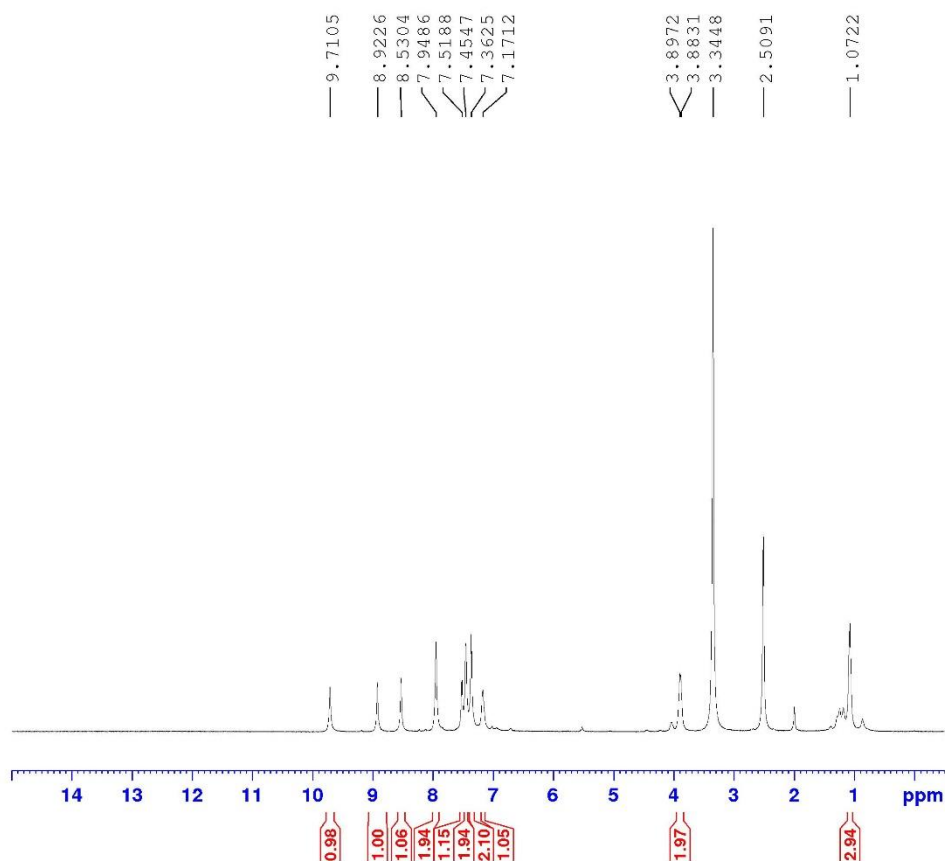
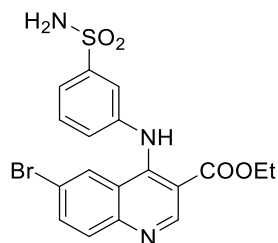


# <sup>1</sup>H NMR spectrum of compound 5a

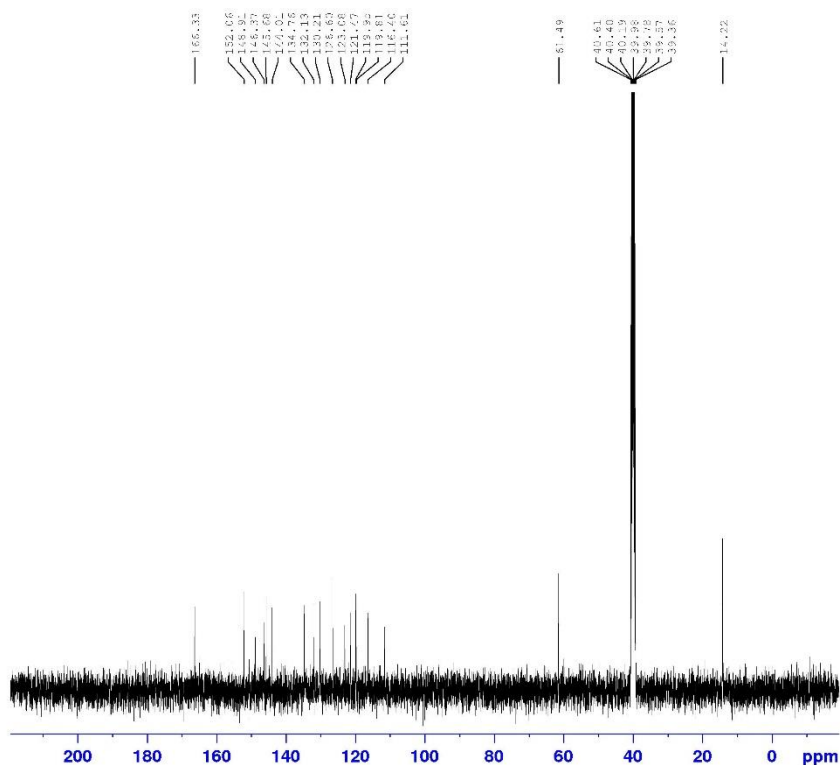
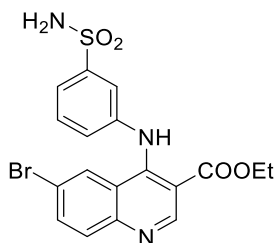


Current Data Parameters  
NAME 5b  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171107  
Time 17.10 h  
INSTRUM spect  
PROBHD Z108618\_0941 ( )  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 142.45  
DW 62.400 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 -  
SFO1 400.1324708 MHz  
NUC1 1H  
P1 14.00 usec  
PLW1 13.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>13</sup>C NMR spectrum of compound 5a



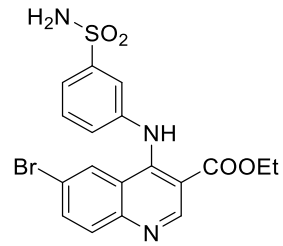
```

Current Data Parameters
NAME          5a_13C
EXPNO         1
PROCNO        1

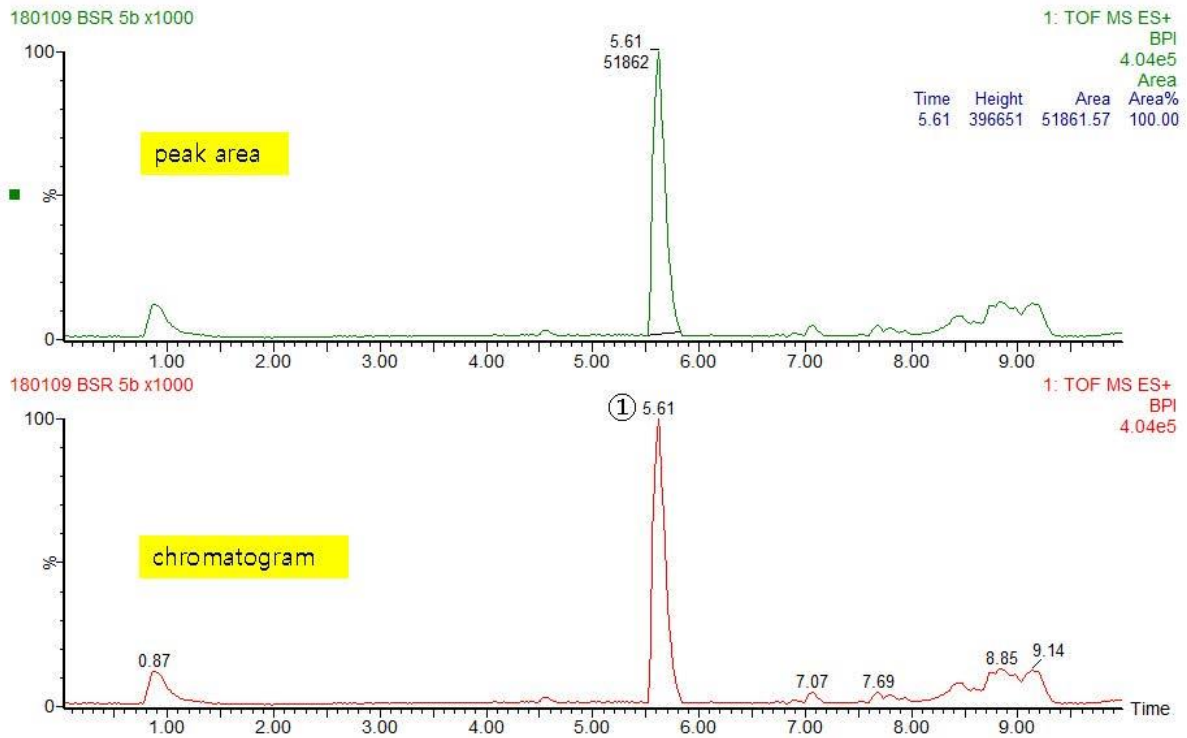
F2 - Acquisition Parameters
Date_         20171110
Time          14.11 h
INSTRUM       spect
PROBHD        Z108618_0941 (
PULPROG       zgpg30
TD            65536
SOLVENT       DMSC
NS            181
DS            4
SHE           24038.461 Hz
FIDRES        0.733596 Hz
AQ            1.3631488 sec
RG            198.73
DW            20.800 usec
DE            6.50 usec
TE            296.2 K
D1            2.0000000 sec
D11           0.0300000 sec
DDO           1
SFO1          100.6228298 MHz
NUC1          13C
P1            10.00 usec
PLM1          47.0000000 W
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          13.0000000 W
PLM12         0.31457001 W
PLM13         0.15623001 W

F2 - Processing parameters
SI            32768
SF            100.6127685 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

## Purity and HRMS of compound 5a



### 2. 5b : chromatogram / area



2. 5b : mass spectrum

Molecular formula:  $C_{18}H_{16}BrN_3O_4S$

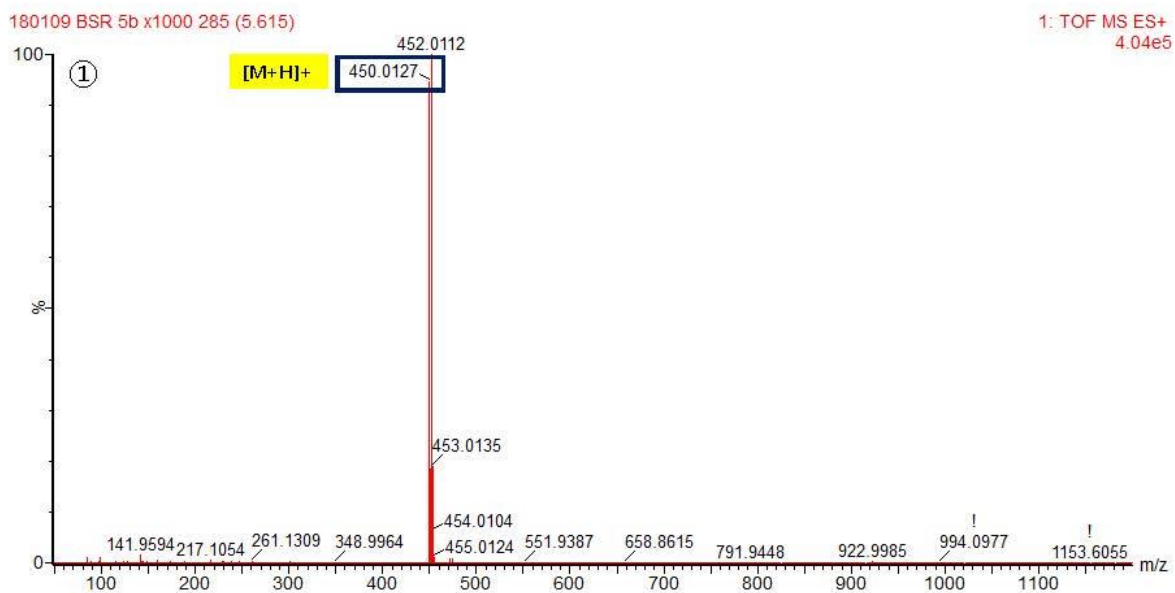
Exact mass: 449.0045

113.2589 (4+)

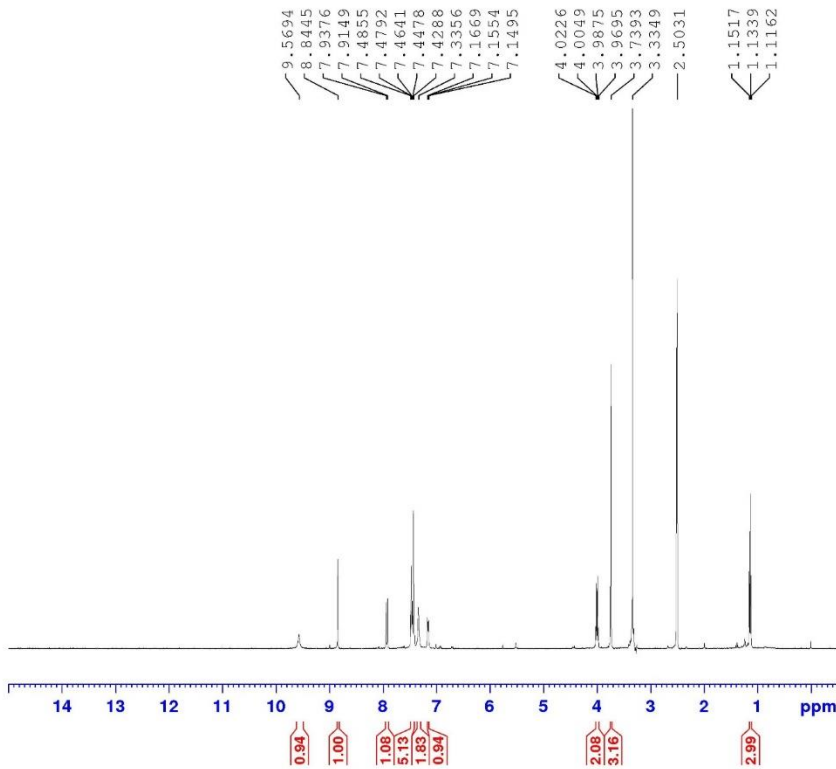
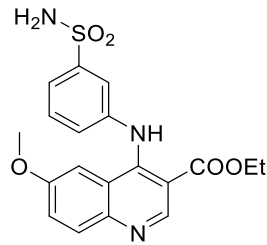
150.6760 (3+)

225.5101 (2+)

450.0123 (1+)



# <sup>1</sup>H NMR spectrum of compound **5b**

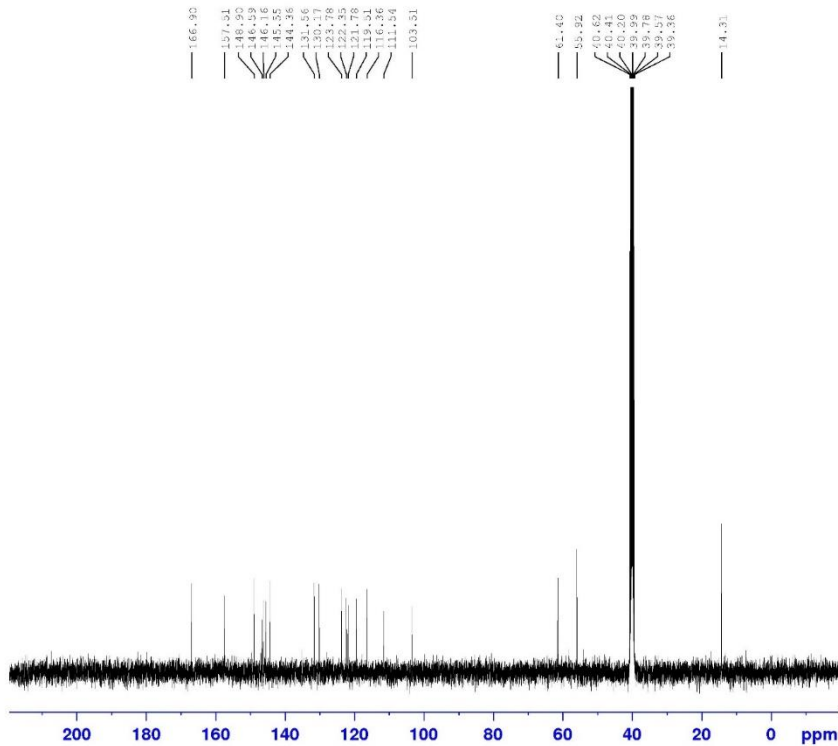
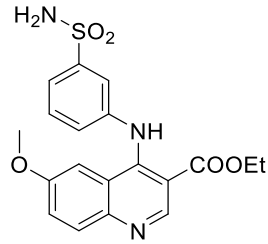


Current Data Parameters  
NAME 5d  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171108  
Time 10.03 h  
INSTRUM spect  
PROBHD z108618\_0941 (1  
PULPROG zg30  
TD 65536  
SOLVENT DM60  
NS 4  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 156.81  
DW 62.400 usec  
DE 6.50 usec  
TE 296.0 K  
D1 1.00000000 sec  
IDG 1  
SFO1 400.1324706 MHz  
NUC1 1H  
P1 14.00 usec  
PLW1 13.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300022 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>13</sup>C NMR spectrum of compound **5b**



Current Data Parameters  
NAME 5d\_13c  
EXPNO 1  
PROCNO 1

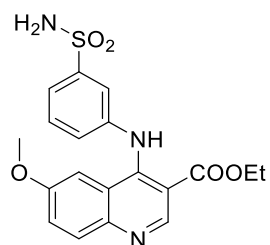
F2 - Acquisition Parameters  
Date\_ 20171113  
Time 13.40  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 311  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 190.62  
DW 20.800 usec  
DE 6.50 usec  
TE 298.6 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

----- CHANNEL f1 -----  
SFO1 100.6229474 MHz  
NUC1 13c  
P1 10.00 usec  
PLW1 52.0000000 W

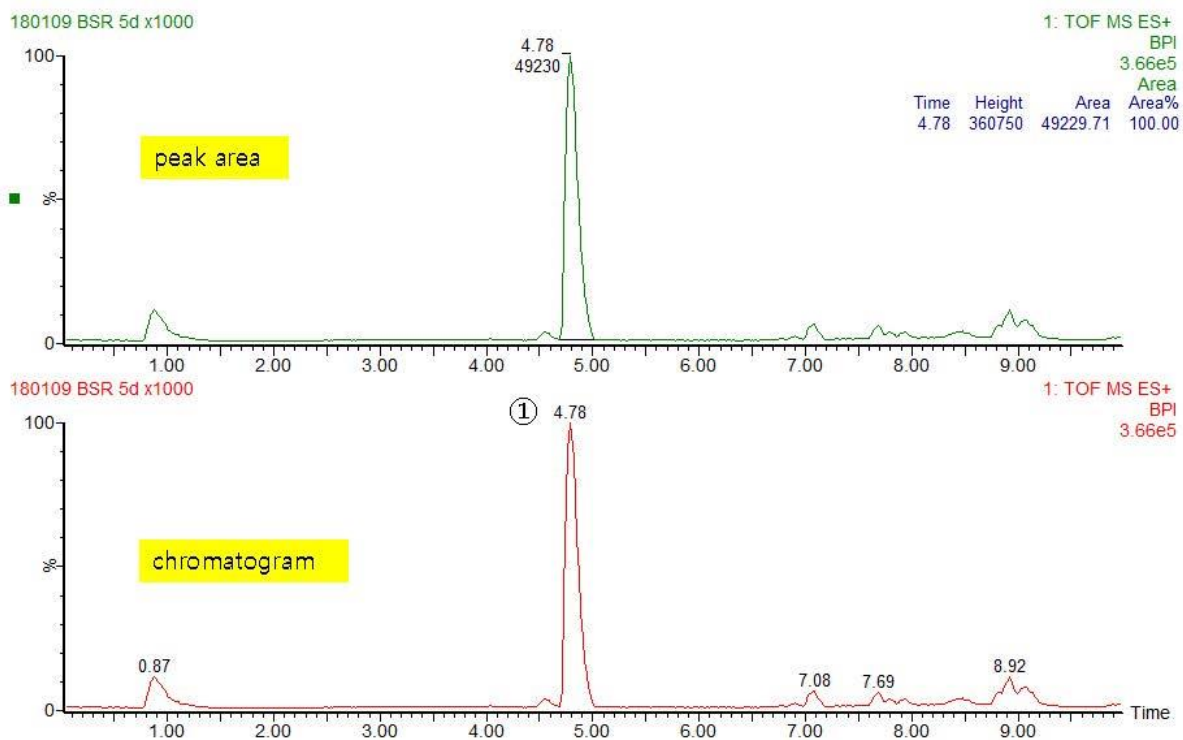
----- CHANNEL f2 -----  
SFO2 400.2116008 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.0000000 W  
PLW12 0.3377000 W  
PLW13 0.2897900 W

F2 - Processing parameters  
SI 32768  
SF 100.6228860 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
FC 1.40

## Purity and HRMS of compound **5b**



### 4. 5d : chromatogram / area



4. 5d : mass spectrum

Molecular formula:  $C_{19}H_{19}N_3O_5S$

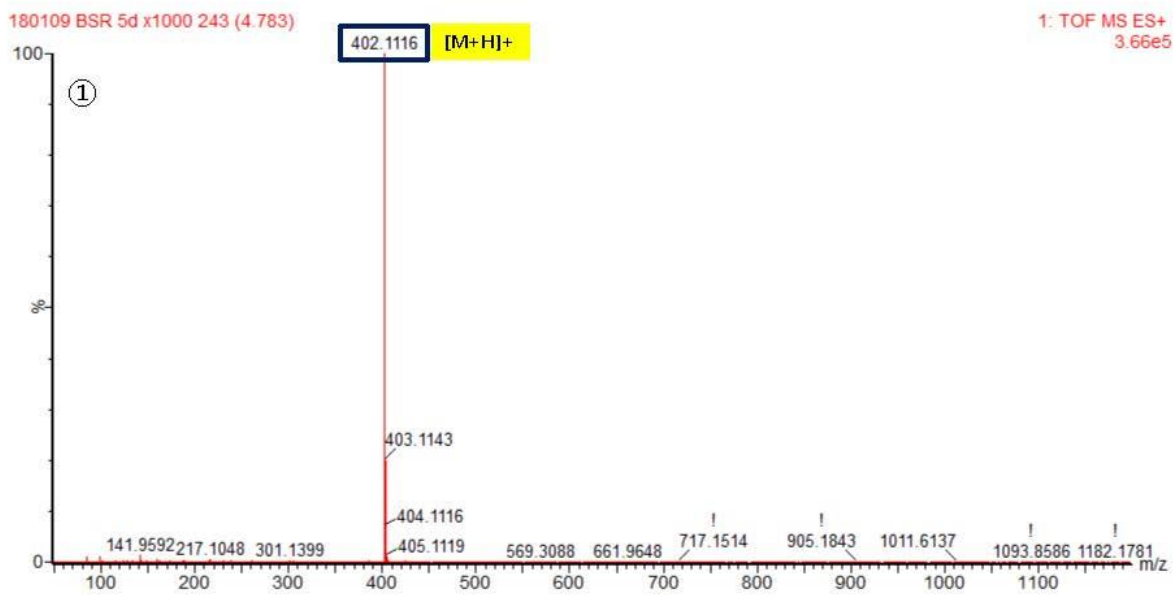
Exact mass: 401.1045

101.2840 (4+)

134.7093 (3+)

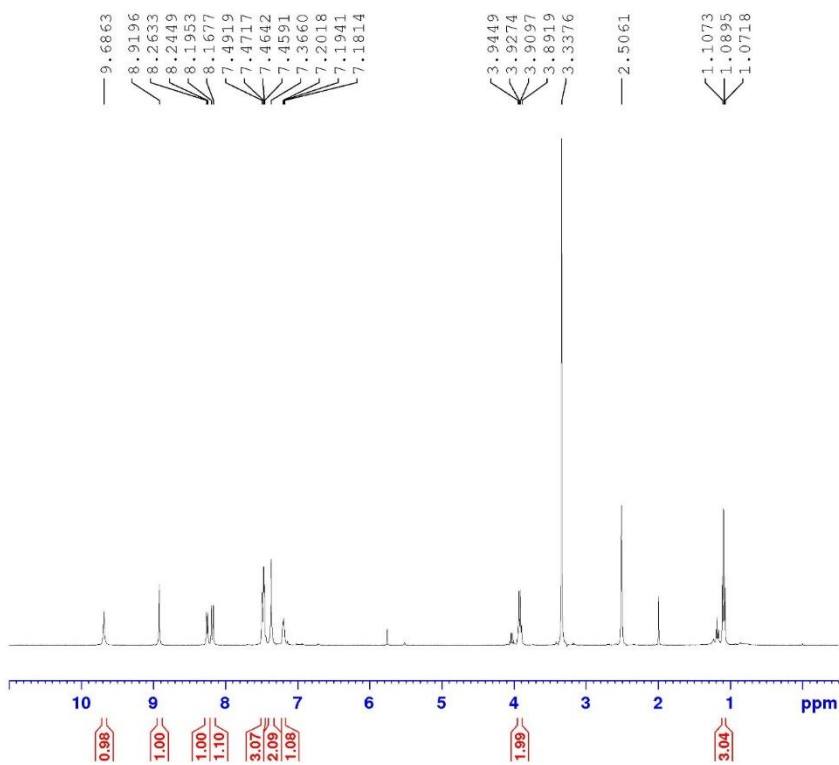
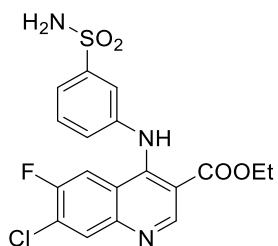
201.5601 (2+)

402.1124 (1+)





# <sup>1</sup>NMR spectrum of compound 5c

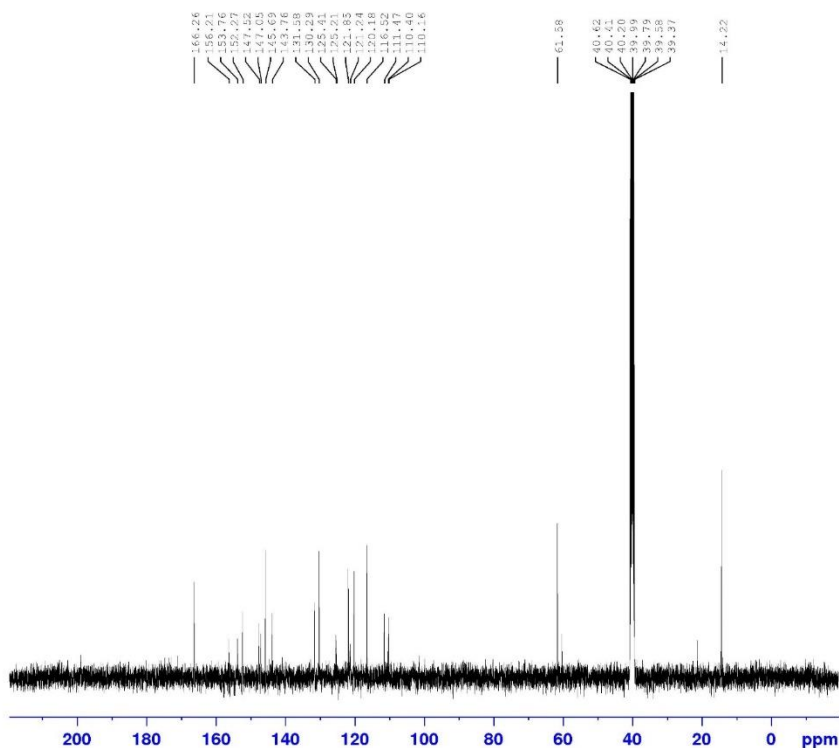
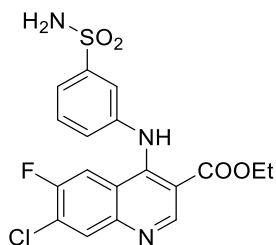


Current Data Parameters  
NAME 5f  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171109  
Time 10.04 h  
INSTRUM spect  
PROBHD Z108618\_0941 (4  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 4  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244832 Hz  
AQ 4.0894465 sec  
RG 142.45  
DW 62.400 usec  
DE 6.50 usec  
TE 296.5 K  
D1 1.0000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P1 14.00 usec  
PLW1 13.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300010 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

# <sup>13</sup>C NMR spectrum of compound 5c

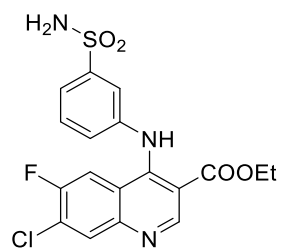


Current Data Parameters  
NAME Sf\_13c  
EXPNO 1  
PROCNO 1

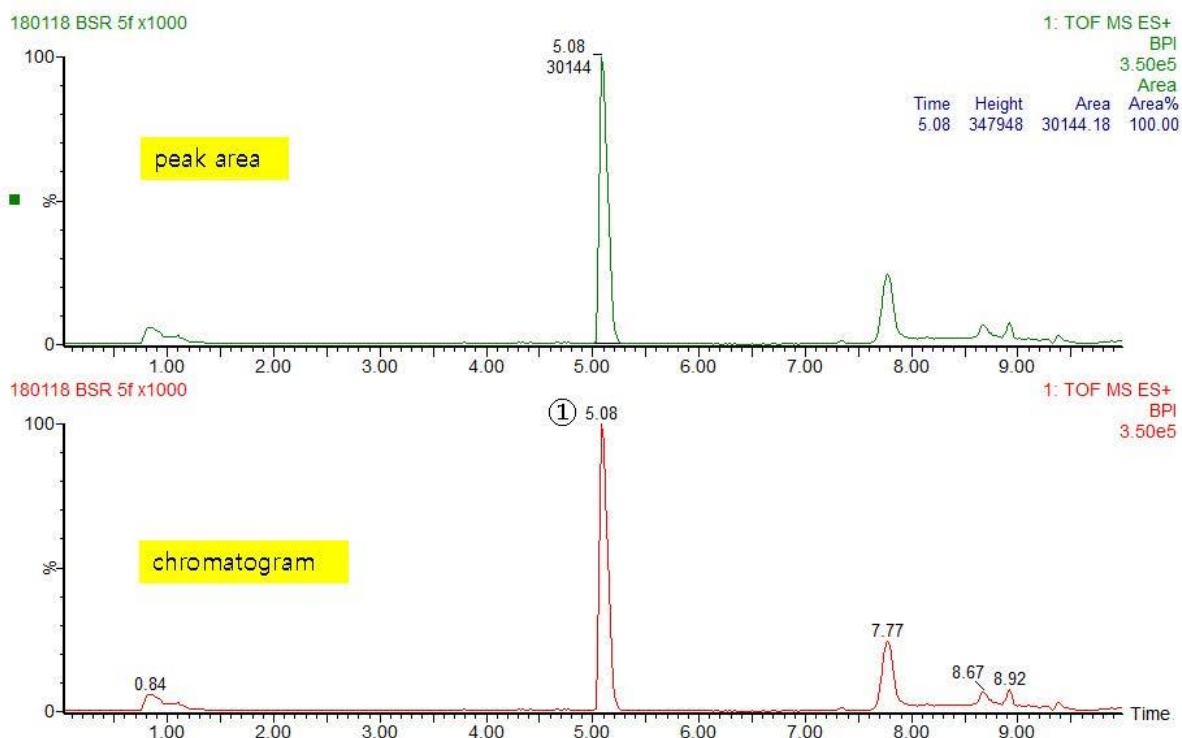
F2 - Acquisition Parameters  
Date\_ 20171109  
Time 10.28 h  
INSTRUM spect  
PROBHD Z108618\_0941 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 381  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 198.73  
DW 20.800 usec  
DE 6.50 usec  
TE 297.5 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13c  
P1 10.00 usec  
PLW1 47.0000000 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.0000000 W  
PLW12 0.31457001 W  
PLW13 0.15823001 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## Purity and HRMS of compound **5c**



### 6. 5f : chromatogram / area



6. 5f : mass spectrum

Molecular formula:  $C_{18}H_{15}ClFN_3O_4S$

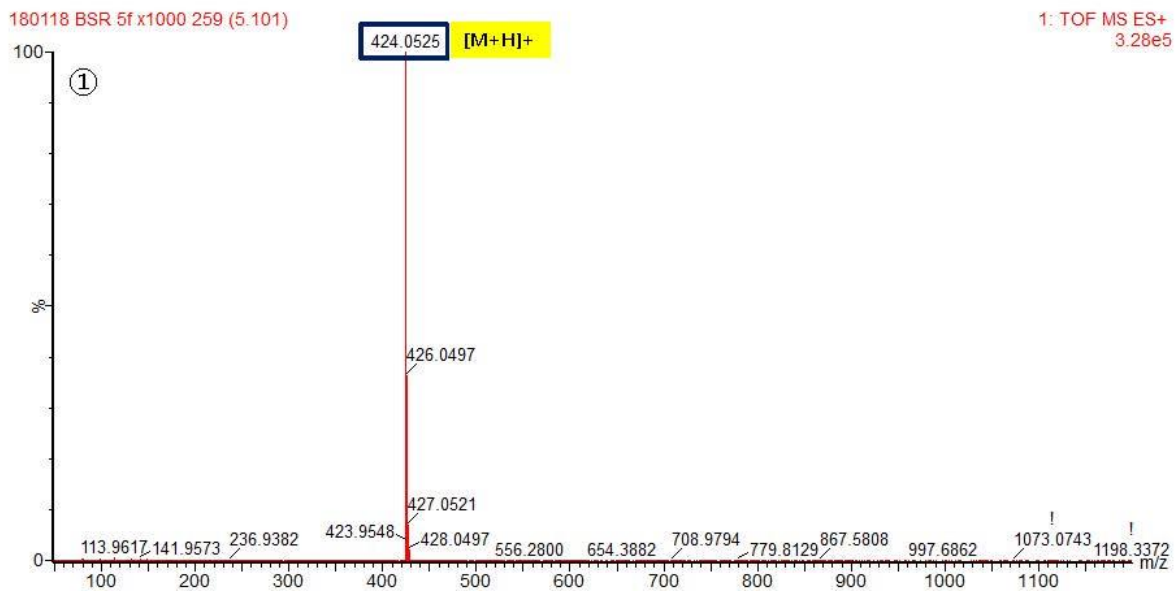
Exact mass: 423.0456

106.7692 (4+)

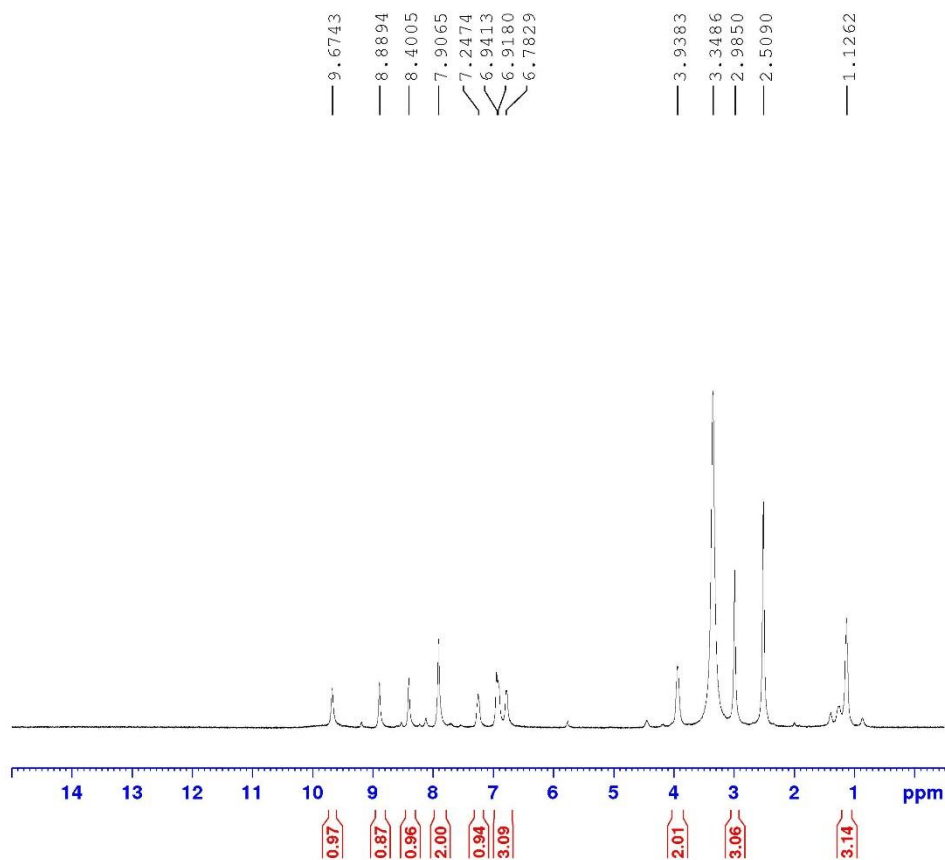
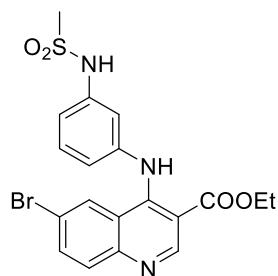
142.0230 (3+)

212.5306 (2+)

424.0534 (1+)



# <sup>1</sup>H NMR spectrum of compound 5d

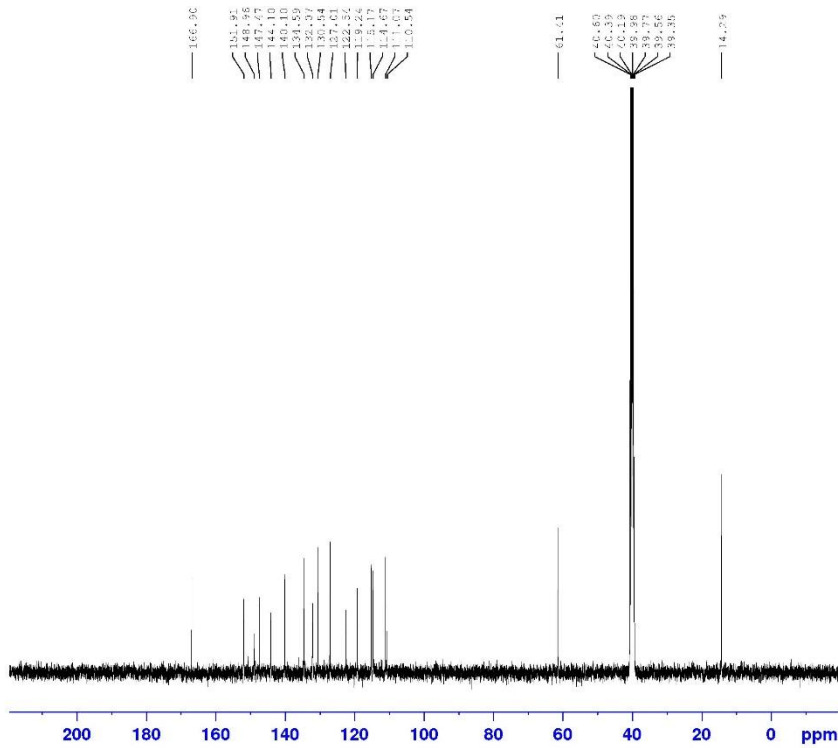
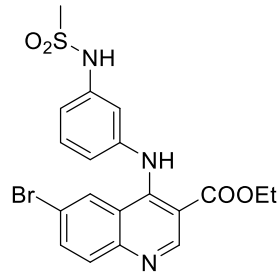


Current Data Parameters  
NAME Saudi\_6b  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171128  
Time 18.38 h  
INSTRUM spect  
PROBHD Z108618\_0341 ( )  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 2  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 126.56  
DW 62.400 usec  
DE 6.50 usec  
TE 296.0 K  
D1 1.00030000 sec  
TDO -  
SF01 400.1324708 MHz  
NUC1 1H  
P1 14.00 usec  
PLW1 13.00000003 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

# <sup>13</sup>C NMR spectrum of compound 5d

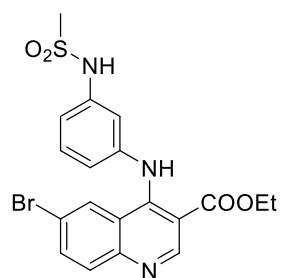


Current Data Parameters  
NAME SAUDI\_6b\_13C  
EXPNO 1  
PROCNO 1

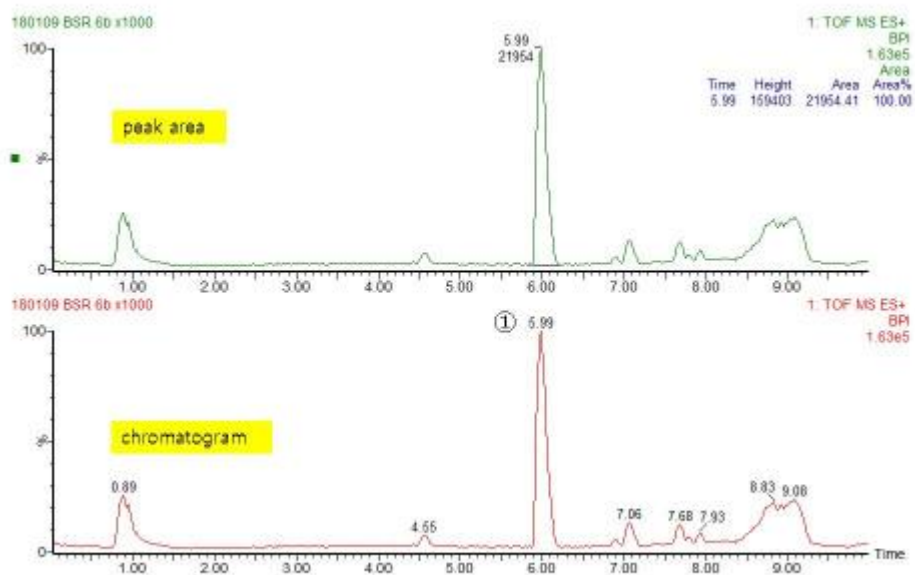
F2 - Acquisition Parameters  
Date\_ 20171218  
Time 16.52 h  
INSTRUM spect  
PROBHD e106618\_094C (4  
PULPROG zgpg30  
ID 65536  
SOLVENT DMSO  
NS 809  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 298.73  
DW 20.800 usec  
DE 8.50 usec  
IE 296.9 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDC 1  
SFO1 100.6228298 MHz  
NUC1 13C  
F1 10.00 usec  
PLW1 47.0000000 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 13.0000000 W  
PLW12 0.31457001 W  
PLW13 0.25823001 W

F2 - Processing parameters  
SI 32768  
SF 100.6227685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
FC 1.40

## Purity and HRMS of compound **5d**



### 8. 5b : chromatogram / area



8. 6b : mass spectrum

Molecular formula:  $C_{19}H_{18}BrN_3O_4S$

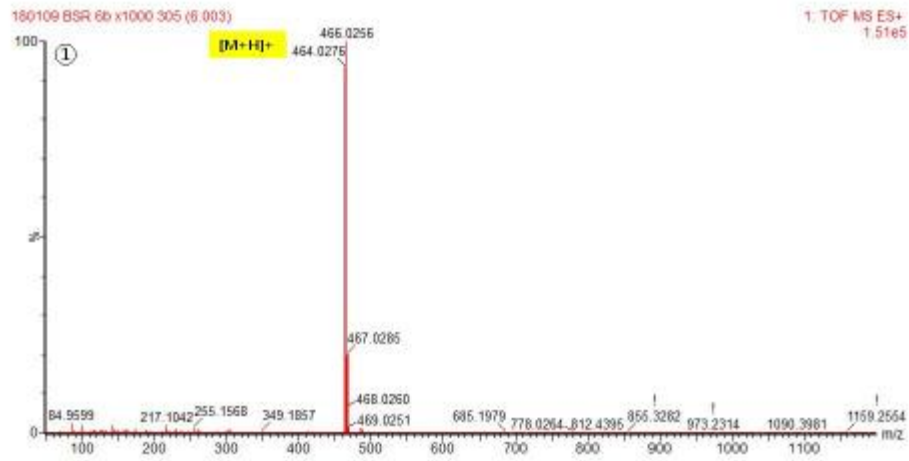
Exact mass: 463.0201

116.7623 (4+)

155.3479 (3+)

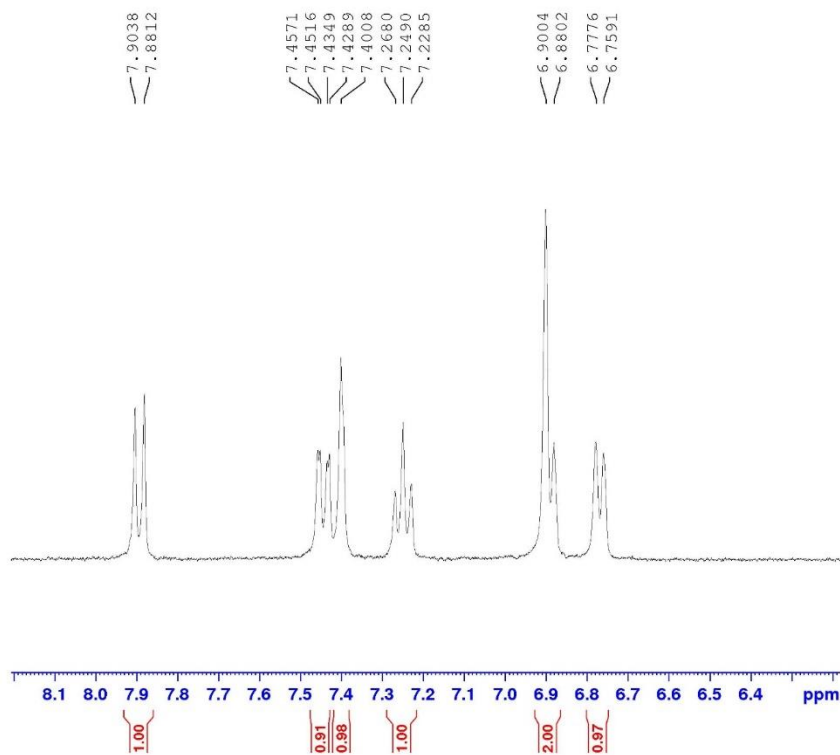
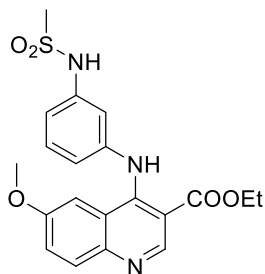
232.5179 (2+)

464.0280 (1+)





# <sup>1</sup>H NMR spectrum of compound 5e

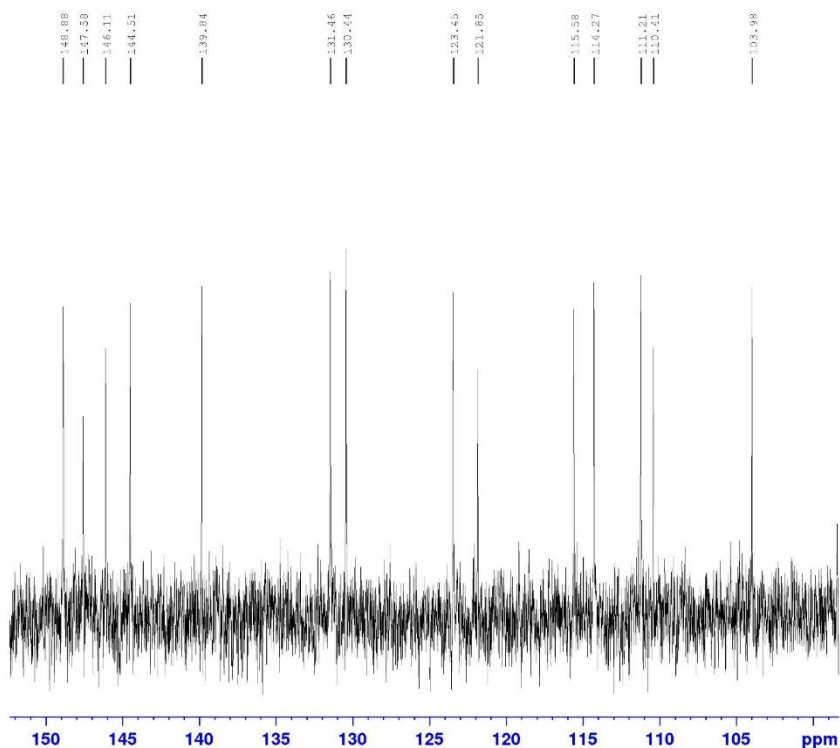
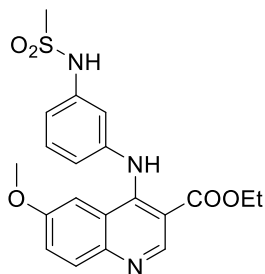


Current Data Parameters  
NAME SAUDI\_6d  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171206  
Time 17.03 h  
INSTRUM spect  
PROBHD Z109618\_0941 ( )  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 6  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 156.81  
DW 62.400 usec  
DE 6.50 usec  
TE 295.7 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
F1 14.00 usec  
PLW1 13.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

# <sup>13</sup>C NMR spectrum of compound **5e**

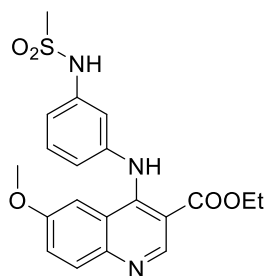


Current Data Parameters  
NAME SAUDI\_6d\_13c  
EXPNO 1  
PROCNO 1

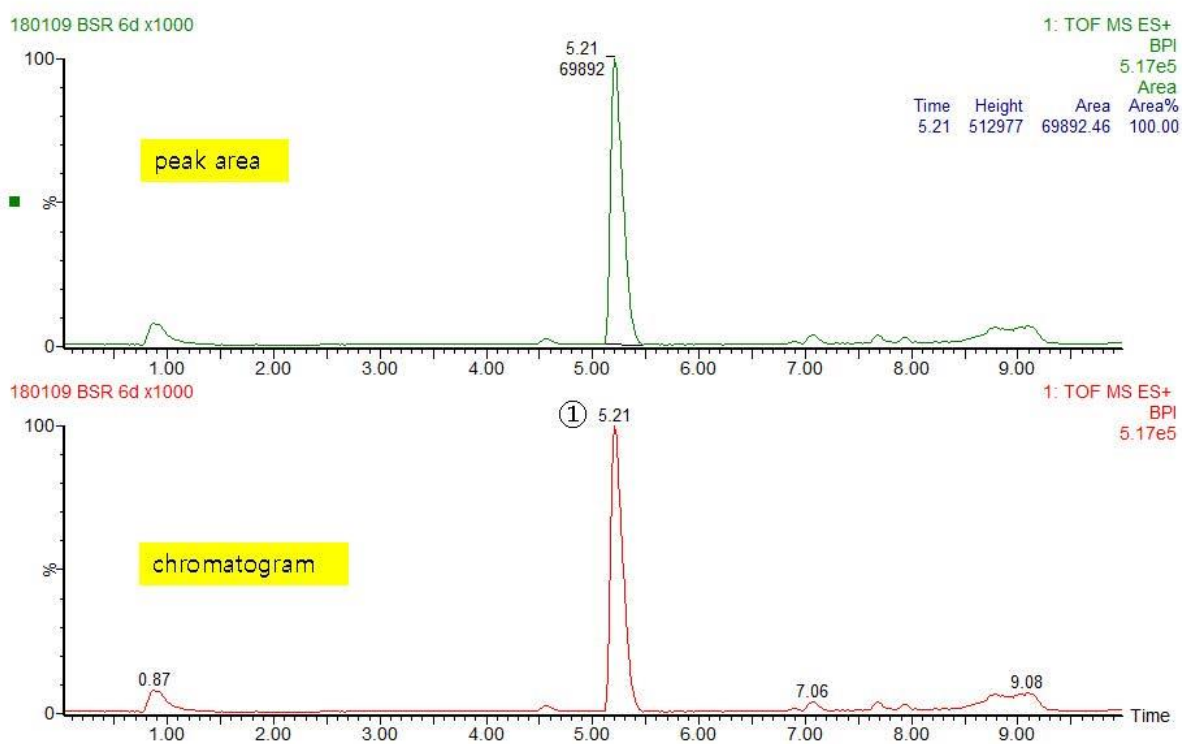
F2 - Acquisition Parameters  
Date\_ 20171219  
Time 15.22 h  
INSTRUM spect  
PROBHD Z108618\_0941 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 289  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733396 Hz  
AQ 1.3631488 sec  
RG 198.73  
DW 20.800 usec  
DE 6.50 usec  
TE 296.8 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
F1 10.00 usec  
PLW1 47.0000000 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 13.0000000 W  
PLW3 0.31457001 W  
PLW13 0.15823001 W

F2 - Processing parameters  
SI 32768  
SF 100.6127688 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## Purity and HRMS of compound 5e



### 10. 6d : chromatogram / area



10. 6d : mass spectrum

Molecular formula:  $C_{20}H_{21}N_3O_5S$

Exact mass: 415.1202

104.7879 (4+)

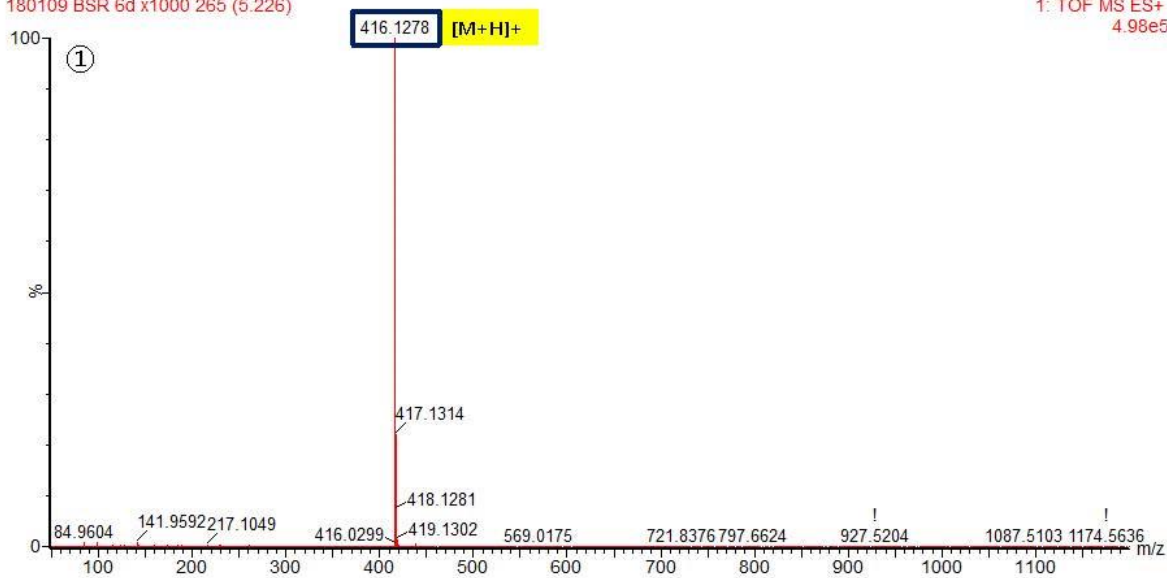
139.3812 (3+)

208.5679 (2+)

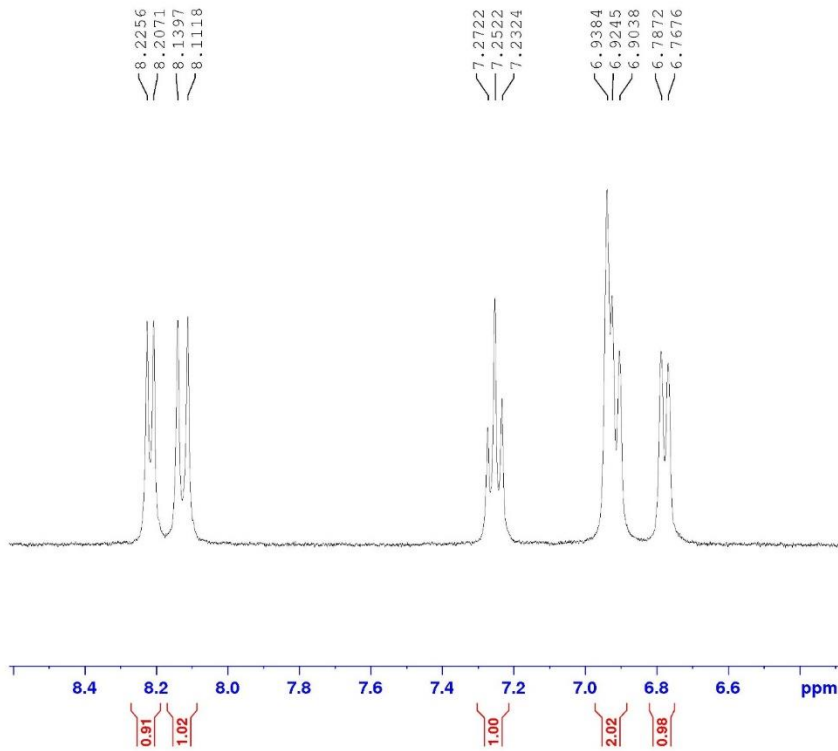
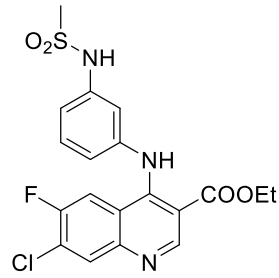
416.1280 (1+)

180109 BSR 6d x1000 265 (5.226)

1: TOF MS ES+  
4.98e5



<sup>1</sup>H NMR spectrum of compound **5f**

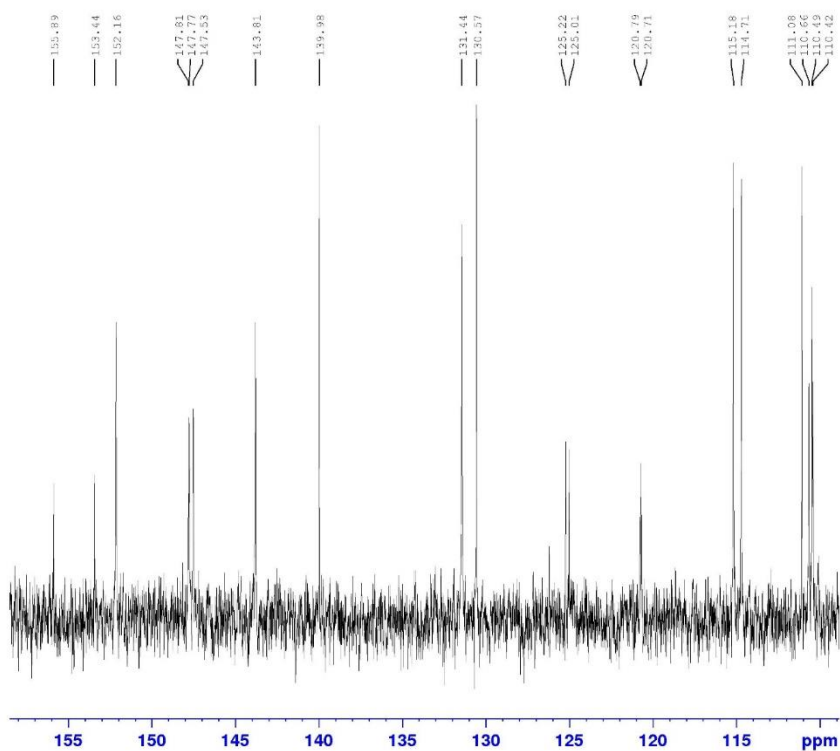
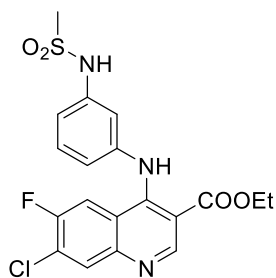


Current Data Parameters  
NAME SAUDI\_6f  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171206  
Time 17.10 h  
INSTRUM spect  
PROBHD Z108618\_0941 ( )  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 3  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244332 Hz  
AQ 4.0894465 sec  
RG 142.45  
DW 62.400 usec  
DE 6.50 usec  
TE 295.5 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P1 14.00 usec  
PLW1 13.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

# <sup>13</sup>C NMR spectrum of compound **5f**

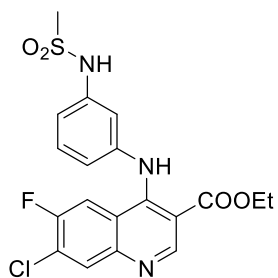


```
Current Data Parameters
NAME      SAUDI_gf_13C
EXPNO    1
PROCNO   1

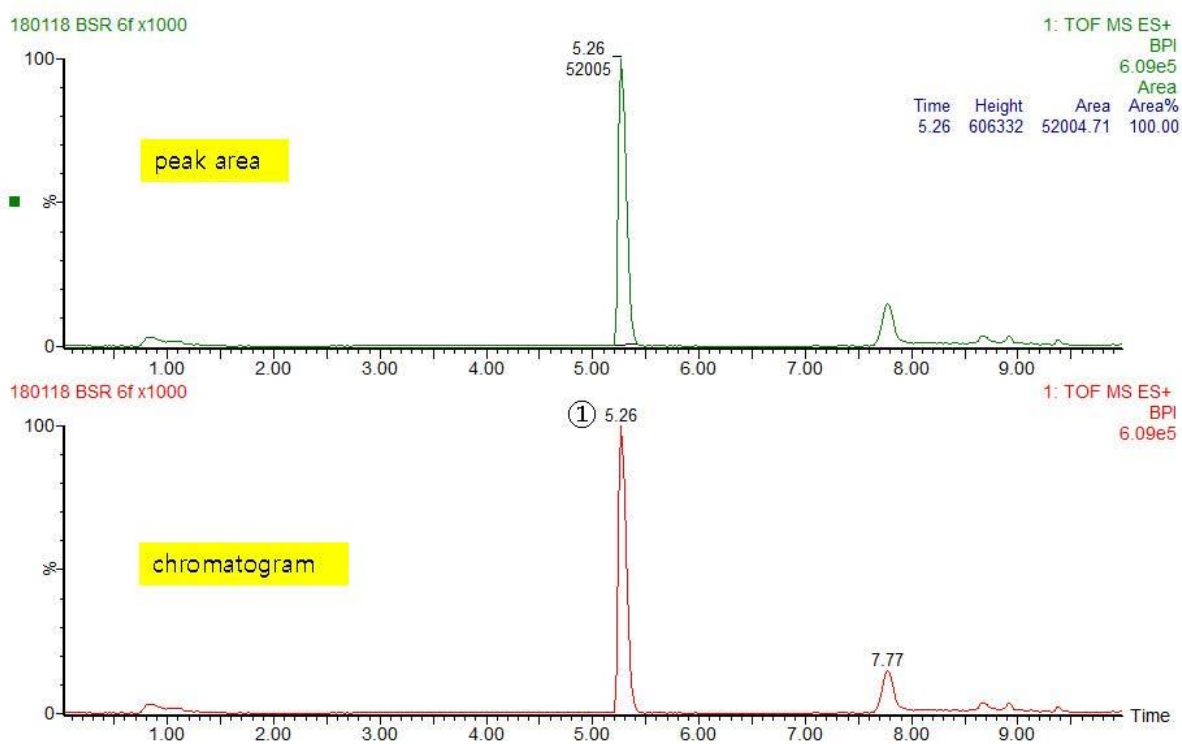
F2 - Acquisition Parameters
Date_    20171221
Time     9.56 h
INSTRUM  spect
PROBHD   Z108618_0941 (
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       514
DS       4
SWH      24038.461 Hz
FIDRES   0.733596 Hz
AQ       1.3631488 sec
RG       198.73
DW       20.800 usec
DE       6.50 usec
TE       296.6 K
DL       2.0000000 sec
D11      0.03000000 sec
TDC      1
SFO1     100.6228296 MHz
NUC1     13C
P1       10.00 usec
PLW1     47.00000000 W
SFO2     400.1316005 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLW2     13.00000000 W
PLW12    0.31437001 W
PLW13    0.15623001 W

F2 - Processing parameters
SI       32768
SF       100.6127685 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

## Purity and HRMS of compound **5f**



### 12. 6f : chromatogram / area



## 12. 6f : mass spectrum

Molecular formula:  $C_{19}H_{17}ClFN_3O_4S$

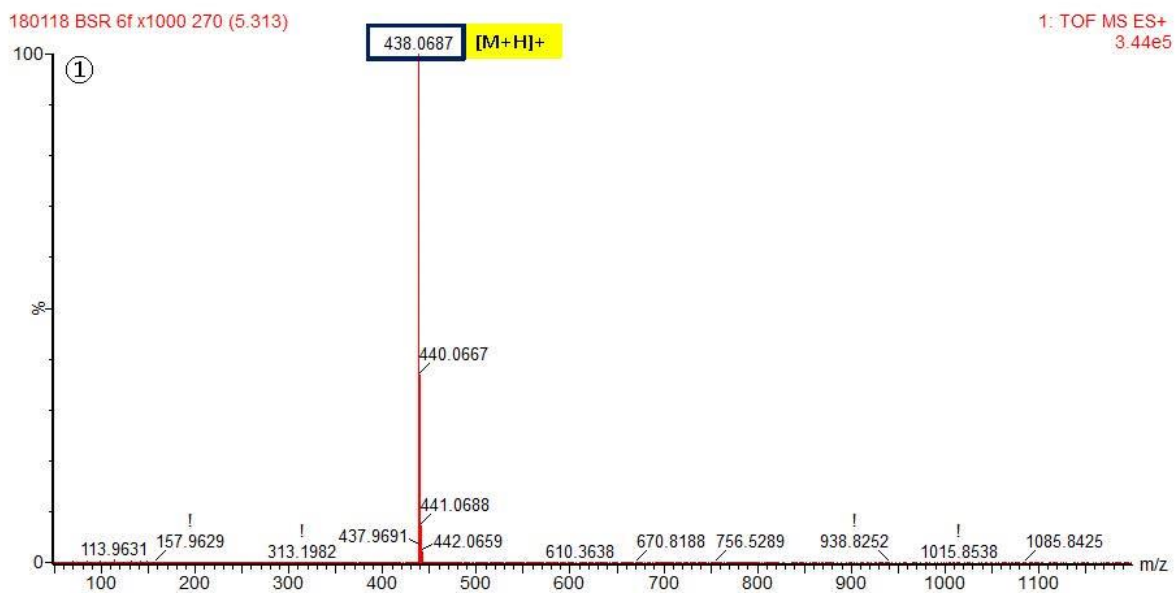
Exact mass: 437.0612

110.2731 (4+)

146.6949 (3+)

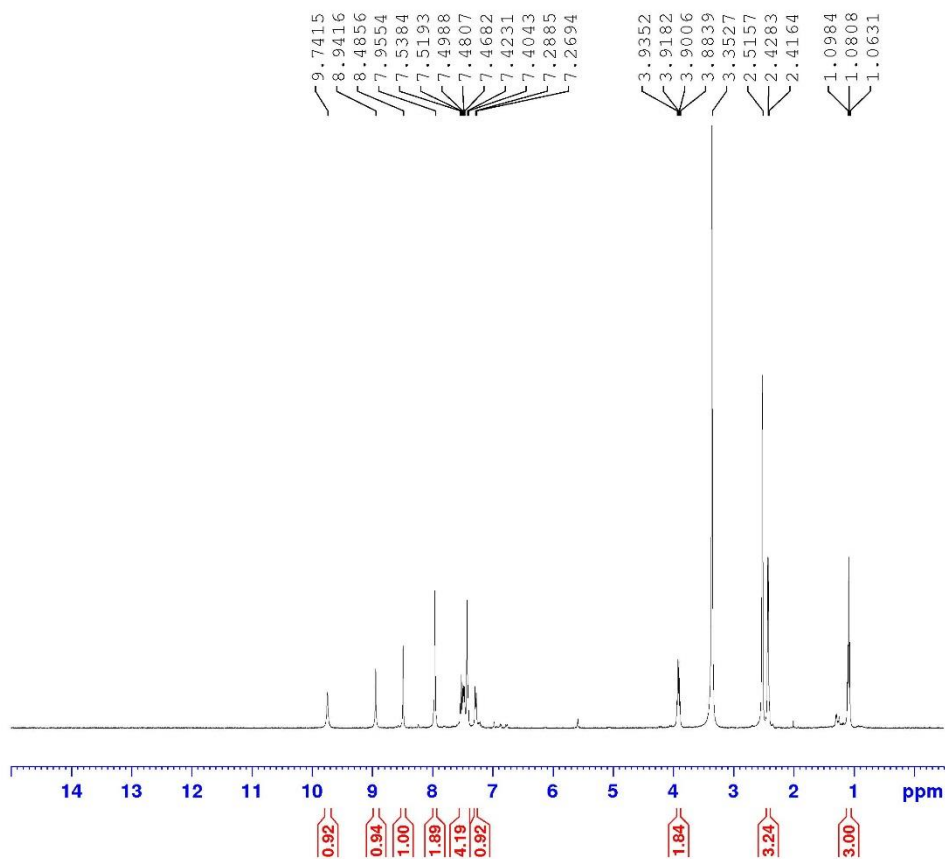
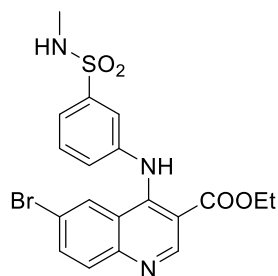
219.5384 (2+)

438.0691 (1+)





<sup>1</sup>H NMR spectrum of compound 5g



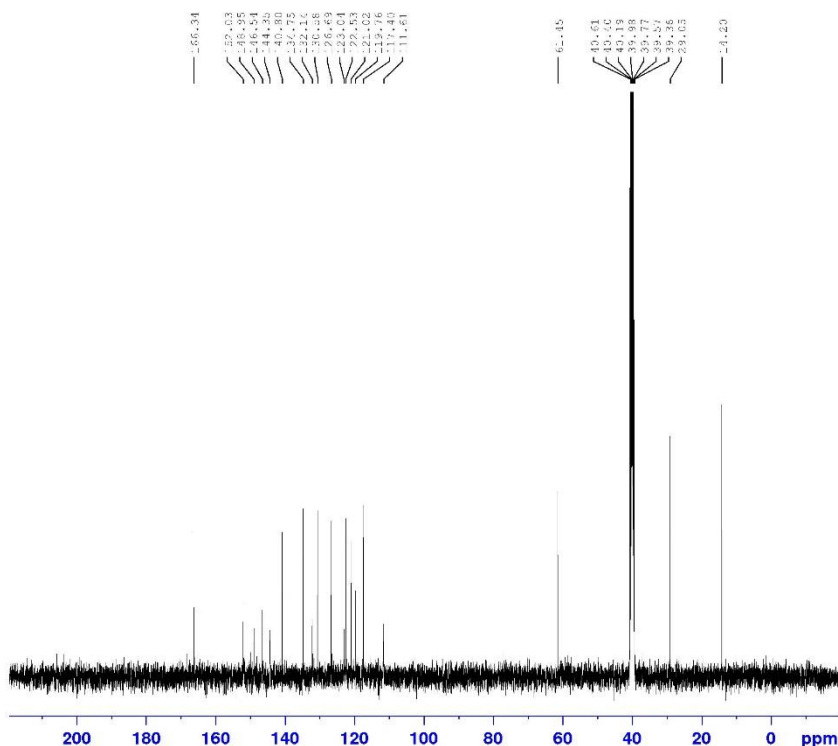
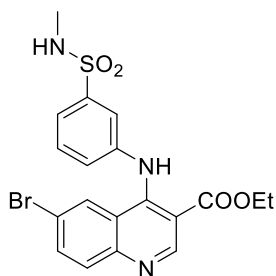
Current Data Parameters  
NAME SAUDI\_7b  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171212  
Time 10.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 4  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 190.62  
DW 62.400 usec  
DE 6.50 usec  
TE 297.0 K  
D1 1.0000000 sec  
TDC 1

===== CHANNEL f1 =====  
SFO1 400.2124715 MHz  
NUC1 1H  
P1 18.34 usec  
PLW1 12.0000000 W

F2 - Processing parameters  
SI 65536  
SF 400.2100000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>13</sup>C NMR spectrum of compound 5g



```

Current Data Parameters
NAME      SAUDI_Ta_30
EXPNO    1
PROCNO   1

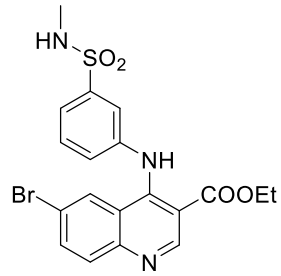
F2 - Acquisition Parameters
Date_    20171227
Time     15.11
INSTRUM  spect
PROBHD   5 mm F400 BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       514
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3921488 sec
RG       190.82
DW       20.800 usec
DE       6.50 usec
TE       298.1 K
D1       2.0000000 sec
D11      0.0500000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    100.628474 MHz
NUC1    13C
P1      10.00 usec
PLW1    52.0000000 W

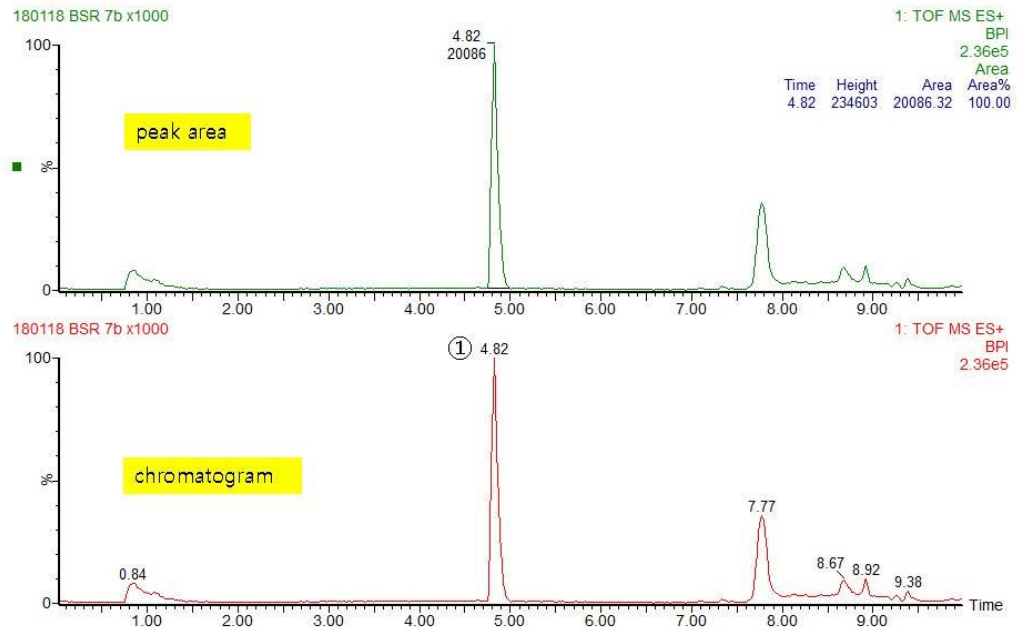
===== CHANNEL f2 =====
SFO2    400.2116008 MHz
NUC2    1H
PCPDPRG2  waltz16
PCPD2    90.00 usec
PLW2    12.0000000 W
PLW12   0.3577000 W
PLW13   0.28979000 W

F2 - Processing parameters
SI      32768
SF      100.6328860 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
    
```

# Purity and HRMS of compound 5g

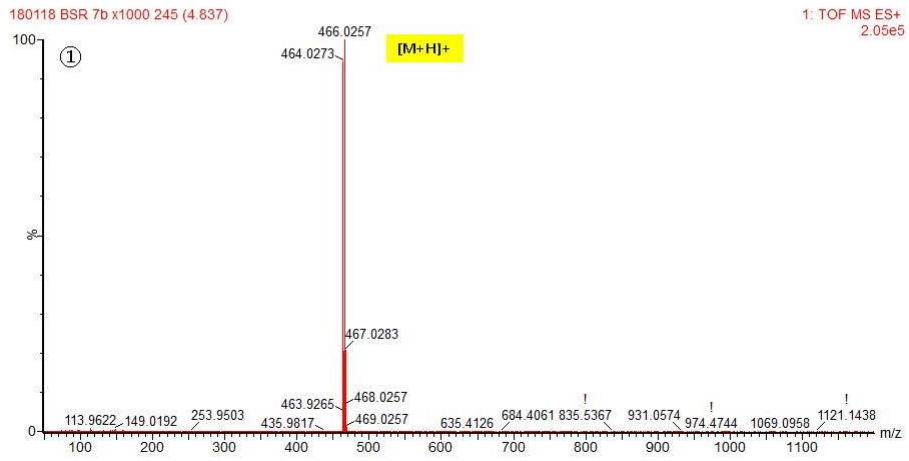


14. 7b : chromatogram / area

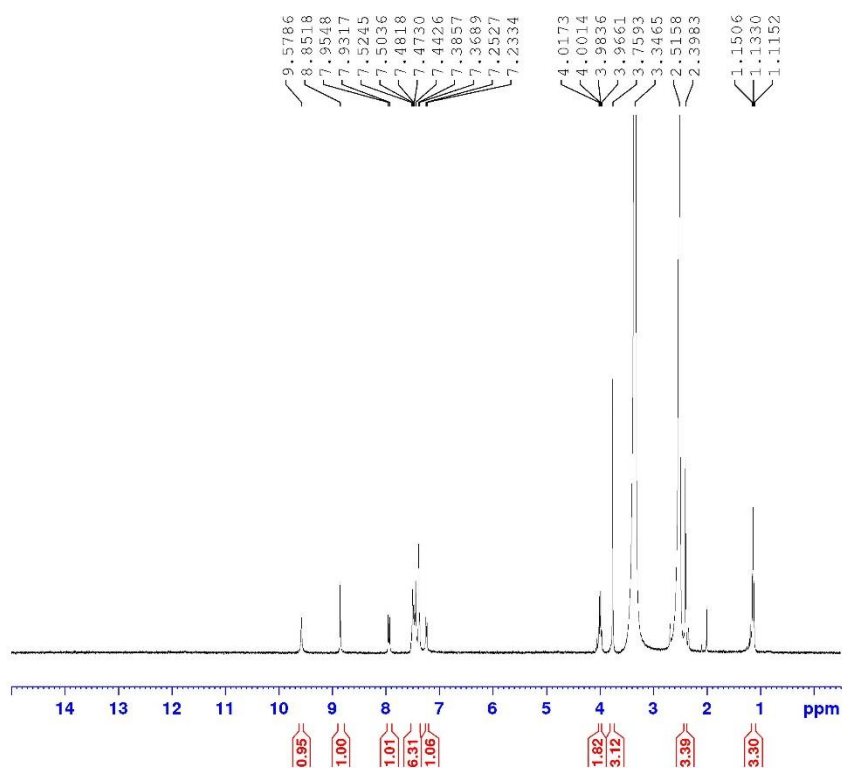
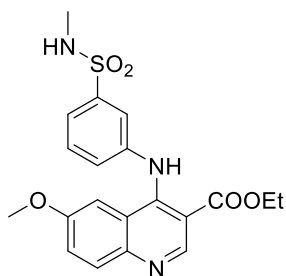


14. 7b : mass spectrum

Molecular formula:  $C_{19}H_{18}BrN_3O_4S$   
Exact mass: 463.0201  
116.7629 (4+)  
155.3479 (3+)  
232.5179 (2+)  
464.0280 (1+)



# <sup>1</sup>H NMR spectrum of compound 5h



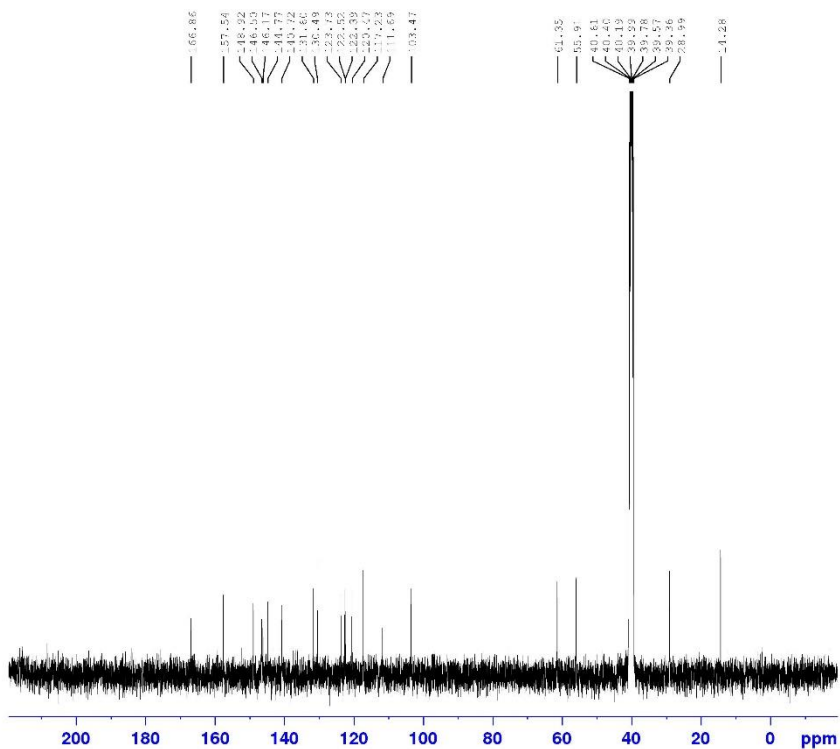
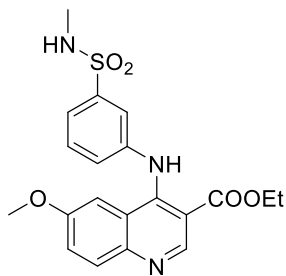
Current Data Parameters  
NAME SAUDI\_7d  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171212  
Time 10.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 85336  
SOLVENT DMSC  
NS 64  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.222266 Hz  
AQ 4.0894465 sec  
RG 190.62  
DW 62.400 usec  
DE 8.56 usec  
TE 297.2 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
SF01 400.2124715 MHz  
NUC1 1H  
P1 15.54 usec  
PLN1 12.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.2100000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

# <sup>13</sup>C NMR spectrum of compound 5h

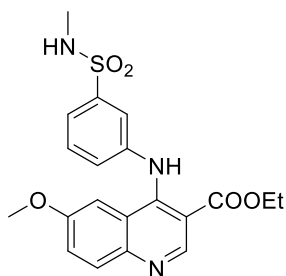


Current Data Parameters  
NAME SAUDI\_7d\_13c  
EXPNO 1  
PROCNO 1

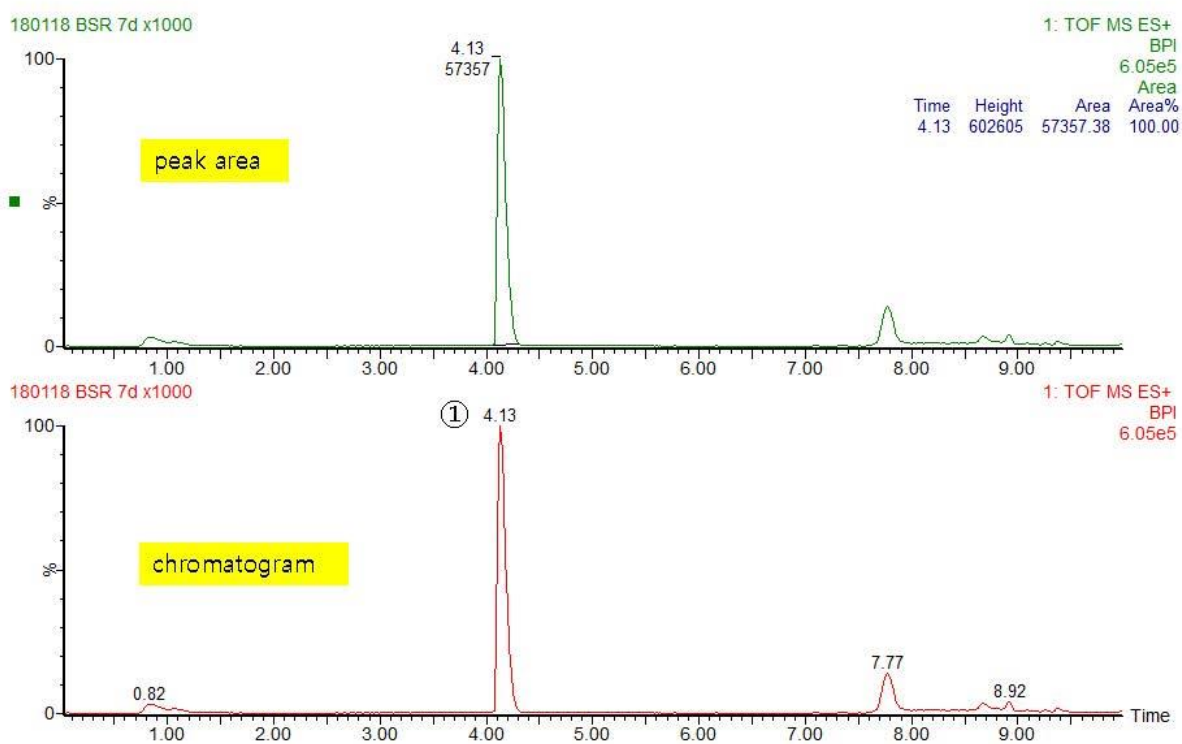
F2 - Acquisition Parameters  
Date\_ 20190117  
Time 8.52 h  
INSTRUM spect  
PROBHD z108618\_0941 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 576  
DS 4  
SWE 24038.461 Hz  
FIDRES 0.733598 Hz  
AQ 1.3631488 sec  
RG 198.73  
DW 20.800 usec  
DE 6.30 usec  
TE 297.2 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P1 10.00 usec  
PLM1 47.0000000 W  
SFO2 400.1316205 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLM2 19.0000000 W  
PLM12 0.31457001 W  
PLM13 0.15823001 W

F2 - Processing parameters  
SI 32768  
SF 100.6127695 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
FC 1.40

## Purity and HRMS of compound **5h**



### 16. 7d : chromatogram / area



16. 7d : mass spectrum

Molecular formula:  $C_{20}H_{21}N_3O_5S$

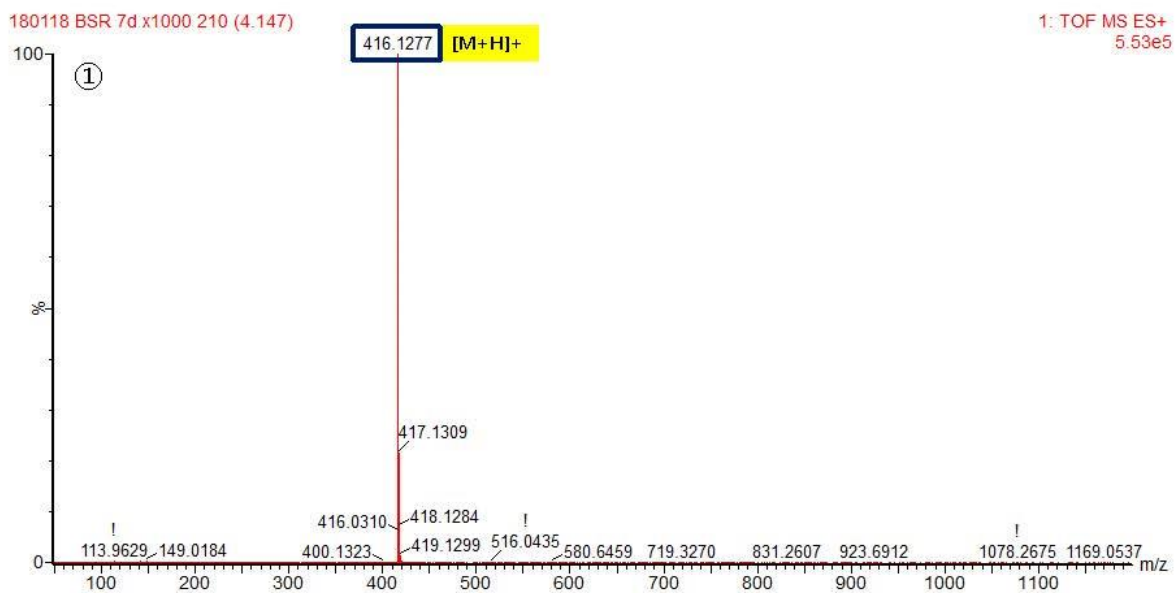
Exact mass: 415.1202

104.7879 (4+)

139.3812 (3+)

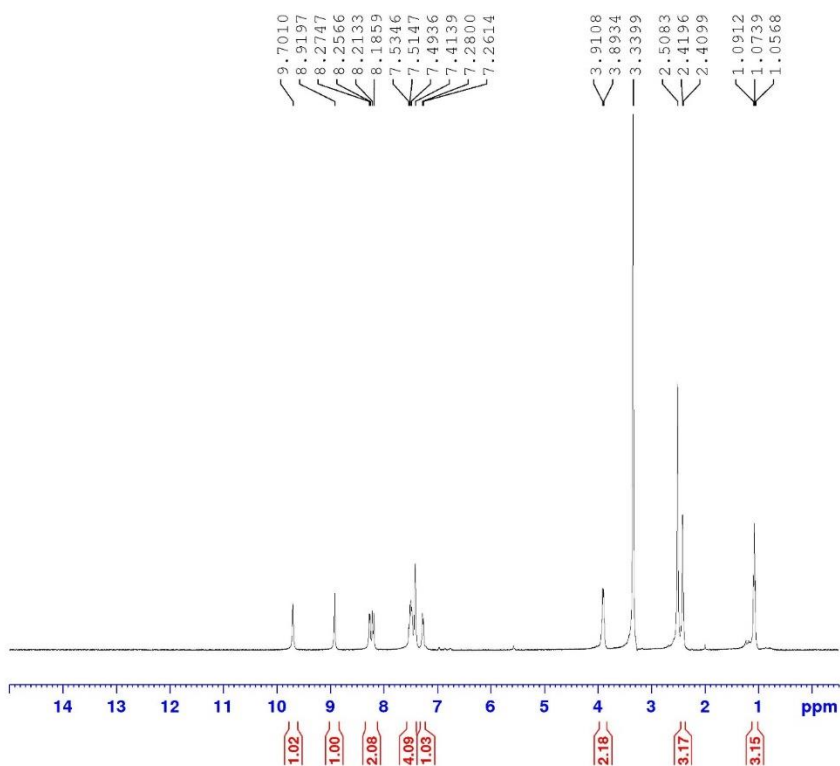
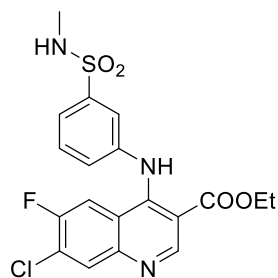
208.5679 (2+)

416.1280 (1+)





# <sup>1</sup>H NMR spectrum of compound **5i**

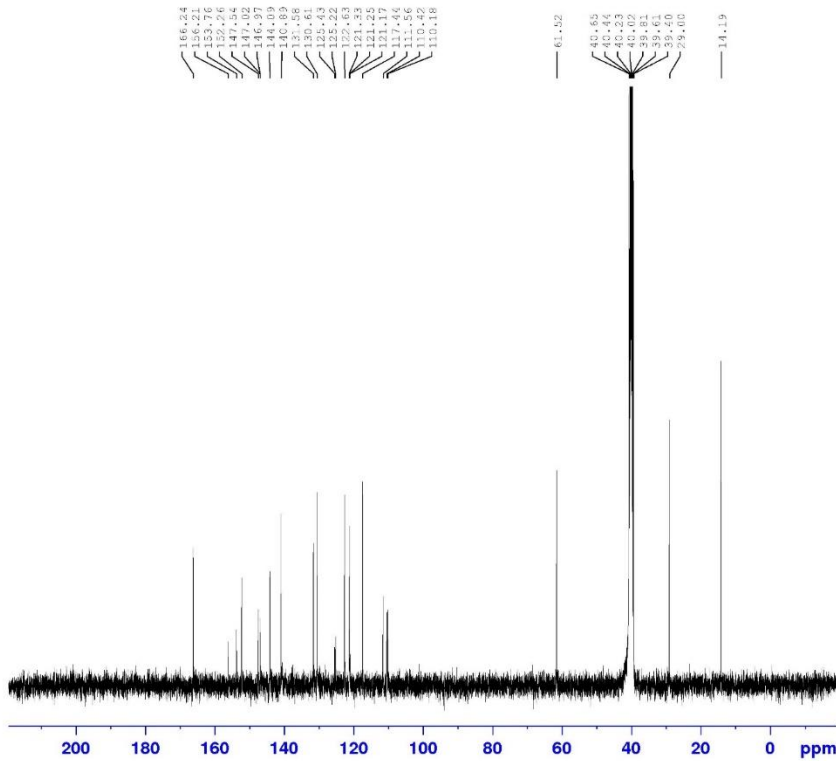
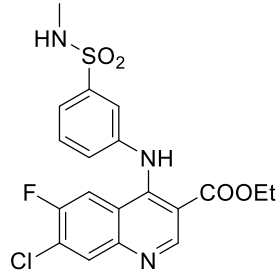


Current Data Parameters  
NAME SAUDI\_7f  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171213  
Time 18.06 h  
INSTRUM spect  
PROBHD Z108618\_0941 (1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 4  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 142.45  
DW 62.400 usec  
DE 6.50 usec  
TE 295.8 K  
D1 1.00000000 sec  
TDC 1  
SFO1 400.1324708 MHz  
NUC1 1H  
PI 14.00 usec  
PLW1 13.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>13</sup>C NMR spectrum of compound **5i**



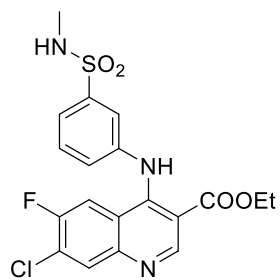
```

Current Data Parameters
NAME      SAUD-7f_13c_final
EXPNO    1
PROCNO   1

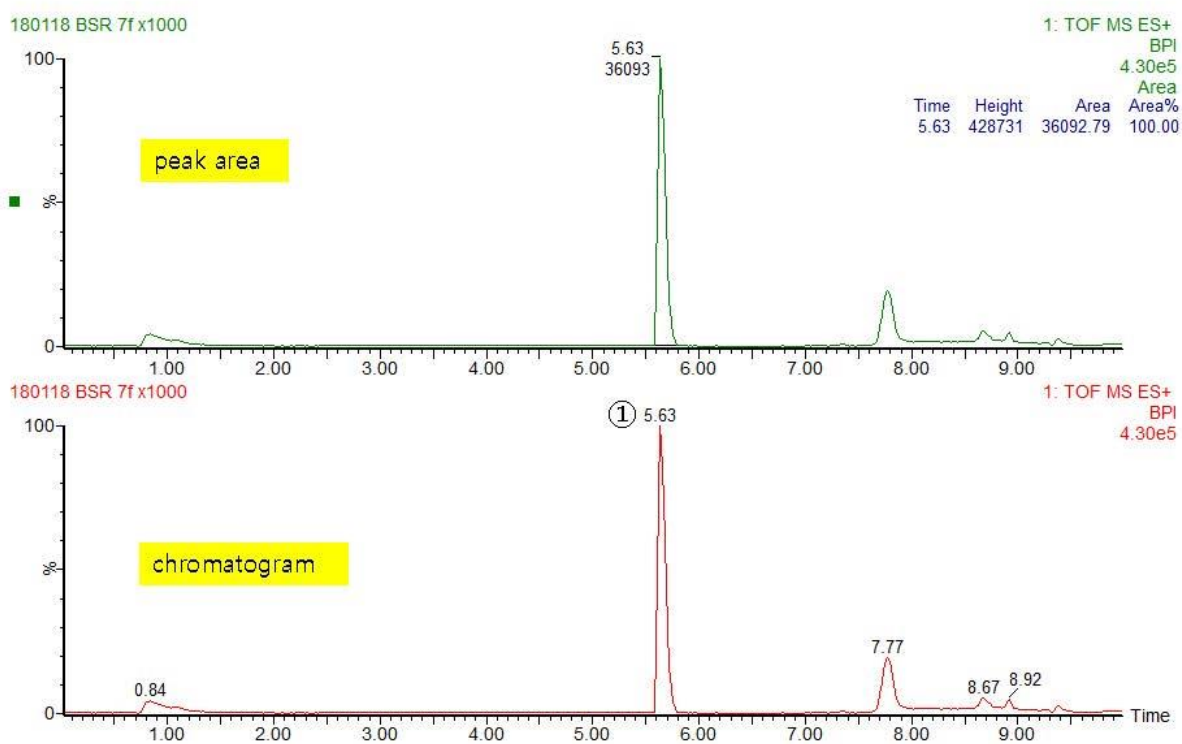
F2 - Acquisition Parameters
Date_    20180129
Time     17.51 h
INSTRUM  spect
PROBHD   E1C8618_0941 (
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        874
DS        4
SWH       24038.461 Hz
FIDRES    0.733598 Hz
AQ         1.3631488 sec
RG         198.73
DW         20.800 usec
DE         6.50 usec
TE         301.7 K
D1         2.0000000 sec
d11       0.0300000 sec
TD0       1
SFO1      100.6228298 MHz
NUC1      13c
P1         10.00 usec
PLW1      47.0000000 W
SFO2      400.1316005 MHz
NUC2      1H
CPDPRG2   waltz16
PCPD2     90.00 usec
PLW2      13.0000000 W
PLW12     0.31457001 W
PLW13     0.15823001 W

F2 - Processing parameters
SI         32768
SF         100.6127685 MHz
WCM       EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

# Purity and HRMS of compound **5i**



## 18. 7f : chromatogram / area



18. 7f : mass spectrum

Molecular formula:  $C_{19}H_{17}ClFN_3O_4S$

Exact mass: 437.0612

110.2731 (4+)

146.6949 (3+)

219.5384 (2+)

438.0691 (1+)

