.01 h
INSTRUM                spect
PROBHD   Z113652_0266 (
PULPROG                 jmod
TD                     65536
SOLVENT                DMSO
NS                      1024
DS                         4
SWH                29761.904 Hz
FIDRES              0.908261 Hz
AQ                 1.1010048 sec
RG                    189.93
DW                   16.800 usec
DE                    6.50 usec
TE                   295.2 K
CNST2             145.0000000
CNST11              1.0000000
D1                2.00000000 sec
D20               0.00689655 sec
TD0                        1
SFO1             125.7703643 MHz
NUC1                     13C
P1                    10.00 usec
P2                    20.00 usec
PLW1              74.29499817 W
SFO2             500.1320005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 80.00 usec
PLW2              21.58600044 W
PLW12              0.33728001 W

F2 - Processing parameters
SI                     32768
SF               125.7577885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

HPLC

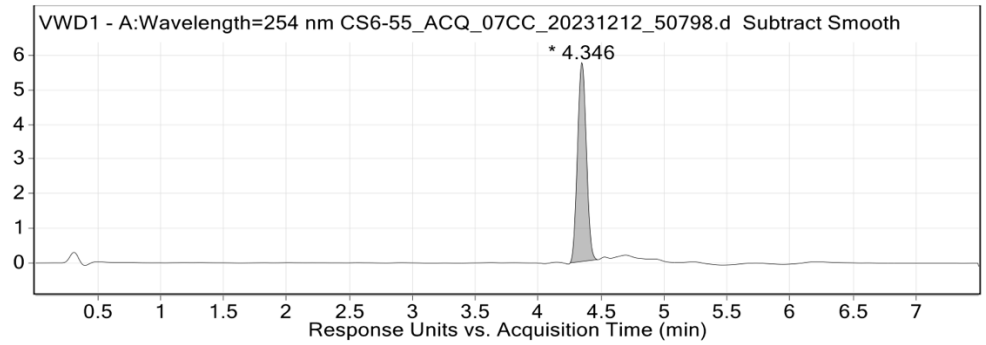


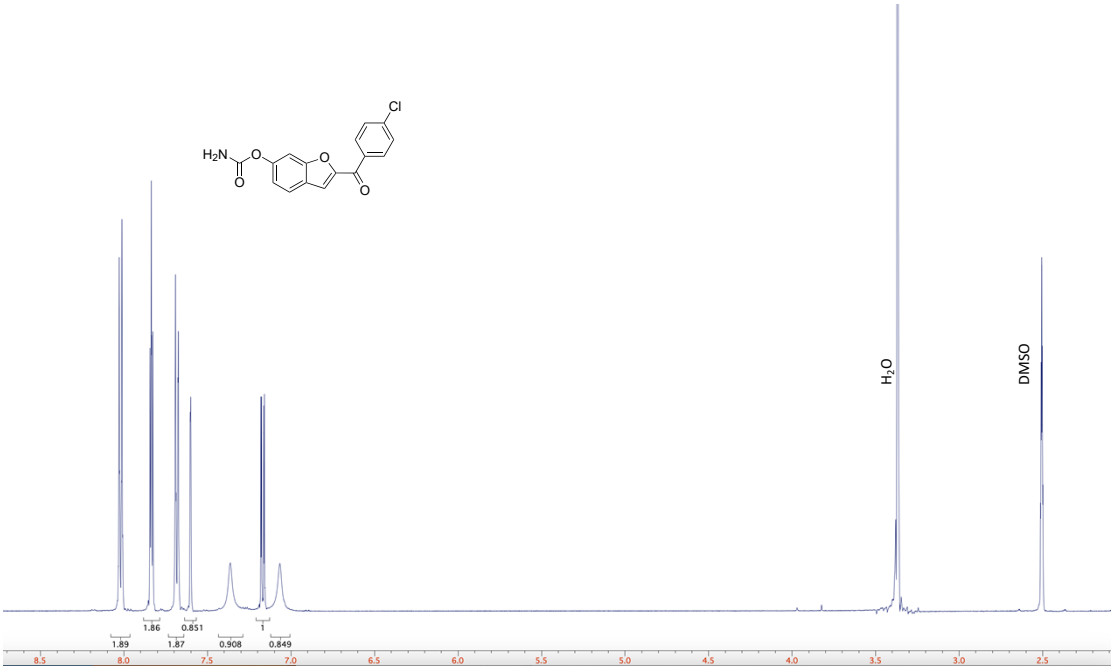
Figure: Base peak or HPLC chromatogram (indicated in left hand corner)

User Chromatogram Peak List

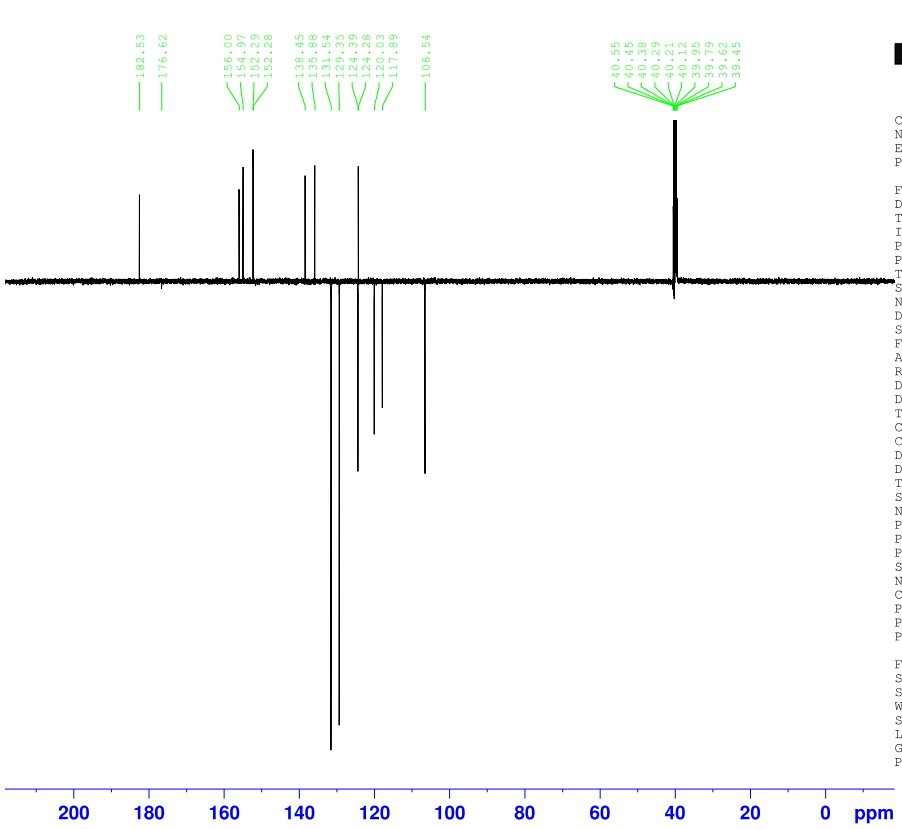
RT (min)	Area	Area %	Area Sum (%)	Symmetry	Width (min)
4.35	28.19	100.00	100.00	1.16	0.217

Compound **20**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)



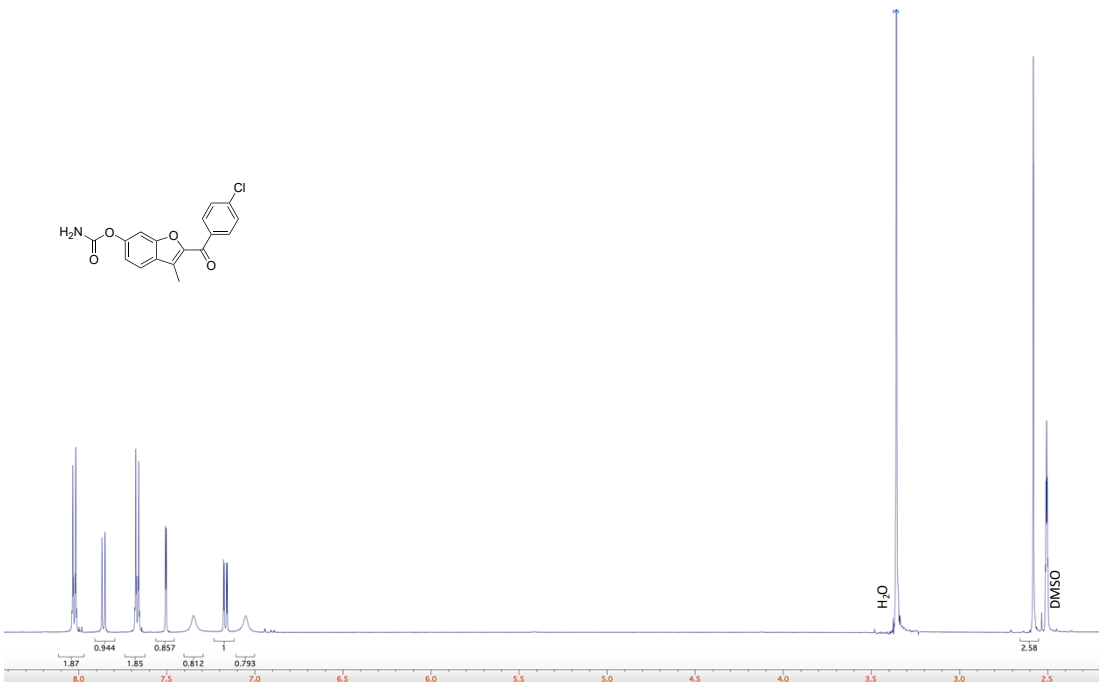
```
Current Data Parameters
NAME                   HAB3
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_               20230729
Time                    3.29 h
INSTRUM                spect
PROBHD    Z113652_0266 (
PULPROG                 jmod
TD                     65536
SOLVENT                 DMSO
NS                      1024
DS                         4
SWH                29761.904 Hz
FIDRES             0.908261 Hz
AQ                 1.1010048 sec
RG                    189.93
DW                    16.800 usec
DE                     6.50 usec
TE                    295.5 K
CNST2             145.0000000
CNST11              1.0000000
D1                  2.00000000 sec
D20                 0.00689655 sec
TD0                        1
SFO1              125.7703643 MHz
NUC1                     13C
P1                    10.00 usec
P2                    20.00 usec
PLW1              74.29499817 W
SFO2              500.1320005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 80.00 usec
PLW2              21.58600044 W
PLW12              0.33728001 W

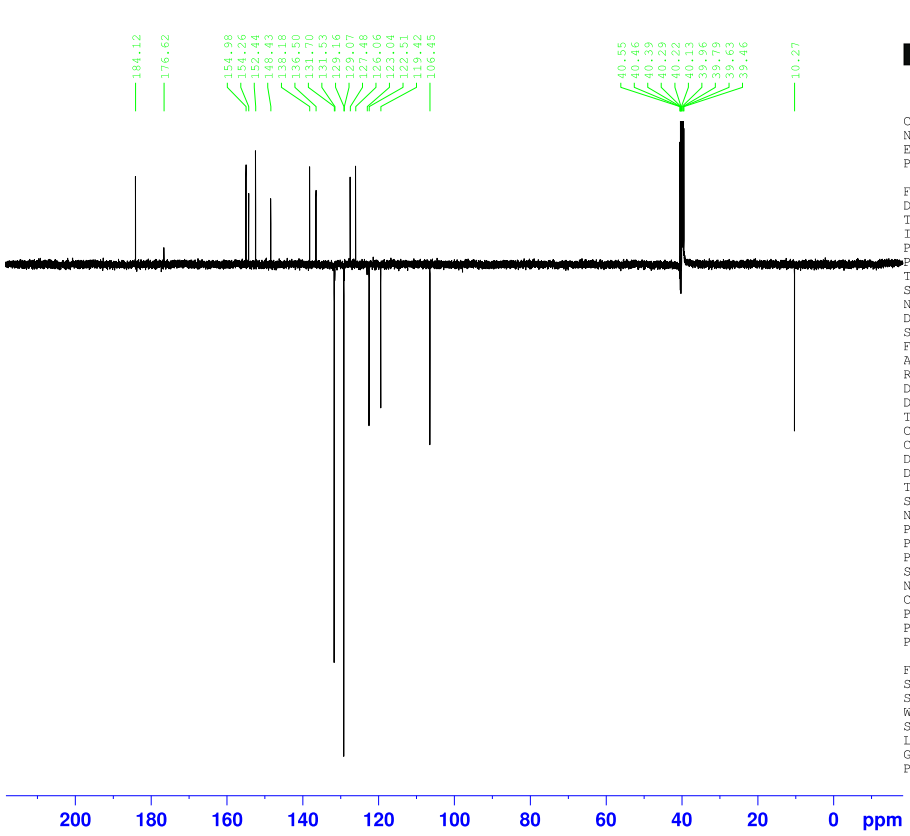
F2 - Processing parameters
SI                        32768
SF                125.7577885 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

Compound **21**

^{1}H NMR (DMSO-d_6)



^{13}C NMR (DMSO-d_6)

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Current Data Parameters
NAME                  HAB2-C
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20230727
Time                 22.43 h
INSTRUM                spect
PROBHD    Z113652_0266 (
PULPROG                jmod
TD                    65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH               29761.904 Hz
FIDRES             0.908261 Hz
AQ                1.1010048 sec
RG                   189.93
DW                   16.800 usec
DE                    6.50 usec
TE                   295.1 K
CNST2           145.0000000
CNST11            1.0000000
D1                2.00000000 sec
D20               0.00689655 sec
TD0                       1
SFO1           125.7703643 MHz
NUC1                    13C
P1                    10.00 usec
P2                    20.00 usec
PLW1           74.29499817 W
SFO2           500.1320005 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                 80.00 usec
PLW2           21.58600044 W
PLW12           0.33728001 W

F2 - Processing parameters
SI                    32768
SF             125.7577885 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```