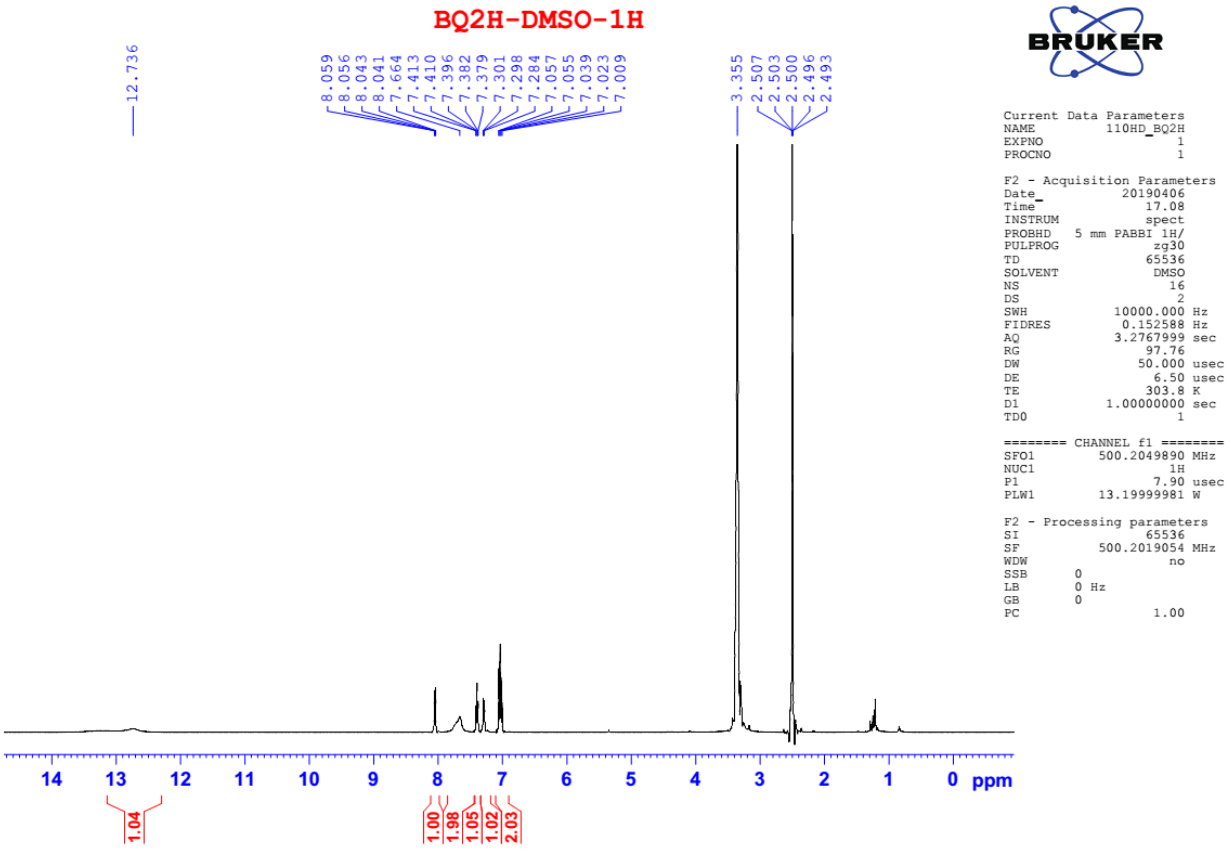
2-(5-Chloro-1H-benzoimidazol-2-yl)-phenol (**15**):

^{1}H – NMR

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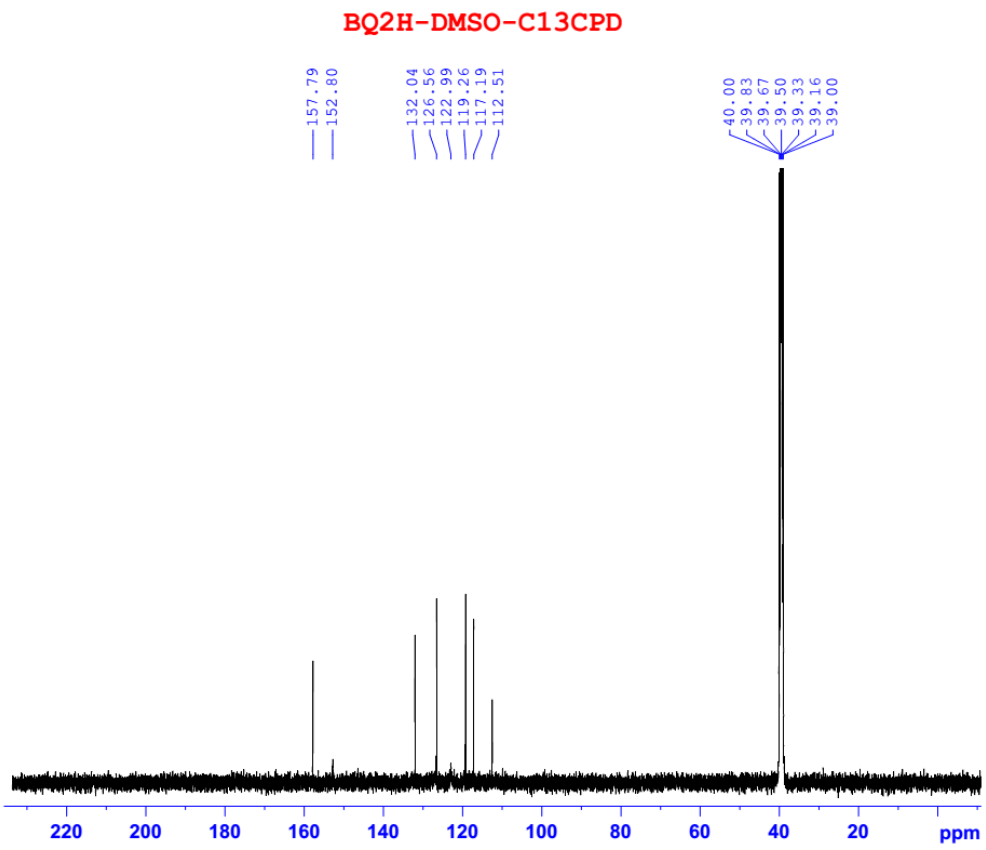
Current Data Parameters
NAME          110HD_BQ2H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190406
Time              17.08
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                97.76
DW               50.000 usec
DE                6.50 usec
TE               303.8 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        500.2049890 MHz
NUC1               1H
P1                7.90 usec
PLW1        13.19999981 W

F2 - Processing parameters
SI               65536
SF          500.2019054 MHz
WDW                no
SSB       0
LB        0 Hz
GB        0
PC                1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME            110HD_BQ2H
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20190409
Time                 7.05
INSTRUM             spect
PROBHD    5 mm PABBI 1H/
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   2048
DS                      4
SWH             31250.000 Hz
FIDRES          0.476837 Hz
AQ              1.0485760 sec
RG                 198.57
DW                 16.000 usec
DE                  6.50 usec
TE                 305.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          125.7897032 MHz
NUC1                  13C
P1                  15.40 usec
PLW1          81.00000000 W

======== CHANNEL f2 ========
SFO2          500.2039008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          13.19999981 W
PLW12          0.12872000 W
PLW13          0.08238100 W

F2 - Processing parameters
SI                   32768
SF            125.7759310 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

HRMS

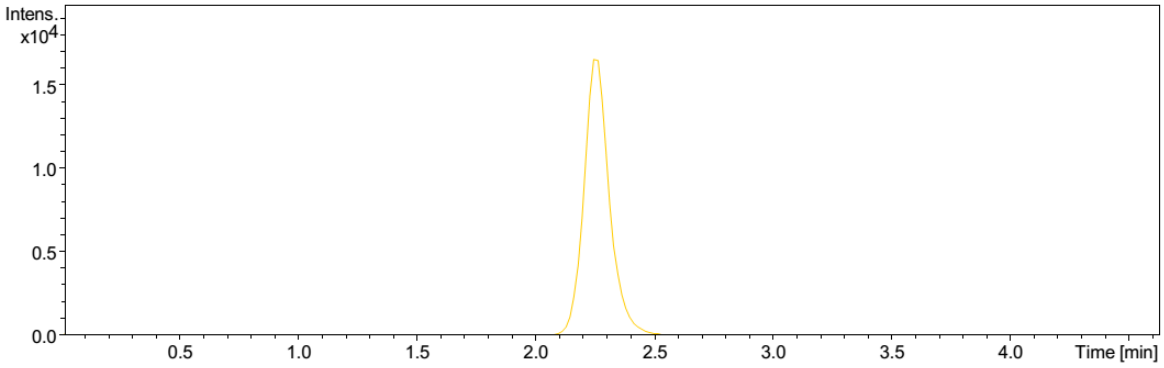
Display Report

Analysis Info

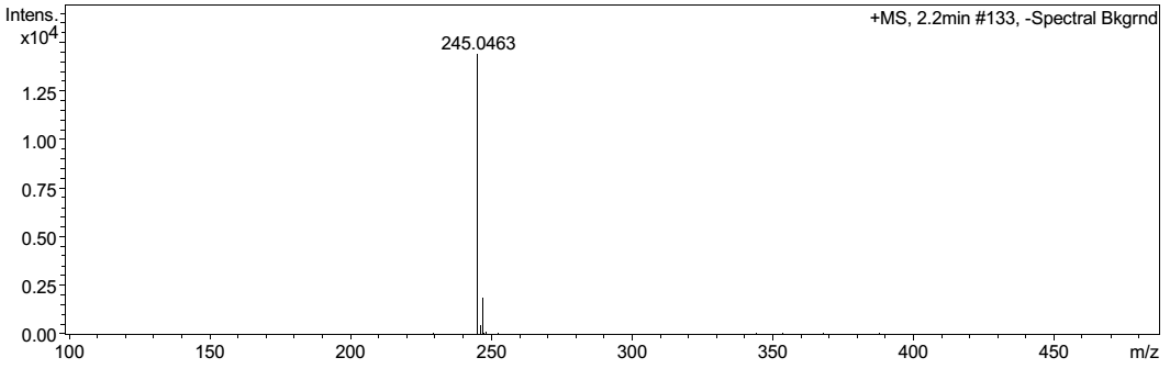
Analysis Name	D:\Data\2019\thang 05\BQ2H_1-F,4_01_1753.d	Acquisition Date	6/21/2019 7:30:49 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BQ2H	Instrument	micrOTOF-Q 10187
Comment			

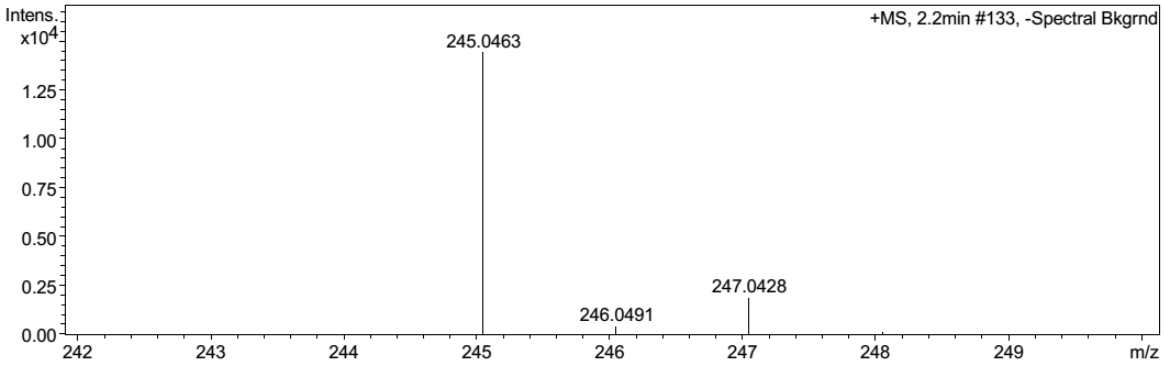
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



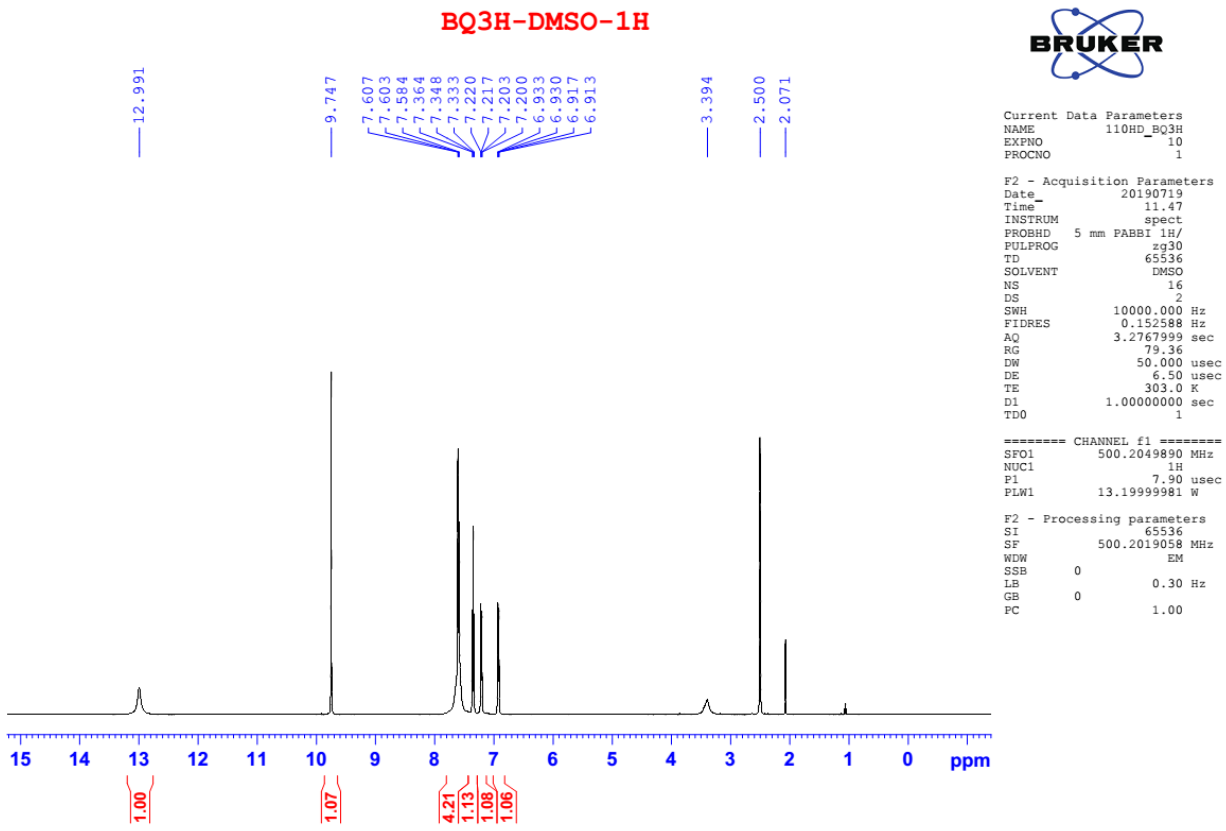
EIC 245.0000 +All MS, -Spectral Bkgrnd





3-(5-Chloro-1H-benzoimidazol-2-yl)-phenol (**16**):

^{1}H – NMR



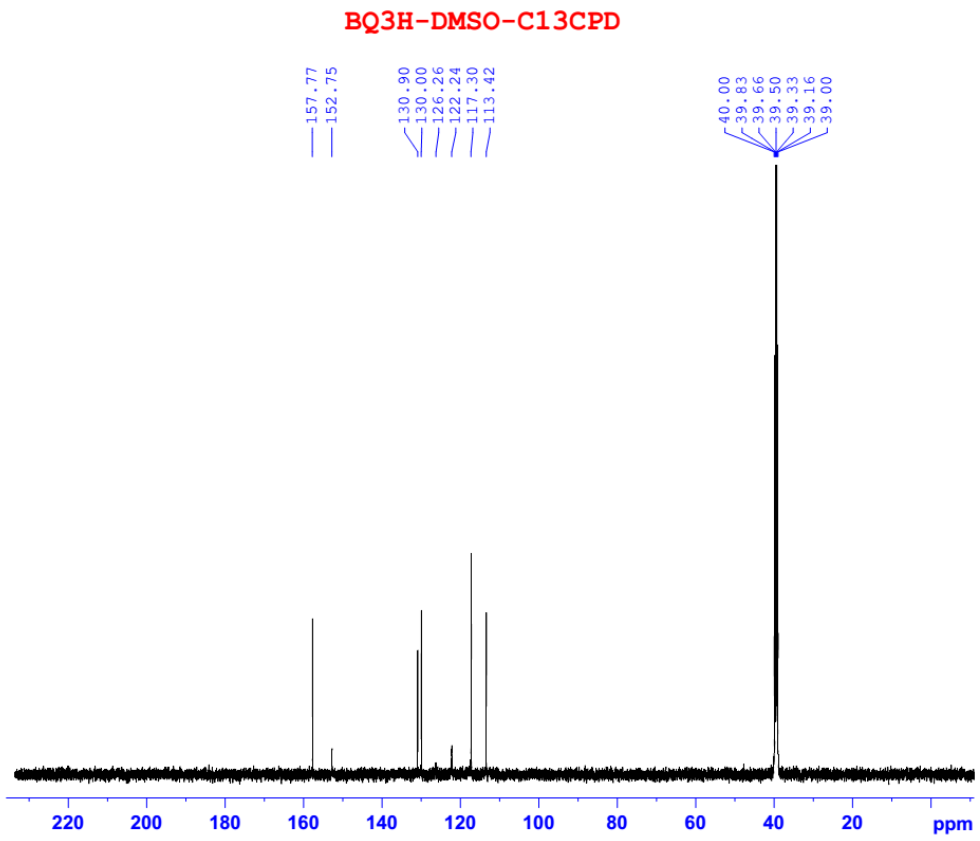

```
Current Data Parameters
NAME          110HD_BQ3H
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190719
Time              11.47
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                79.36
DW               50.000 usec
DE                6.50 usec
TE               303.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.2049890 MHz
NUC1                1H
P1                 7.90 usec
PLW1        13.19999981 W

F2 - Processing parameters
SI               65536
SF           500.2019058 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BQ3H
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190720
Time               22.20
INSTRUM            spect
PROBHD    5 mm PABBI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                   128
DS                     4
SWH            31250.000 Hz
FIDRES          0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW                16.000 usec
DE                 6.50 usec
TE                303.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7897032 MHz
NUC1                 13C
P1                15.40 usec
PLW1         81.00000000 W

======== CHANNEL f2 ========
SFO2         500.2039008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         13.19999981 W
PLW12         0.12872000 W
PLW13         0.08238100 W

F2 - Processing parameters
SI                 32768
SF           125.7759325 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HRMS

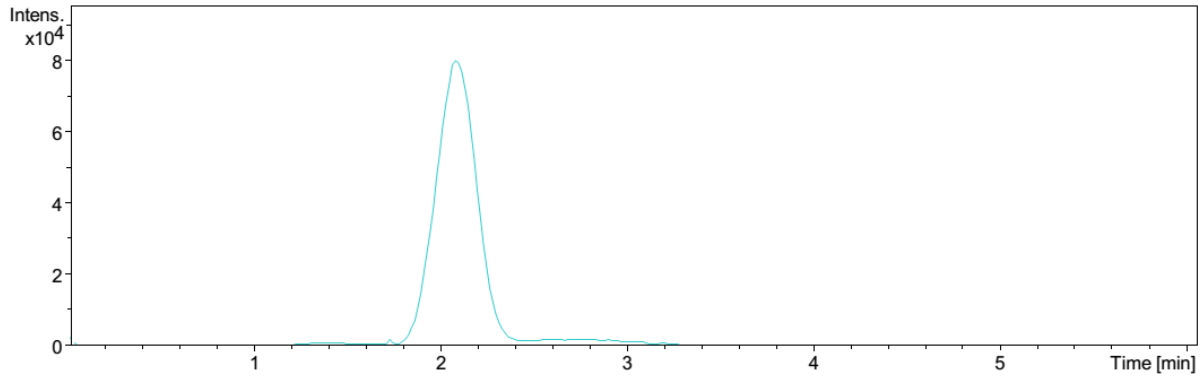
Display Report

Analysis Info

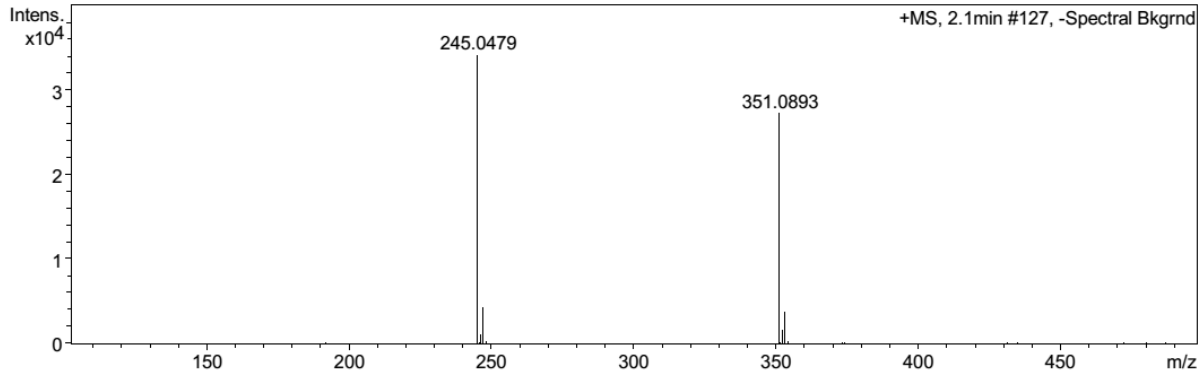
Analysis Name	D:\Data\2019\thang 05\BQ3H_2-E,8_01_1724.d	Acquisition Date	6/20/2019 10:00:09 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BQ3H	Instrument	micrOTOF-Q 10187
Comment			

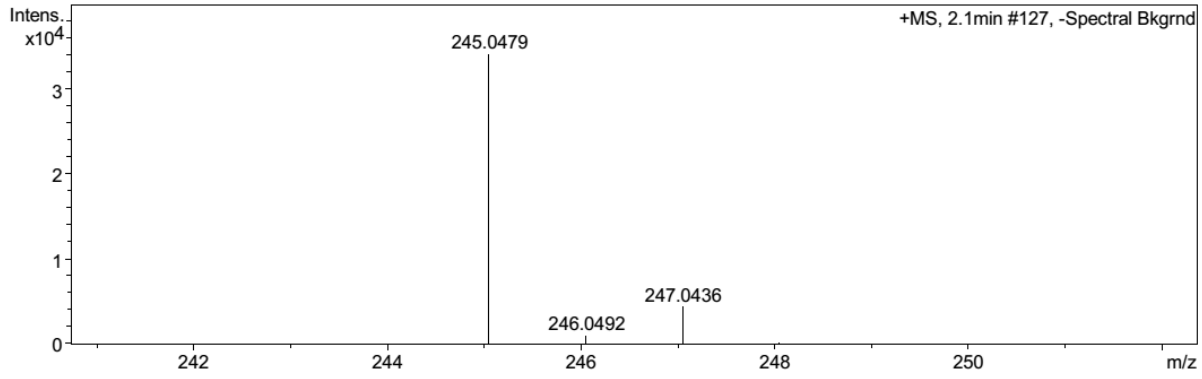
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



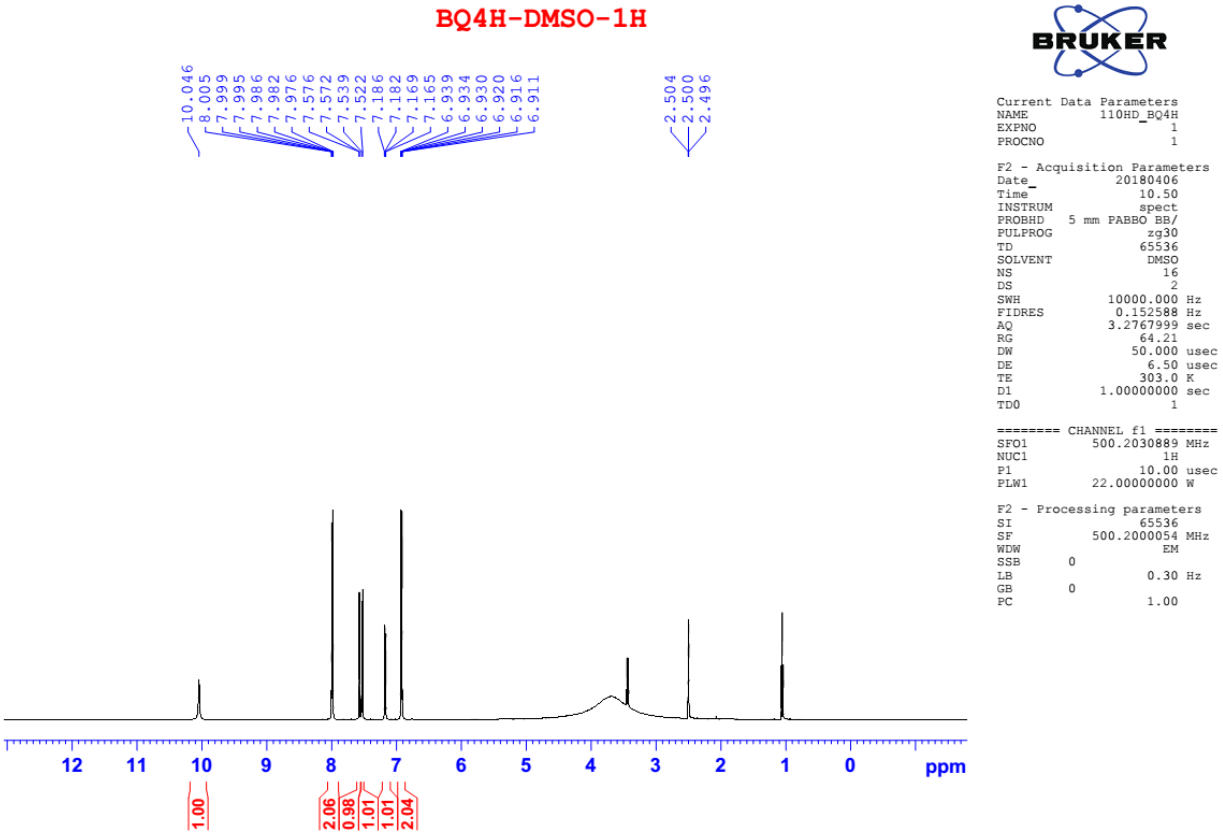
TIC +All MS, -Spectral Bkgrnd





3-(5-Chloro-1H-benzoimidazol-2-yl)-phenol (**17**):

^{1}H – NMR



BRUKER

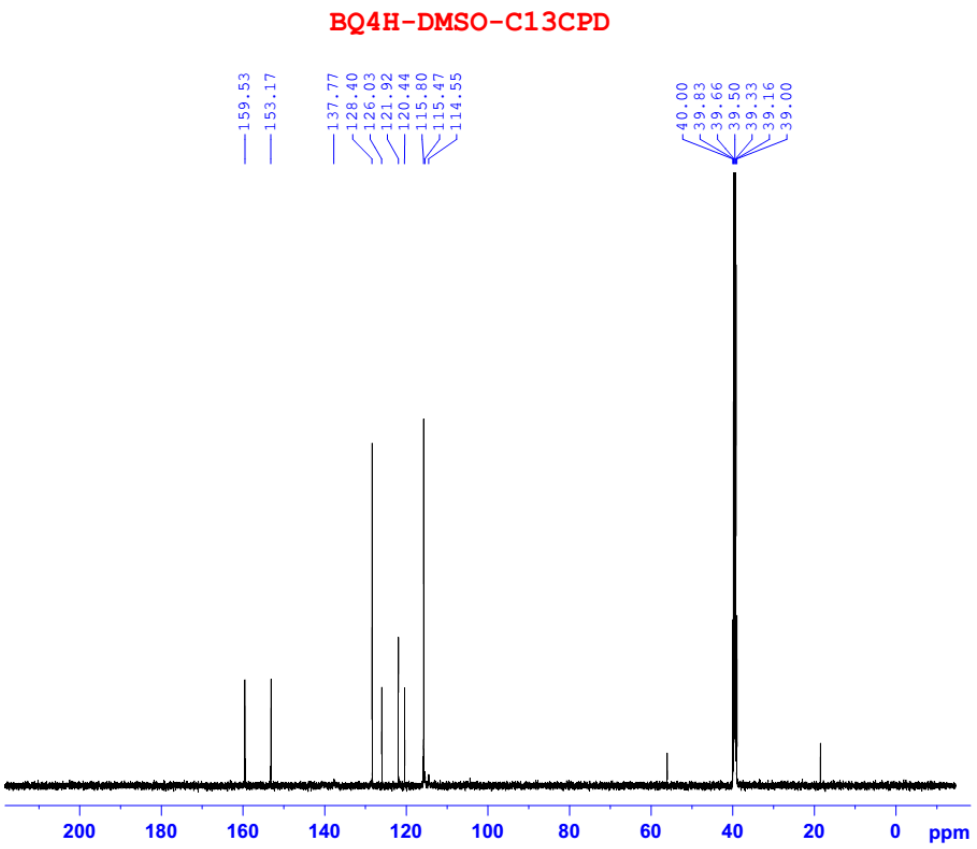
```
Current Data Parameters
NAME          110HD_BQ4H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180406
Time              10.50
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                64.21
DW               50.000 usec
DE                6.50 usec
TE               303.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                   1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.2000054 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BQ4H
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180406
Time              12.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT            DMSO
NS                   256
DS                     4
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG                198.57
DW               16.000 usec
DE                6.50 usec
TE                303.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        125.7892253 MHz
NUC1                  13C
P1                  10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

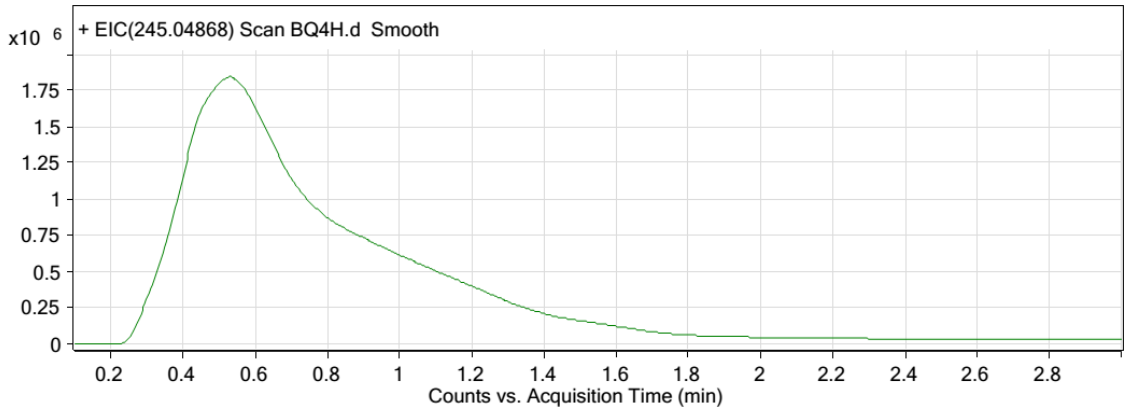
F2 - Processing parameters
SI                 32768
SF          125.7754470 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

Qualitative Analysis Report

Data File	BQ4H.d	**Sample Name**	BQ4H
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	20/05/2018 6:00:21 PM
IRM Calibration Status	Success	**DA Method**	default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

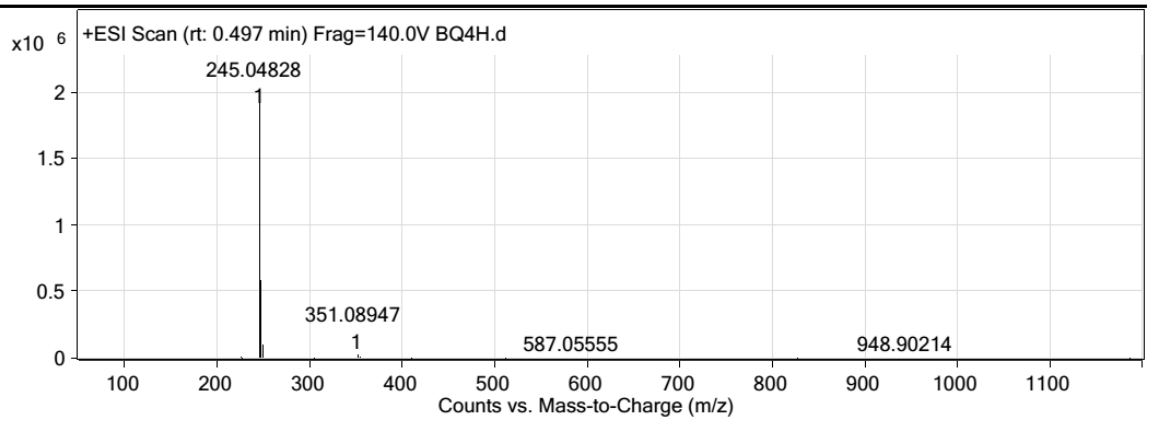
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



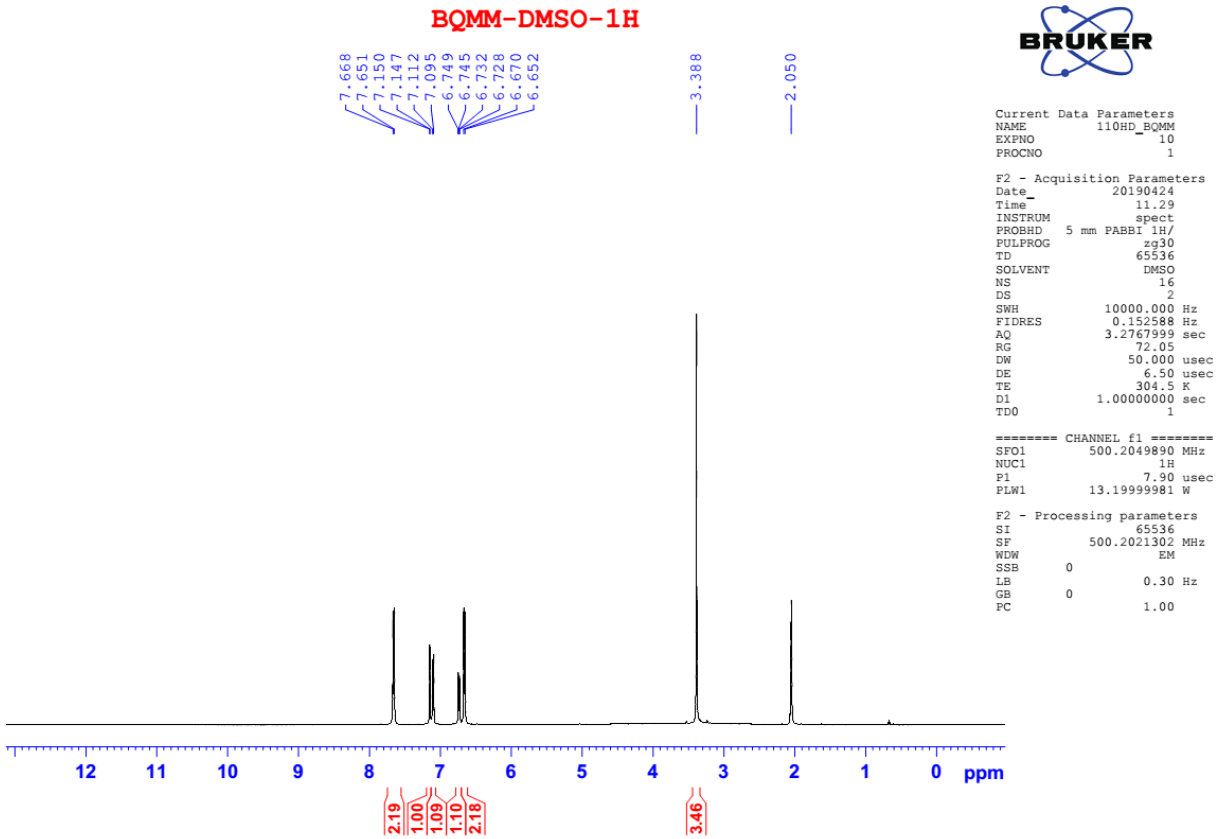
Peak List

m/z	z	Abund
225.10201	1	13228.71
245.04828	1	1961348.38
245.10911	1	145892.56
246.05177	1	254148.91
246.11394	1	17142.88
247.04558	1	586516.38
247.10827	1	45219.25
248.04842	1	92818.61
351.08947	1	28901.58
353.08737	1	8437.04

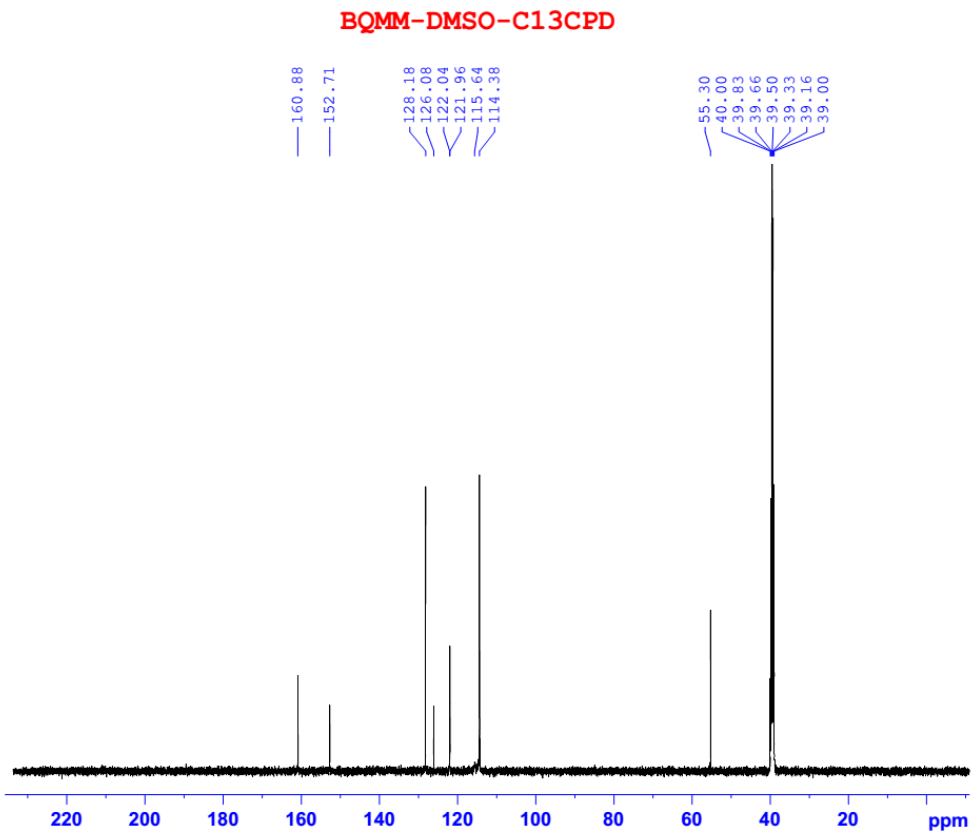
--- End Of Report ---

5-Chloro-2-(4-methoxy-phenyl)-1H-benzoimidazole (**18**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME            110HD_BQMM
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20190424
Time                15.02
INSTRUM             spect
PROBHD   5 mm PABBI 1H/
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                     256
DS                       4
SWH            31250.000 Hz
FIDRES          0.476837 Hz
AQ             1.0485760 sec
RG                 198.57
DW                 16.000 usec
DE                   6.50 usec
TE                  305.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         125.7897032 MHz
NUC1                  13C
P1                  15.40 usec
PLW1         81.00000000 W

======== CHANNEL f2 ========
SFO2         500.2039008 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2         13.19999981 W
PLW12         0.12872000 W
PLW13         0.08238100 W

F2 - Processing parameters
SI                   32768
SF           125.7759340 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

HRMS

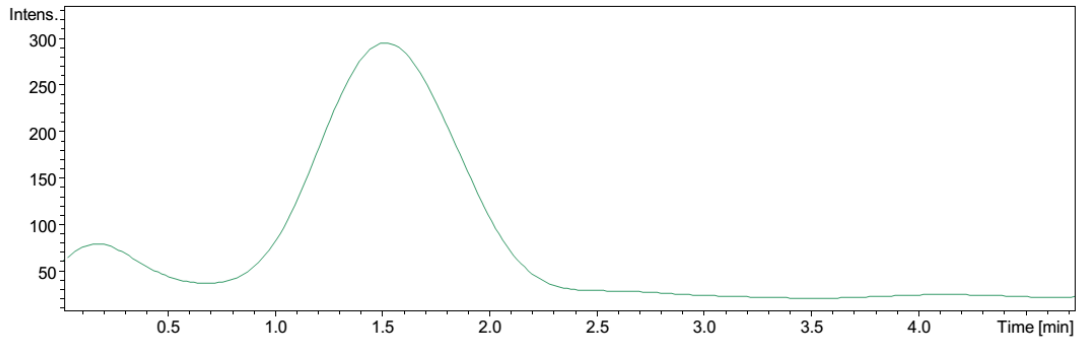
Display Report

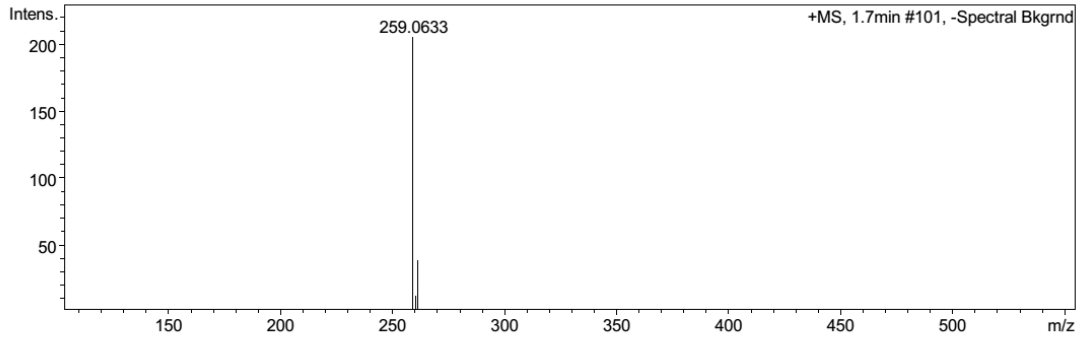
Analysis Info

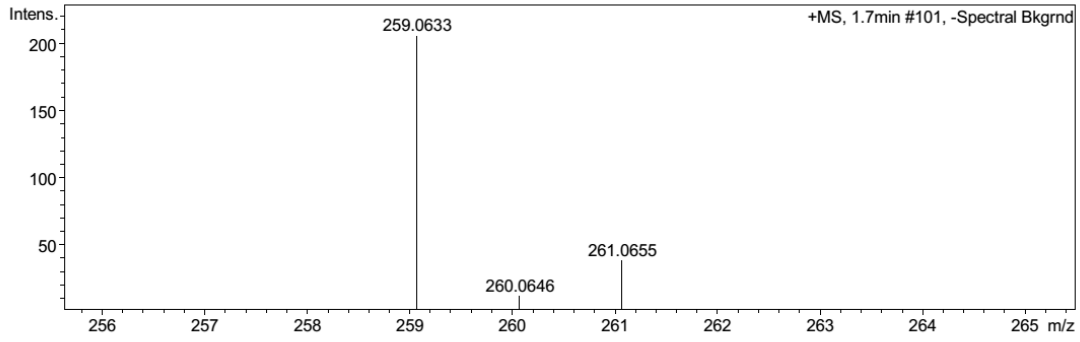
Analysis Name	D:\Data\2019\thang 05\BQMM_1-C,7_01_1714.d	Acquisition Date	6/20/2019 8:53:02 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BQMM	Instrument	micrOTOF-Q 10187
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

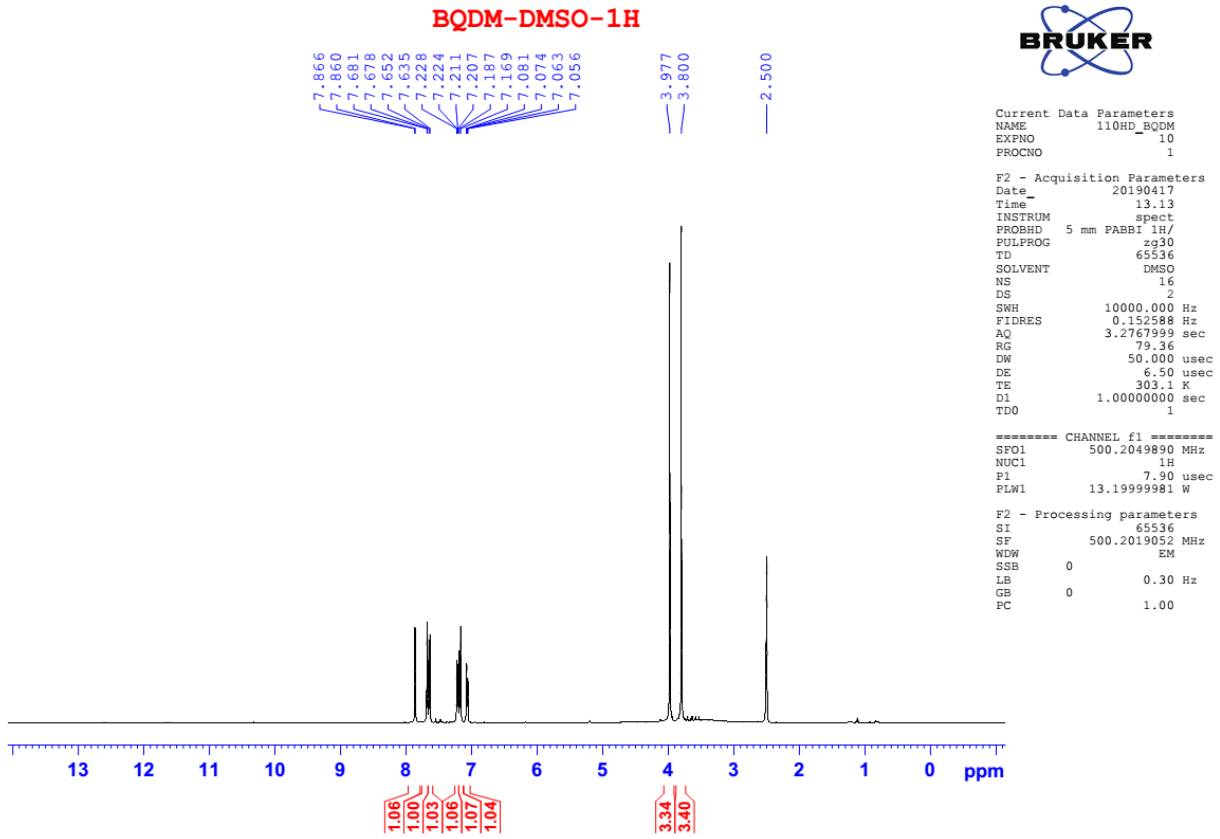




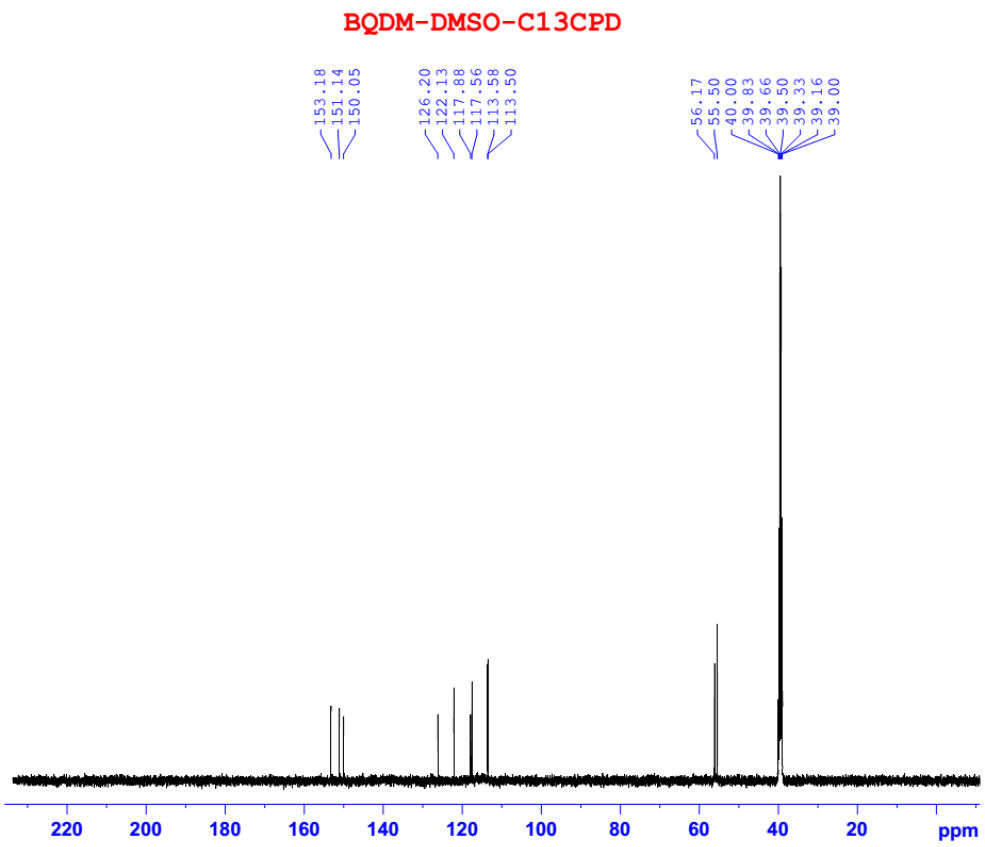


5-Chloro-2-(2,5-methoxy-phenyl)-1H-benzoimidazole (**19**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME              110HD_BQDM
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190417
Time                 17.09
INSTRUM              spect
PROBHD   5 mm PABBI 1H/
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                     256
DS                       4
SWH              31250.000 Hz
FIDRES           0.476837 Hz
AQ               1.0485760 sec
RG                  198.57
DW                  16.000 usec
DE                    6.50 usec
TE                   303.8 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            125.7897032 MHz
NUC1                    13C
P1                    15.40 usec
PLW1           81.00000000 W

======== CHANNEL f2 ========
SFO2            500.2039008 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 80.00 usec
PLW2           13.19999981 W
PLW12           0.12872000 W
PLW13           0.08238100 W

F2 - Processing parameters
SI                     32768
SF              125.7759344 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

HRMS

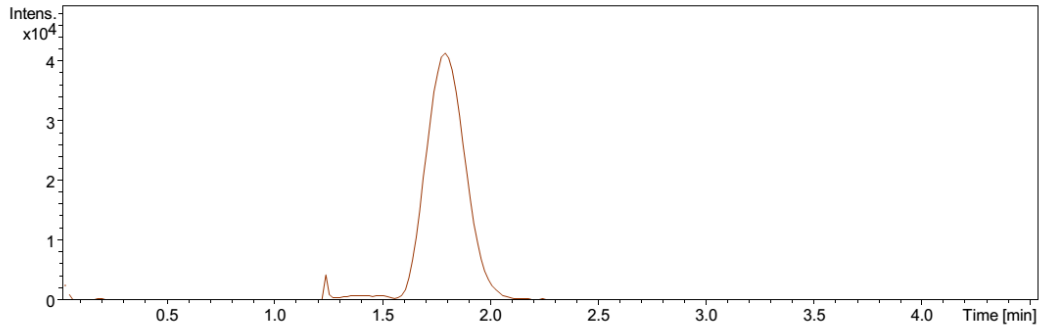
Display Report

Analysis Info

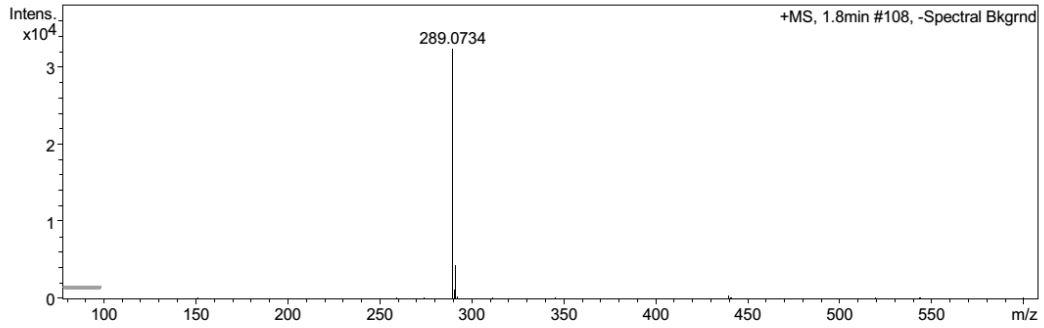
Analysis Name	D:\Data\2019\thang 05\BQDM_2-C,9_01_1727.d	Acquisition Date	6/20/2019 10:20:19 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BQDM	Instrument	micrOTOF-Q 10187
Comment			

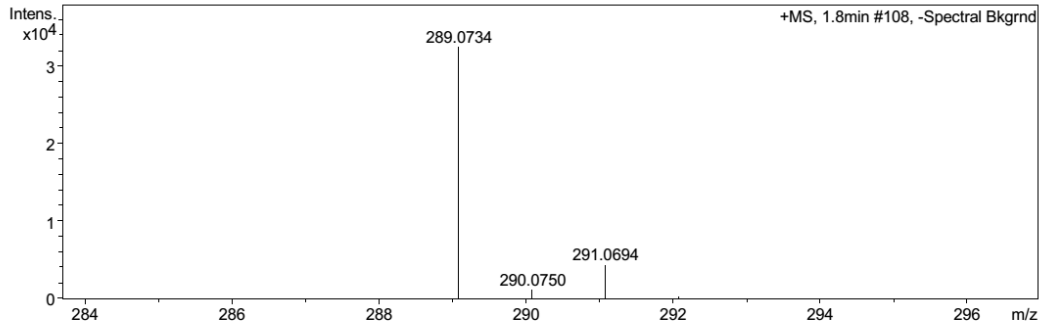
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



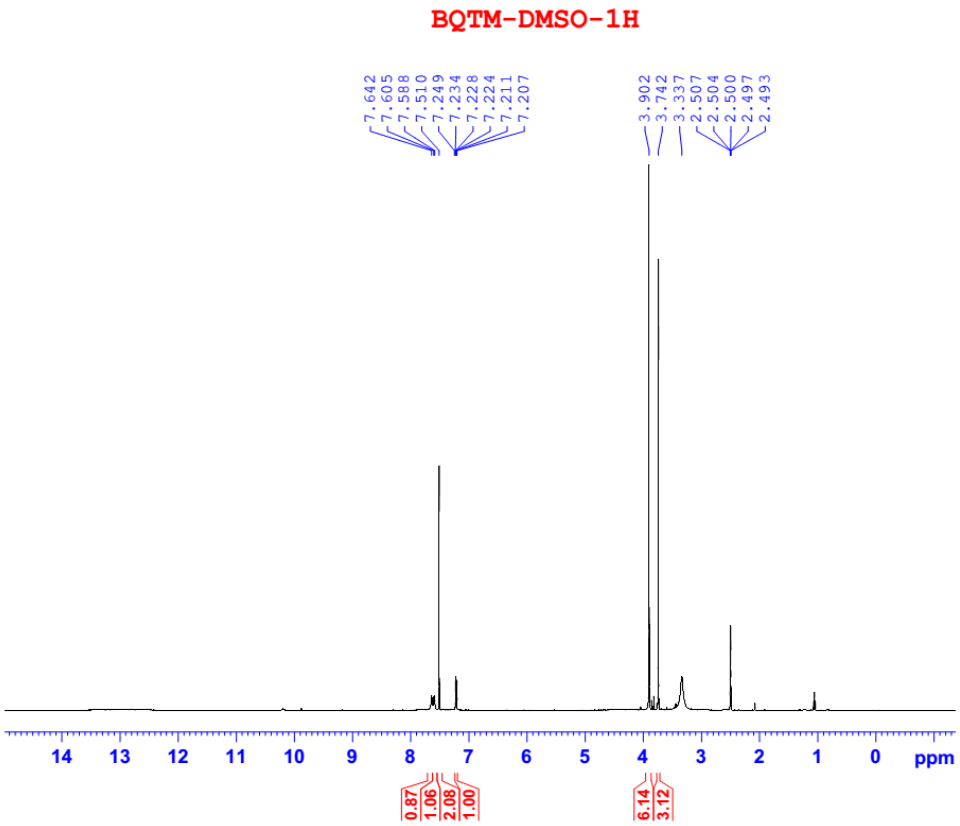
TIC +All MS, -Spectral Bkgrnd





5-Chloro-2-(3,4,5-trimethoxy-phenyl)-1H-benzoimidazole (**20**):

^{1}H – NMR



BRUKER

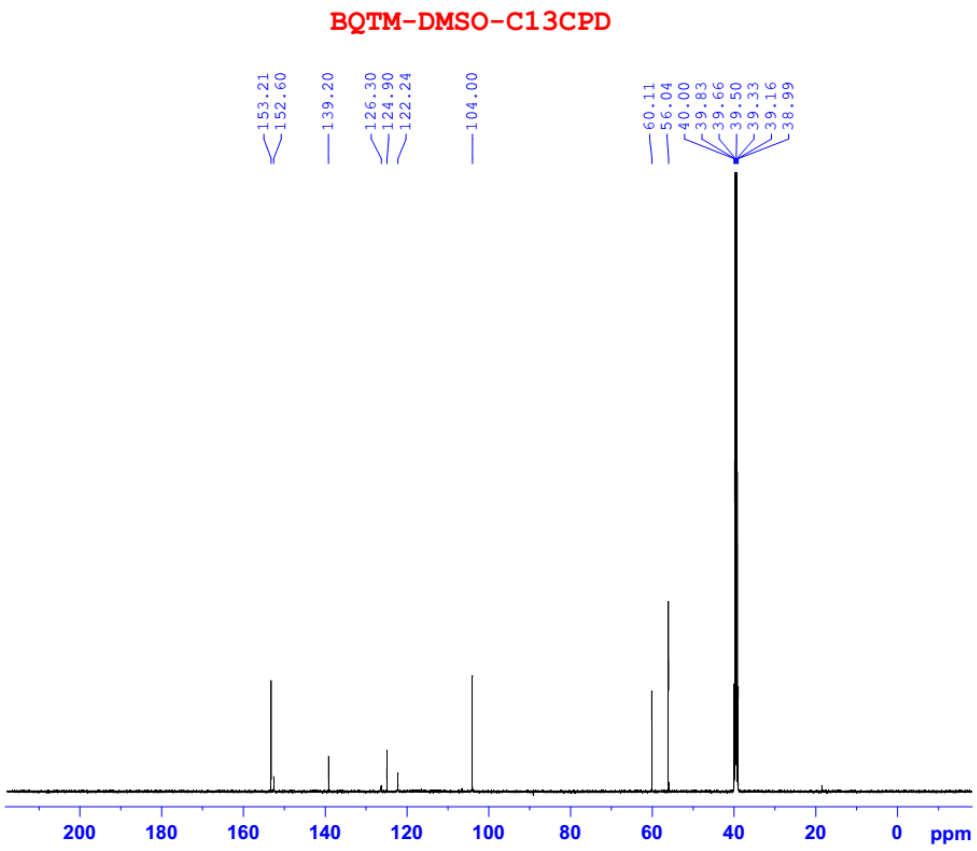
```
Current Data Parameters
NAME          110HD_BQTM
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171224
Time                6.23
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ              3.2767999 sec
RG                 89.63
DW                 50.000 usec
DE                  6.50 usec
TE                303.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000054 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME         110HD_BQTM
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20171224
Time               7.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1               13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                32768
SF          125.7754557 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

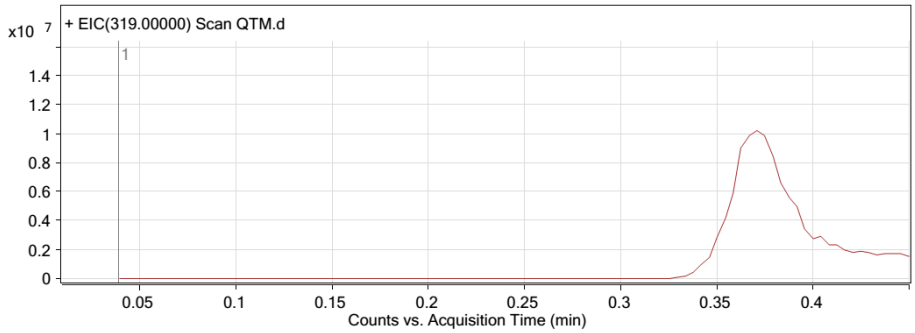
HRMS

Qualitative Analysis Report

Data File	QTM.d	**Sample Name**	QTM
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	17/01/2018 2:29:47 PM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

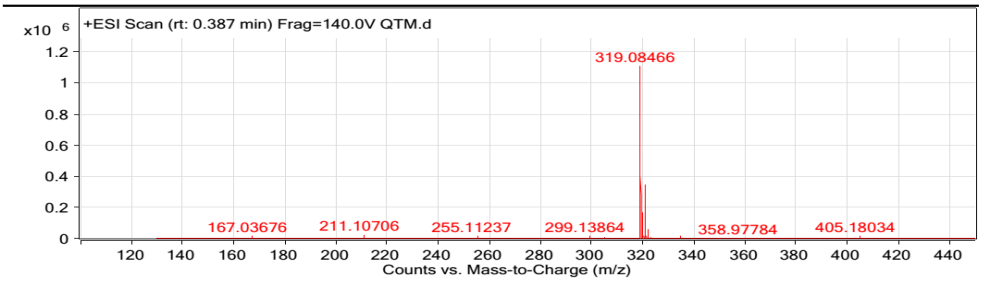
Fragmentor Voltage	14 0	**Collision Energy**	0	**Ionization Mode**	ES I



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



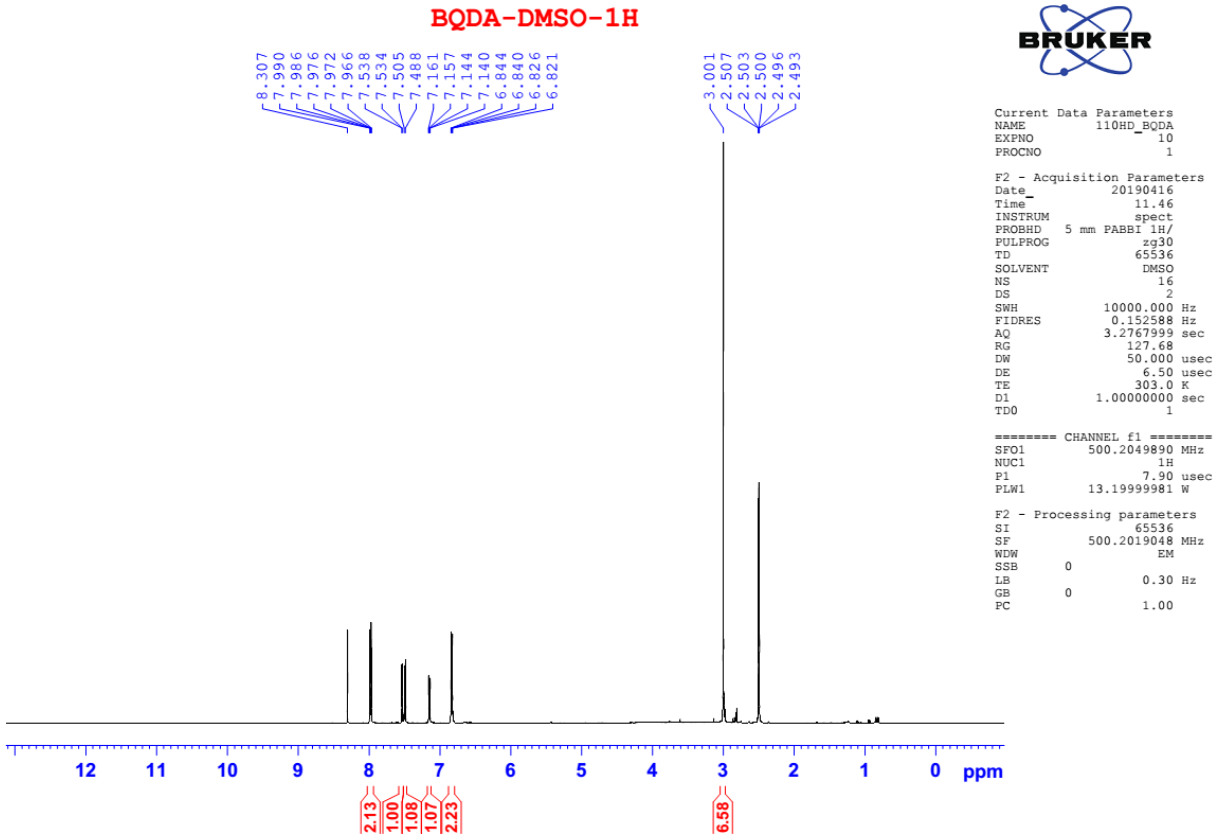
Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
S	0	5
Cl	0	3

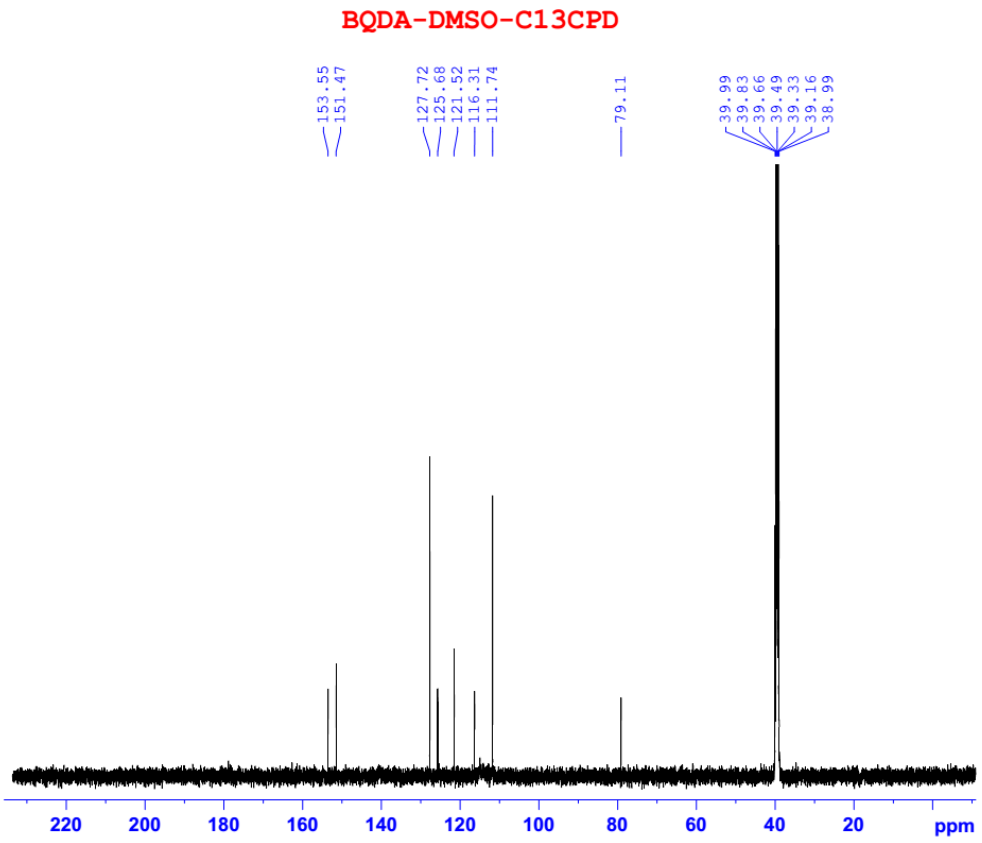
--- End Of Report ---

4-(5-Chloro-1H-benzoimidazol-2-yl)-N,N-dimethylaniline (**21**):

^{1}H – NMR



^{13}C – NMR




```
Current Data Parameters
NAME          110HD_BQDA
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190416
Time               12.35
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                  512
DS                    4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW                16.000 usec
DE                 6.50 usec
TE                303.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7897032 MHz
NUC1                 13C
P1                15.40 usec
PLW1         81.00000000 W

======== CHANNEL f2 ========
SFO2         500.2039008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         13.19999981 W
PLW12         0.12872000 W
PLW13         0.08238100 W

F2 - Processing parameters
SI                32768
SF           125.7759363 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HRMS

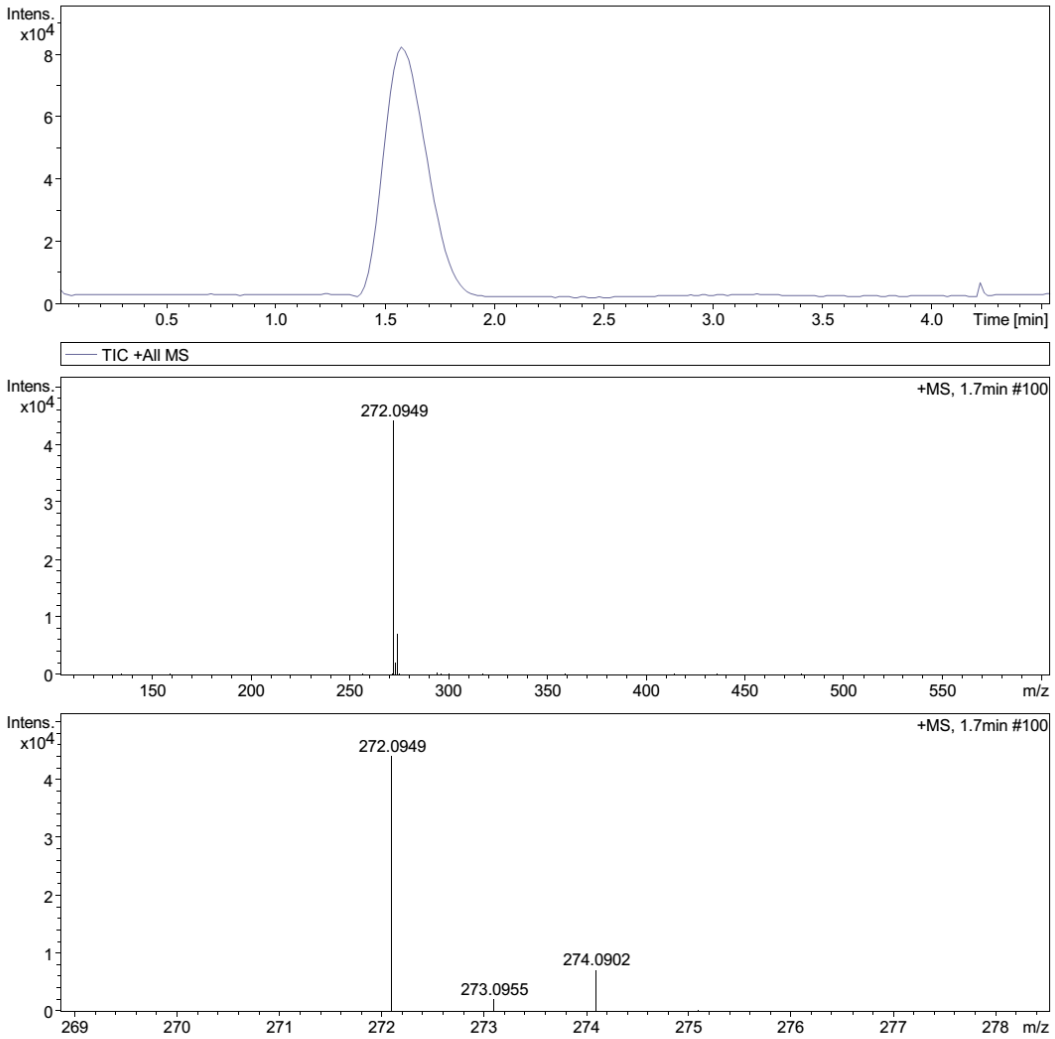
Display Report

Analysis Info

Analysis Name	D:\Data\2019\thang 05\BQDA_2-C,8_01_1728.d	Acquisition Date	6/20/2019 10:27:02 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BQDA	Instrument	micrOTOF-Q 10187
Comment			

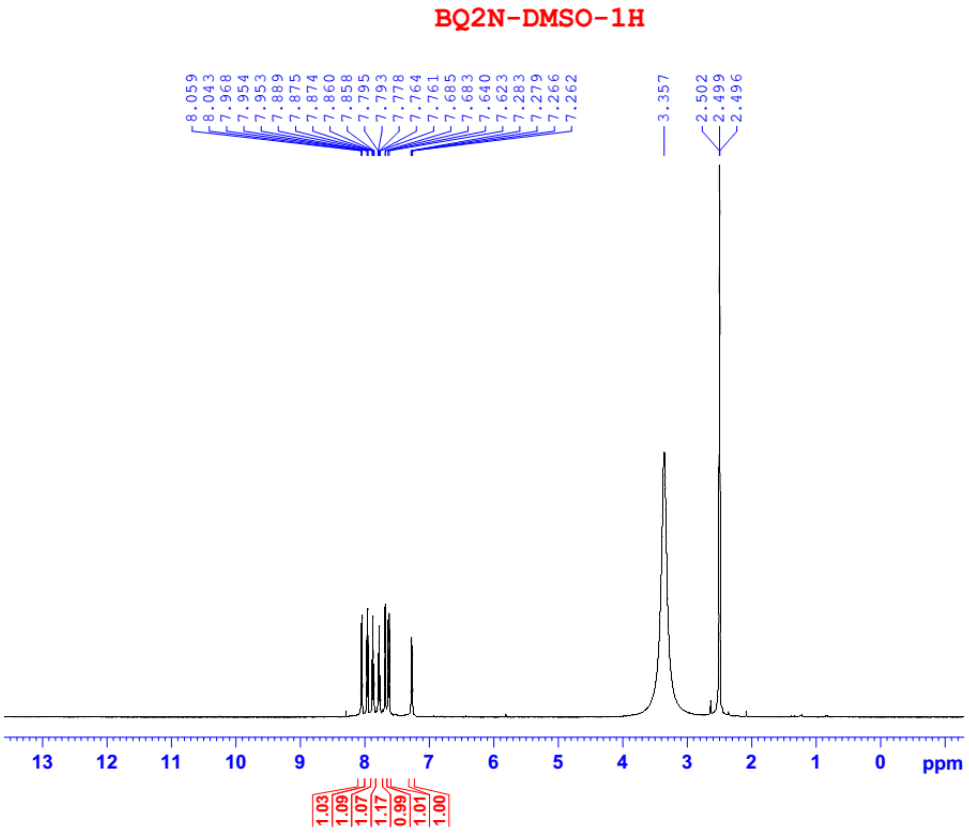
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



5-Chloro-2-(2-nitro-phenyl)-1H-benzoimidazole (**22**):

^{1}H – NMR



BRUKER

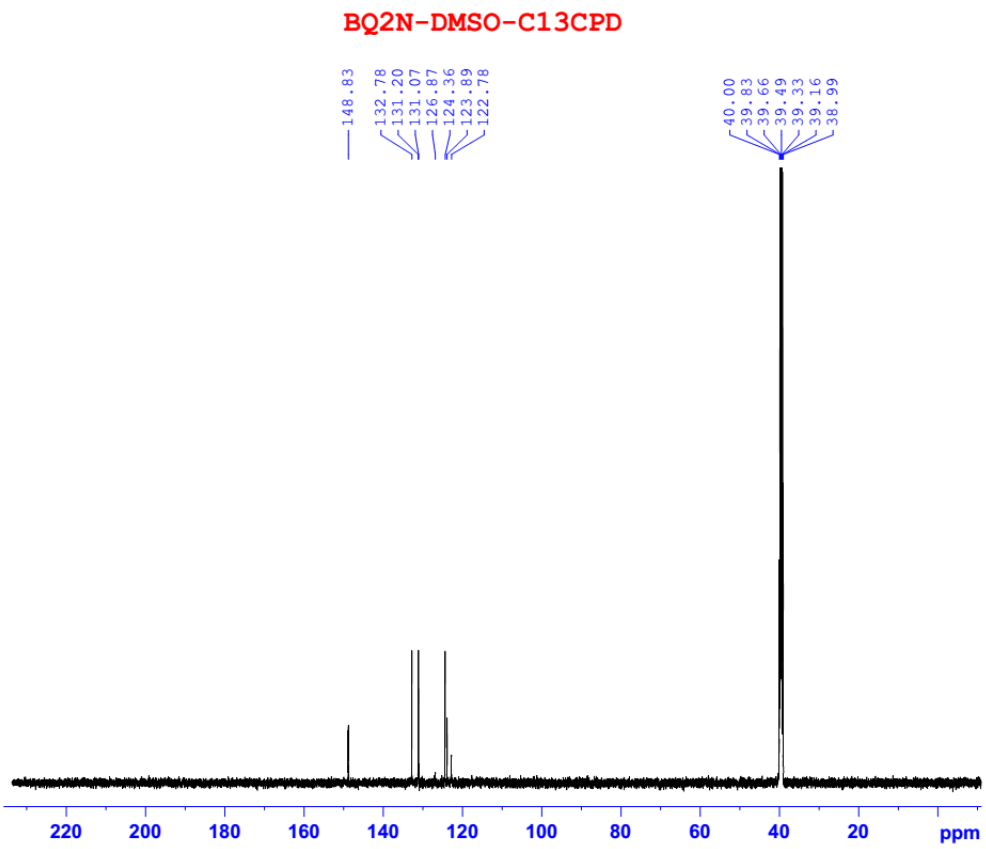
```
Current Data Parameters
NAME          110HD_BQ2N
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181005
Time               18.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ             3.2767999 sec
RG                 89.63
DW                 50.000 usec
DE                  6.50 usec
TE                304.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000067 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BQ2N
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181006
Time                9.45
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  2048
DS                     4
SWH            31250.000 Hz
FIDRES          0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW                16.000 usec
DE                 6.50 usec
TE                304.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7892253 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                 32768
SF           125.7754540 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HRMS

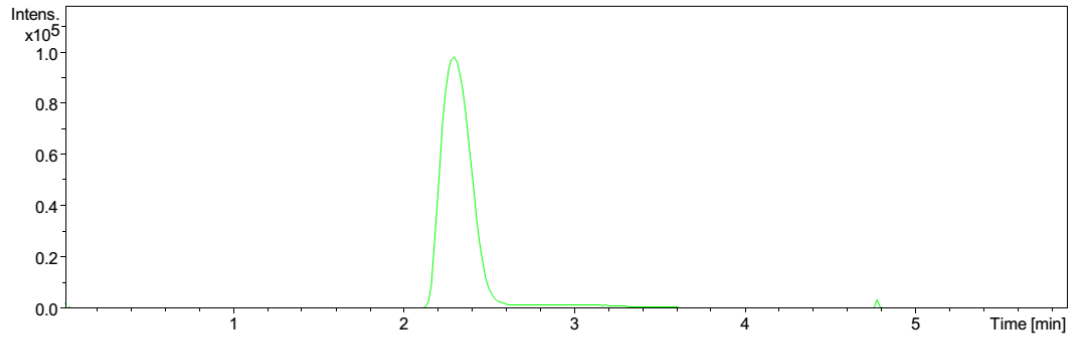
Display Report

Analysis Info

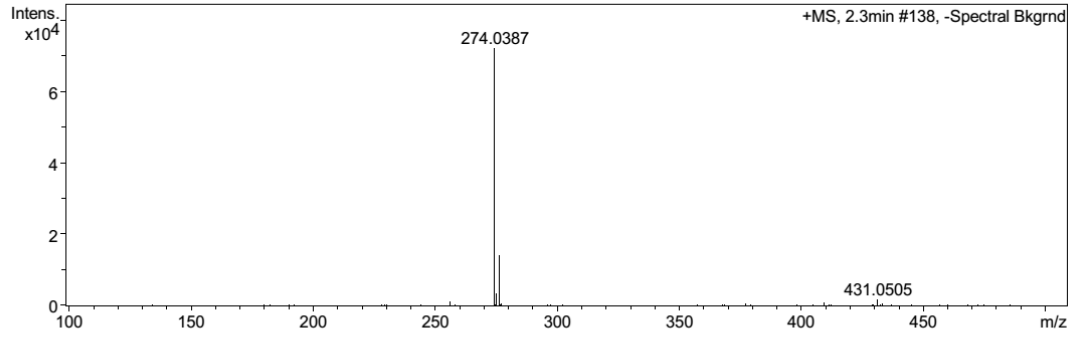
Analysis Name	D:\Data\2019\thang 05\BQ2N_1-F,5_01_1751.d	Acquisition Date	6/21/2019 7:19:05 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BQ2N	Instrument	micrOTOF-Q 10187
Comment			

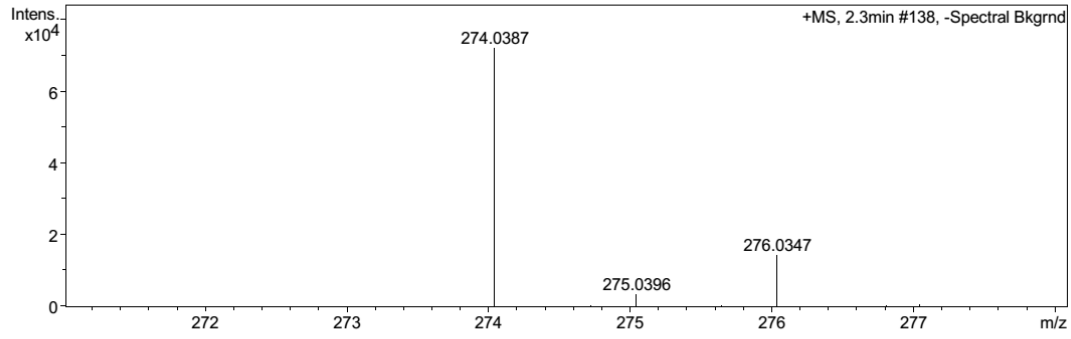
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



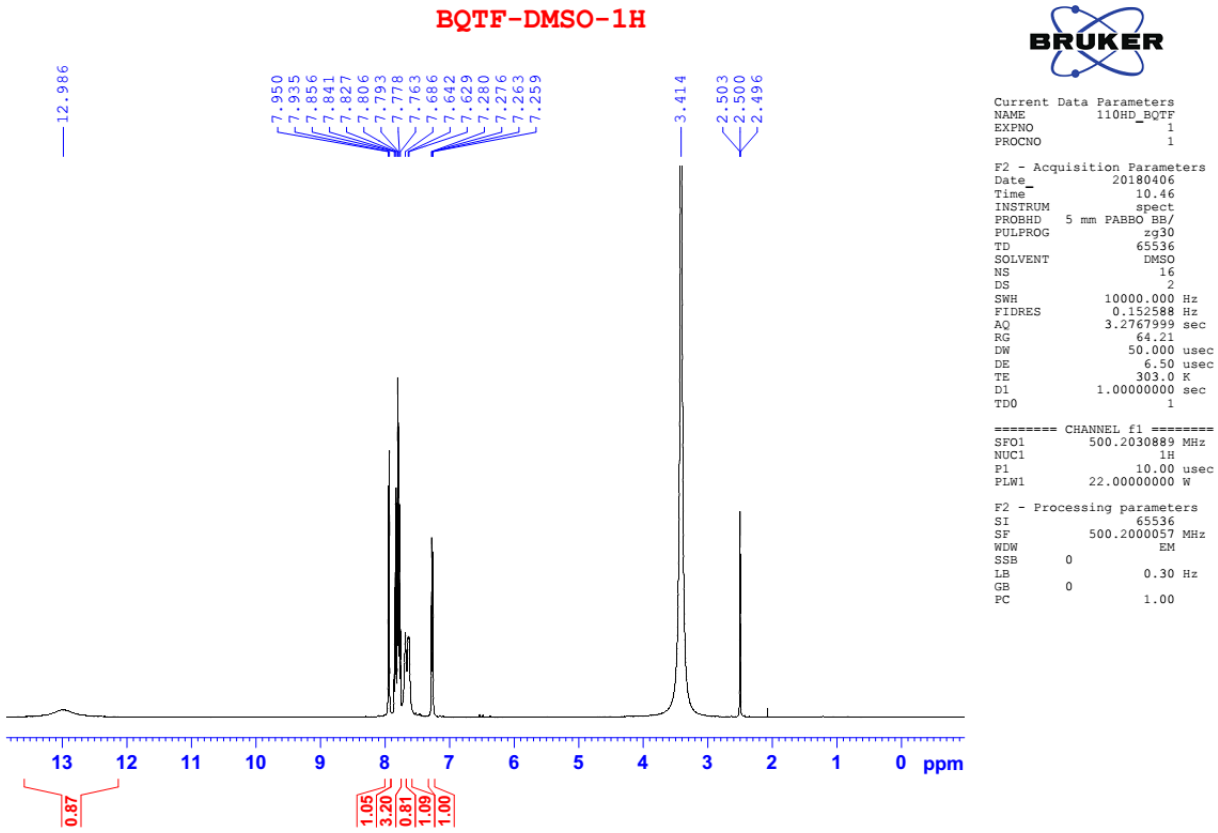
TIC +All MS, -Spectral Bkgrnd



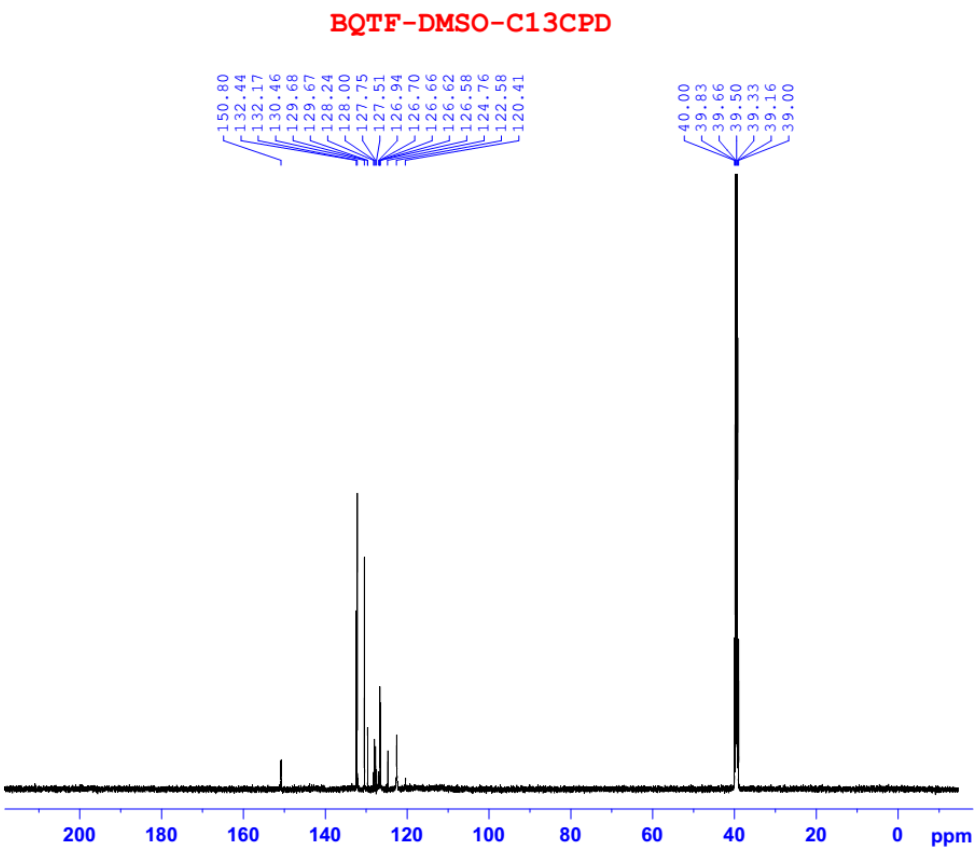


5-Chloro-2-(2-trifluoromethyl-phenyl)-1H-benzoimidazole (**23**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BQTF
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180406
Time              11.50
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT             DMSO
NS                    512
DS                      4
SWH           31250.000 Hz
FIDRES            0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW               16.000 usec
DE                6.50 usec
TE               303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7892253 MHz
NUC1                 13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                   32768
SF           125.7754478 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

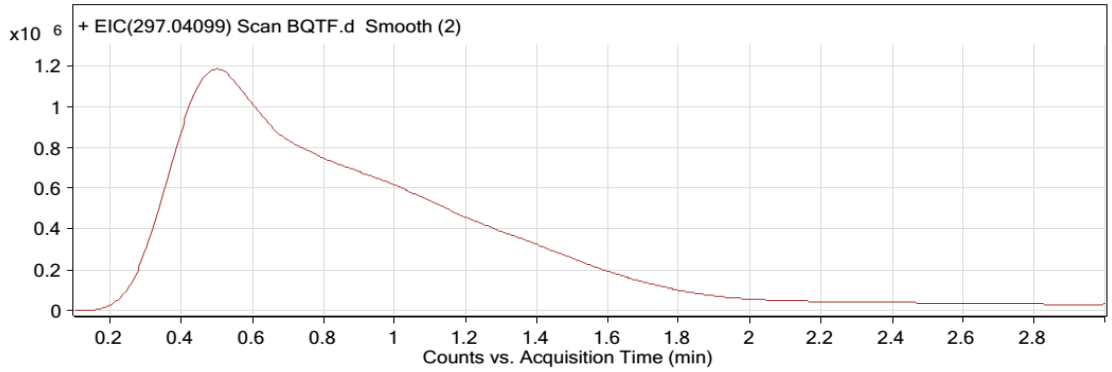
HRMS

Qualitative Analysis Report

Data File	BQTF.d	**Sample Name**	BQTF
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	20/05/2018 5:54:42 PM
IRM Calibration Status	Success	**DA Method**	default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

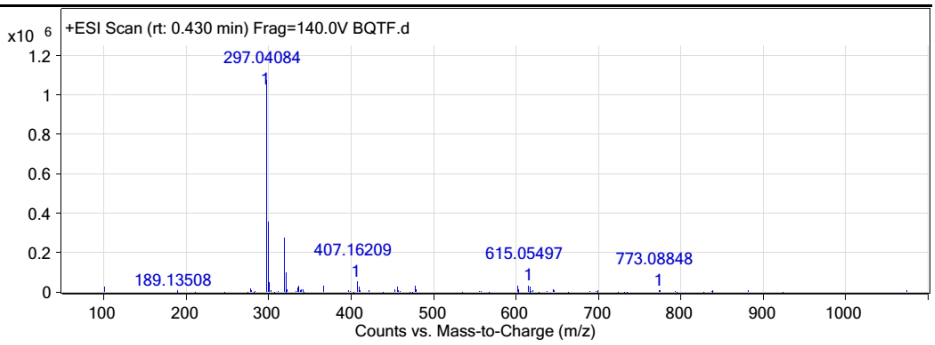
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



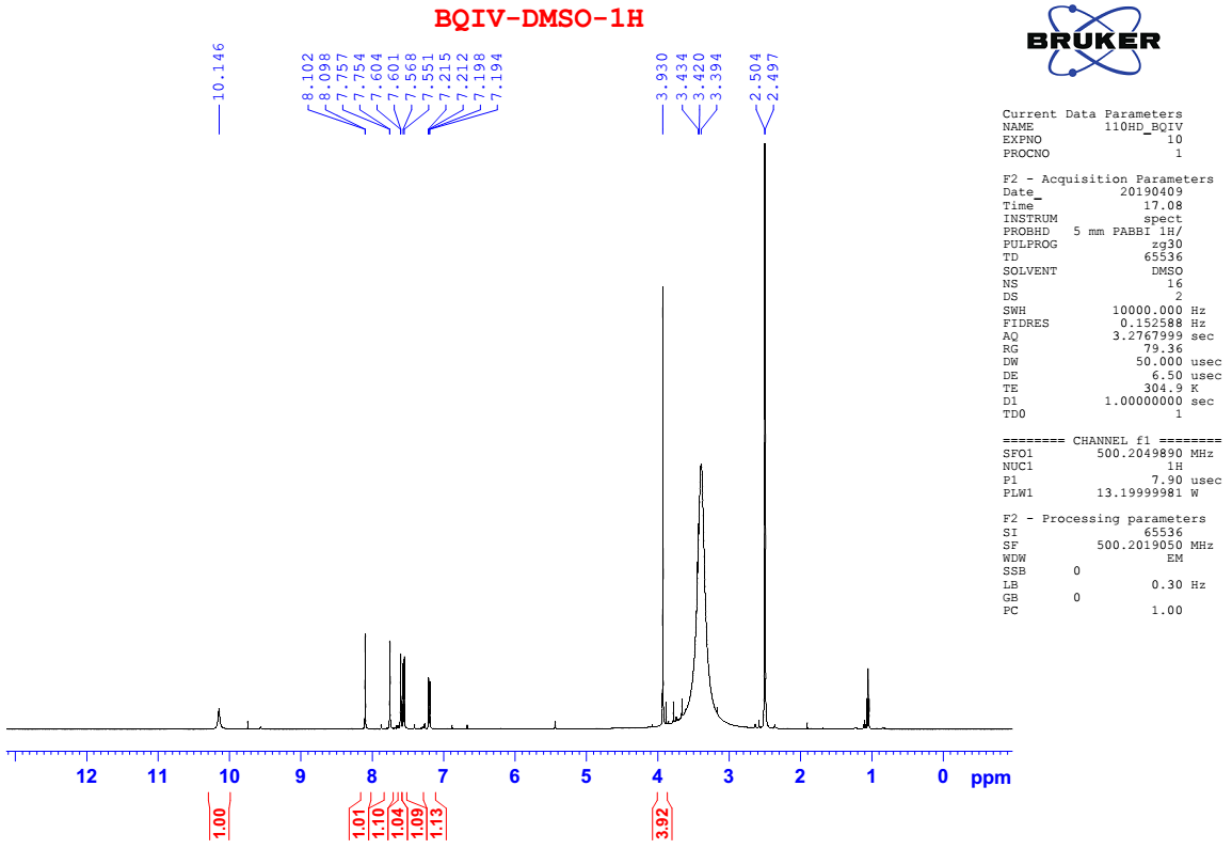
Peak List

m/z	z	Abund
297.04084	1	1081155.5
297.10731	1	84229.26
298.04399	1	158833.36
299.03864	1	357333.19
300.04083	1	55277.56
319.02346	1	278978.38
319.08468	1	49764.92
320.02548	1	47005.36
321.01983	1	98334.5
407.16209	1	54262.3

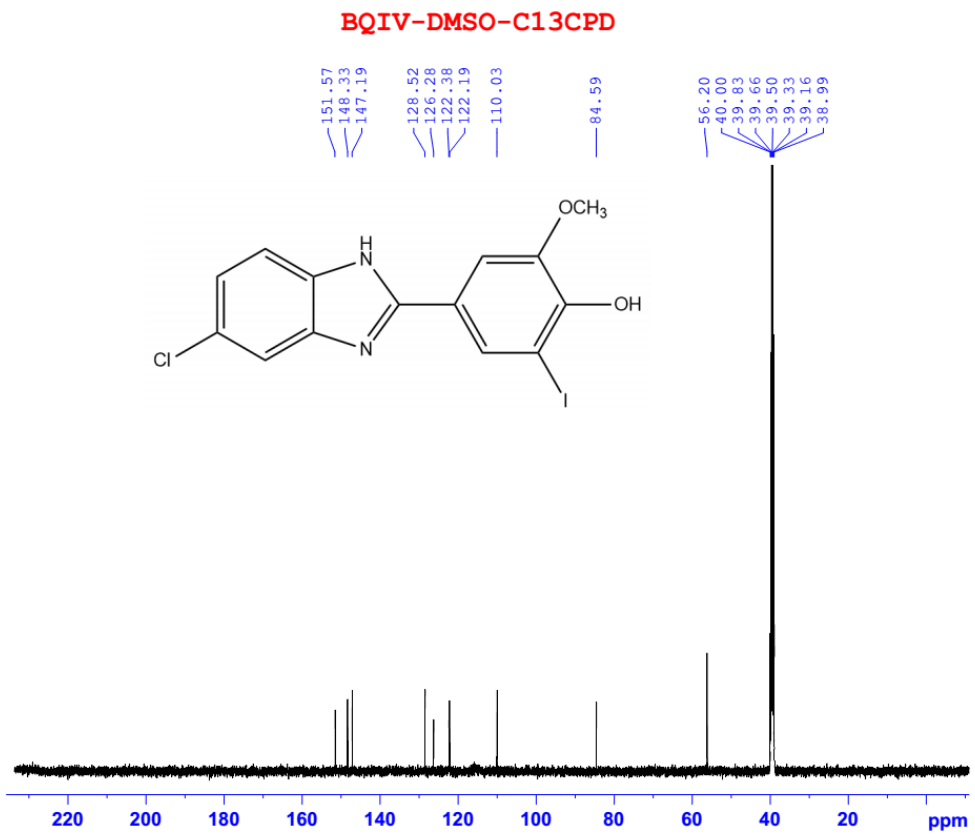
--- End Of Report ---

4-(5-Chloro-1H-Benzoimidazole-2-yl)-2 iodo-6-methoxy-phenol (**24**):

^{1}H – NMR



^{13}C – NMR




```
Current Data Parameters
NAME                 110HD_BQIV
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20190509
Time                      6.18
INSTRUM                 spect
PROBHD    5 mm PABBI 1H/
PULPROG                 zgpg30
TD                       65536
SOLVENT                    DMSO
NS                          512
DS                            4
SWH                 31250.000 Hz
FIDRES                0.476837 Hz
AQ                    1.0485760 sec
RG                       198.57
DW                       16.000 usec
DE                        6.50 usec
TE                       303.5 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1               125.7897032 MHz
NUC1                        13C
P1                        15.40 usec
PLW1               81.00000000 W

======== CHANNEL f2 ========
SFO2               500.2039008 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2               13.19999981 W
PLW12               0.12872000 W
PLW13               0.08238100 W

F2 - Processing parameters
SI                        32768
SF                 125.7759348 MHz
WDW                          EM
SSB             0
LB                        1.00 Hz
GB              0
PC                        1.40
```

HRMS

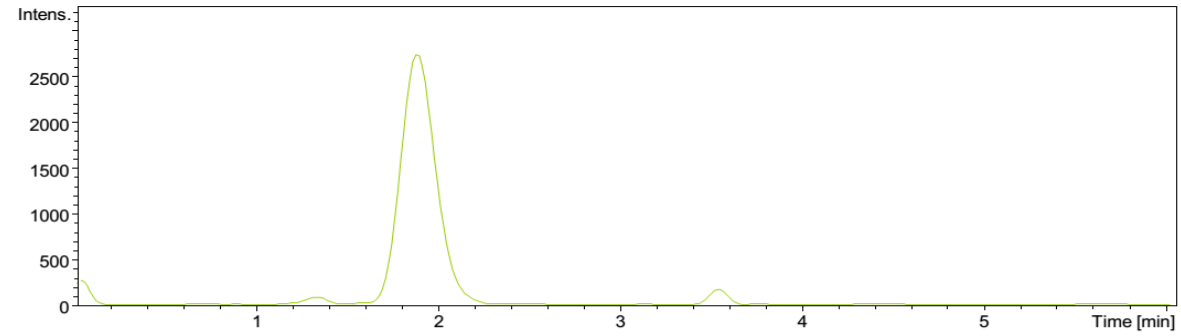
Display Report

Analysis Info

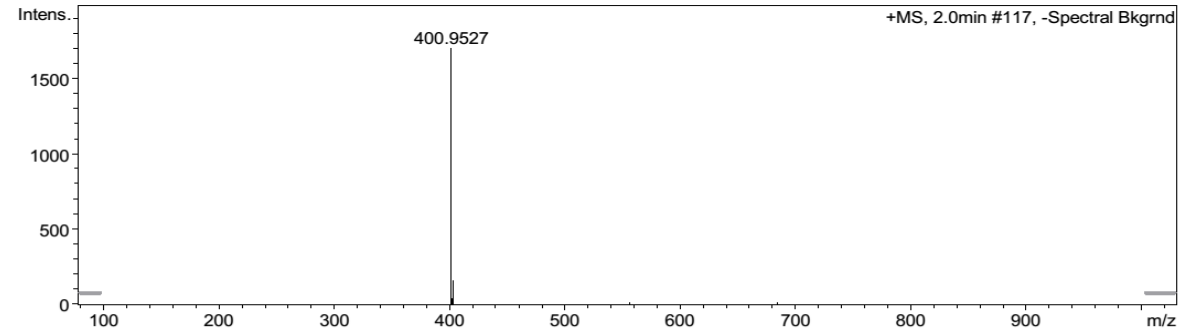
Analysis Name	D:\Data\2019\thang 05\BQIV_2-E,7_01_1723.d	Acquisition Date	6/20/2019 9:53:26 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BQIV	Instrument	micrOTOF-Q 10187
Comment			

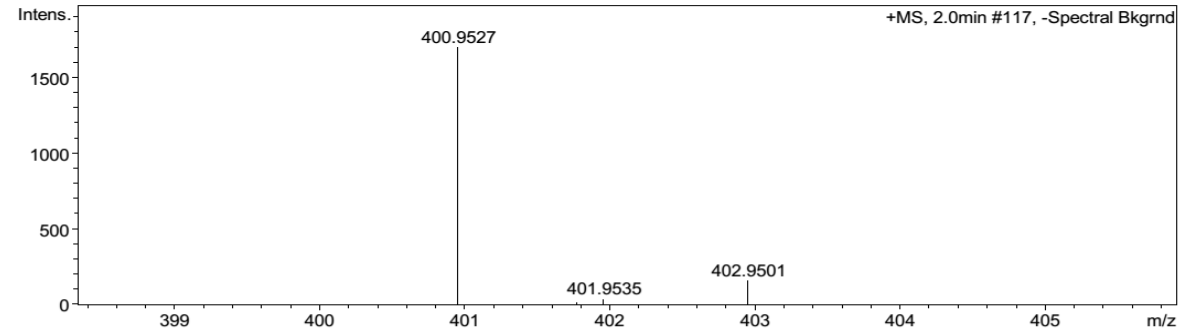
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



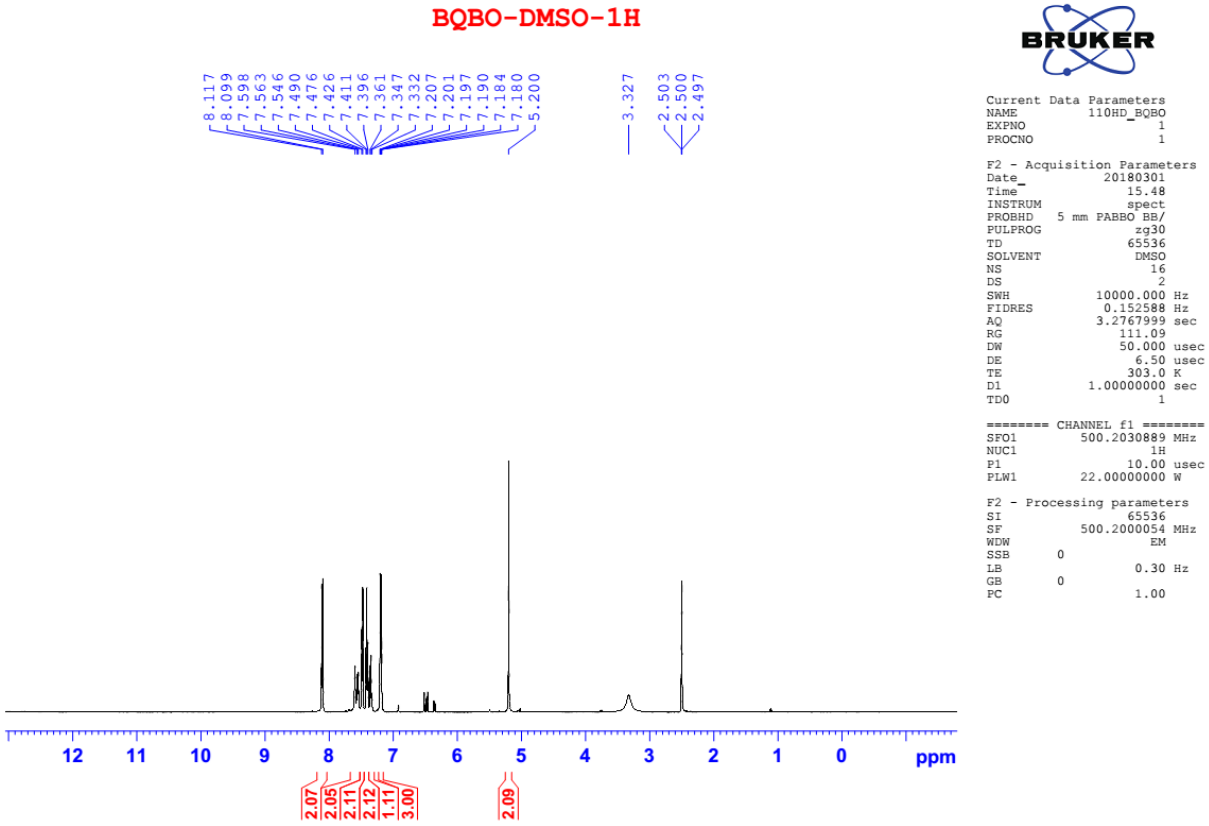
TIC +All MS, -Spectral Bkgrnd, Smoothed (2.01,2,GA)





2-(4-(Benzyloxy)phenyl)-5-chloro-1H-benzoimidazole (**25**):

^{1}H – NMR



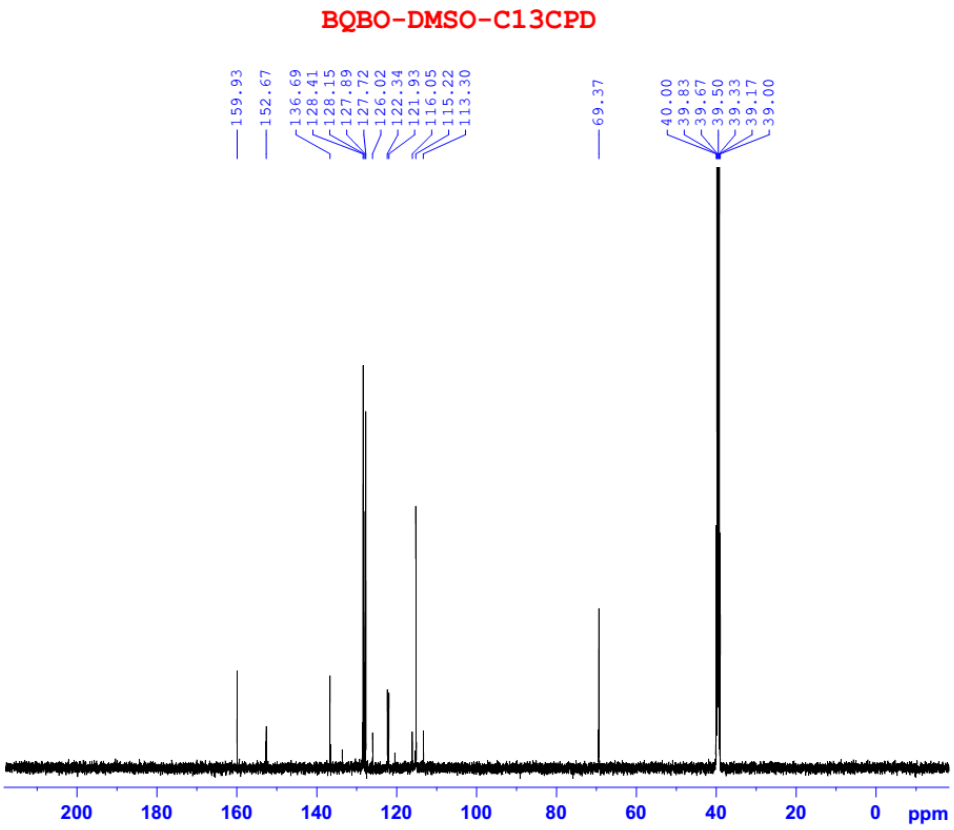

```
Current Data Parameters
NAME          110HD_BQBO
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180301
Time              15.48
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               111.09
DW              50.000 usec
DE               6.50 usec
TE               303.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                   1H
P1                 10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000054 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BQBO
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180301
Time              17.31
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW              16.800 usec
DE               6.50 usec
TE               303.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1                13C
P1                10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

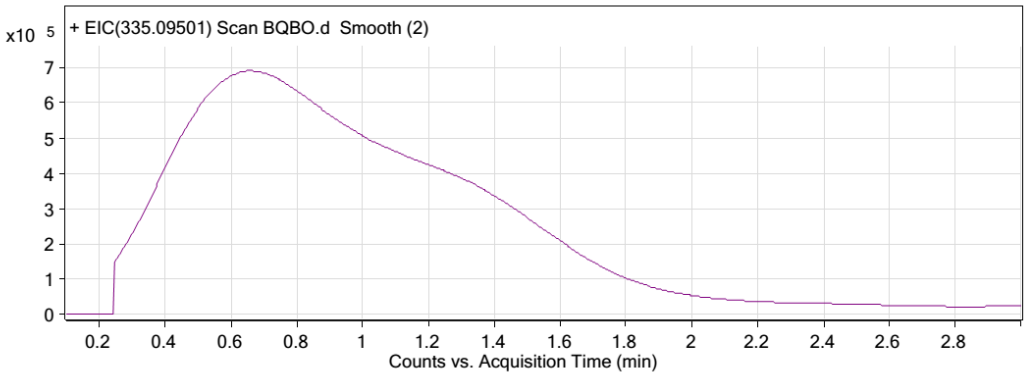
F2 - Processing parameters
SI                 32768
SF          125.7754574 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Qualitative Analysis Report

Data File	BQBO.d	**Sample Name**	BQBO
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	20/05/2018 6:05:59 PM
IRM Calibration Status	Success	**DA Method**	default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

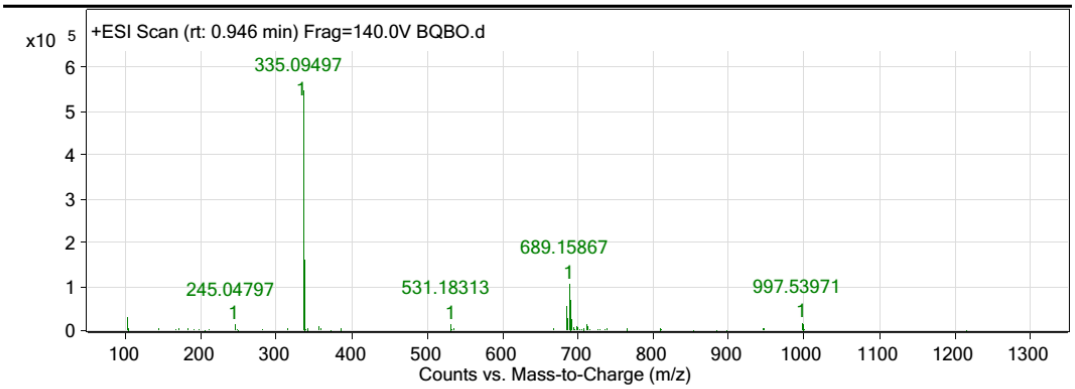
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



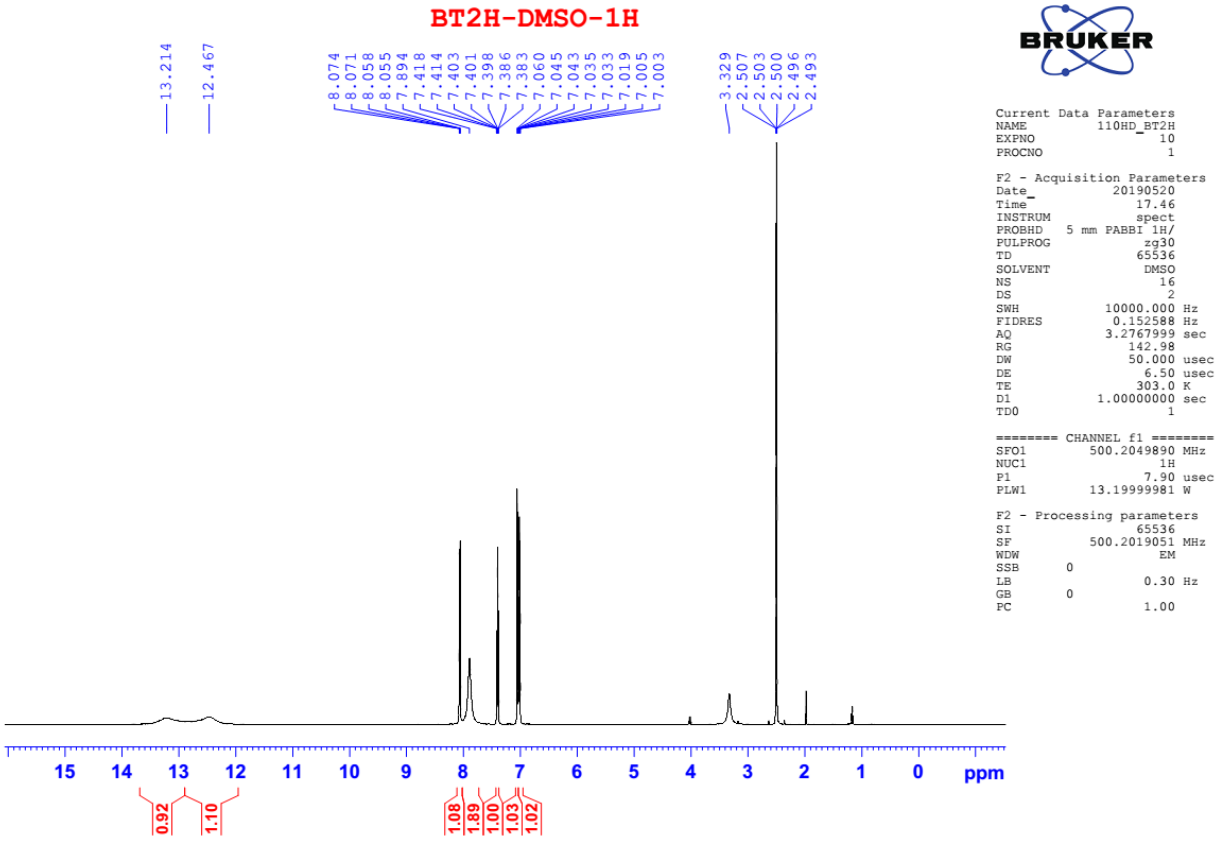
Peak List

m/z	z	Abund
335.09497	1	548406.63
335.1659		37280.09
336.09795	1	118707.34
337.0935	1	160673.69
338.09532	1	40312.67
684.20316	1	55062.52
685.20353	1	36772.19
689.15867	1	106520.9
690.15905	1	69930.52
691.15876	1	66357.37

--- End Of Report ---

5,6-Dichloro-2-(4-trimethoxy-phenyl)-1H-benzoimidazole (**26**):

^{1}H – NMR



BRUKER

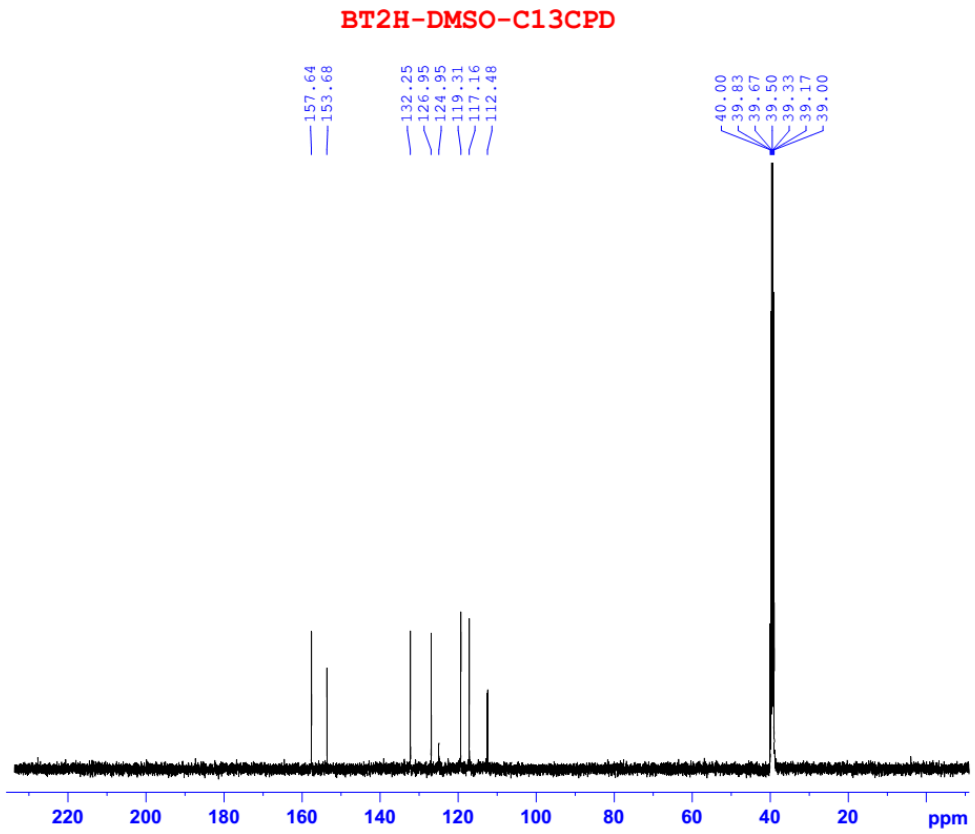
```
Current Data Parameters
NAME          110HD_BT2H
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_          20190520
Time              17.46
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               142.98
DW               50.000 usec
DE                6.50 usec
TE               303.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          500.2049890 MHz
NUC1                  1H
P1                 7.90 usec
PLW1         13.19999981 W

F2 - Processing parameters
SI               65536
SF          500.2019051 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BT2H
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190521
Time                6.30
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                    256
DS                      4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW                16.000 usec
DE                 6.50 usec
TE                303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7897032 MHz
NUC1                  13C
P1                  15.40 usec
PLW1         81.00000000 W

======== CHANNEL f2 ========
SFO2         500.2039008 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         13.19999981 W
PLW12         0.12872000 W
PLW13         0.08238100 W

F2 - Processing parameters
SI                 32768
SF           125.7759350 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

HRMS

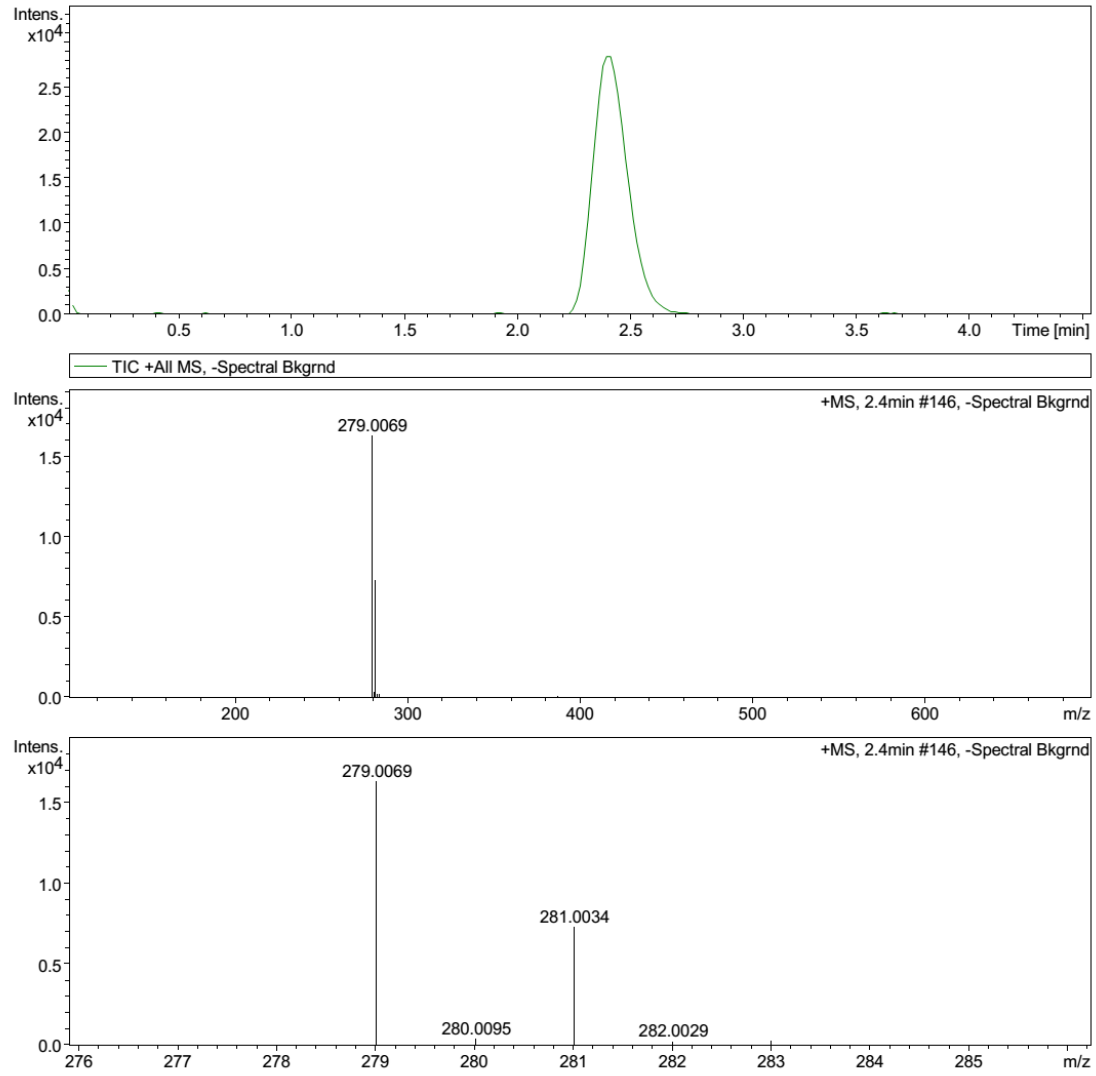
Display Report

Analysis Info

Analysis Name	D:\Data\2019\thang 05\BT2H-XT_2-D,8_01_1725.d	Acquisition Date	6/20/2019 10:06:53 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BT2H-XT	Instrument	micrOTOF-Q 10187
Comment			

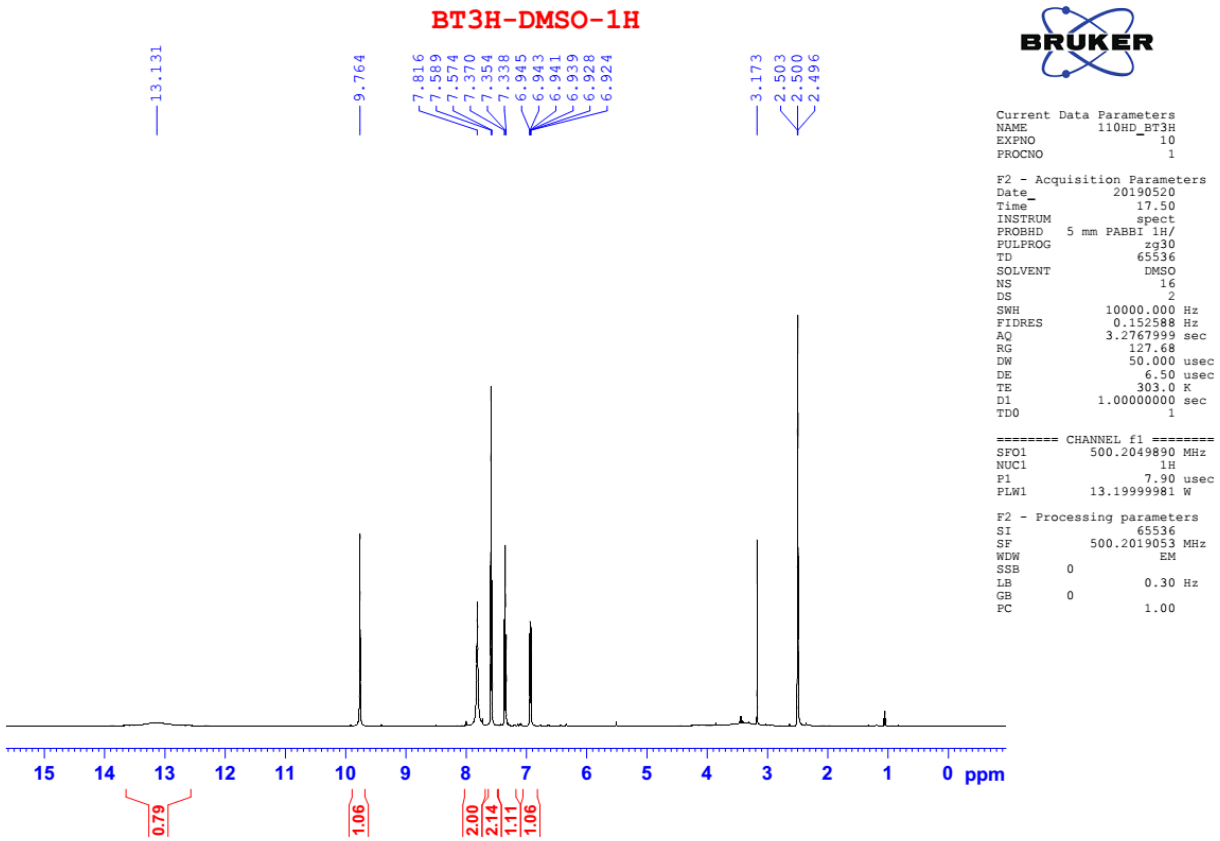
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

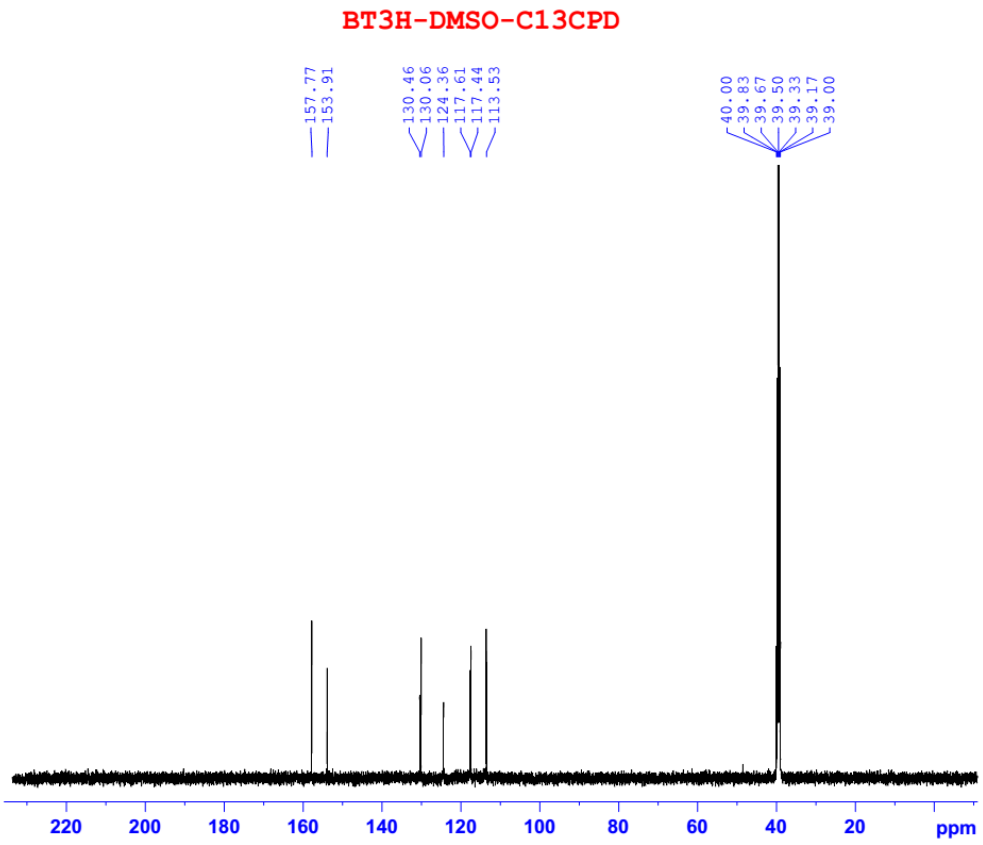


3-(5,6-Dichloro-1H-benzoimidazol-2-yl)phenol (**27**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME                 110HD_BT3H
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20190521
Time                    9.16
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                     256
DS                       4
SWH              31250.000 Hz
FIDRES               0.476837 Hz
AQ                1.0485760 sec
RG                   198.57
DW                   16.000 usec
DE                    6.50 usec
TE                   303.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            125.7897032 MHz
NUC1                    13C
P1                   15.40 usec
PLW1           81.00000000 W

======== CHANNEL f2 ========
SFO2            500.2039008 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                80.00 usec
PLW2           13.19999981 W
PLW12           0.12872000 W
PLW13           0.08238100 W

F2 - Processing parameters
SI                   32768
SF              125.7758678 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

HRMS

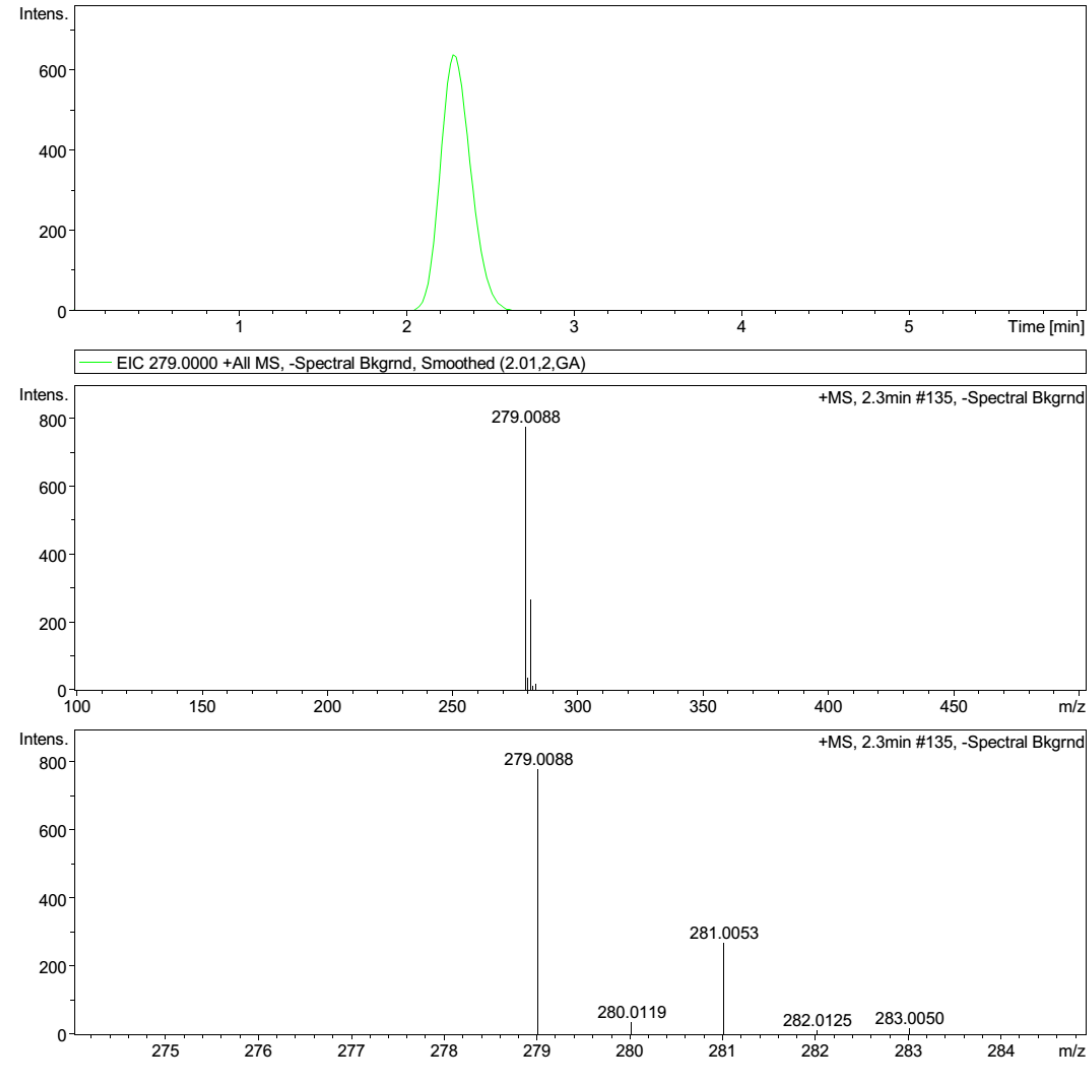
Display Report

Analysis Info

Analysis Name	D:\Data\2019\thang 05\BT3H-XT_1-C,9_01_1716.d	Acquisition Date	6/20/2019 9:06:28 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BT3H-XT	Instrument	micrOTOF-Q 10187
Comment			

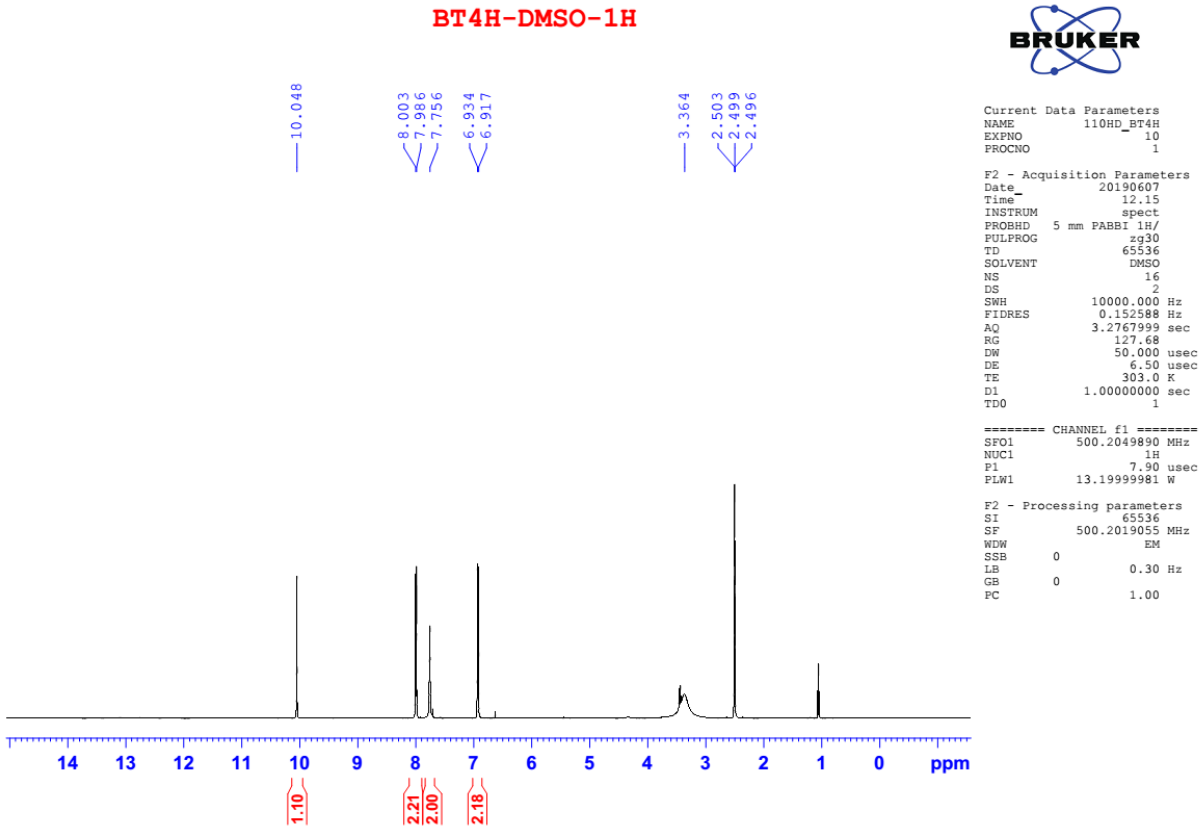
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



4-(5,6-Dichloro-1H-benzoimidazol-2-yl)phenol (**28**):

^{1}H – NMR



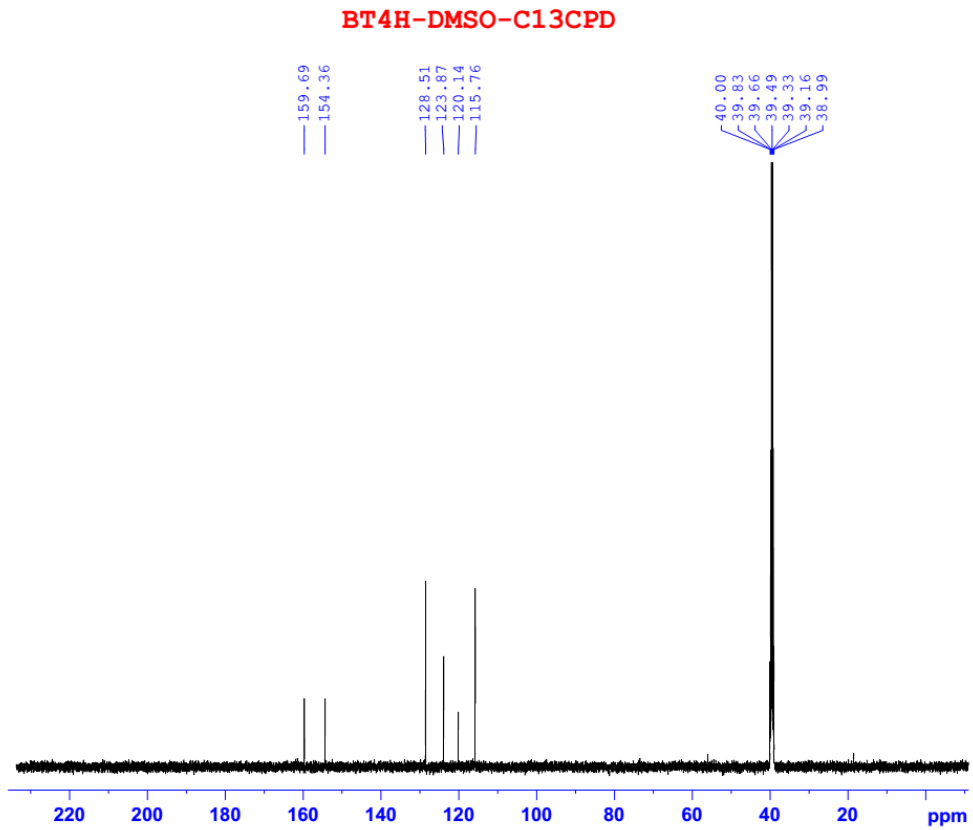

```
Current Data Parameters
NAME          110HD_BT4H
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190607
Time               12.15
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                127.68
DW                50.000 usec
DE                 6.50 usec
TE                303.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2049890 MHz
NUC1                  1H
P1                 7.90 usec
PLW1        13.19999981 W

F2 - Processing parameters
SI                 65536
SF          500.2019055 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BT4H
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190607
Time               15.22
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG         zgpg30
TD                65536
SOLVENT             DMSO
NS                    256
DS                      4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW                16.000 usec
DE                 6.50 usec
TE                303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7897032 MHz
NUC1                  13C
P1                  15.40 usec
PLW1         81.00000000 W

======== CHANNEL f2 ========
SFO2         500.2039008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2               80.00 usec
PLW2         13.19999981 W
PLW12         0.12872000 W
PLW13         0.08238100 W

F2 - Processing parameters
SI                 32768
SF           125.7759325 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

HRMS

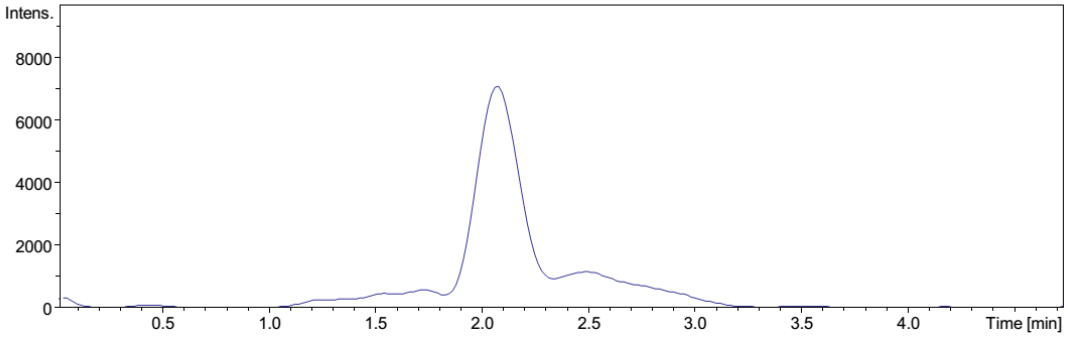
Display Report

Analysis Info

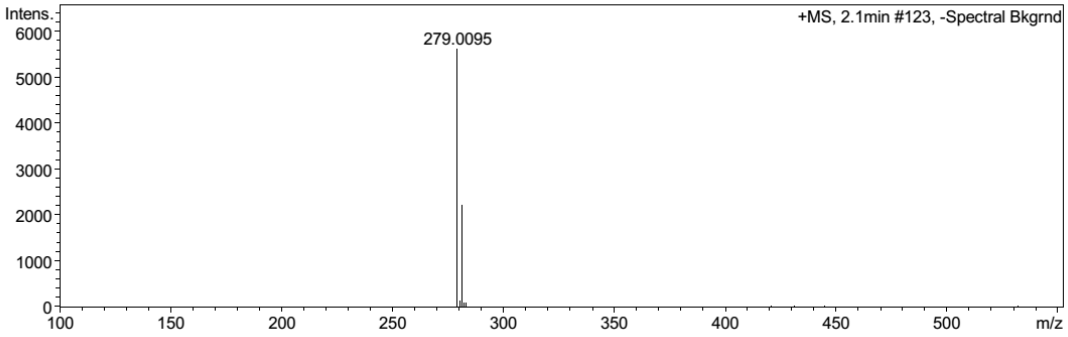
Analysis Name	D:\Data\2019\thang 05\BT4H_1-C,8_01_1715.d	Acquisition Date	6/20/2019 8:59:45 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BT4H	Instrument	micrOTOF-Q 10187
Comment			

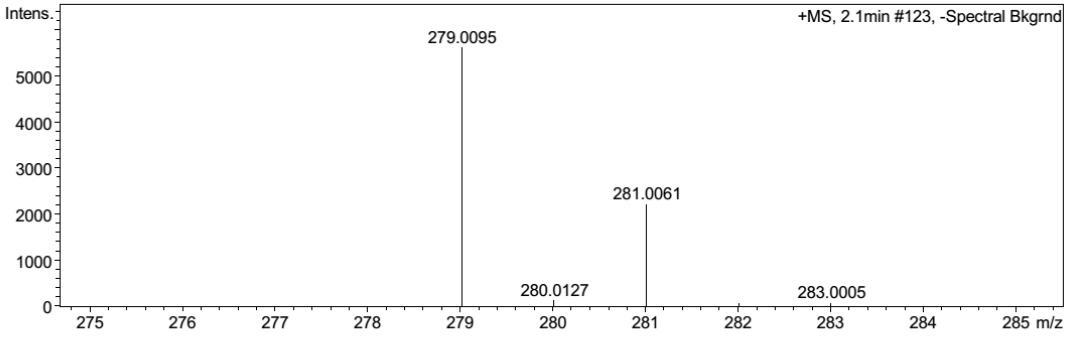
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



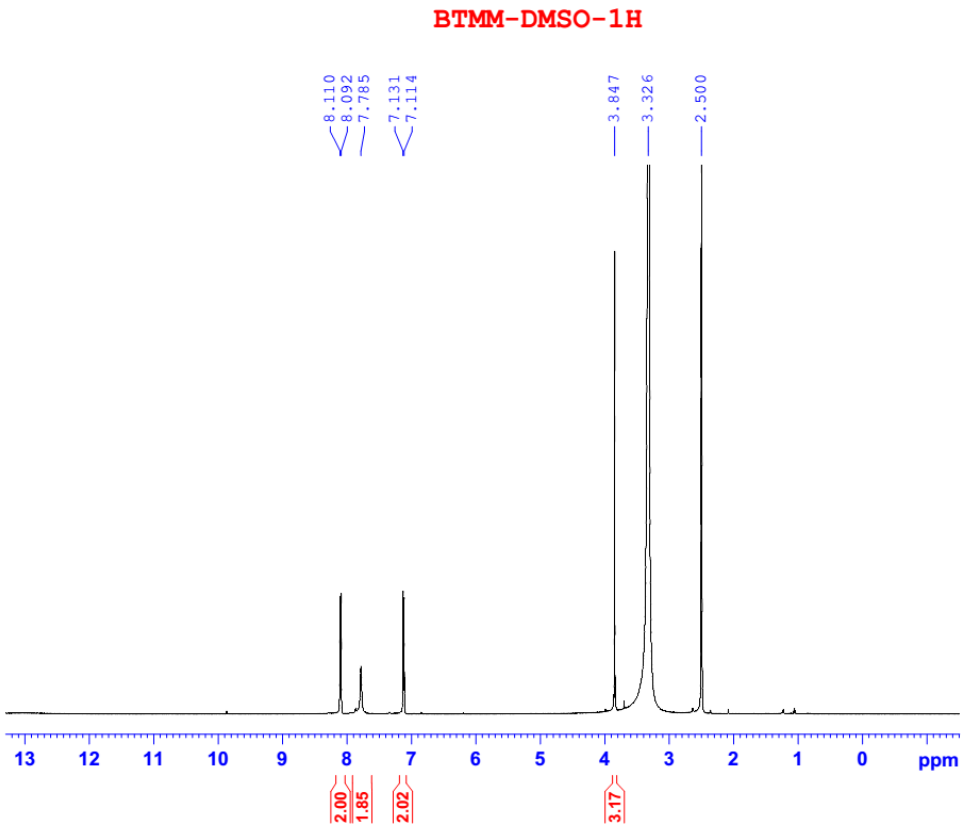
TIC +All MS, -Spectral Bkgrnd, Smoothed (2.01,2,GA)





5,6-Dichloro-2-(4-methoxy-phenyl)-1H-benzoimidazole (**29**):

^{1}H – NMR



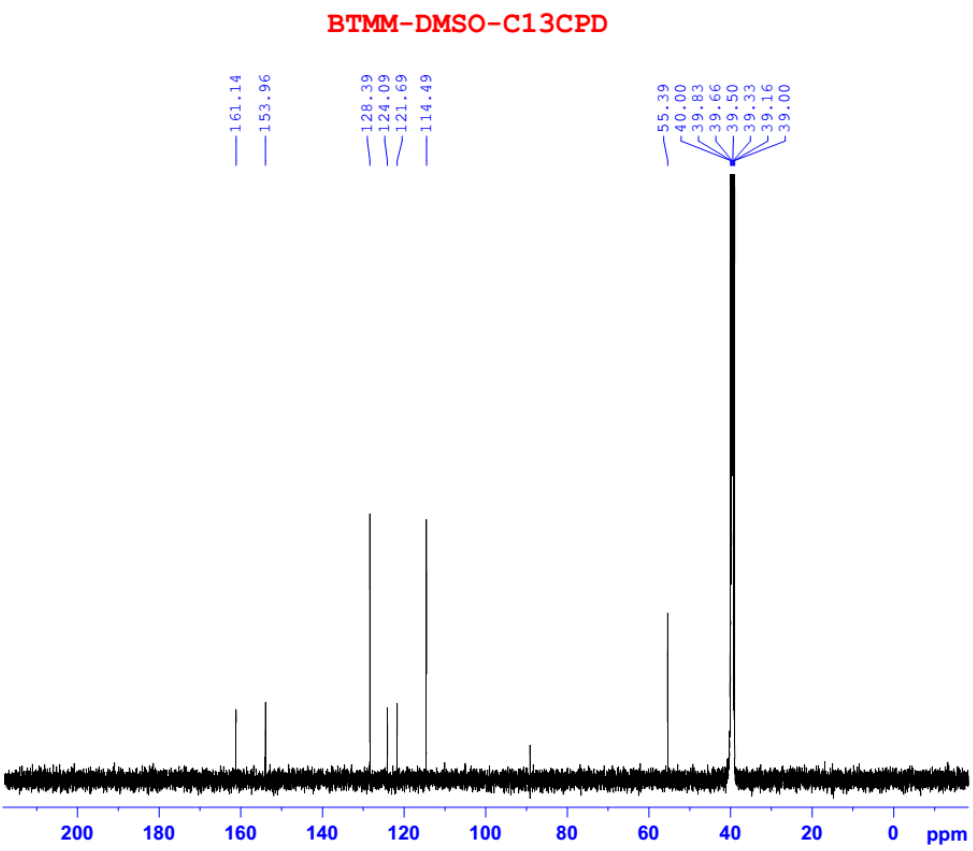

```
Current Data Parameters
NAME          110HD_BTMM
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171116
Time_              10.36
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ             3.2767999 sec
RG                 97.76
DW                 50.000 usec
DE                  6.50 usec
TE                308.8 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000054 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BTMM
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20171116
Time              12.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                2048
DS                   4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               198.57
DW               16.800 usec
DE                6.50 usec
TE               304.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         125.7879670 MHz
NUC1                13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                32768
SF           125.7753900 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

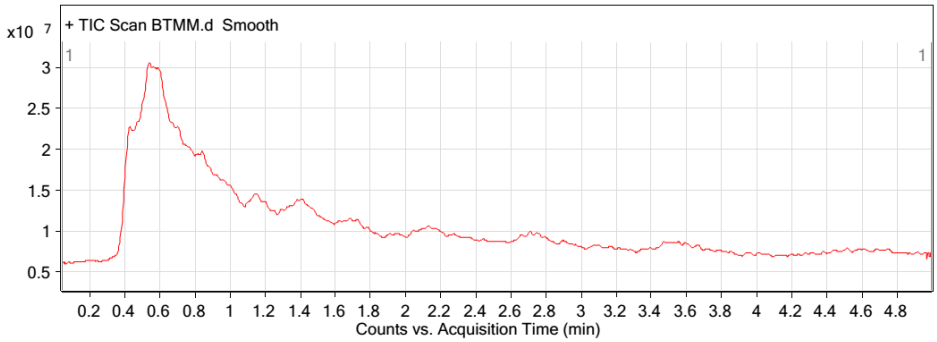
HRMS

Qualitative Analysis Report

Data File	BTMM.d	**Sample Name**	BTMM
Sample Type	Sample	**Position**	P1-D3
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	25/11/2017 12:11:11 PM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

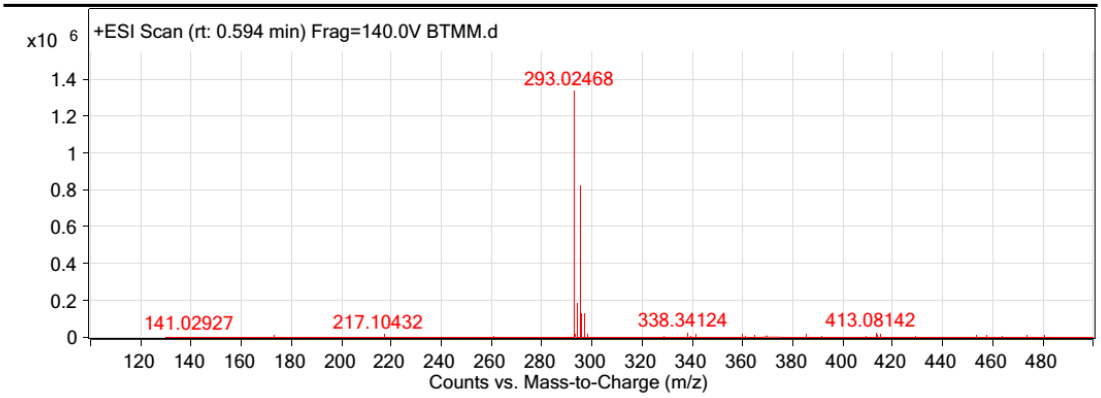
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



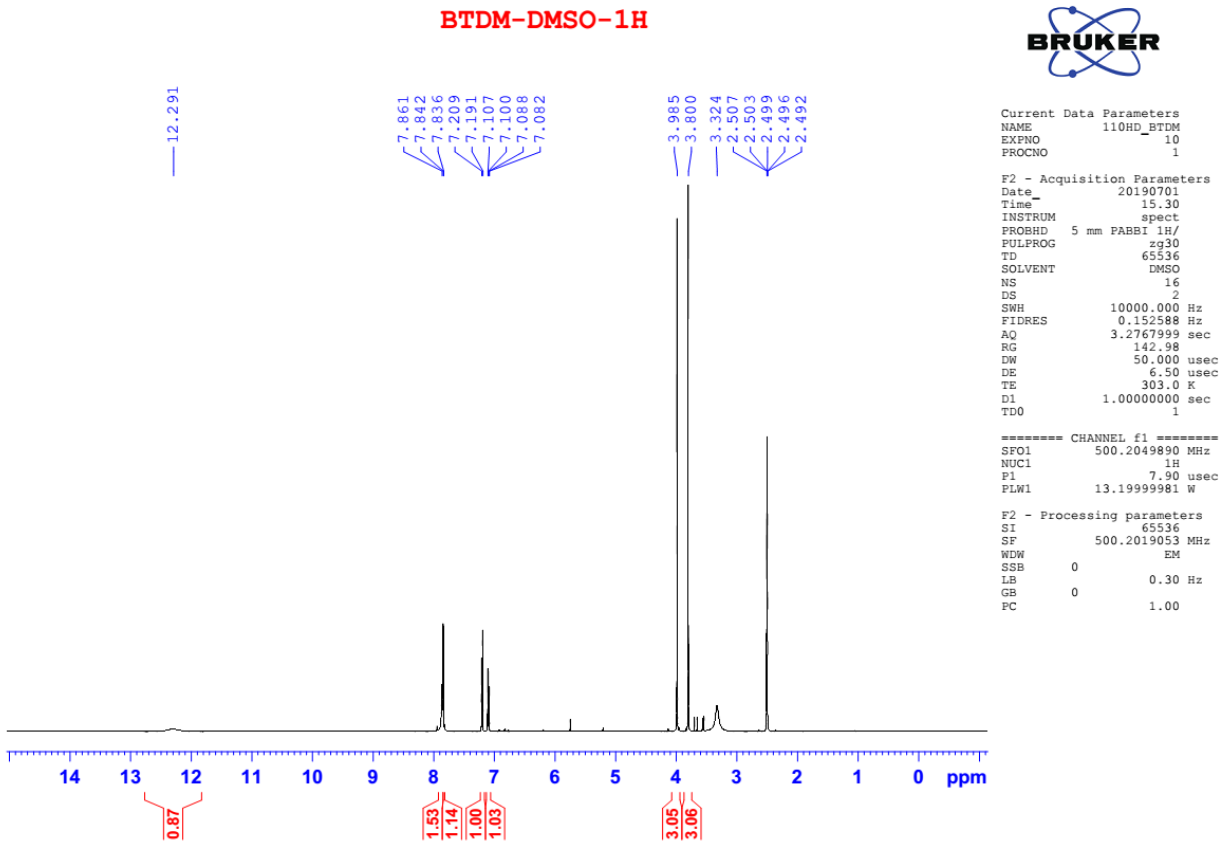
Peak List

m/z	z	Abund
293.02468	1	1334829.86
293.09217	1	102394.43
294.02821	1	182840.32
295.02184	1	832993.17
295.08953	1	62855.29
296.02483	1	138426.77
297.01924	1	134981.24
413.08142	1	27598.3
683.30097	1	41716.35
685.29951	1	29105.92

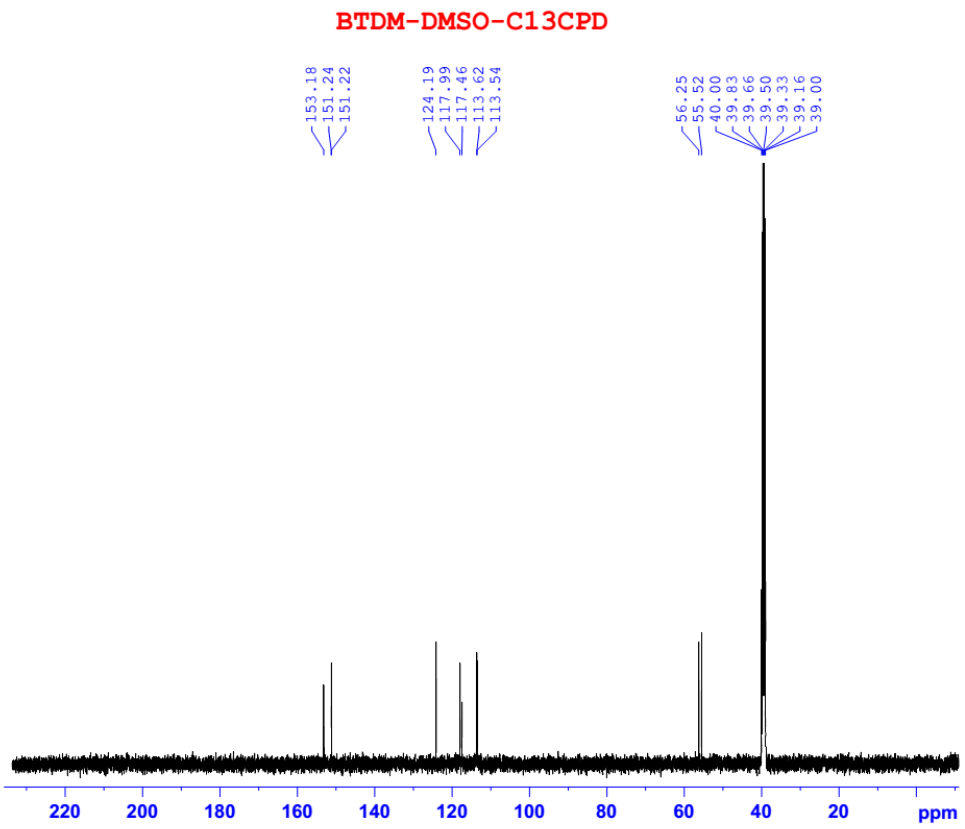
--- End Of Report ---

5,6-Dichloro-2-(2,5-dimethoxyphenyl)-1H-benzo[d]imidazole (**30**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BTDM
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190702
Time               13.56
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                    256
DS                      4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW                16.000 usec
DE                 6.50 usec
TE                303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7897032 MHz
NUC1                 13C
P1                15.40 usec
PLW1         81.00000000 W

======== CHANNEL f2 ========
SFO2         500.2039008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         13.19999981 W
PLW12         0.12872000 W
PLW13         0.08238100 W

F2 - Processing parameters
SI                  32768
SF           125.7759349 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HRMS

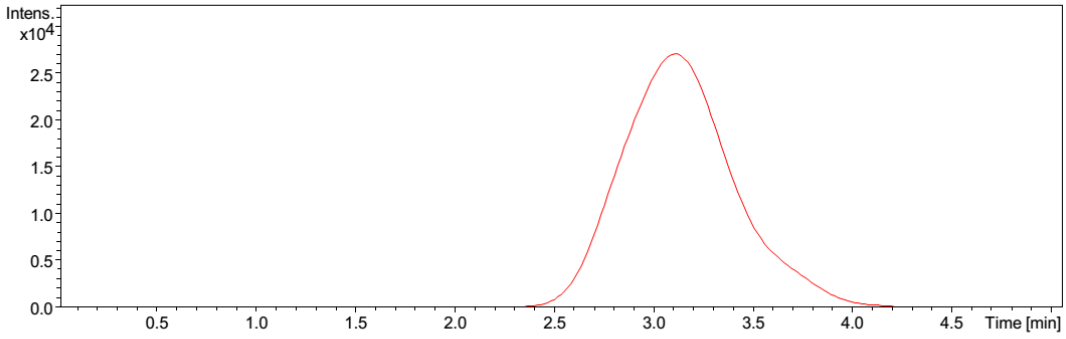
Display Report

Analysis Info

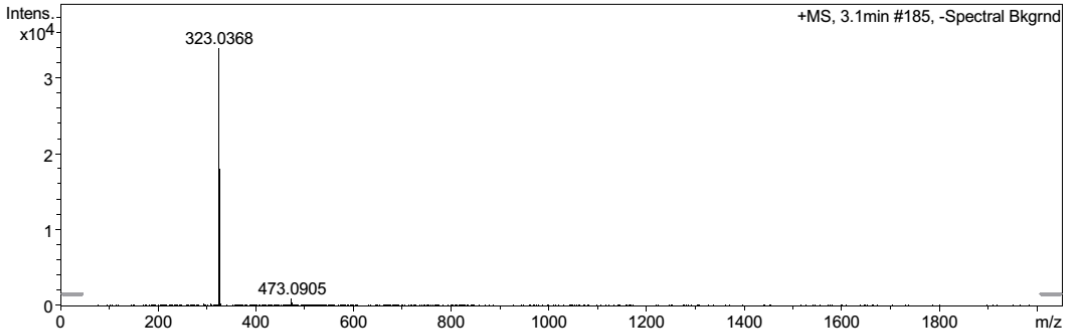
Analysis Name	D:Data2019thang 05BTDM_1-D,5_01_2200.d	Acquisition Date	7/30/2019 4:31:26 PM
Method	dmm 2016 low mass.m	Operator	ANH MAI
Sample Name	BTDM	Instrument	micrOTOF-Q 10187
Comment			

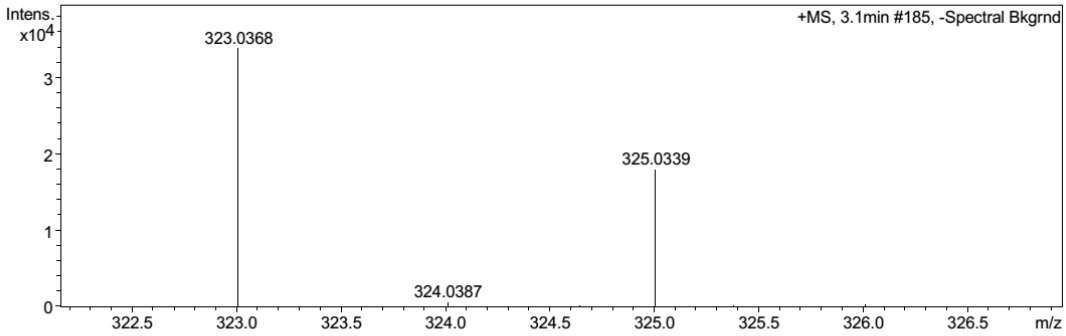
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	2000 m/z	Set Collision Cell RF	520.0 Vpp	Set Divert Valve	Source



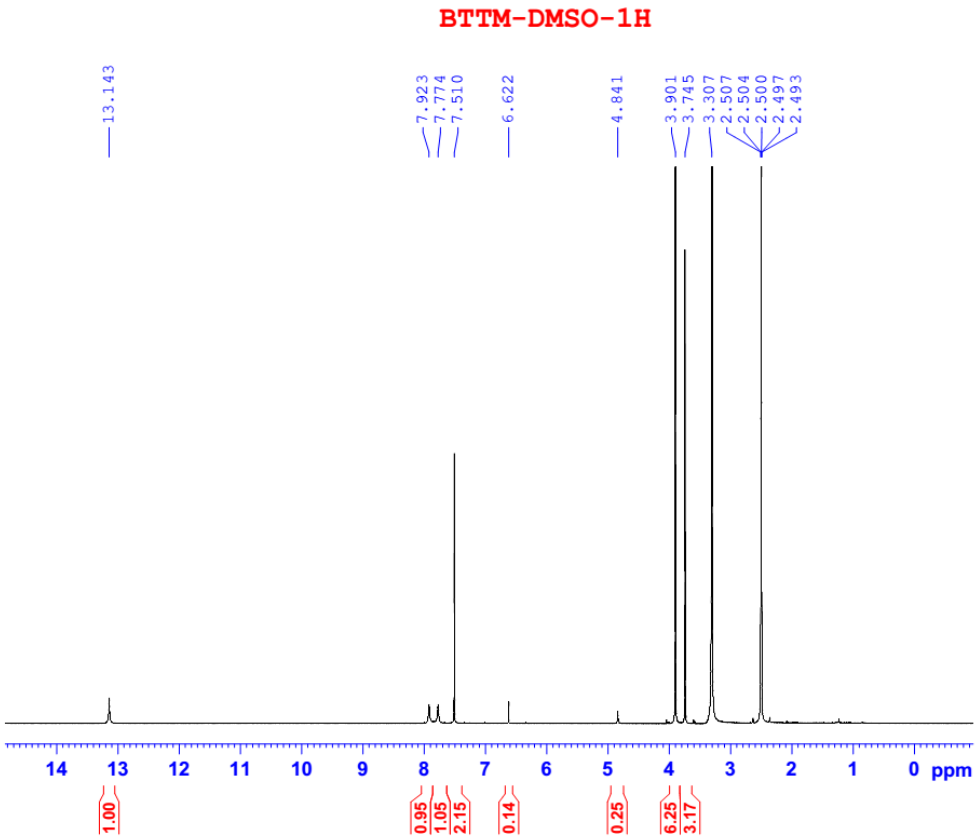
EIC 323.0000 +All MS, -Spectral Bkgrnd, Smoothed 5.03,2,GA)





5,6-Dichloro-2-(3,4,5-trimethoxy-phenyl)-1H-benzoimidazole (**31**):

^{1}H – NMR



BRUKER

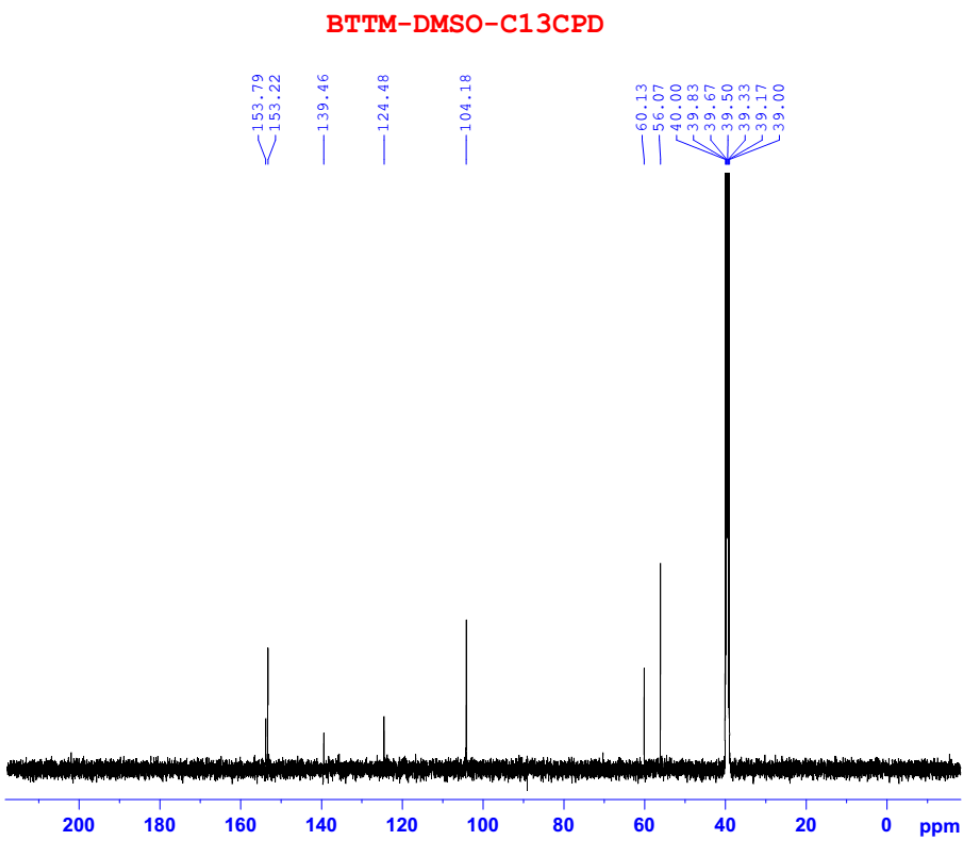
```
Current Data Parameters
NAME          110HD_BTTM
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171030
Time               9.36
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                175.34
DW                50.000 usec
DE                 6.50 usec
TE                303.4 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1        22.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000059 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BTTM
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171102
Time               9.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              65536
SOLVENT          DMSO
NS                2048
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               198.57
DW               16.800 usec
DE                6.50 usec
TE               303.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

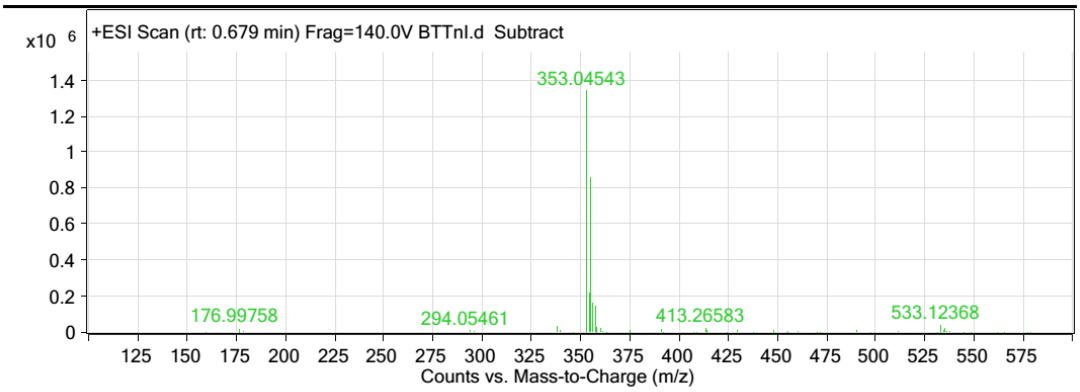
======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1               13C
P1               10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                32768
SF          125.7754560 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

HRMS

Qualitative Analysis Report



Peak List

m/z	z	Abund
338.34079	1	31623.74
353.04543	1	1341906.5
353.11725		103068.48
354.04934	1	216297.97
355.04278	1	859096.25
356.04577	1	158752.89
357.04048	1	146714.36
533.12368	1	37446.61
743.3228	1	51240.3
745.32098	1	36014.19

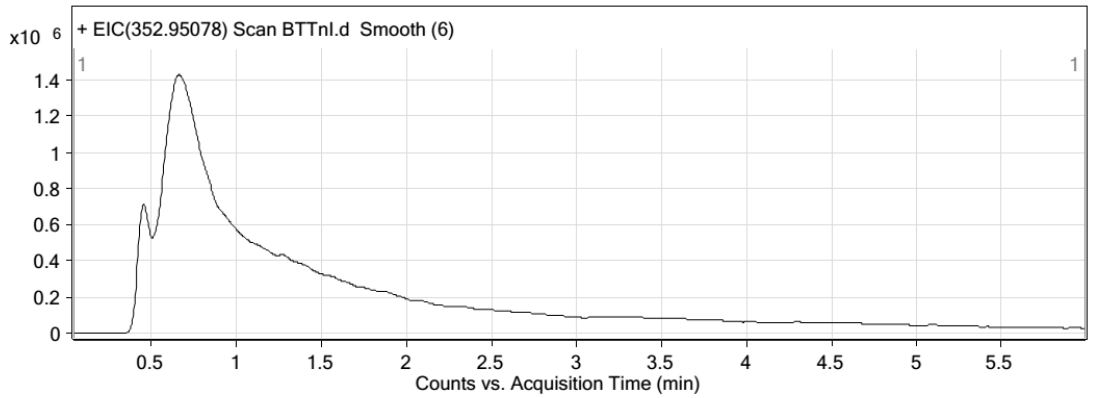
--- End Of Report ---

Qualitative Analysis Report

Data File	BTTnI.d	**Sample Name**	BTTnI
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	11/2/2017 3:25:28 PM
IRM Calibration Status	Success	**DA Method**	Khao sat ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI

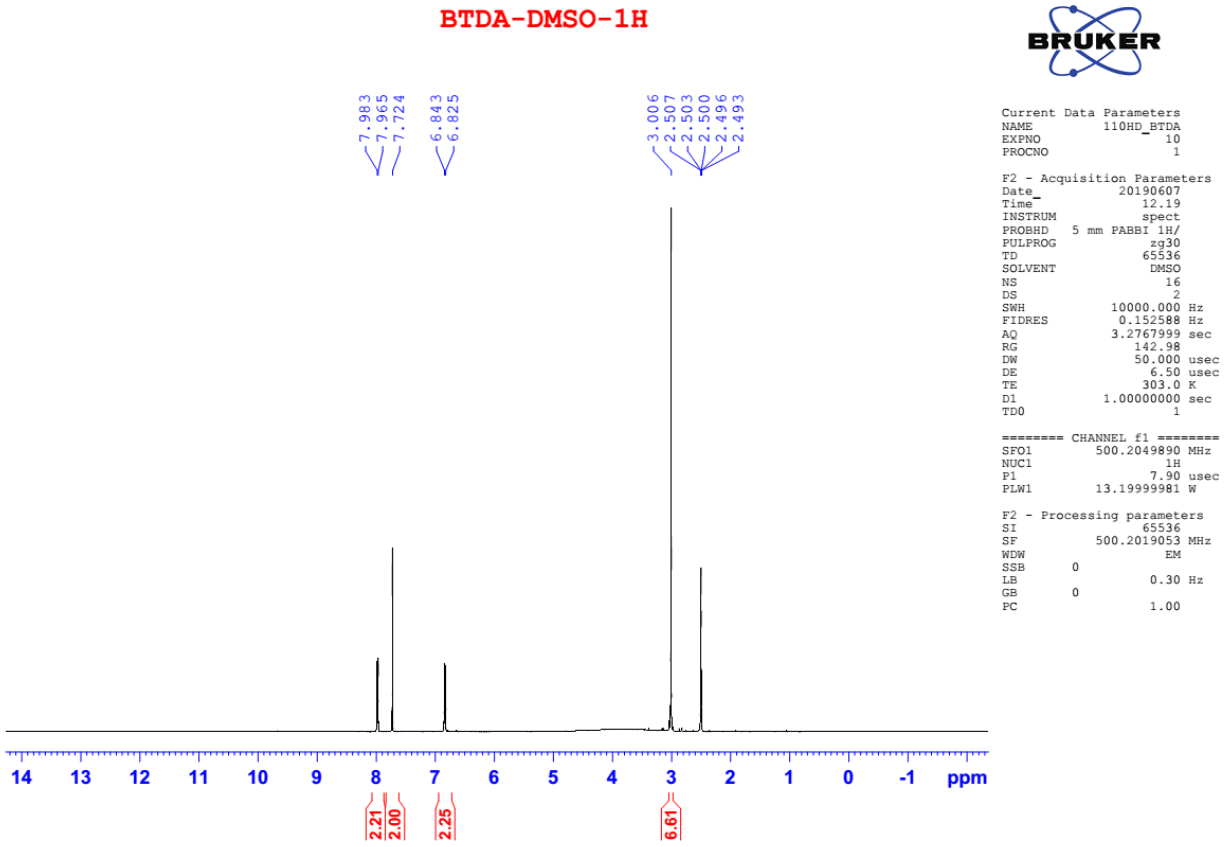


User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

4-(5,6-Dichloro-1H-benzo[d]imidazol-2-yl)-N,N-dimethylaniline (**32**):

^{1}H – NMR



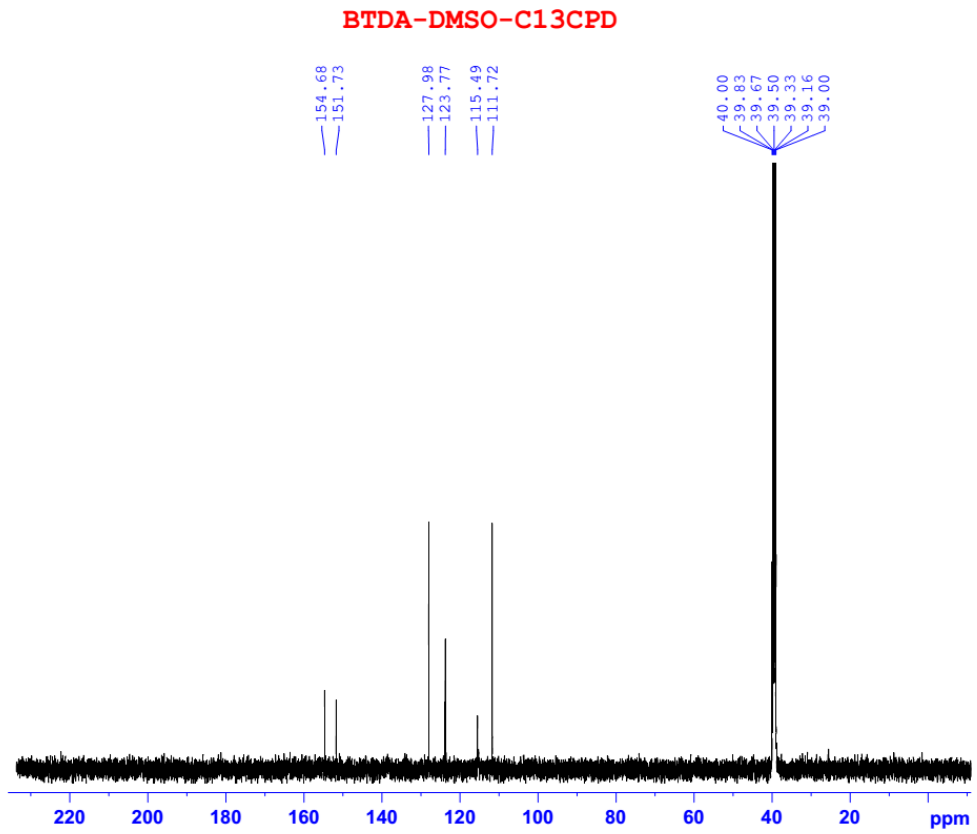

```
Current Data Parameters
NAME          110HD_BTDA
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190607
Time              12.19
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               142.98
DW               50.000 usec
DE                6.50 usec
TE               303.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2049890 MHz
NUC1                  1H
P1                 7.90 usec
PLW1        13.19999981 W

F2 - Processing parameters
SI                 65536
SF          500.2019053 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BTDA
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20190607
Time              15.34
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG         zgpg30
TD                65536
SOLVENT             DMSO
NS                    256
DS                      4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW                16.000 usec
DE                 6.50 usec
TE                303.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7897032 MHz
NUC1                 13C
P1                 15.40 usec
PLW1         81.00000000 W

======== CHANNEL f2 ========
SFO2         500.2039008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         13.19999981 W
PLW12         0.12872000 W
PLW13         0.08238100 W

F2 - Processing parameters
SI                 32768
SF           125.7759335 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HRMS

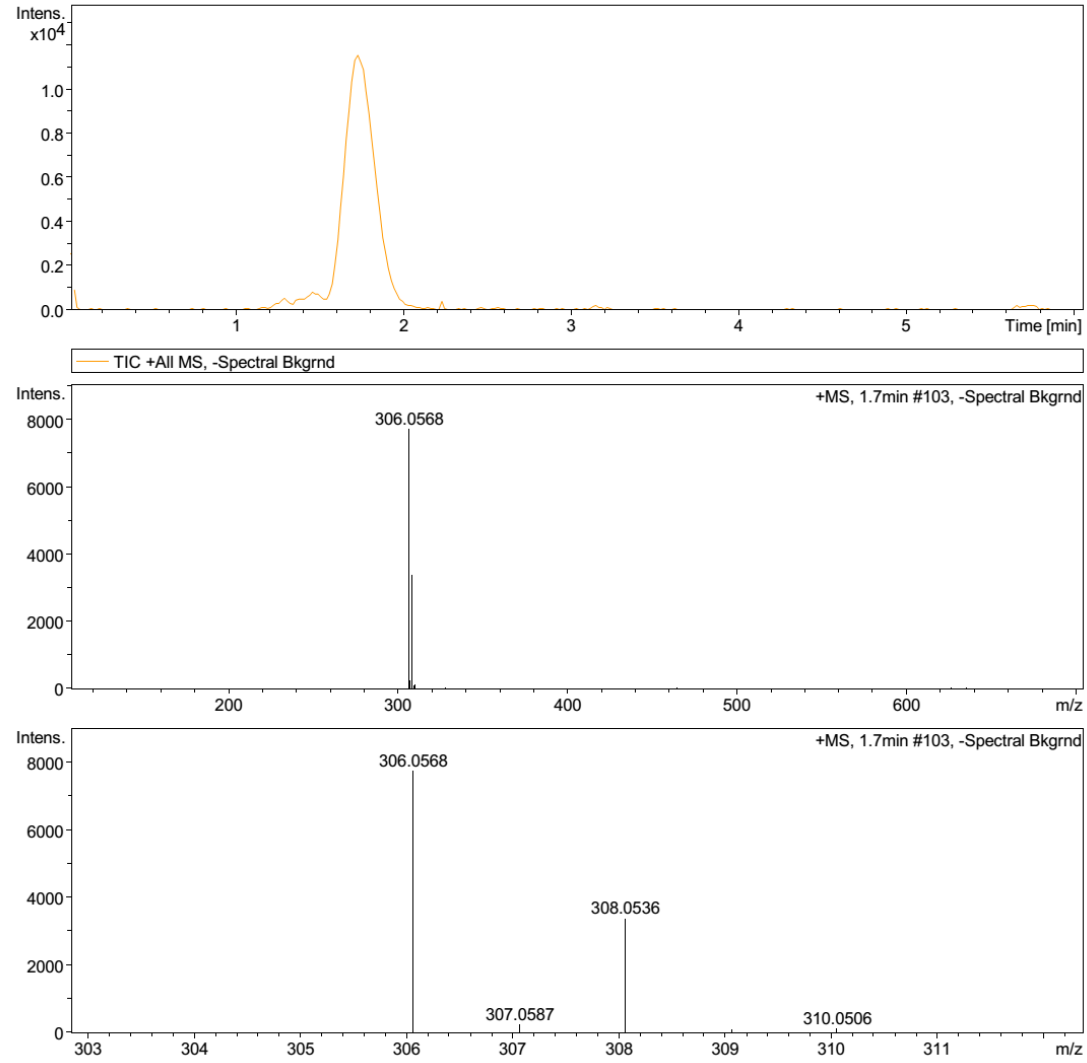
Display Report

Analysis Info

Analysis Name	D:\Data\2019\thang 05\BTDA_1-C,6_01_1713.d	Acquisition Date	6/20/2019 8:46:19 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BTDA	Instrument	micrOTOF-Q 10187
Comment			

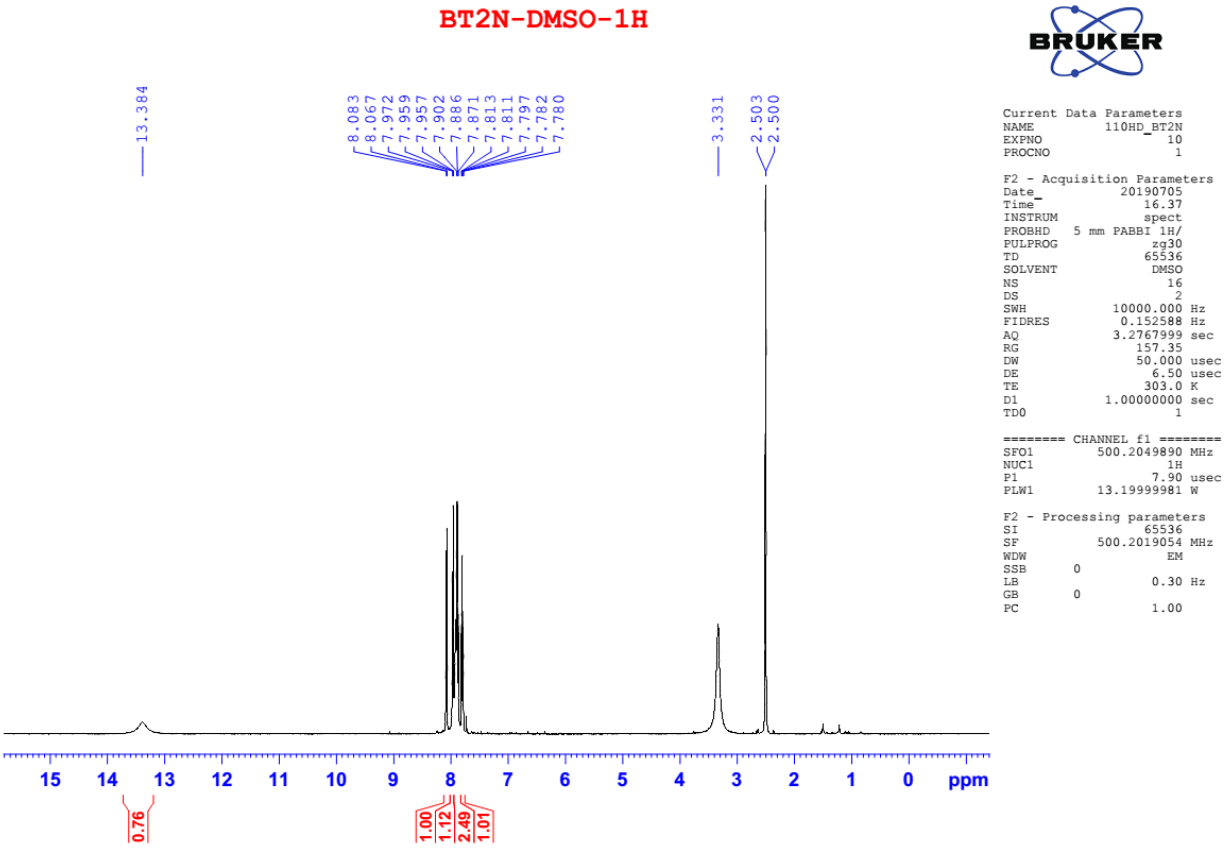
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



5,6-Dichloro-2-(2-nitrophenyl)-1H-benzoimidazole (**33**):

^{1}H – NMR



BRUKER

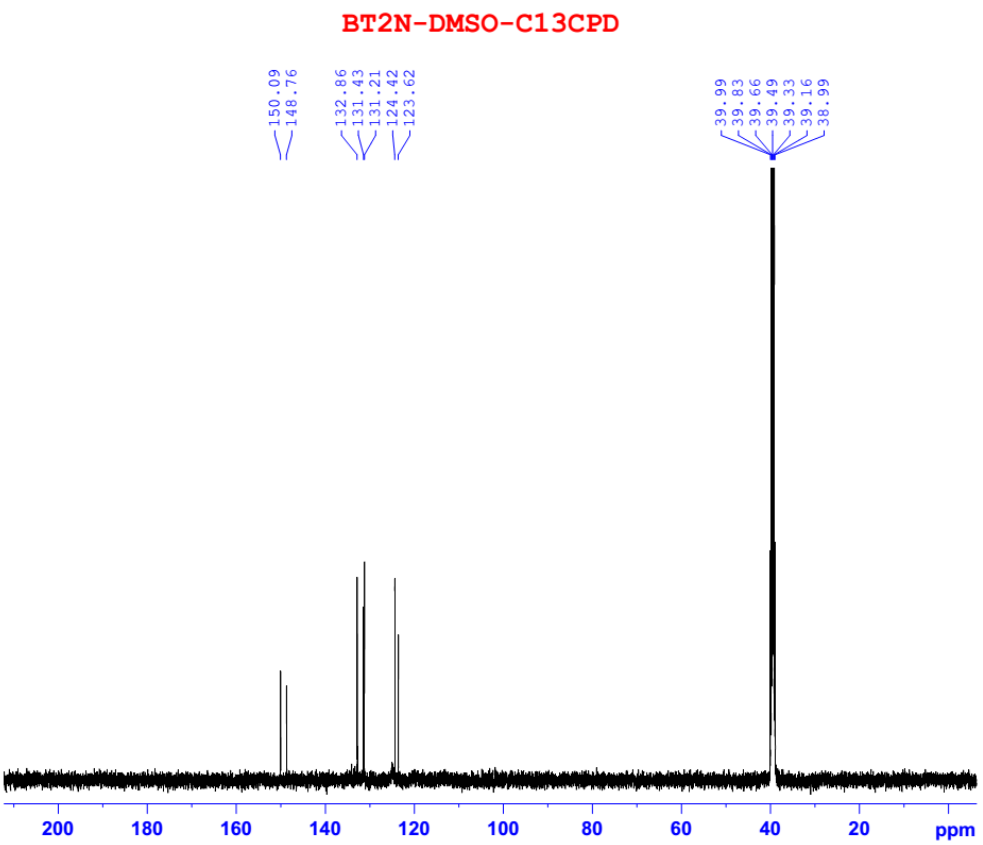
```
Current Data Parameters
NAME          110HD_BT2N
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190705
Time              16.37
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               157.35
DW               50.000 usec
DE                6.50 usec
TE               303.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        500.2049890 MHz
NUC1                   1H
P1                  7.90 usec
PLW1        13.19999981 W

F2 - Processing parameters
SI                 65536
SF          500.2019054 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BT2N
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190708
Time               19.10
INSTRUM            spect
PROBHD   5 mm PABBI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                   512
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                303.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7884448 MHz
NUC1                 13C
P1                15.40 usec
PLW1         81.00000000 W

======== CHANNEL f2 ========
SFO2         500.2039008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         13.19999981 W
PLW12         0.12872000 W
PLW13         0.08238100 W

F2 - Processing parameters
SI                   32768
SF           125.7759344 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

HRMS

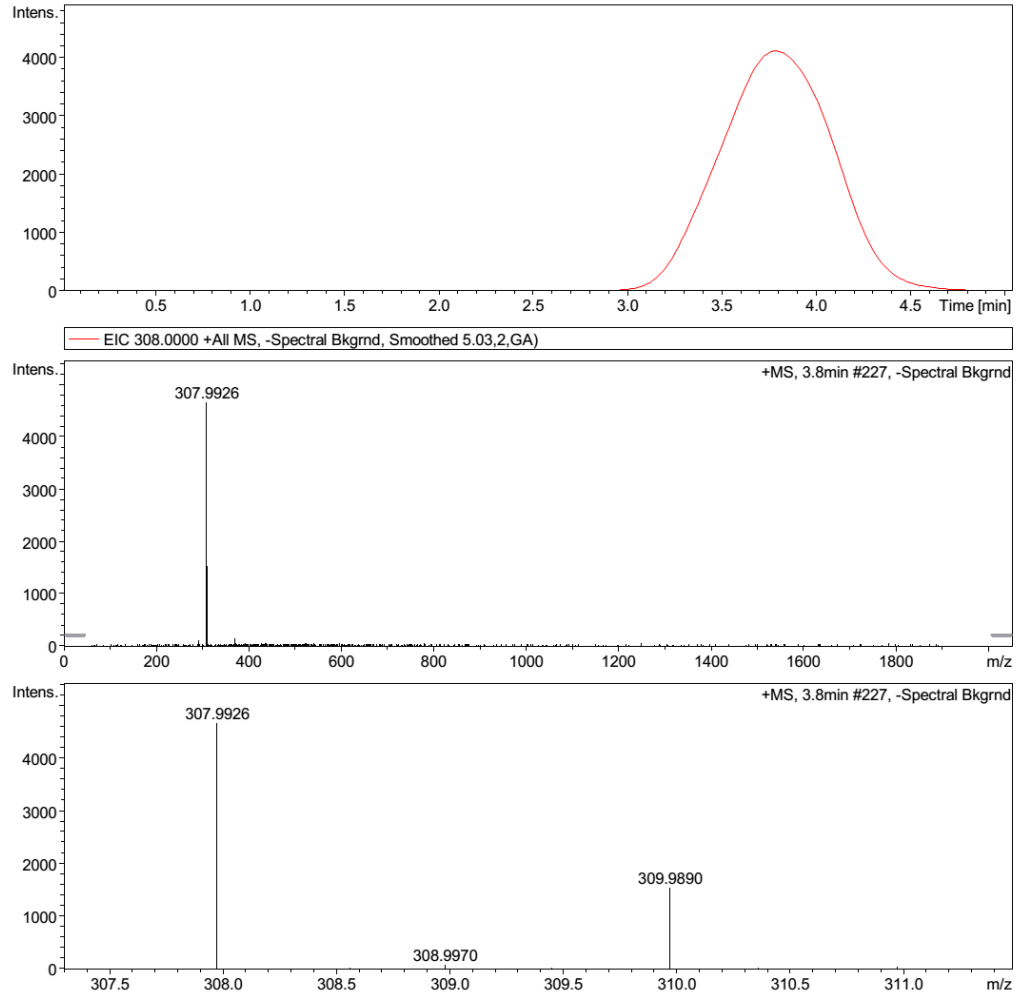
Display Report

Analysis Info

Analysis Name	D:Data2019thang 05BT2N_1-D,5_01_2201.d	Acquisition Date	7/30/2019 4:47:55 PM
Method	dmm 2016 low mass.m	Operator	ANH MAI
Sample Name	BT2N	Instrument	micrOTOF-Q 10187
Comment			

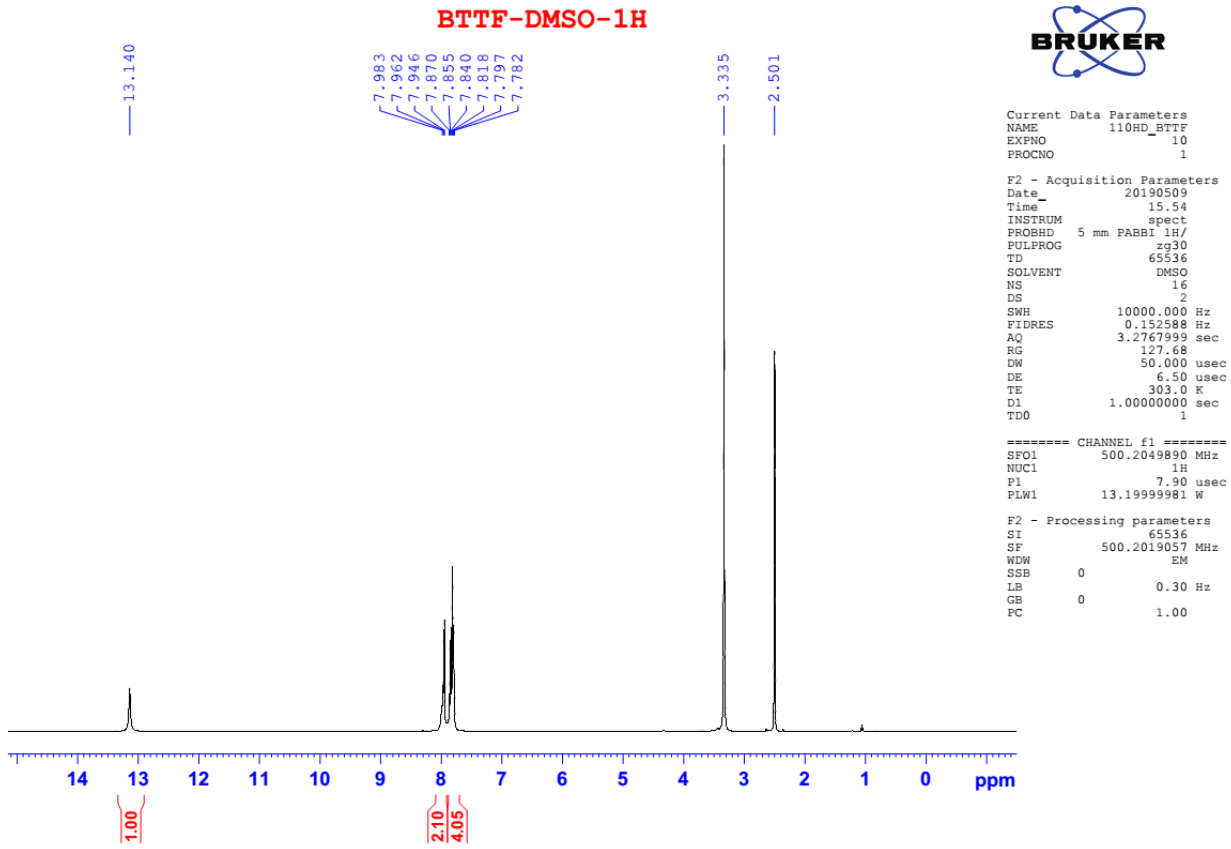
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	2000 m/z	Set Collision Cell RF	520.0 Vpp	Set Divert Valve	Source

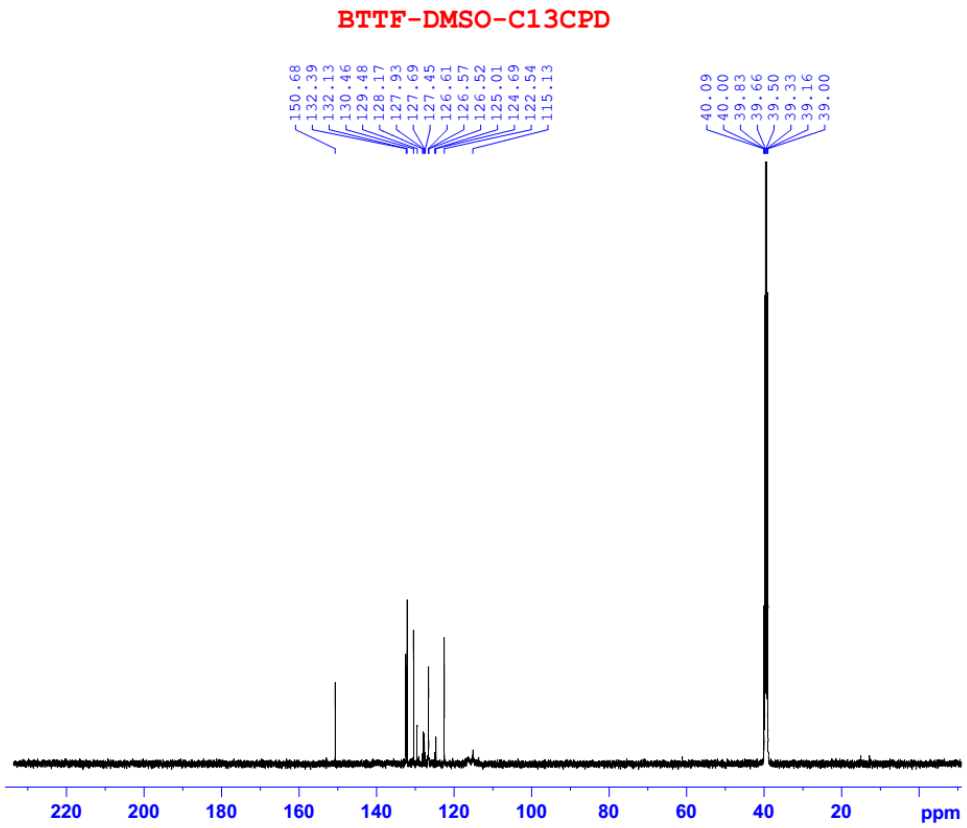


5,6-Dichloro-2-(2-trifluoromethyl-phenyl)-1H-benzoimidazole (**34**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME                 110HD_BTTF
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20190510
Time                    8.01
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     2048
DS                        4
SWH                31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.0485760 sec
RG                    198.57
DW                   16.000 usec
DE                    6.50 usec
TE                   303.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1              125.7897032 MHz
NUC1                     13C
P1                    15.40 usec
PLW1              81.00000000 W

======== CHANNEL f2 ========
SFO2              500.2039008 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 80.00 usec
PLW2              13.19999981 W
PLW12              0.12872000 W
PLW13              0.08238100 W

F2 - Processing parameters
SI                       32768
SF                125.7759341 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

HRMS

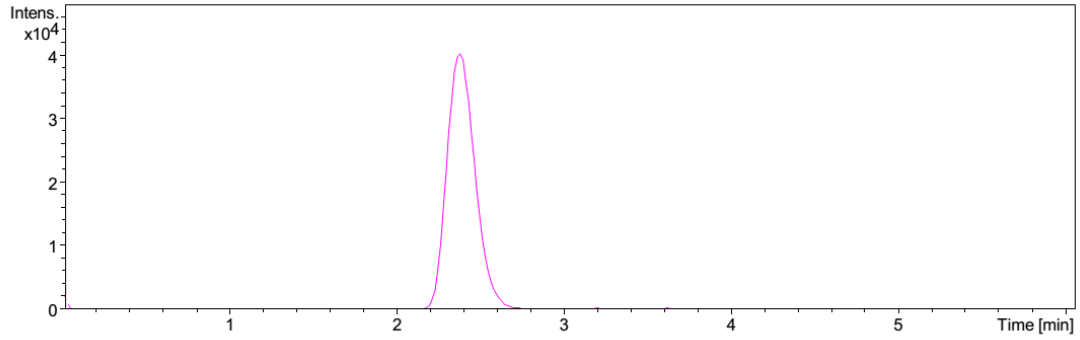
Display Report

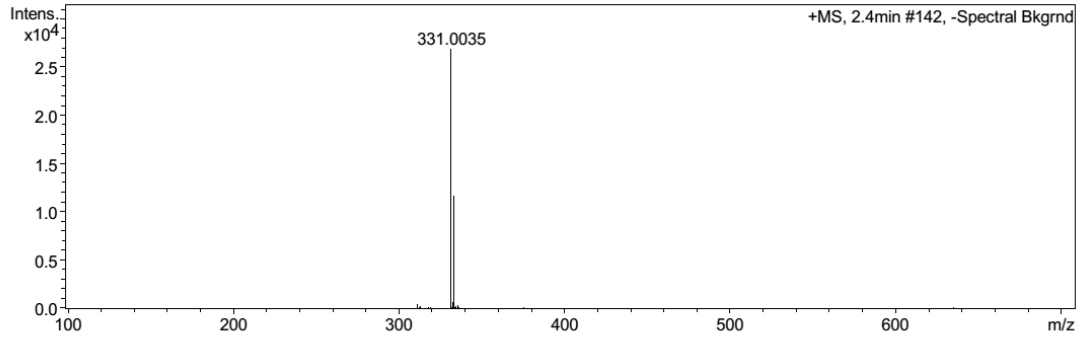
Analysis Info

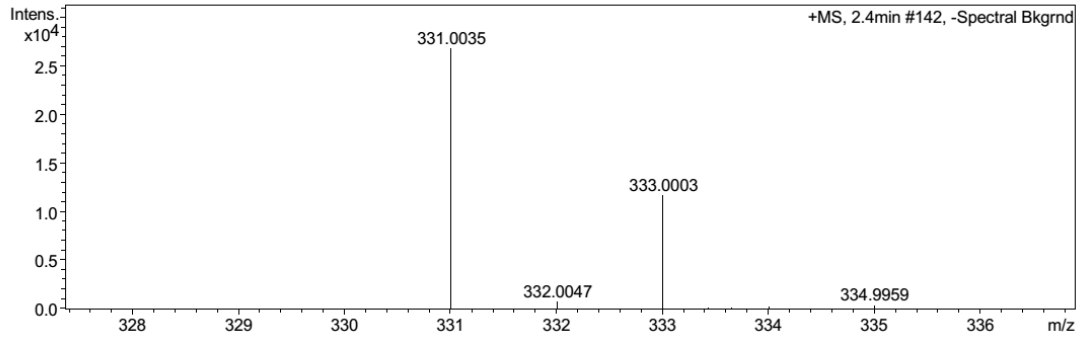
Analysis Name	D:\Data\2019\thang 05\BTTF_1-B,9_01_1717.d	Acquisition Date	6/20/2019 9:13:10 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BTTF	Instrument	micrOTOF-Q 10187
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

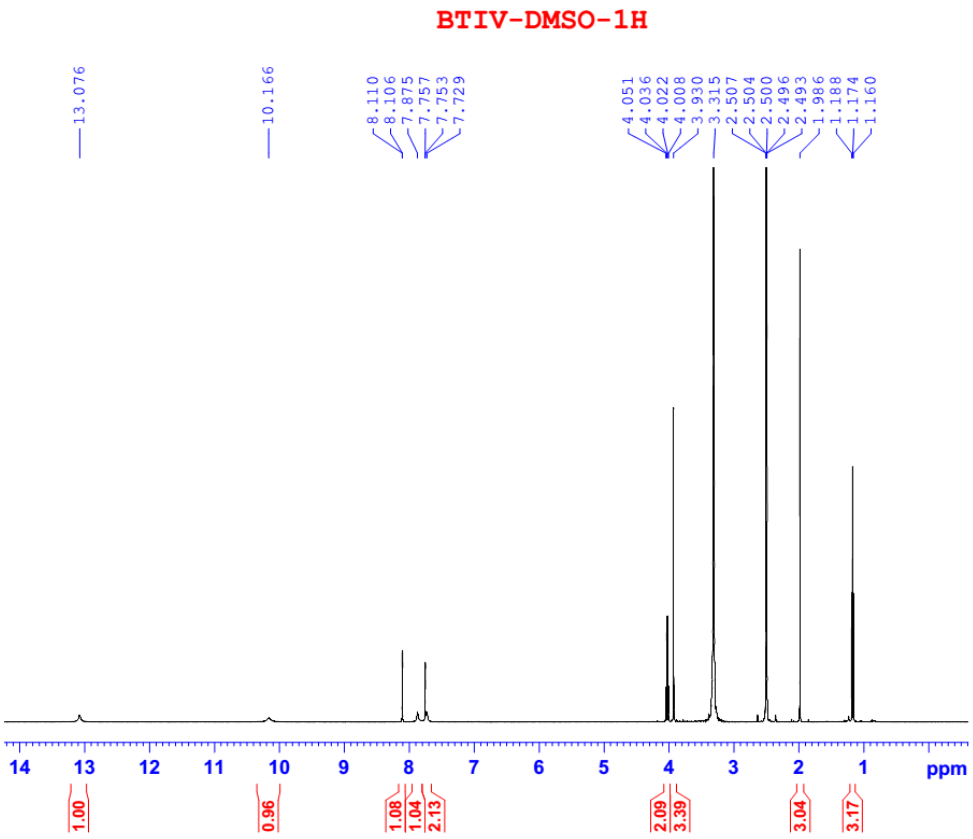






4-(5,6-Dichloro-1H-benzoimidazol-2-yl)-2-iodo-6-methoxy-phenol (**35**):

^{1}H – NMR



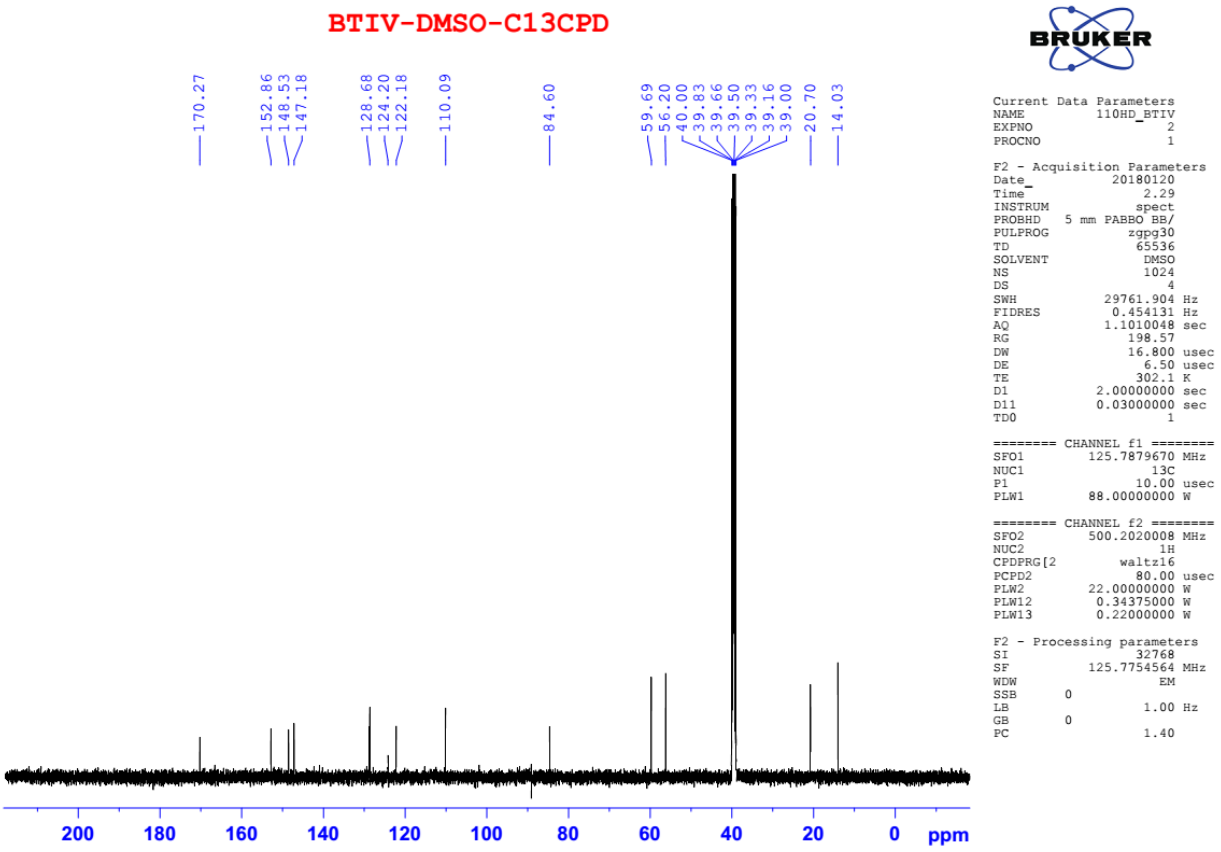

```
Current Data Parameters
NAME          110HD_BTIV
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180111
Time              10.05
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ            3.2767999 sec
RG                157.35
DW                50.000 usec
DE                 6.50 usec
TE                303.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                   1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000057 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR




```
Current Data Parameters
NAME          110HD_BTIV
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180120
Time               2.29
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                1024
DS                   4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                302.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7879670 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                  32768
SF           125.7754564 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

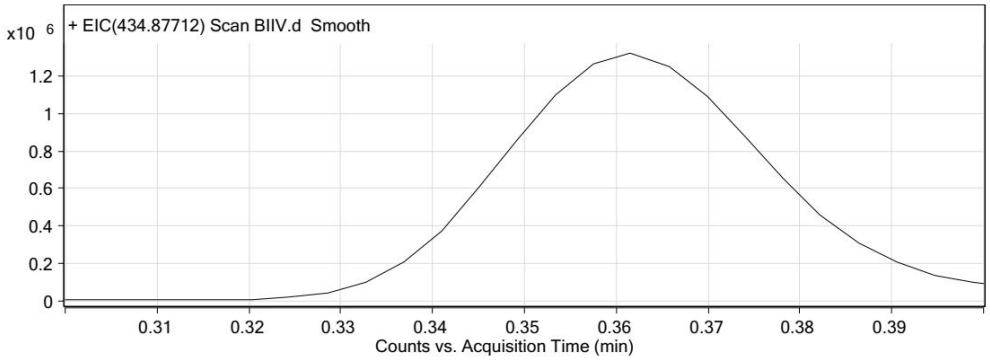
HRMS

Qualitative Analysis Report

Data File	BIIV.d	**Sample Name**	BIIV
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	26/01/2018 10:05:47 AM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

Fragmentor Voltage	14 0	**Collision Energy**	0	**Ionization Mode**	ES I

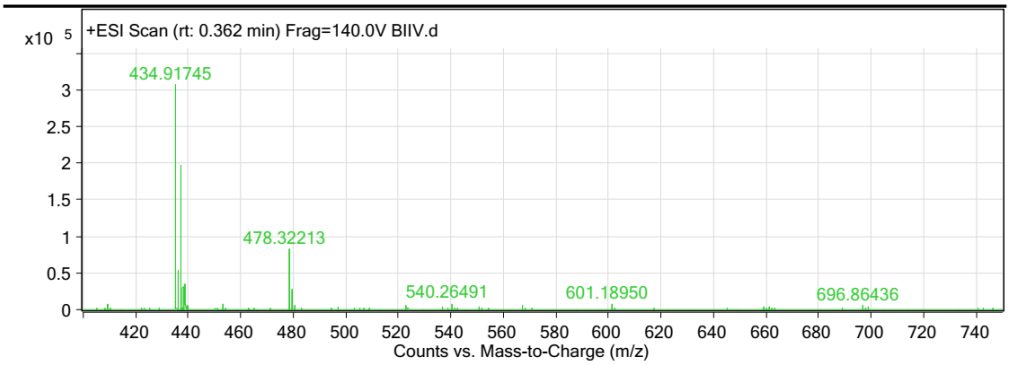


User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Agilent Technologies

Qualitative Analysis Report



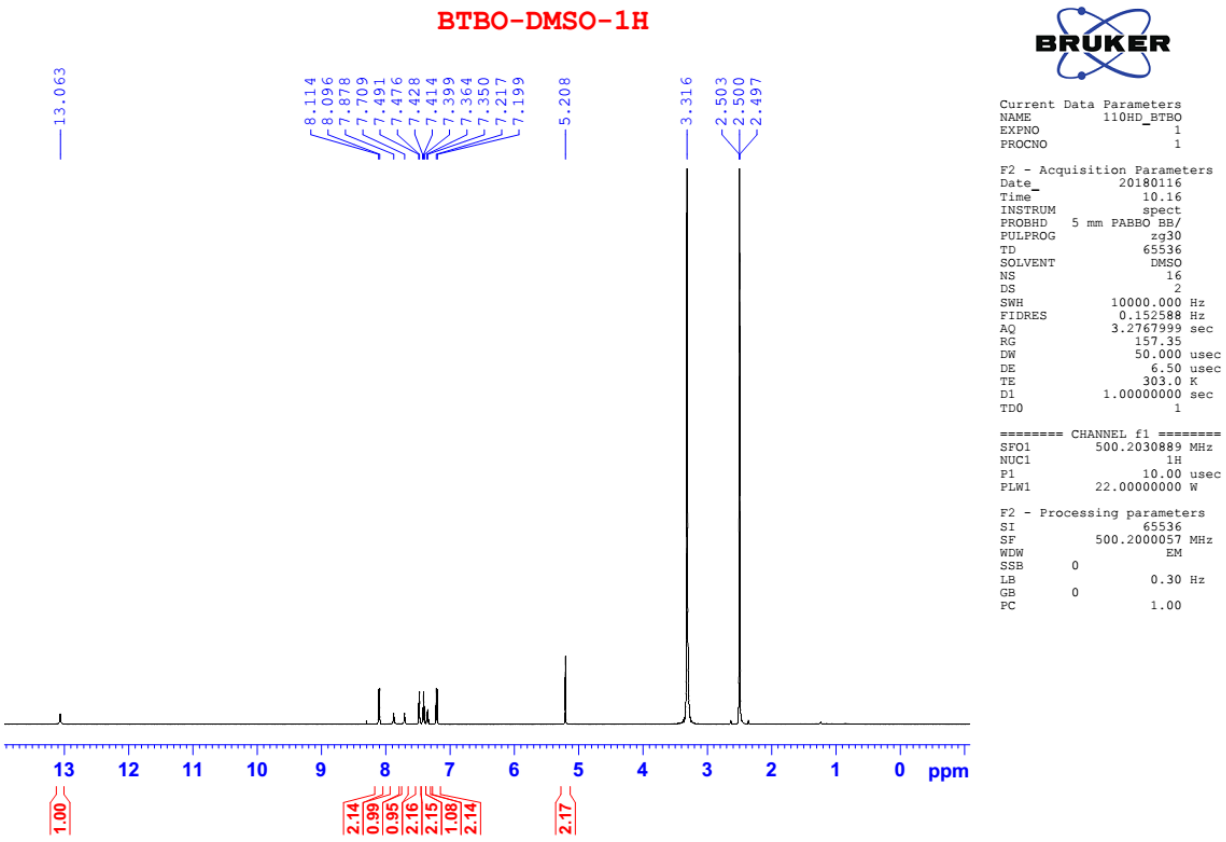
Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
S	0	5
Cl	0	3

--- End Of Report ---

2-(4-Benzyloxy-phenyl)-5,6-dichloro-1H- benzoimidazole (**36**):

^{1}H – NMR



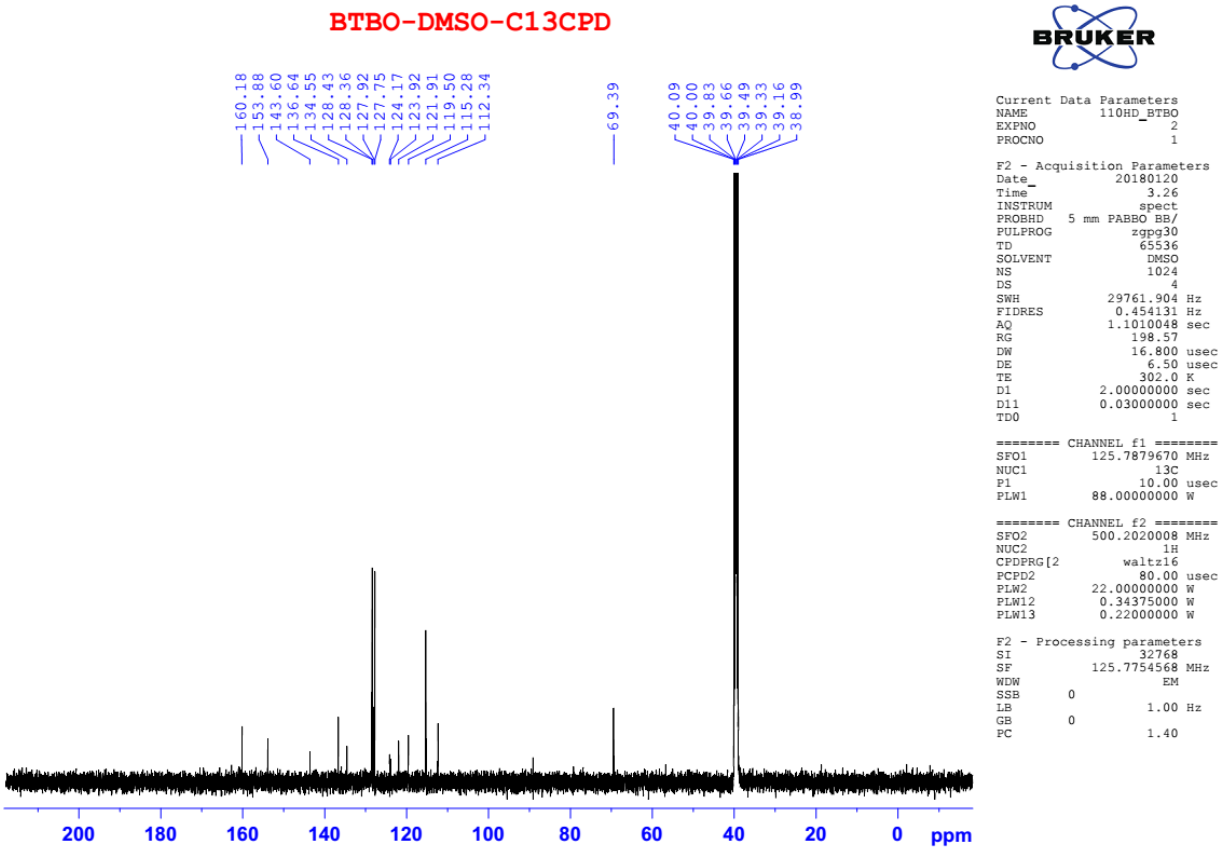

```
Current Data Parameters
NAME          110HD_BTBO
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180116
Time              10.16
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                157.35
DW               50.000 usec
DE                6.50 usec
TE                303.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                 1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                  65536
SF           500.2000057 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C – NMR




```
Current Data Parameters
NAME                 110HD_BTBO
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20180120
Time                    3.26
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       1024
DS                          4
SWH                 29761.904 Hz
FIDRES              0.454131 Hz
AQ                  1.1010048 sec
RG                     198.57
DW                     16.800 usec
DE                      6.50 usec
TE                     302.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1              125.7879670 MHz
NUC1                      13C
P1                      10.00 usec
PLW1              88.00000000 W

======== CHANNEL f2 ========
SFO2              500.2020008 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                  80.00 usec
PLW2              22.00000000 W
PLW12              0.34375000 W
PLW13              0.22000000 W

F2 - Processing parameters
SI                        32768
SF                125.7754568 MHz
WDW                         EM
SSB           0
LB                      1.00 Hz
GB            0
PC                      1.40
```

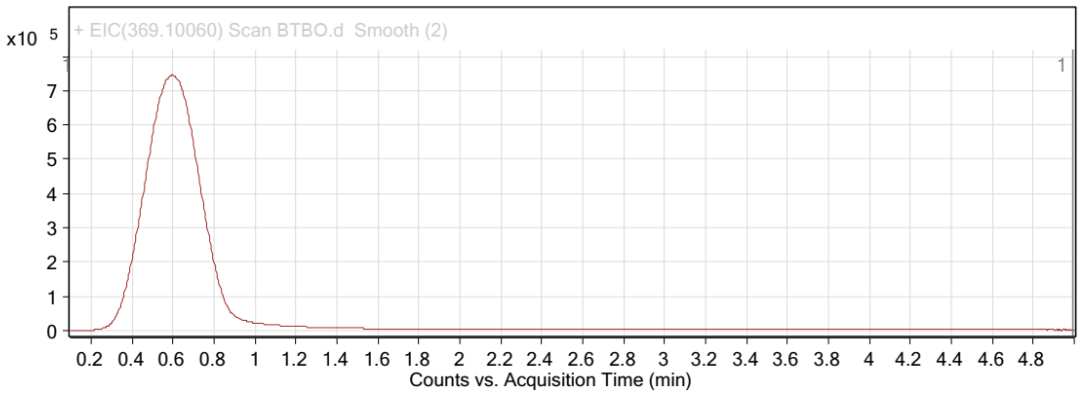
HRMS

Qualitative Analysis Report

Data File	BTBO.d	**Sample Name**	BTBO
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	08/02/2018 9:25:41 AM
IRM Calibration Status	Success	**DA Method**	Pos MS method.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

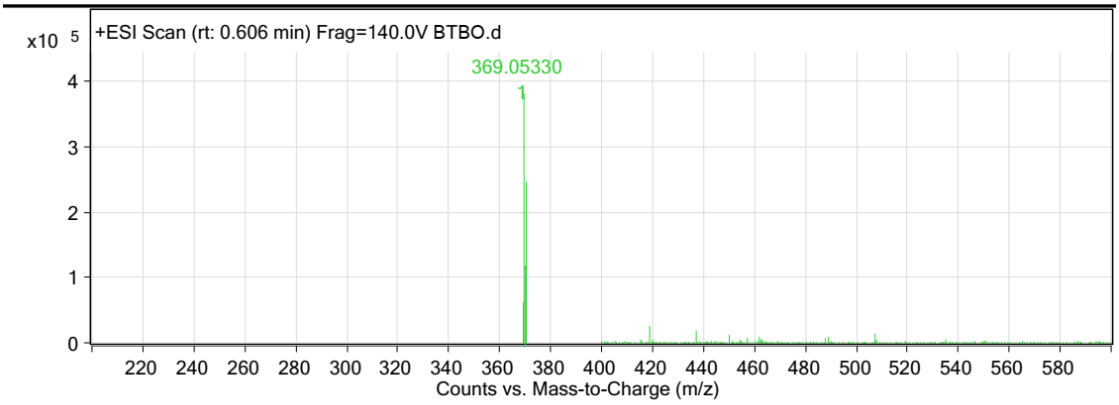
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

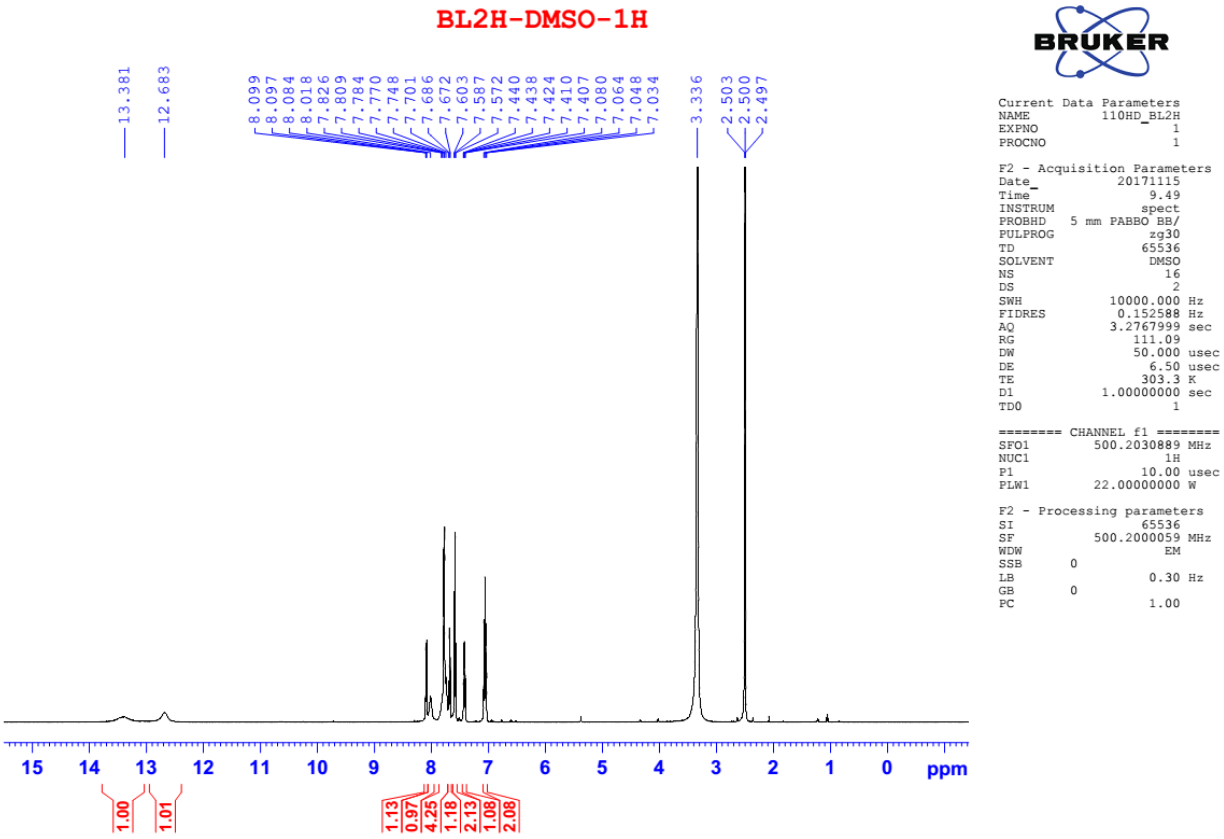
Qualitative Analysis Report



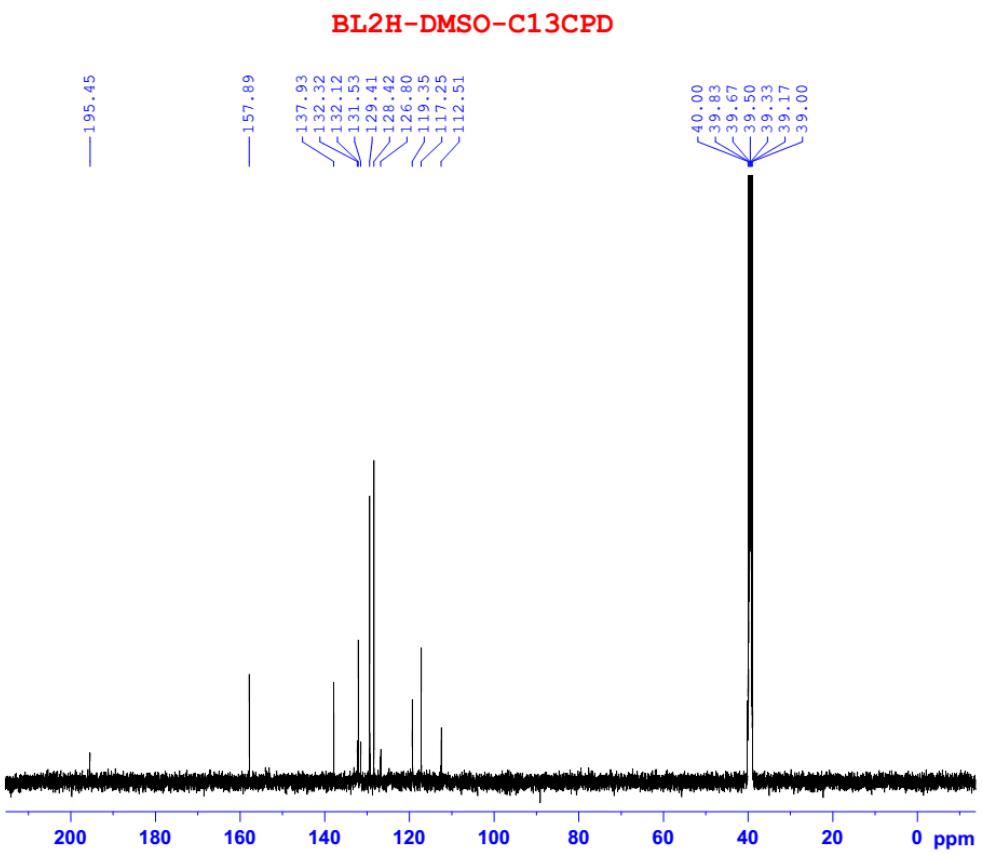
--- End Of Report ---

[2-(2-Hydroxy-phenyl)-1H-benzoimidazol-5-yl]-phenyl-methanone (**37**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BL2H
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20171115
Time              11.49
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  2048
DS                     4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                305.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7879670 MHz
NUC1                  13C
P1                  10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                 32768
SF           125.7754554 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

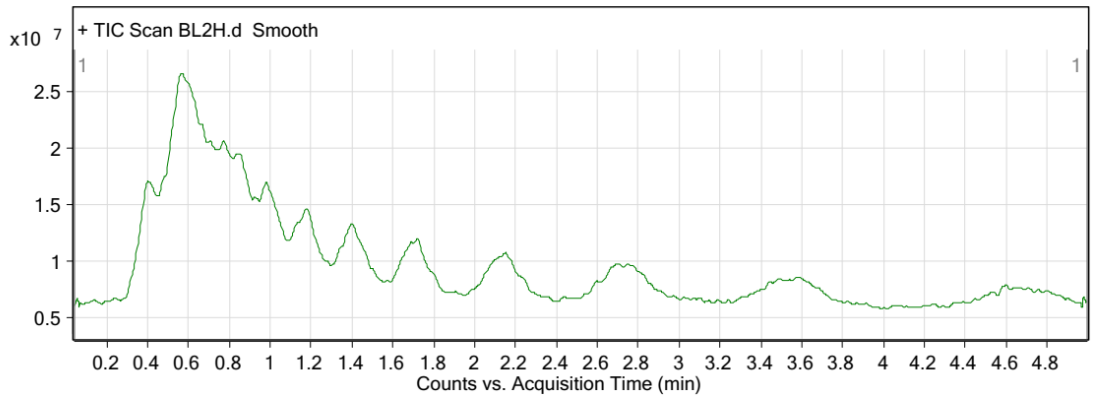
HRMS

Qualitative Analysis Report

Data File	BL2H.d	**Sample Name**	BL2H
Sample Type	Sample	**Position**	P1-C8
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	25/11/2017 11:48:13 AM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

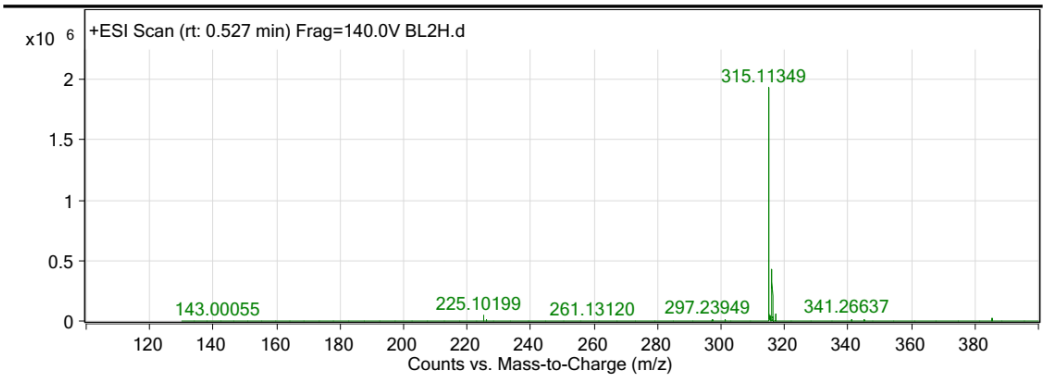
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



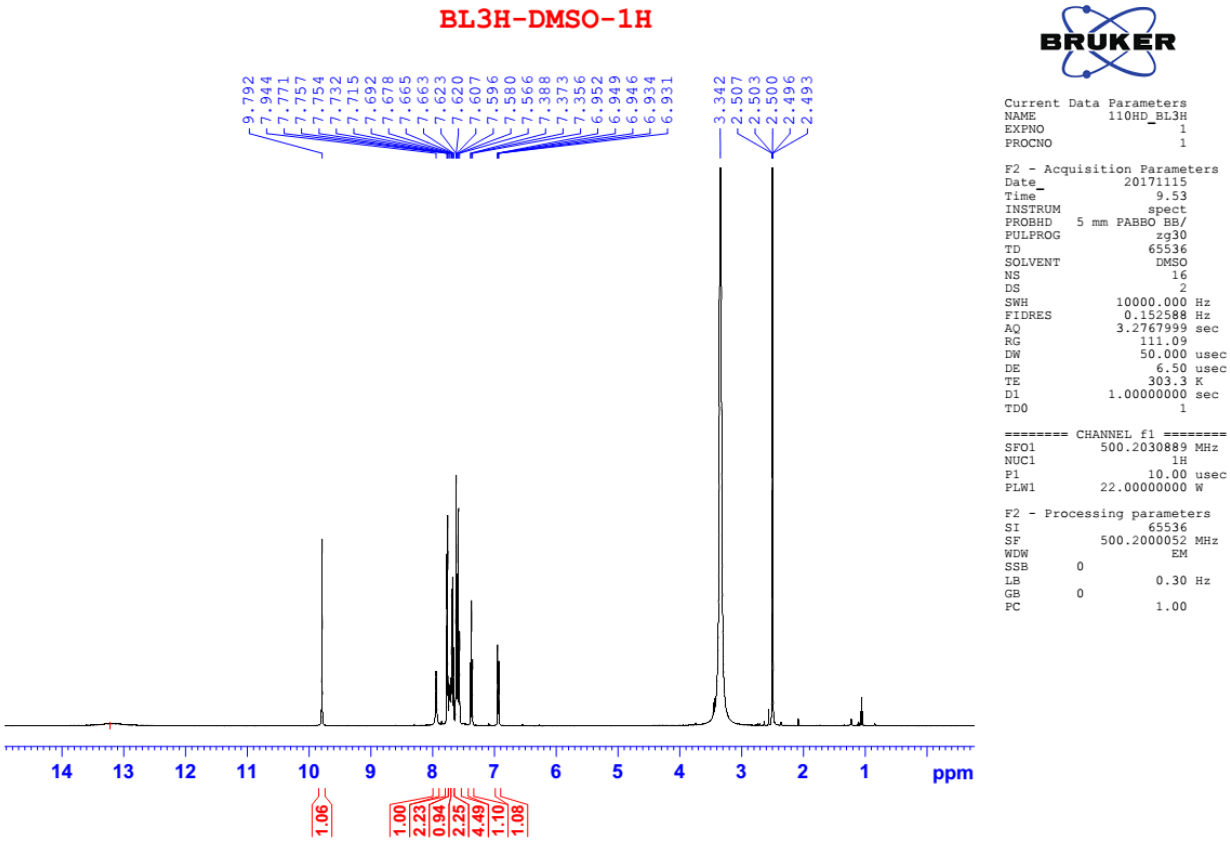
Peak List

m/z	z	Abund
225.10199	1	43673.96
315.11349	1	1945796.14
315.1838	1	155060.81
316.11665	1	425079.72
317.11944	1	54049.19
341.26637	1	18886.38
345.15947	1	14357.27
385.29211	1	21470.3
421.15472	1	54460.97
629.2175	1	27399.69

--- End Of Report ---

[2-(3-Hydroxy-phenyl)-1H-benzoimidazol-5-yl]-phenyl-methanone (**38**):

^{1}H – NMR



BRUKER

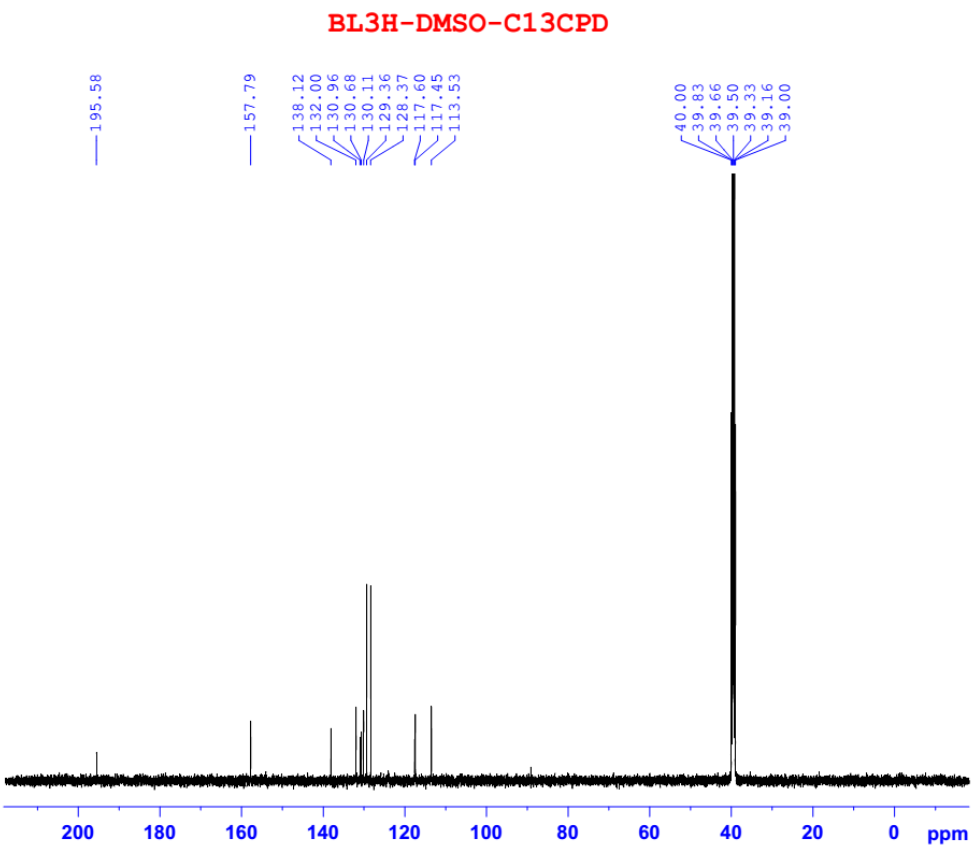
```
Current Data Parameters
NAME          110HD_BL3H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20171115
Time               9.53
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                111.09
DW                50.000 usec
DE                 6.50 usec
TE                303.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000052 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BL3H
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171115
Time              14.16
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT             DMSO
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               198.57
DW               16.800 usec
DE                6.50 usec
TE                305.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1                13C
P1                10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                 32768
SF          125.7754552 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

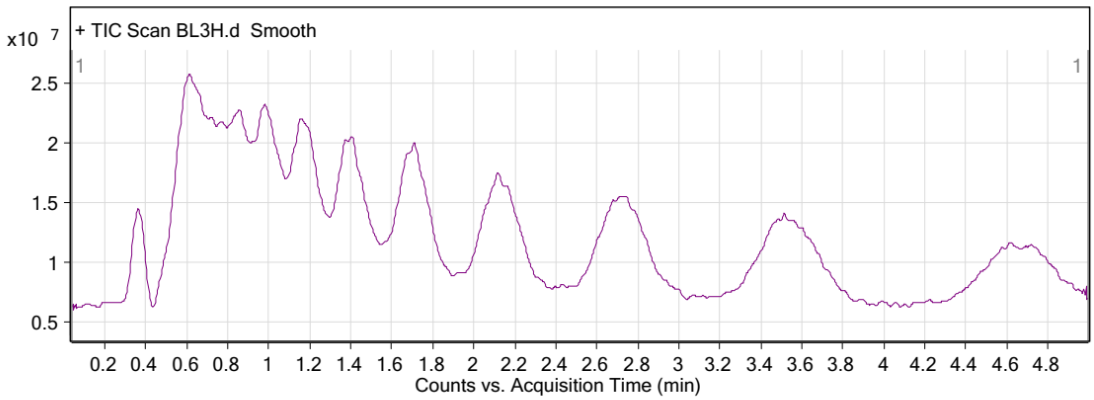
HRMS

Qualitative Analysis Report

Data File	BL3H.d	**Sample Name**	BL3H
Sample Type	Sample	**Position**	P1-C9
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	25/11/2017 11:53:58 AM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI

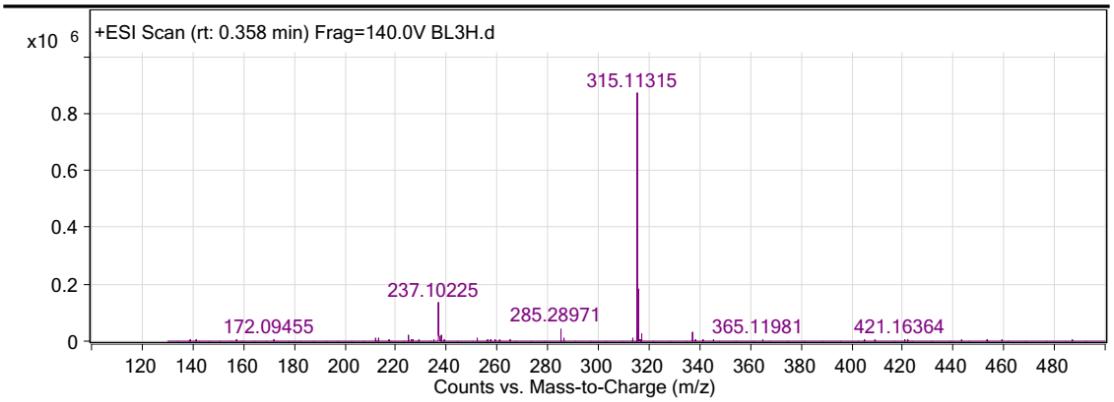


User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Agilent Technologies

Qualitative Analysis Report



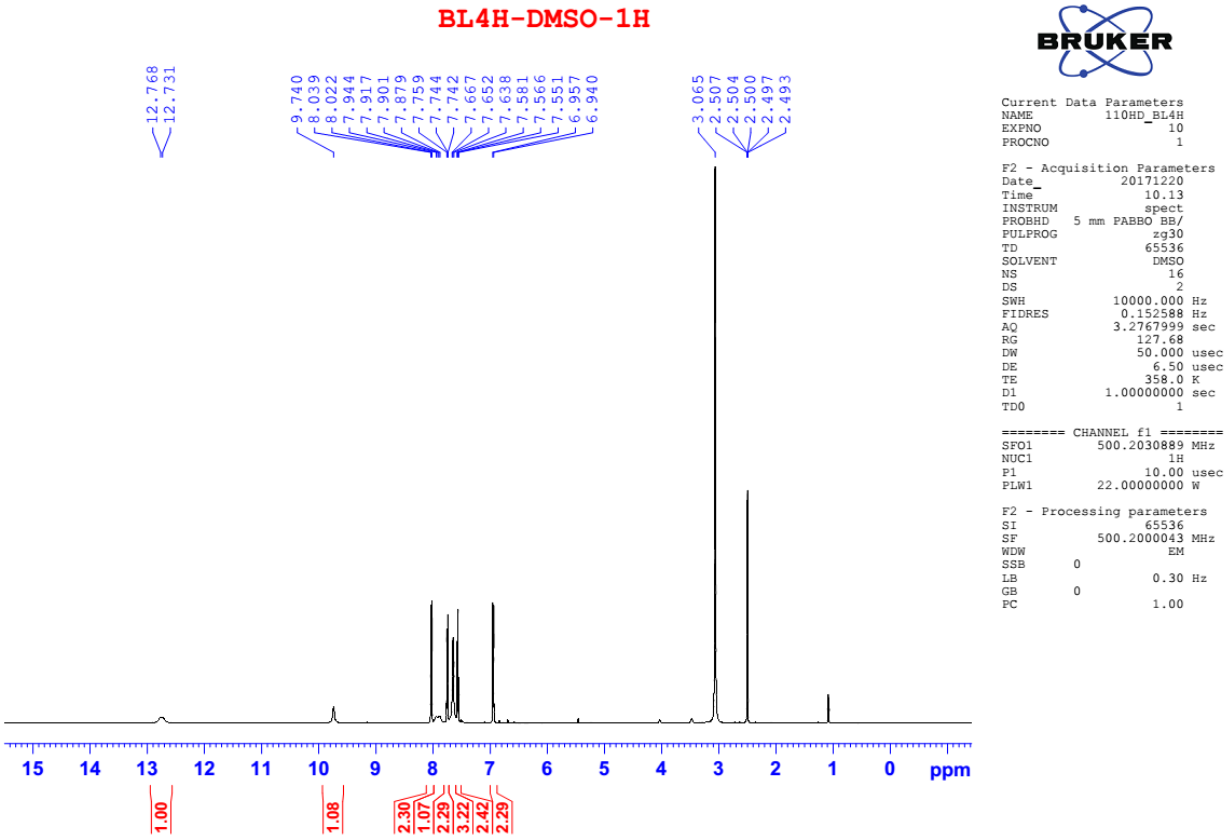
Peak List

m/z	z	Abund
237.10225	1	136281.41
285.28971	1	47357.44
315.11315	1	882123.01
315.18337	1	65545.56
316.1163	1	184772.19
337.09473	1	35600.84
629.21833	1	103159.31
630.22106	1	42897.26
651.19947	1	40552.41
965.3048	1	47540.15

--- End Of Report ---

[2-(4-Hydroxy-phenyl)-1H-benzoimidazol-5-yl]-phenyl-methanone (**39**):

^{1}H – NMR



BRUKER

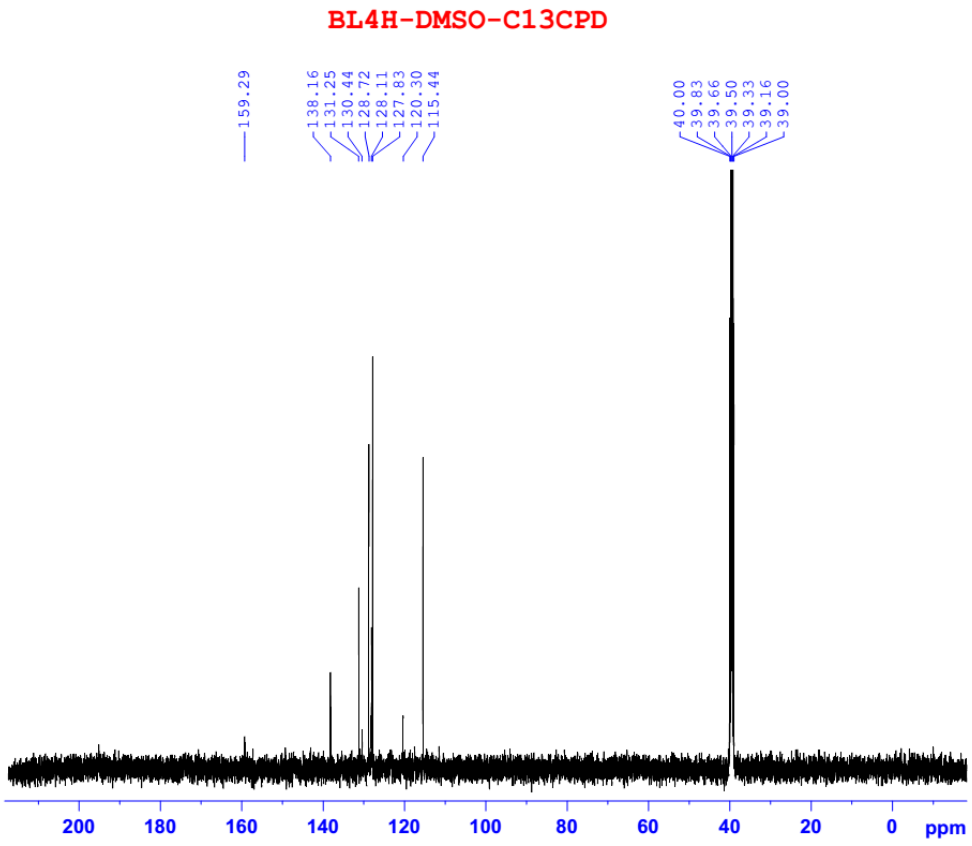
```
Current Data Parameters
NAME            110HD_BL4H
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_            20171220
Time                10.13
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH             10000.000 Hz
FIDRES          0.152588 Hz
AQ              3.2767999 sec
RG                 127.68
DW                 50.000 usec
DE                  6.50 usec
TE                 358.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                    1H
P1                  10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                    65536
SF            500.2000043 MHz
WDW                     EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME                 110HD_BL4H
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20171220
Time                    10.42
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                        1024
DS                           4
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                   1.1010048 sec
RG                      198.57
DW                      16.800 usec
DE                       6.50 usec
TE                      358.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                125.7879670 MHz
NUC1                        13C
P1                        10.00 usec
PLW1                88.00000000 W

======== CHANNEL f2 ========
SFO2                500.2020008 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2                22.00000000 W
PLW12                0.34375000 W
PLW13                0.22000000 W

F2 - Processing parameters
SI                       32768
SF                  125.7753900 MHz
WDW                        EM
SSB              0
LB                        1.00 Hz
GB               0
PC                        1.40
```

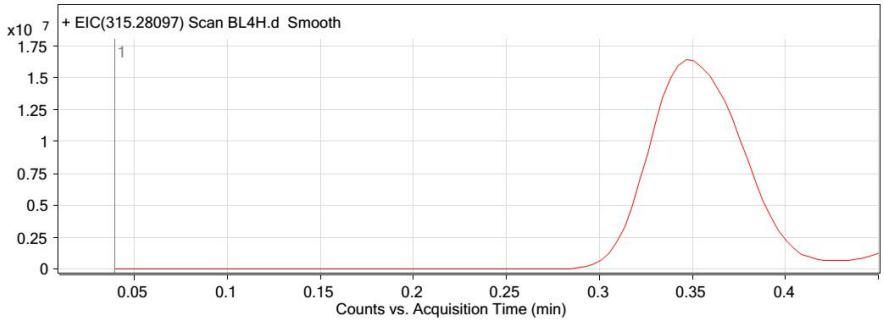
HRMS

Qualitative Analysis Report

Data File	BL4H.d	**Sample Name**	BL4H
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	17/01/2018 2:58:29 PM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

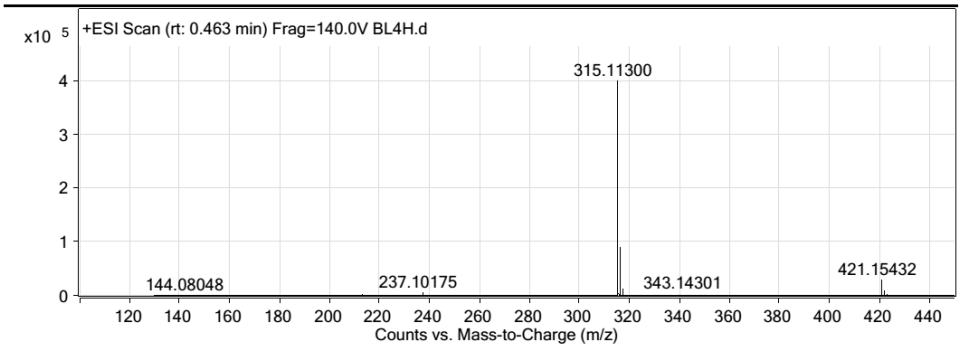
Fragmentor Voltage	14 0	**Collision Energy**	0	**Ionization Mode**	ES I



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



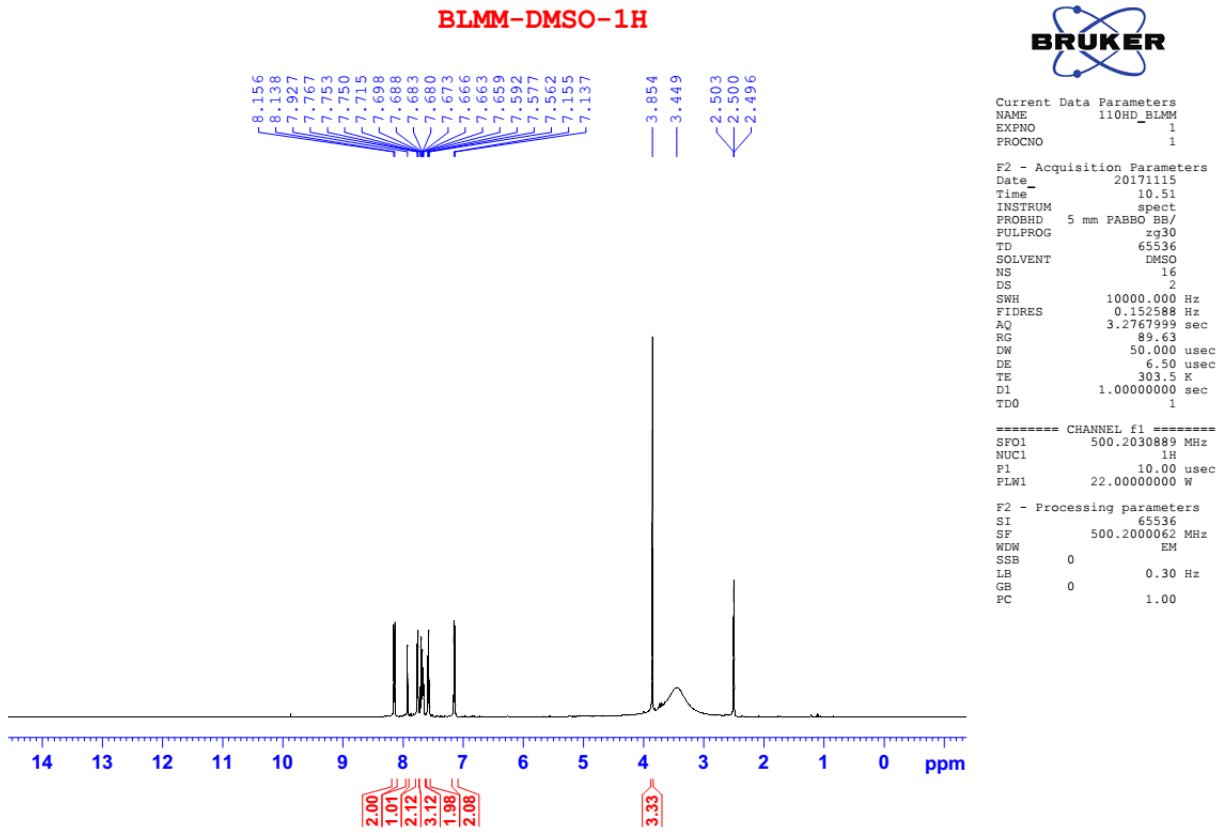
Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
S	0	5
Cl	0	3

--- End Of Report ---

[2-(4-Methoxy-phenyl)-1H-benzoimidazol-5-yl]-phenyl-methanone (**40**):

^{1}H – NMR



BRUKER

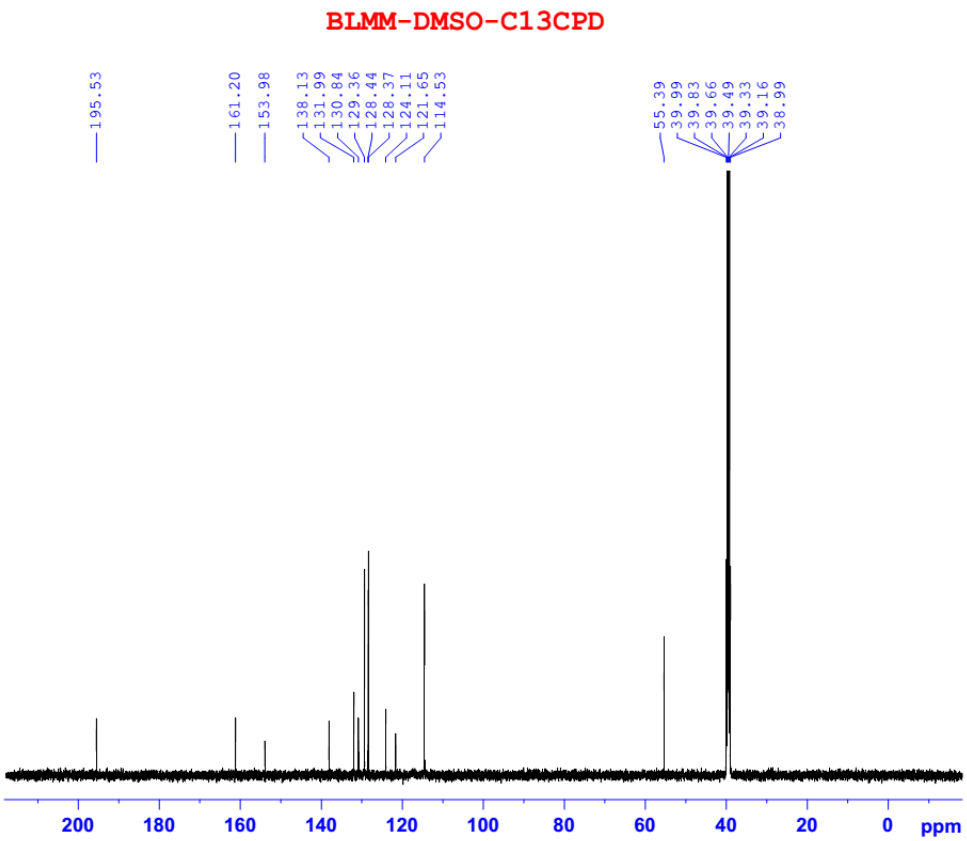
```
Current Data Parameters
NAME          110HD_BLMM
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20171115
Time              10.51
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                89.63
DW               50.000 usec
DE                6.50 usec
TE               303.5 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                 1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.2000062 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BLMM
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20171115
Time              11.09
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT             DMSO
NS                    512
DS                      4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                304.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1                13C
P1                10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                 32768
SF          125.7753900 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

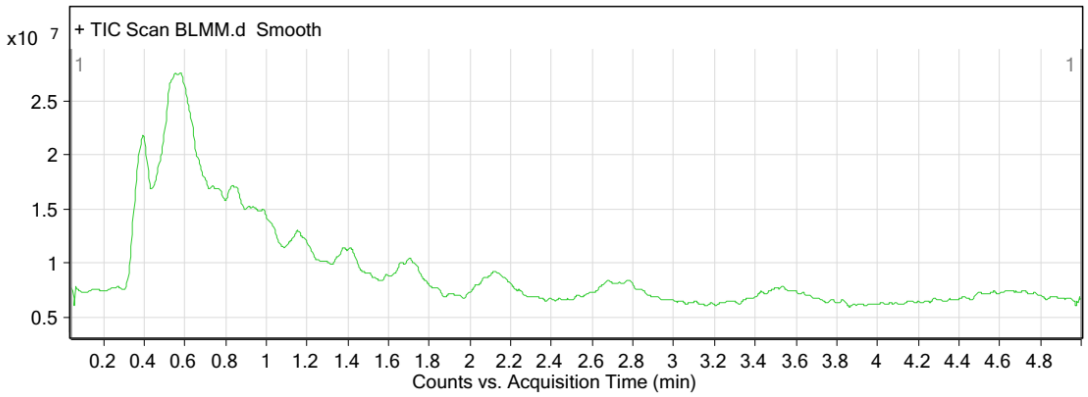
HRMS

Qualitative Analysis Report

Data File	BLMM.d	**Sample Name**	BLMM
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	25/11/2017 12:05:26 PM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

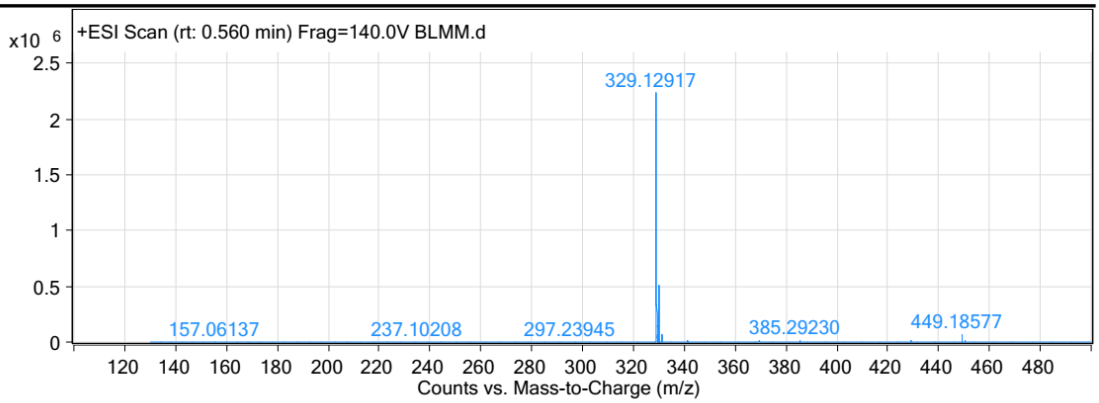
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



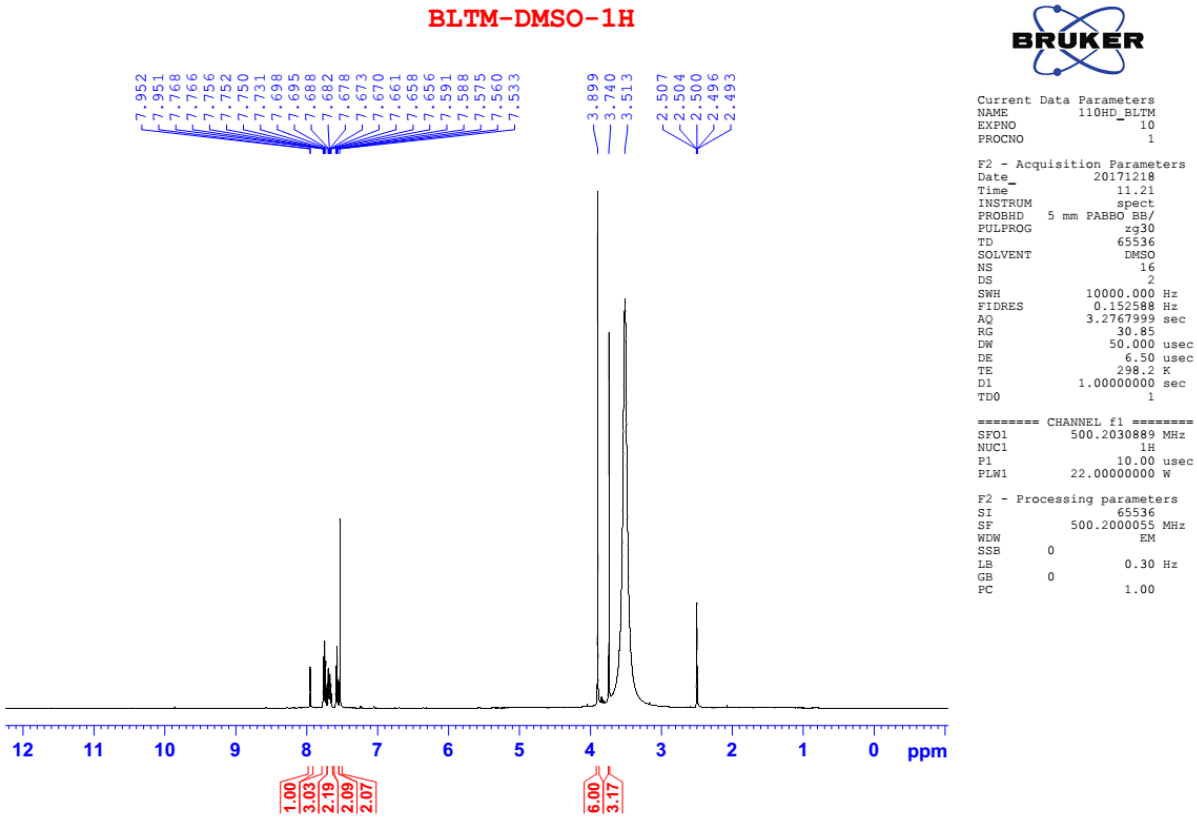
Peak List

m/z	z	Abund
329.12917	1	2268529.31
330.13228	1	515373.98
331.1349	1	65132.97
341.26601	1	21683.95
449.18577	1	66259.56
450.18866	1	20028.15
657.25115	1	153797.56
658.25276	1	78649.23
719.40491	1	43916.58
720.40898	1	22488.36

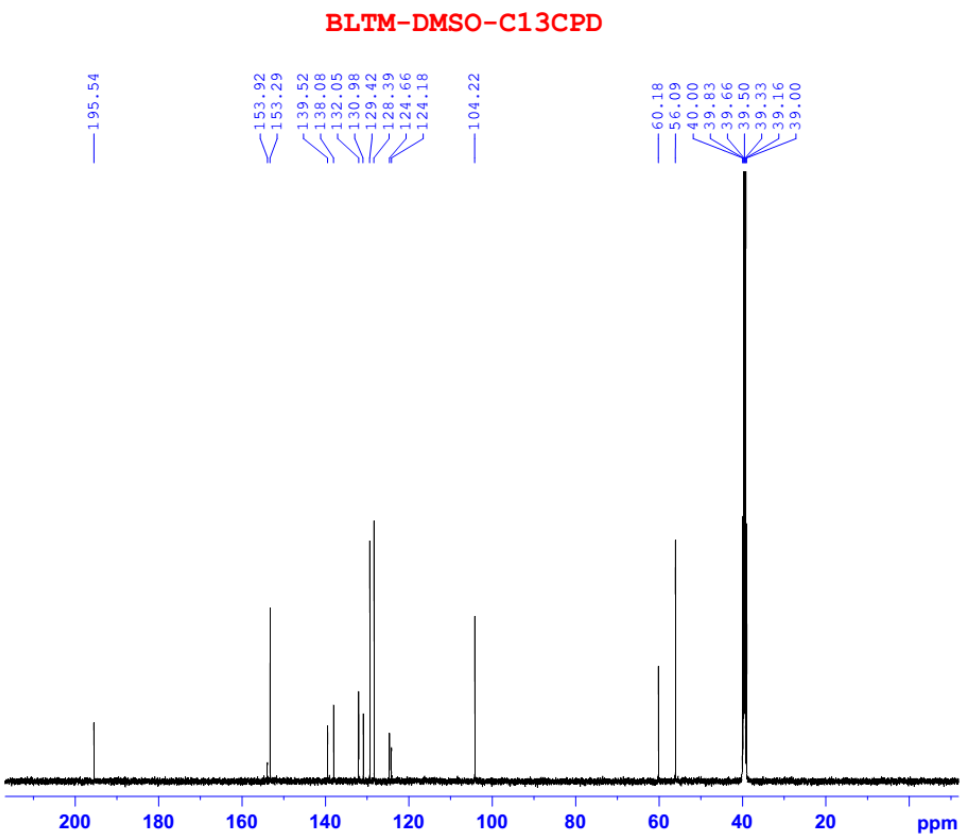
--- End Of Report ---

Phenyl-[2-(3,4,5-trimethoxy-phenyl)-1H-benzoimidazol-5-yl]-methanone (**41**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BLTM
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171117
Time               8.52
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              65536
SOLVENT          DMSO
NS                1024
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              198.57
DW              16.800 usec
DE               6.50 usec
TE              304.5 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1               13C
P1               10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                32768
SF          125.7754519 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

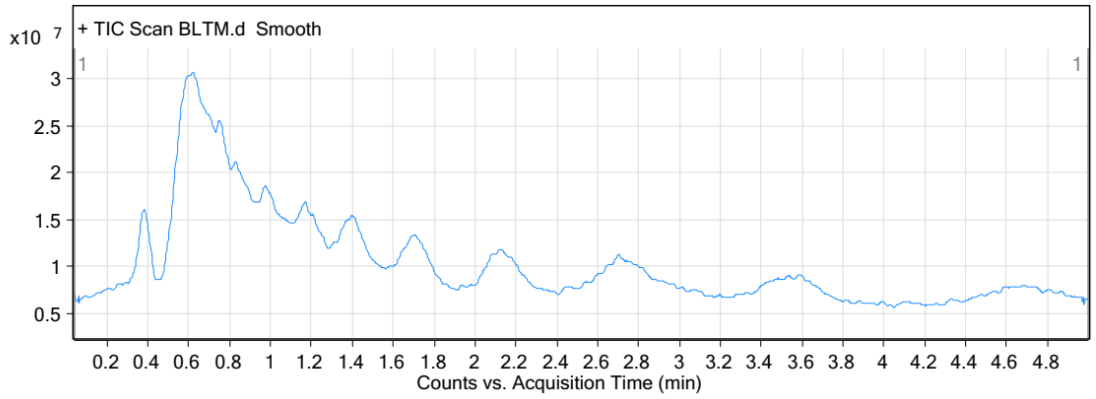
HRMS

Qualitative Analysis Report

Data File	BLTM.d	**Sample Name**	BLTM
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	25/11/2017 11:59:42 AM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

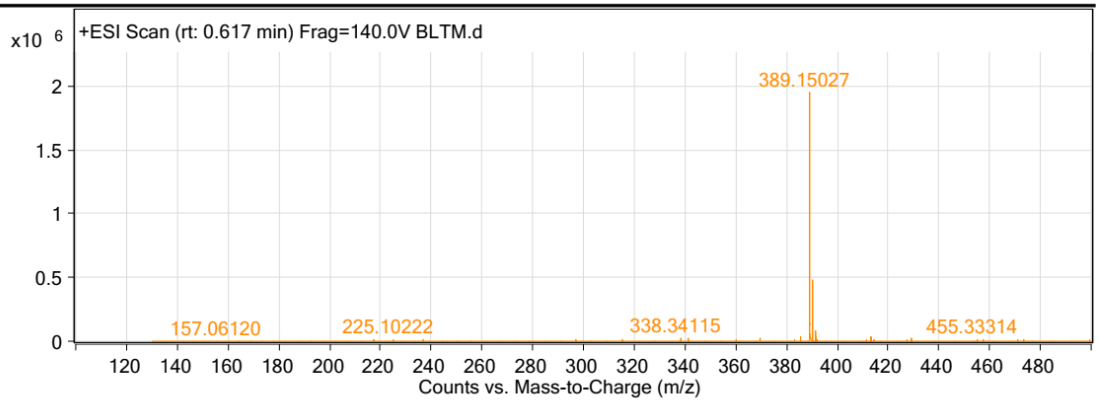
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



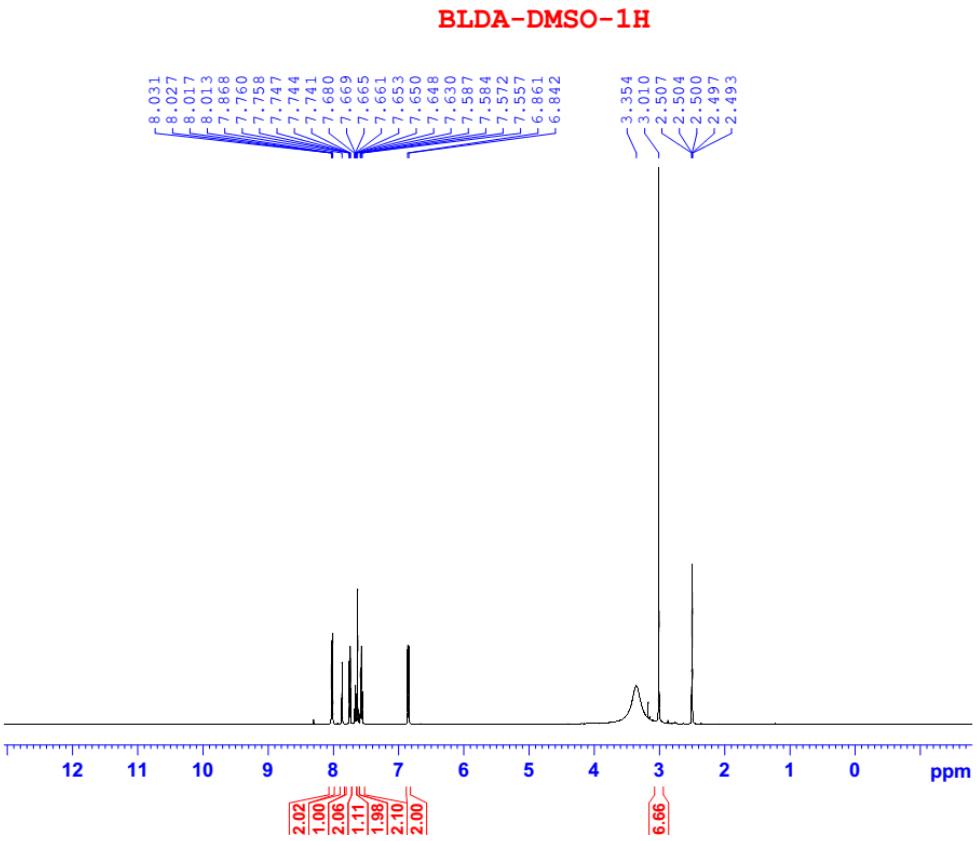
Peak List

m/z	z	Abund
385.2914	1	33517.66
389.15027	1	1999519.47
390.15342	1	490433.2
391.15564	1	78621.57
777.29319	1	218874.84
778.29559	1	126098.91
779.42707	1	143775.93
780.42979	1	74112.81
1165.43339	1	64534.87
1166.43702	1	48734.36

--- End Of Report ---

[2-(4-Dimethylamino-phenyl)-1*H*-benzoimidazol-5-yl](phenyl)methanone (**42**):

^{1}H – NMR



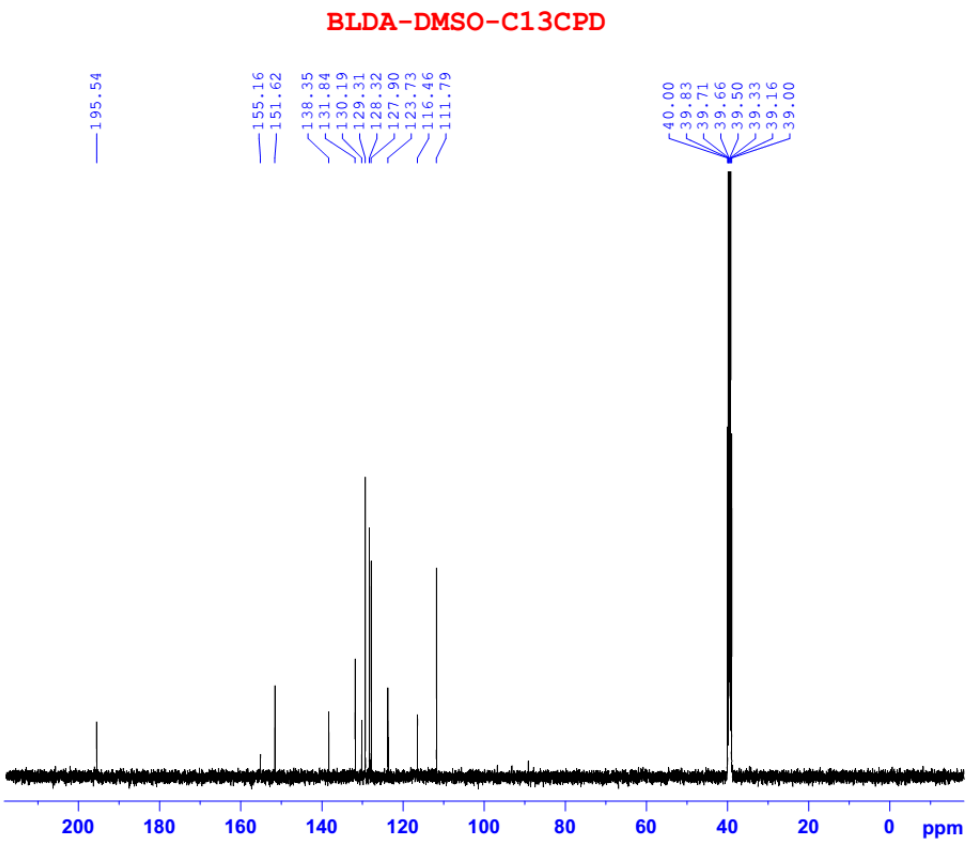
Current Data Parameters
NAME 110HD_BLDA
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180126
Time 16.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 97.76
DW 50.000 usec
DE 6.50 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.2030889 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 500.2000054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME                 110HD_BLDA
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20180126
Time                   18.02
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                    198.57
DW                   16.800 usec
DE                    6.50 usec
TE                   303.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1            125.7879670 MHz
NUC1                       13C
P1                       10.00 usec
PLW1            88.00000000 W

======== CHANNEL f2 ========
SFO2            500.2020008 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                    80.00 usec
PLW2            22.00000000 W
PLW12            0.34375000 W
PLW13            0.22000000 W

F2 - Processing parameters
SI                        32768
SF              125.7753900 MHz
WDW                        EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

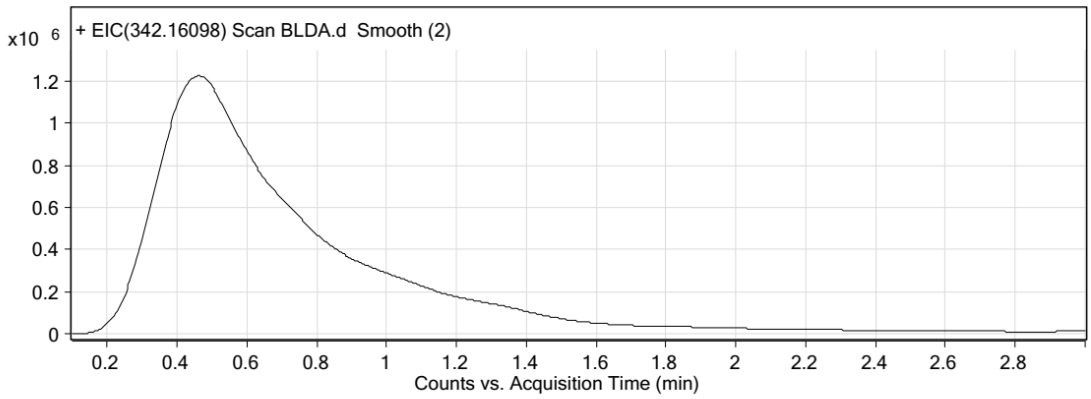
HRMS

Qualitative Analysis Report

Data File	BLDA.d	**Sample Name**	BLDA
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	20/05/2018 6:11:38 PM
IRM Calibration Status	Success	**DA Method**	default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

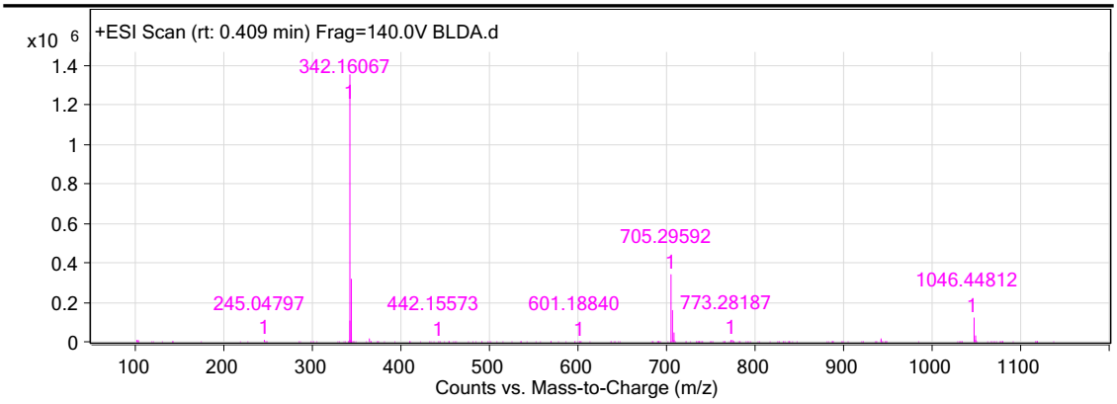
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



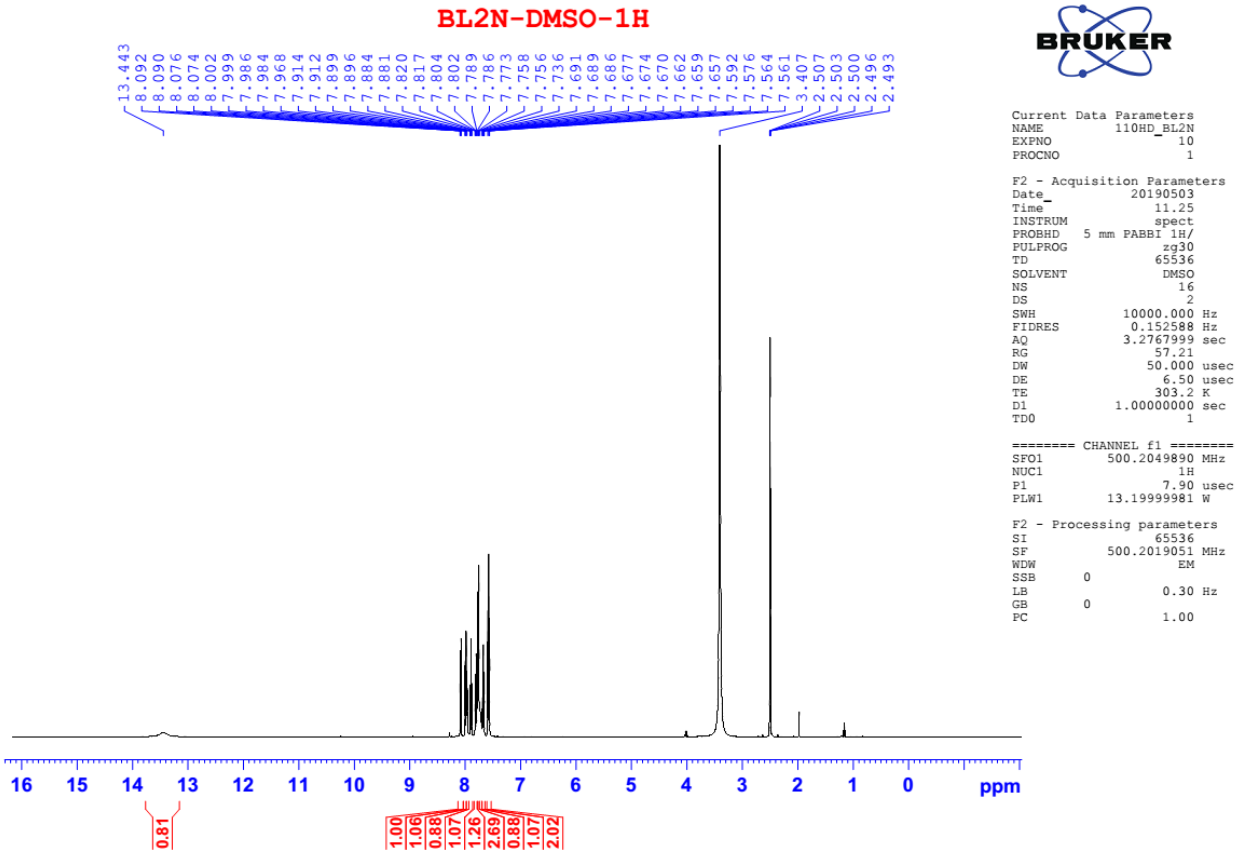
Peak List

m/z	z	Abund
342.16067	1	1348271.75
342.23506	1	106395.44
343.16415	1	317660.97
344.16648	1	43093.84
705.29592	1	342451.22
706.2995	1	162553.94
707.30081	1	43087.26
1046.44812	1	118882.19
1047.45103	1	91199.11
1048.4537	1	33248.23

--- End Of Report ---

[2-(2-Nitrophenyl)-1H-benzoimidazol-5-yl](phenyl)methanone (**43**):

^{1}H – NMR



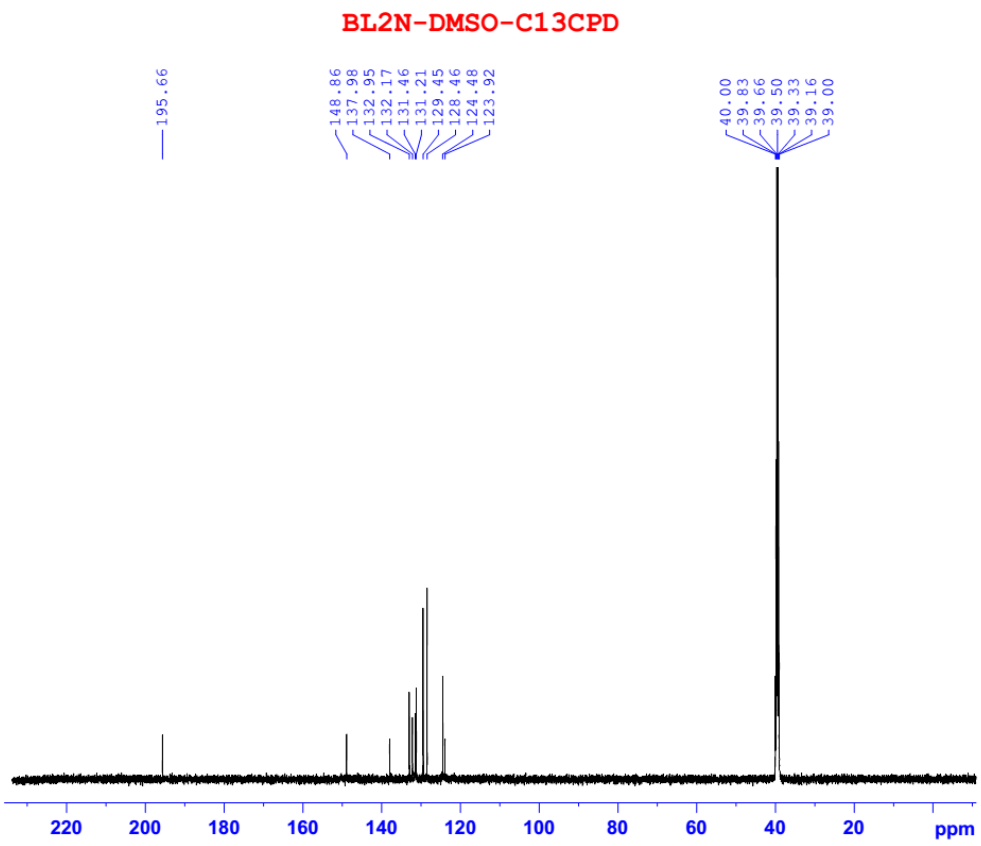

```
Current Data Parameters
NAME          110HD_BL2N
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190503
Time              11.25
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                57.21
DW              50.000 usec
DE               6.50 usec
TE               303.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.2049890 MHz
NUC1                 1H
P1                7.90 usec
PLW1        13.19999981 W

F2 - Processing parameters
SI               65536
SF          500.2019051 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C – NMR



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```
Current Data Parameters
NAME          110HD_BL2N
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190503
Time              17.48
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG         zgpg30
TD               65536
SOLVENT            DMSO
NS                   512
DS                     4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ            1.0485760 sec
RG               198.57
DW               16.000 usec
DE                6.50 usec
TE                307.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        125.7897032 MHz
NUC1                13C
P1                15.40 usec
PLW1        81.00000000 W

======== CHANNEL f2 ========
SFO2        500.2039008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        13.19999981 W
PLW12        0.12872000 W
PLW13        0.08238100 W

F2 - Processing parameters
SI                 32768
SF          125.7759268 MHz
WDW                EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

HRMS

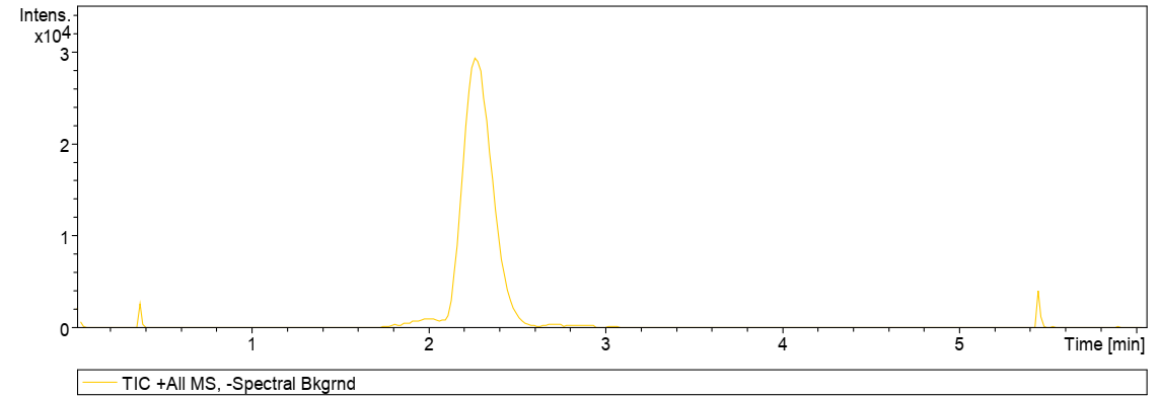
Display Report

Analysis Info

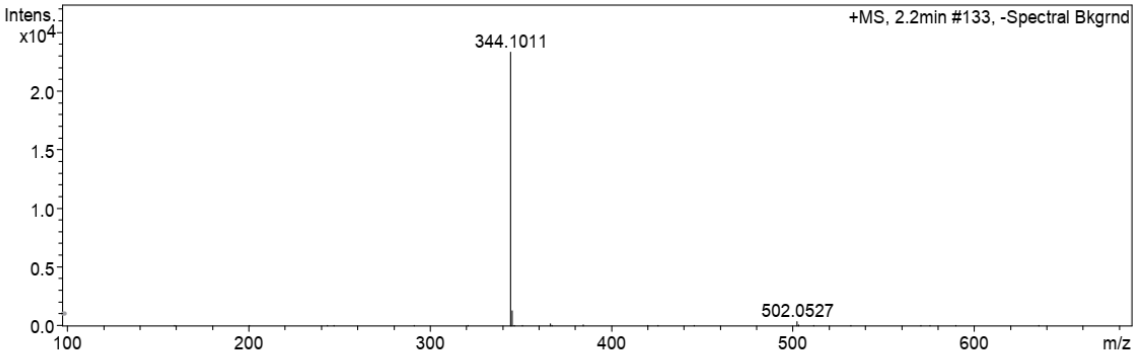
Analysis Name	D:Data2019thang 05BC2N_2-D,1_01_1730.d	Acquisition Date	6/20/2019 10:40:27 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BC2N	Instrument	micrOTOF-Q 10187
Comment			

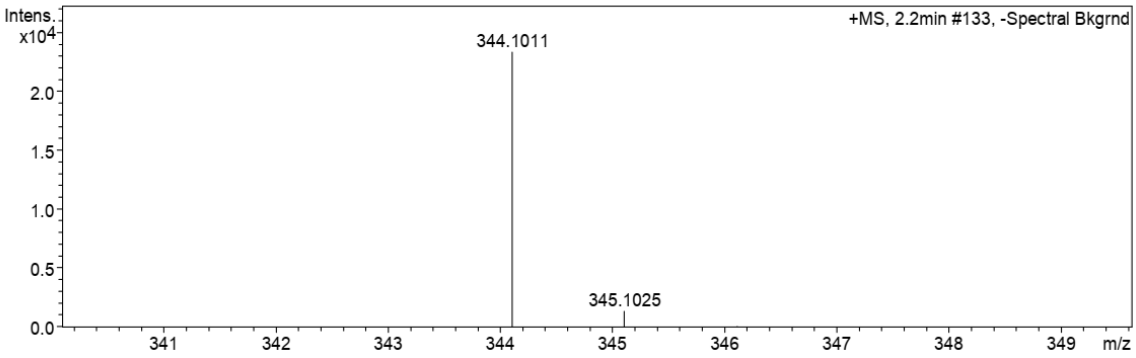
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.5 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



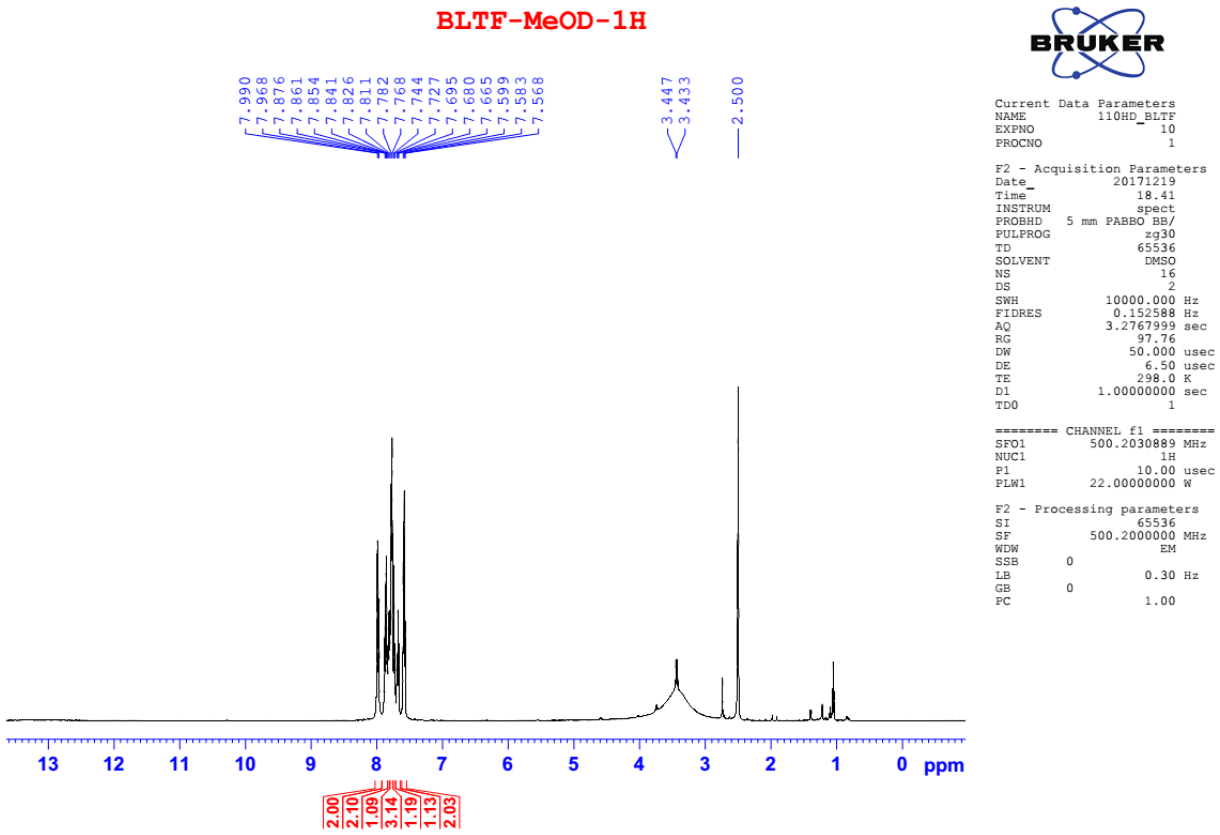
TIC +All MS, -Spectral Bkgrnd





Phenyl(2-(2-(trifluoromethyl)phenyl)-1H-benzo[d]imidazol-5-yl)methanone (**44**):

^{1}H – NMR



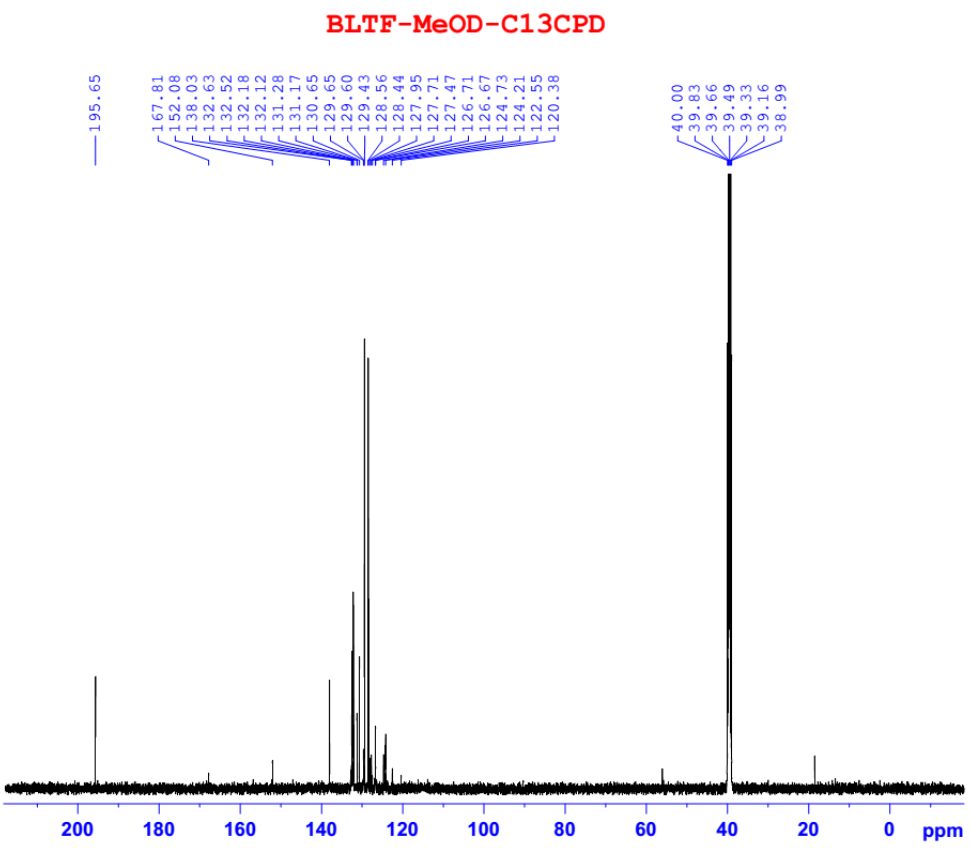

```
Current Data Parameters
NAME          110HD_BLTF
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171219
Time               18.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                 97.76
DW                50.000 usec
DE                 6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR




```
Current Data Parameters
NAME          110HD_BLTF
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171219
Time              19.50
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT             DMSO
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                299.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1                13C
P1                10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                 32768
SF          125.7753900 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

HRMS

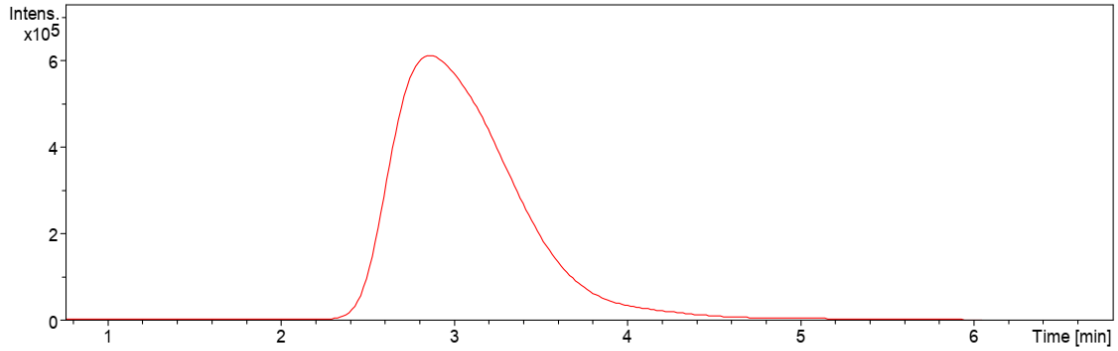
Display Report

Analysis Info

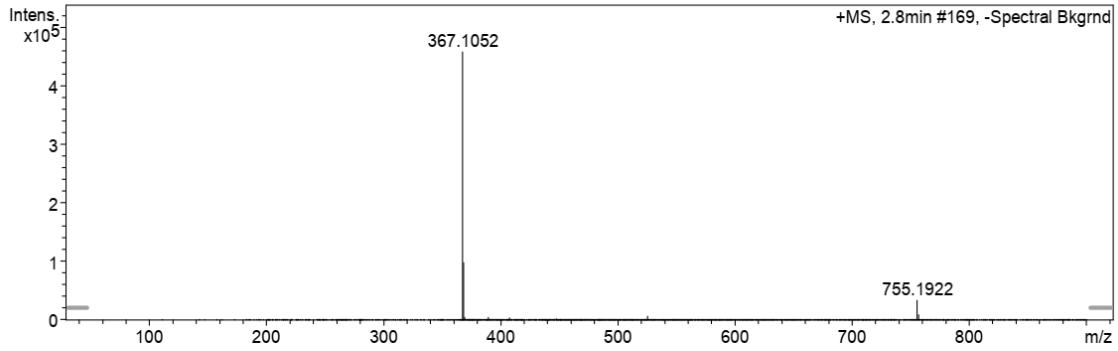
Analysis Name	D:\Data\2019\thang 05\13-05\BLTF_1-B,5_01_1349.d	Acquisition Date	4/19/2019 4:17:07 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BLTF	Instrument	micrOTOF-Q 10187
Comment			

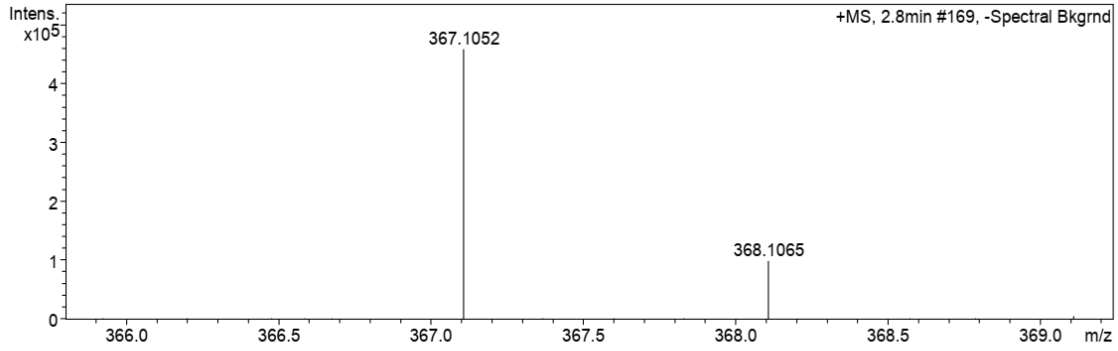
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	900 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



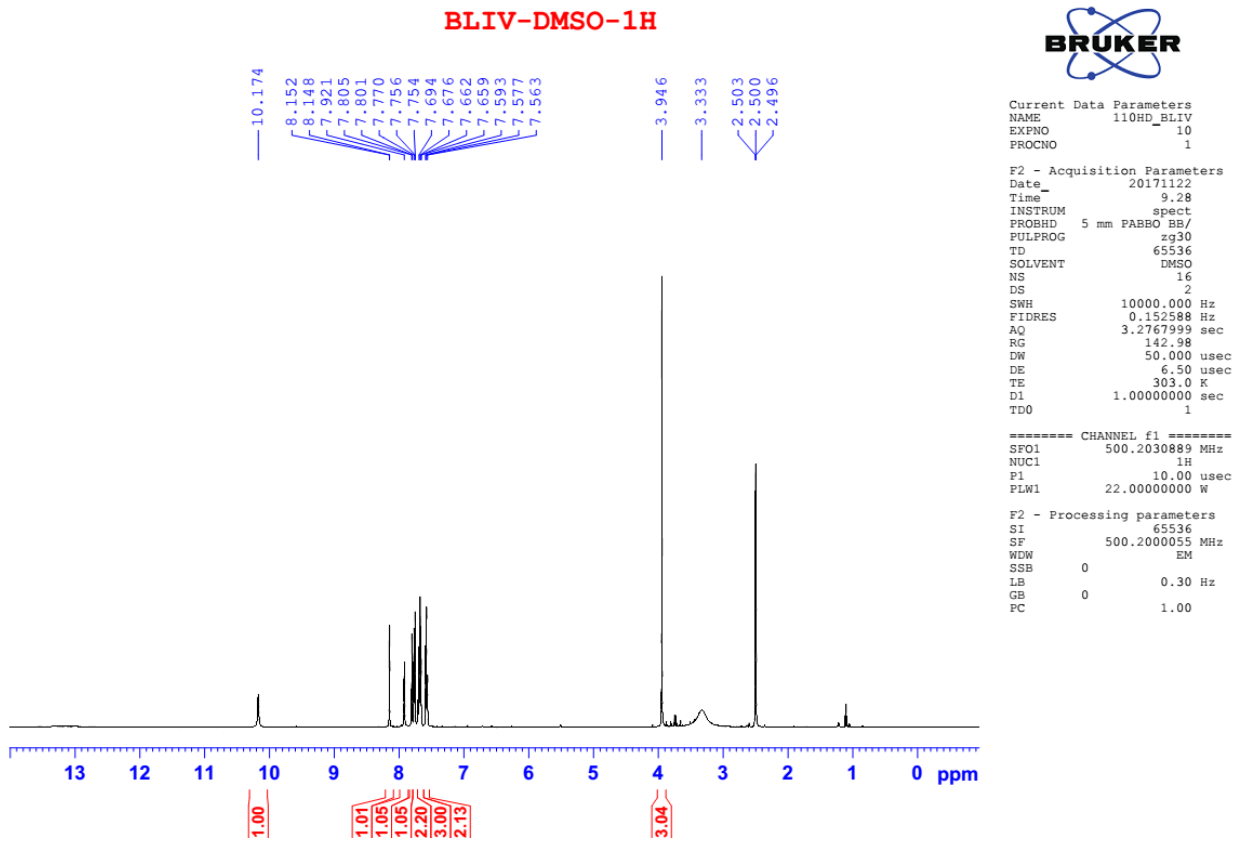
TIC +All MS, -Spectral Bkgrnd, Smoothed (4.01,2,GA)





(2-(4-Hydroxy-3-iodo-5-methoxyphenyl)-1*H*-benzoimidazol-5-yl)(phenyl)methanone (**45**):

^{1}H – NMR



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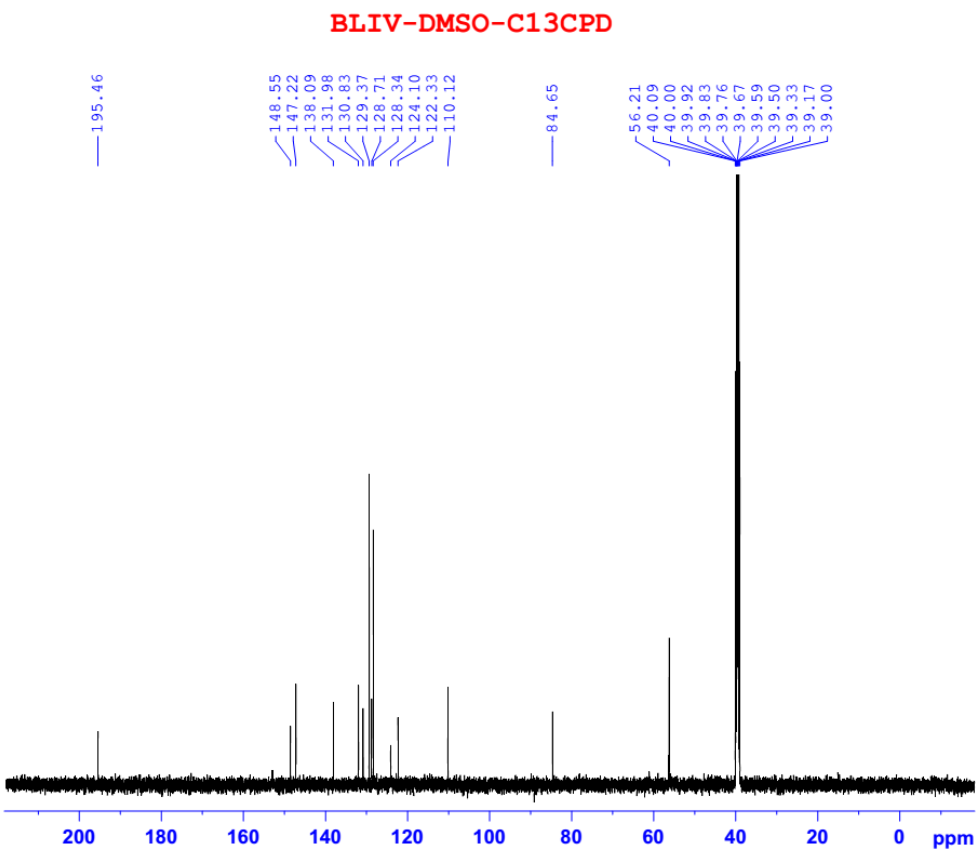
```
Current Data Parameters
NAME          110HD_BLIV
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171122
Time                9.28
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                142.98
DW                50.000 usec
DE                 6.50 usec
TE                303.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                   1H
P1                 10.00 usec
PLW1        22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000055 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BLIV
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171122
Time               9.34
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                 512
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              198.57
DW              16.800 usec
DE               6.50 usec
TE              303.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1               13C
P1               10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                32768
SF          125.7753900 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

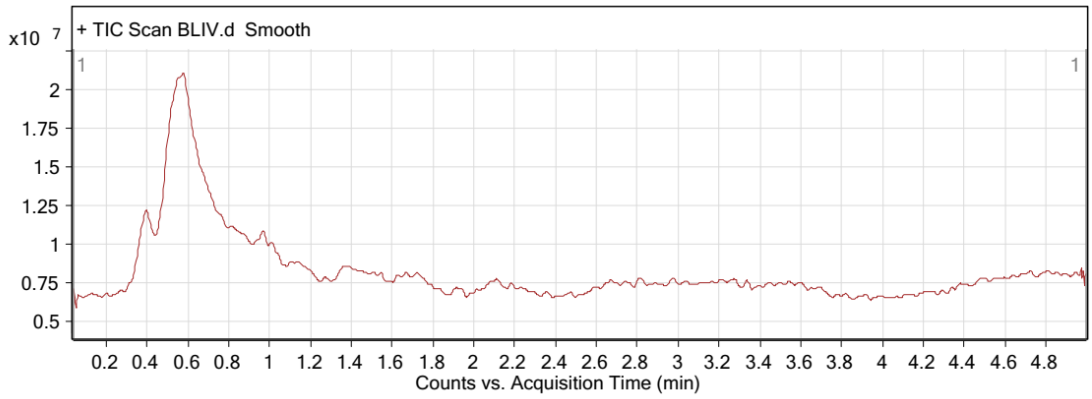
HRMS

Qualitative Analysis Report

Data File	BLIV.d	**Sample Name**	BLIV
Sample Type	Sample	**Position**	P1-D4
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	25/11/2017 12:16:55 PM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI

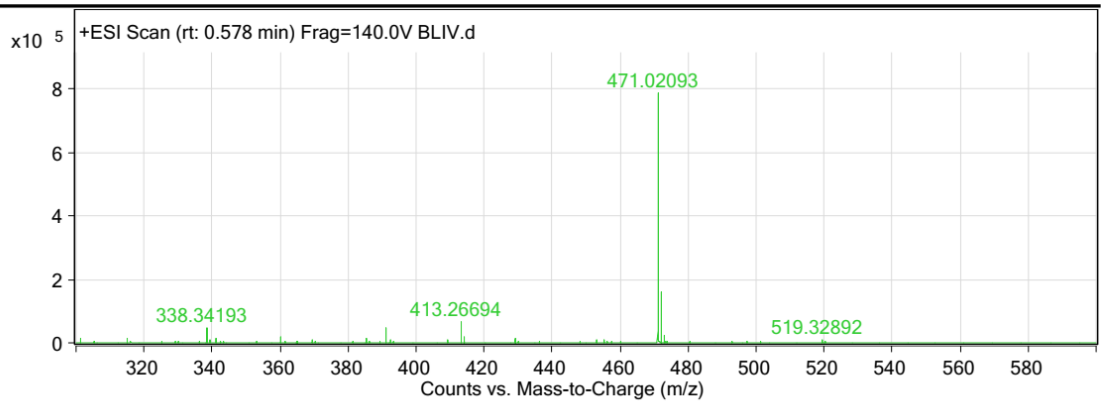


User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Agilent Technologies

Qualitative Analysis Report



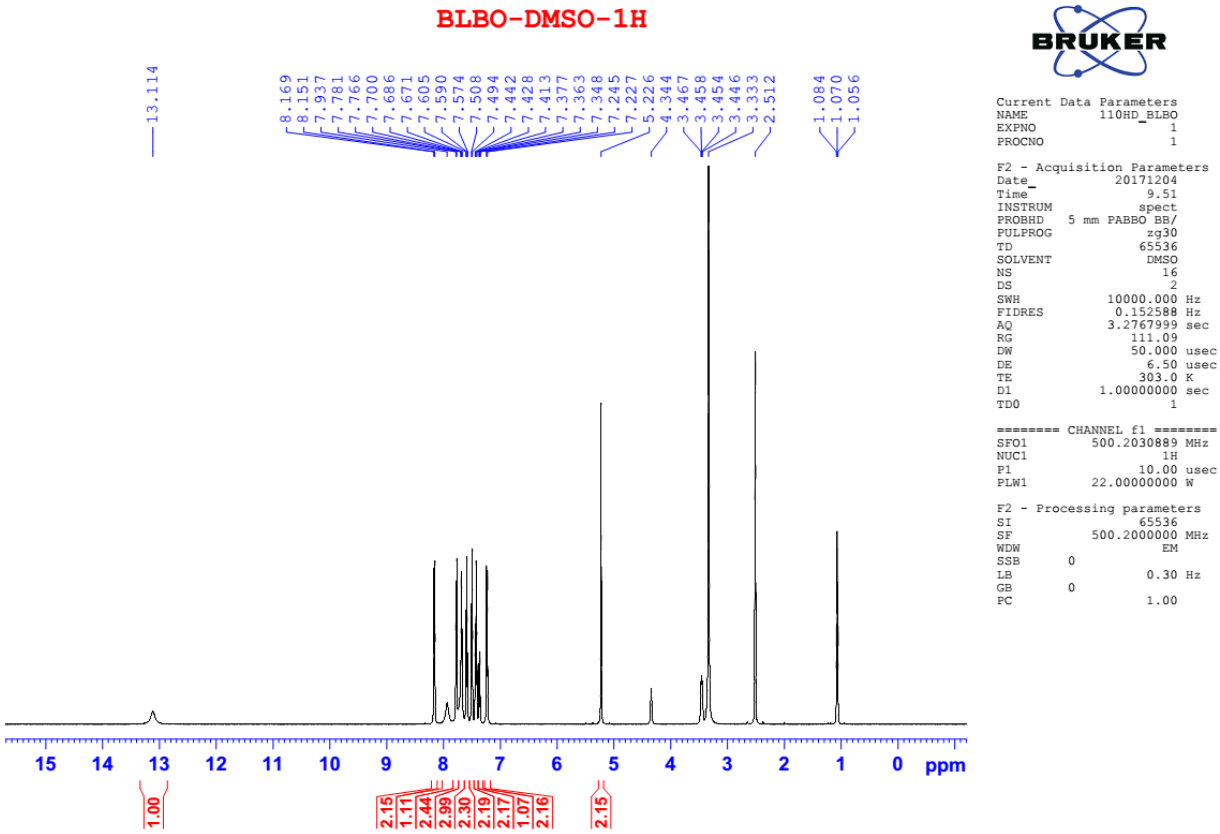
Peak List

m/z	z	Abund
338.34193	1	48250.48
391.28472	1	45739.14
413.26694	1	66204.02
471.02093	1	795408.78
472.02489	1	163875.43
803.54398	1	62083.3
808.35505	1	46611.92
861.29852	1	127180.22
862.30076	1	62932.18
941.03362	1	85225.85

--- End Of Report ---

(2-(4-(Benzyloxy)phenyl)-1*H*-benzoimidazol-5-yl)(phenyl)methanone (**46**):

^{1}H – NMR



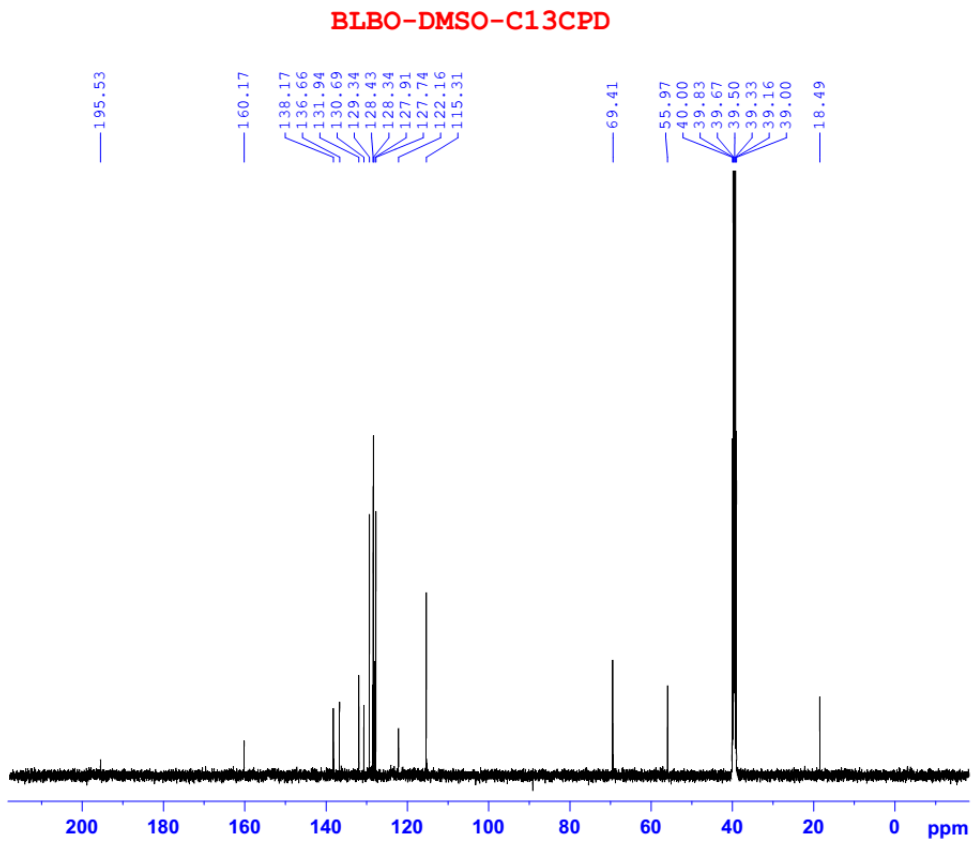

```
Current Data Parameters
NAME          110HD_BLBO
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171204
Time                9.51
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                111.09
DW                50.000 usec
DE                 6.50 usec
TE                303.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BLBO
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171205
Time                9.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                   512
DS                     4
SWH            29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7879670 MHz
NUC1                  13C
P1                  10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2               80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                 32768
SF           125.7754568 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

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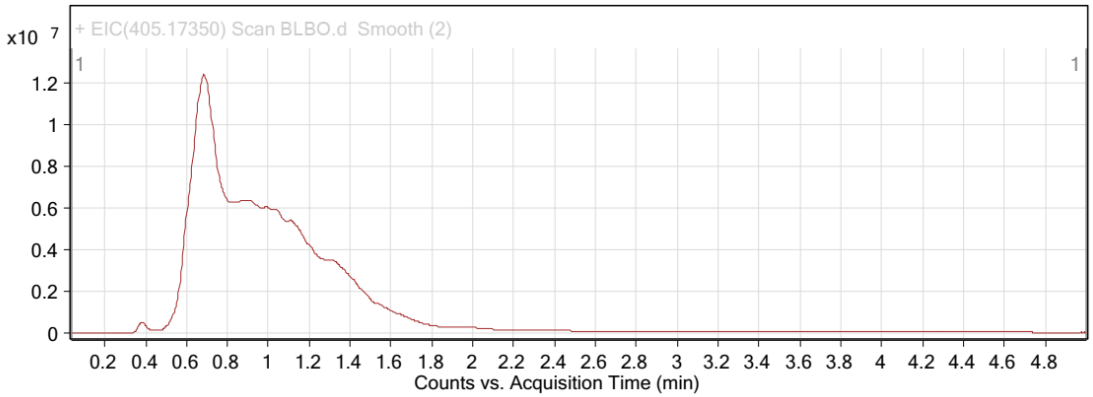
Qualitative Analysis Report

Data File	BLBO.d	**Sample Name**	BLBO
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	All Ion MSMS-Positive-100MeOH.m	**Acquired Time**	21/12/2017 9:17:31 AM
IRM Calibration Status	Success	**DA Method**	GS ton du.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

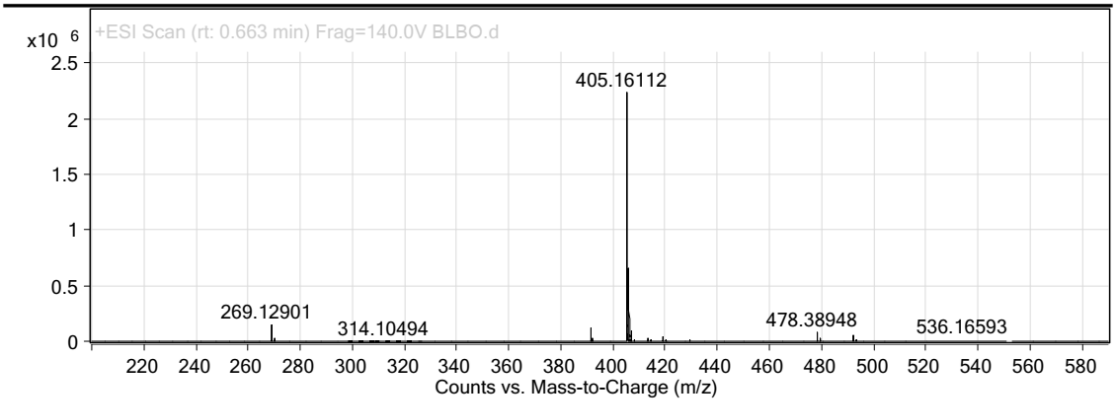
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI

Qualitative Analysis Report



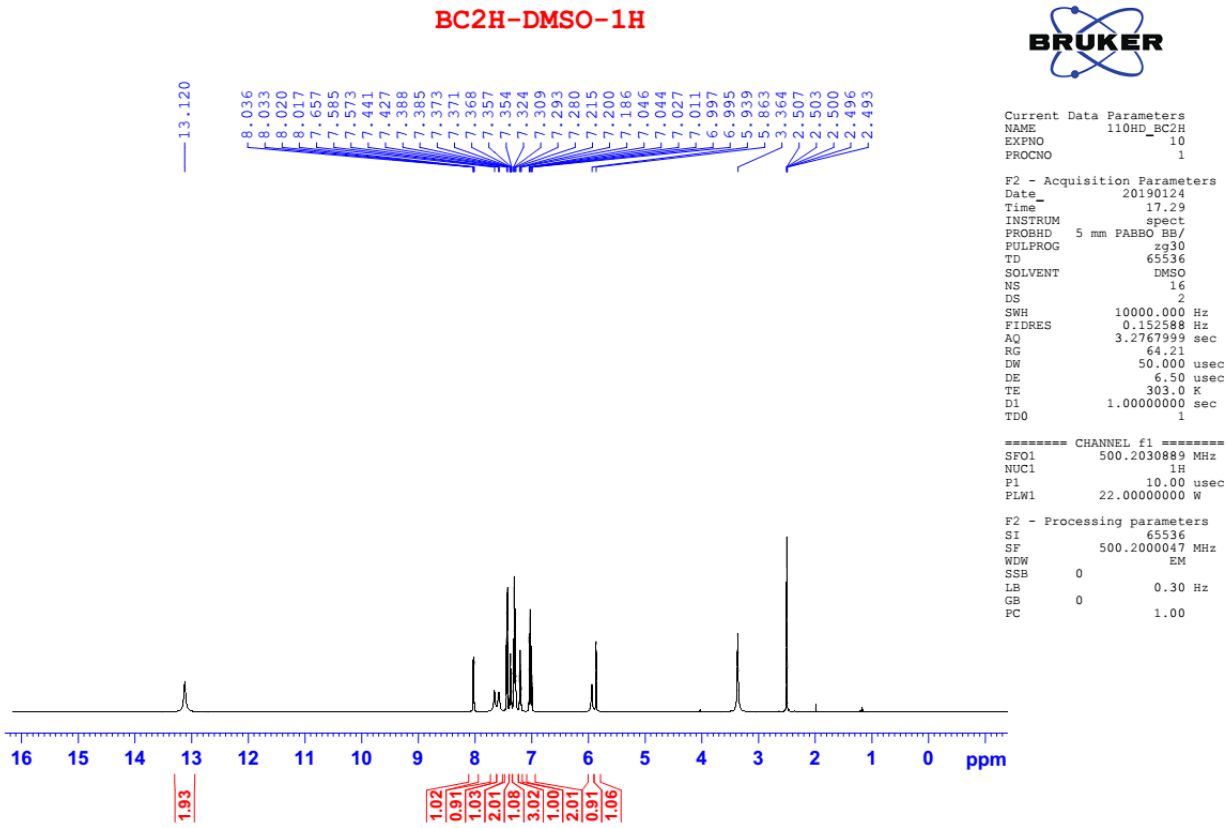
Peak List

m/z	z	Abund
269.12901	1	155937.2
391.28499	1	119469.09
405.16112	1	2256649.23
405.24514	1	148638.71
406.16413	1	661205.91
795.43815	1	633684.02
796.44189	1	350700.3
803.54578	1	256941.48
804.54778	1	150095.15
809.31465	1	151609.46

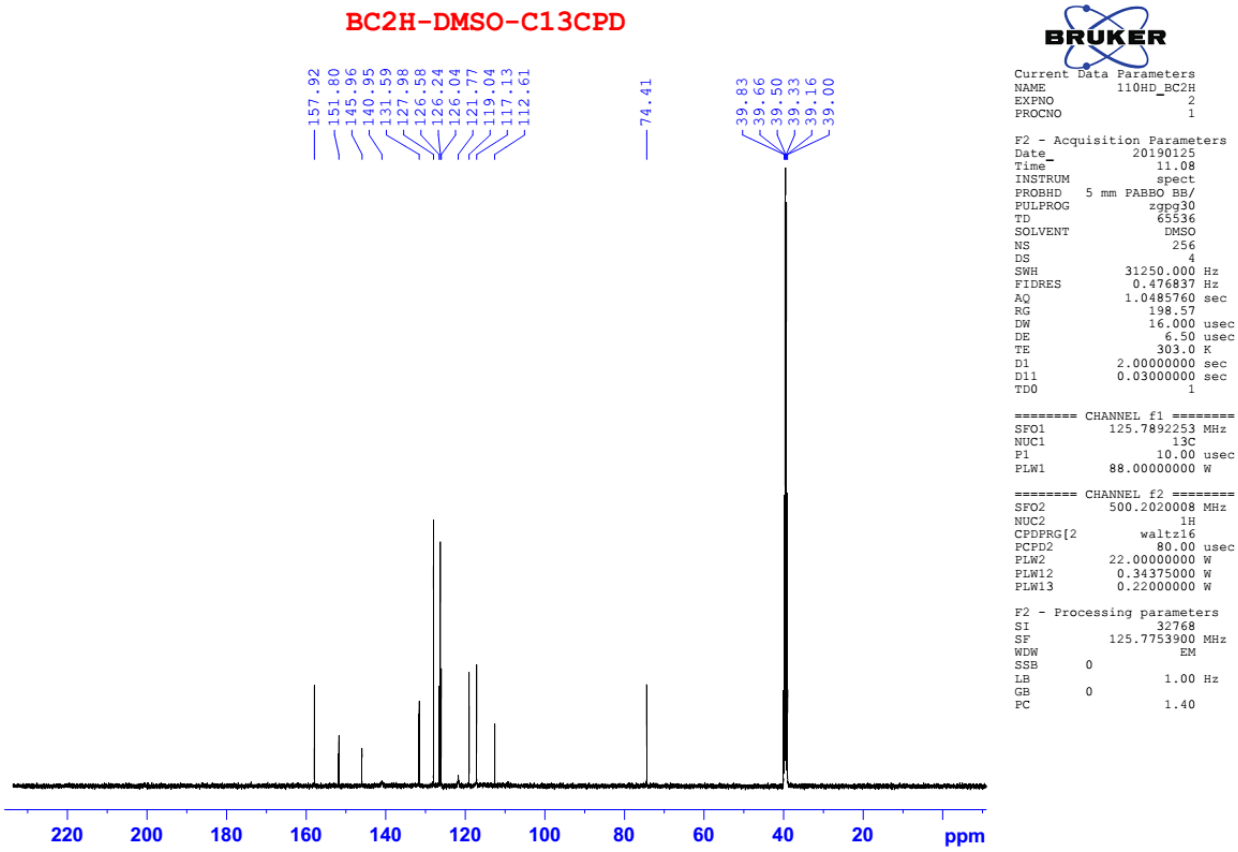
--- End Of Report ---

2-(5-(hydroxy(phenyl)methyl)-1H-benzo[d]imidazol-2-yl)phenol (**47**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BC2H
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190125
Time              11.08
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                 256
DS                   4
SWH          31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG               198.57
DW               16.000 usec
DE                6.50 usec
TE               303.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        125.7892253 MHz
NUC1               13C
P1               10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                 32768
SF          125.7753900 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

HRMS

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PHARMACEUTICAL CHEMISTRY LABORATORY
01, Mac Dinh Chi St., Dist 1, Ho Chi Minh City, Vietnam. Phone: (84) 907 070 939

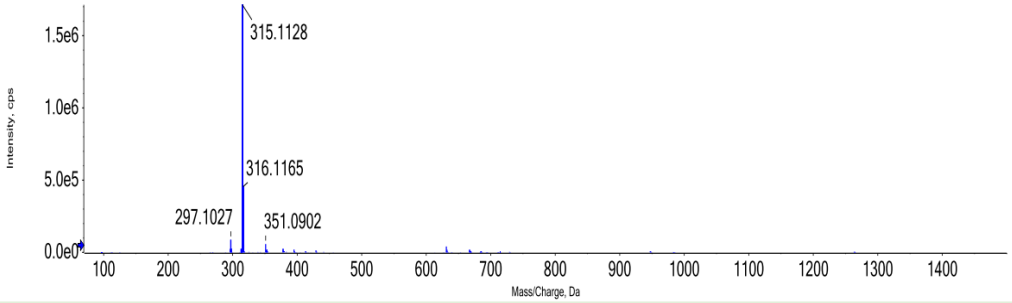
ANALYSIS REPORT

Injection details

Sample name	BC2H	*Vial position*	9
Sample file name	SER. wiff2 – CHI	*Inject volume*	5.00
Acquisition date	23/1/2019 1:04:54 PM	*Acquisition method*	ESI_NEG_SCAN
Operator	CB21261708	*Instrument name*	$X500_R$ QTOF

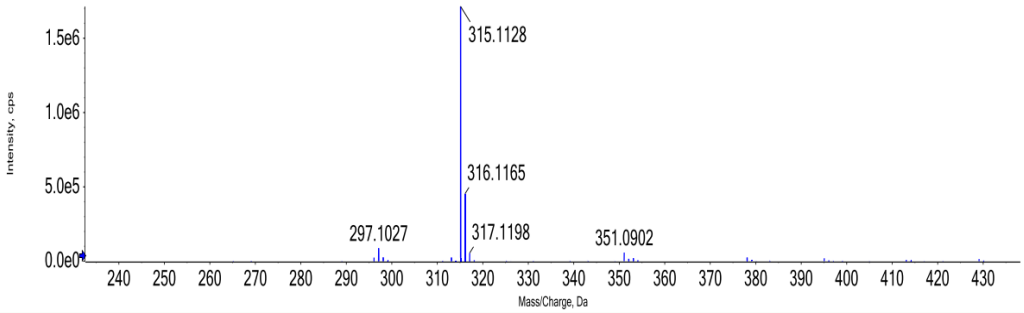
Full mass spectrum

Spectrum from BC2H-ESI.wiff2 (sample 1) - BC2H-ESI, -TOF MS (70 - 1500) from 0.171 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Expanded spectrum

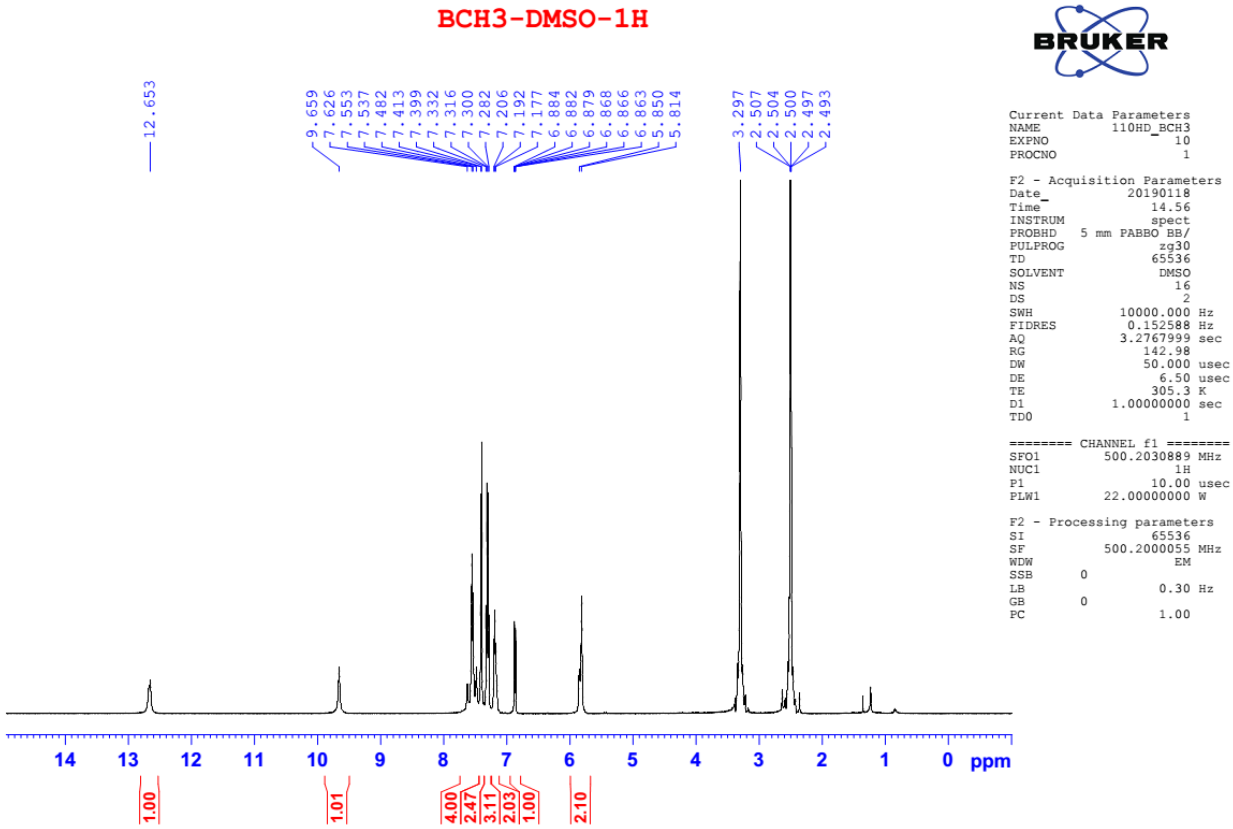
Spectrum from BC2H-ESI.wiff2 (sample 1) - BC2H-ESI, -TOF MS (70 - 1500) from 0.171 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



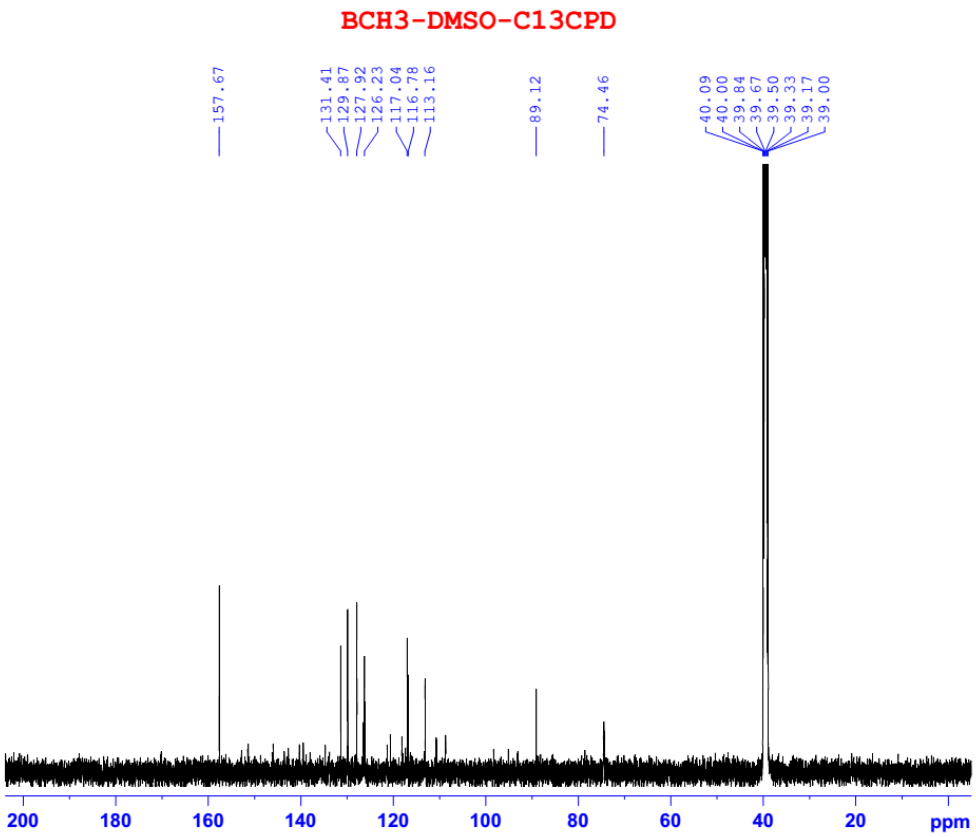
Molecular formula prediction

3-(5-(hydroxy(phenyl)methyl)-1H-benzo[d]imidazol-2-yl)phenol (**48**):

^{1}H – NMR



^{13}C – NMR



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```
Current Data Parameters
NAME          110HD_BCH3
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190119
Time              12.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT            DMSO
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               198.57
DW               16.800 usec
DE                6.50 usec
TE               303.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7879670 MHz
NUC1               13C
P1               10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                32768
SF          125.7754573 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

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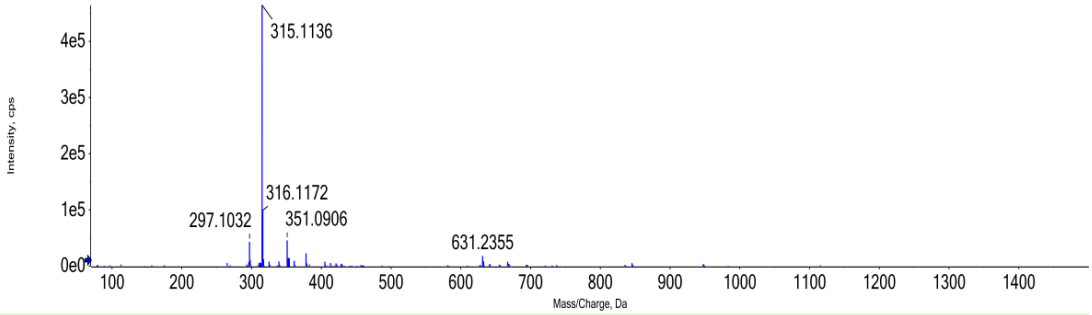
ANALYSIS REPORT

Injection details

Sample name	BC3H	*Vial position*	9
Sample file name	SER. wiff2 – CHI	*Inject volume*	5.00
Acquisition date	23/01/2019 1:04:54 PM	*Acquisition method*	ESI_NEG_SCAN
Operator	CB21261708	*Instrument name*	$X500_R$ QTOF

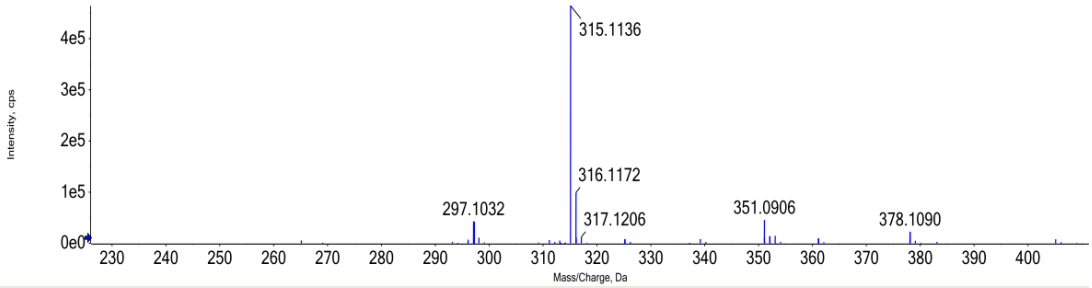
Full mass spectrum

Spectrum from BC3H-ESI.wiff2 (sample 1) - BC3H-ESI, -TOF MS (70 - 1500) from 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Expanded spectrum

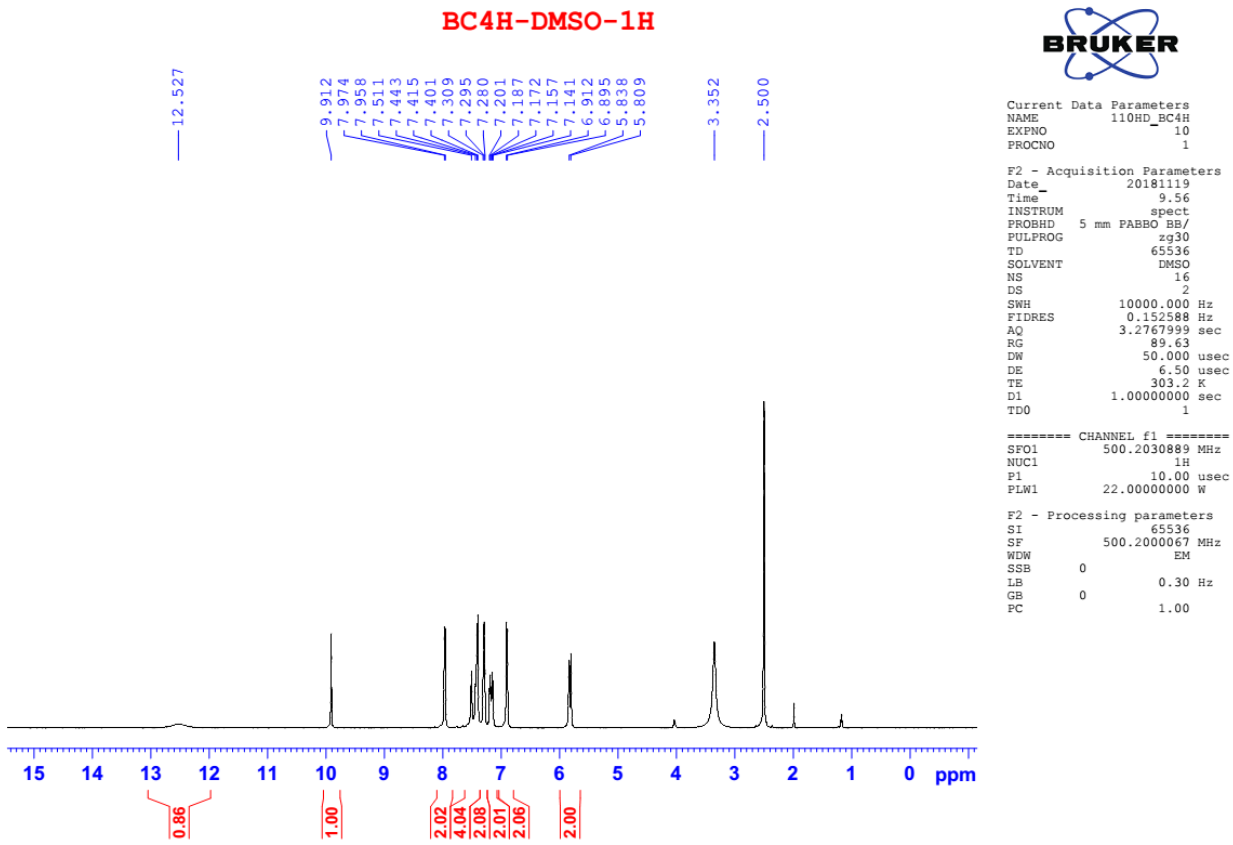
Spectrum from BC3H-ESI.wiff2 (sample 1) - BC3H-ESI, -TOF MS (70 - 1500) from 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Molecular formula prediction

4-(5-(hydroxy(phenyl)methyl)-1H-benzo[d]imidazol-2-yl)phenol (**49**):

^{1}H – NMR

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Current Data Parameters
NAME          110HD_BC4H
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181119
Time               9.56
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                 89.63
DW                50.000 usec
DE                 6.50 usec
TE                303.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000067 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```
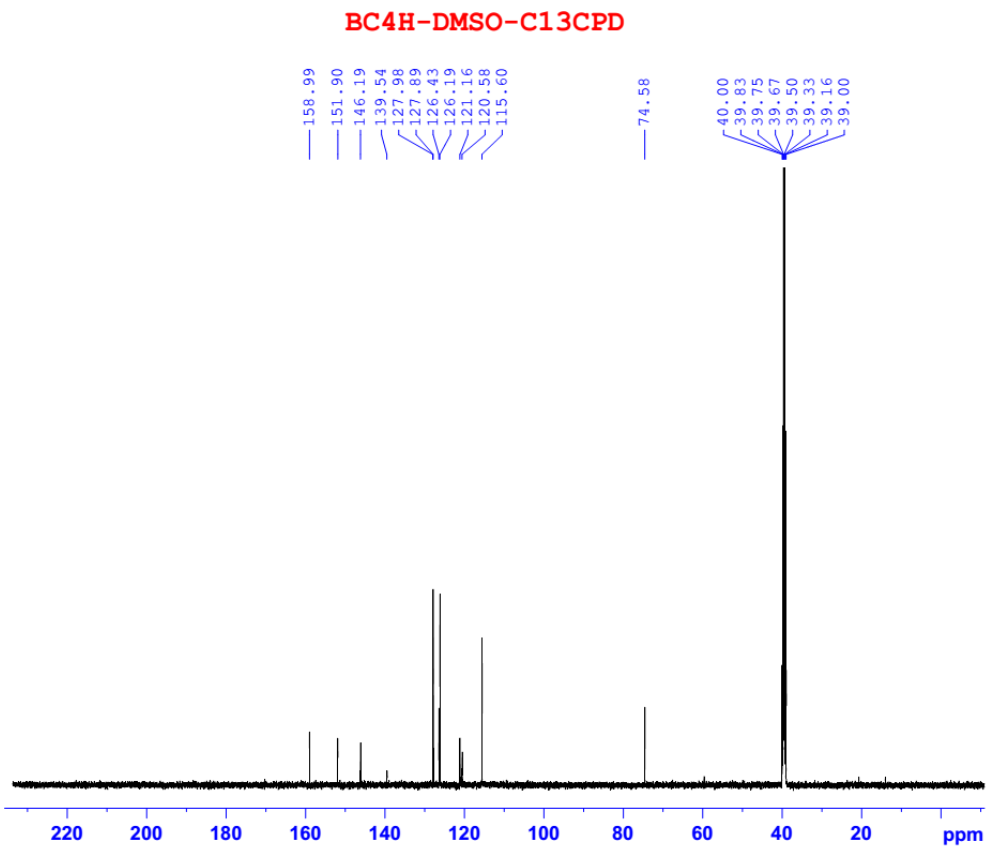

^{13}C – NMR



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```
Current Data Parameters
NAME          110HD_BC4H
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181123
Time                8.36
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                    256
DS                      4
SWH             31250.000 Hz
FIDRES          0.476837 Hz
AQ              1.0485760 sec
RG                 198.57
DW                 16.000 usec
DE                  6.50 usec
TE                 304.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         125.7892253 MHz
NUC1                  13C
P1                  10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                    32768
SF           125.7754568 MHz
WDW                      EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

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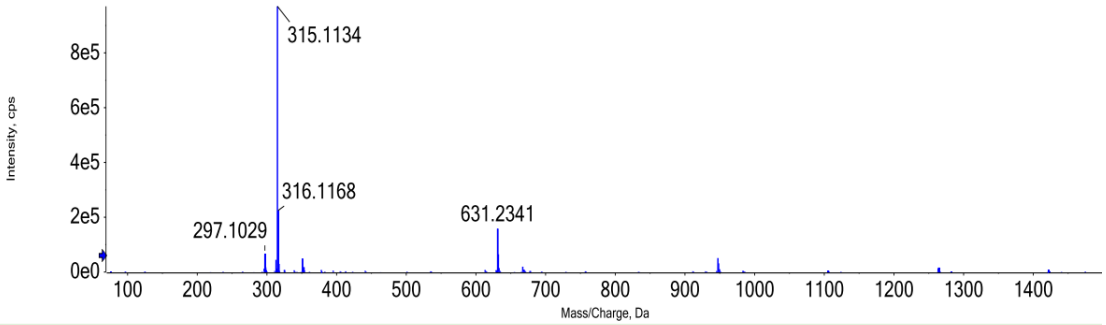
ANALYSIS REPORT

Injection details

Sample name	BC4H	*Vial position*	31
Sample file name	SER. wiff2-CHI	*Inject volume*	5.00
Acquisition date	06/05/2019 1:04:54 PM	*Acquisition method*	**ESI _NEG_SCAN**
Operator	CB21261708	*Instrument name*	$X500_R$ QTOF

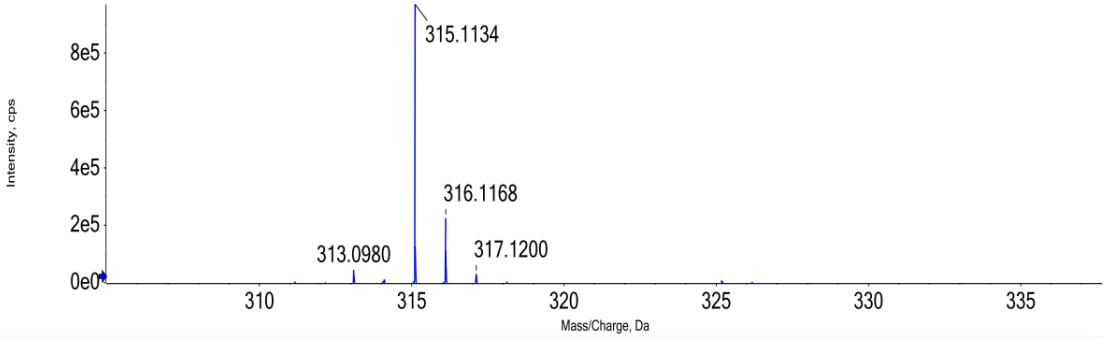
Full mass spectrum

Spectrum from BC4H-ESI.wiff2 (sample 1) - BC4H-ESI, -TOF MS (70 - 1500) from 0.153 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Expanded spectrum

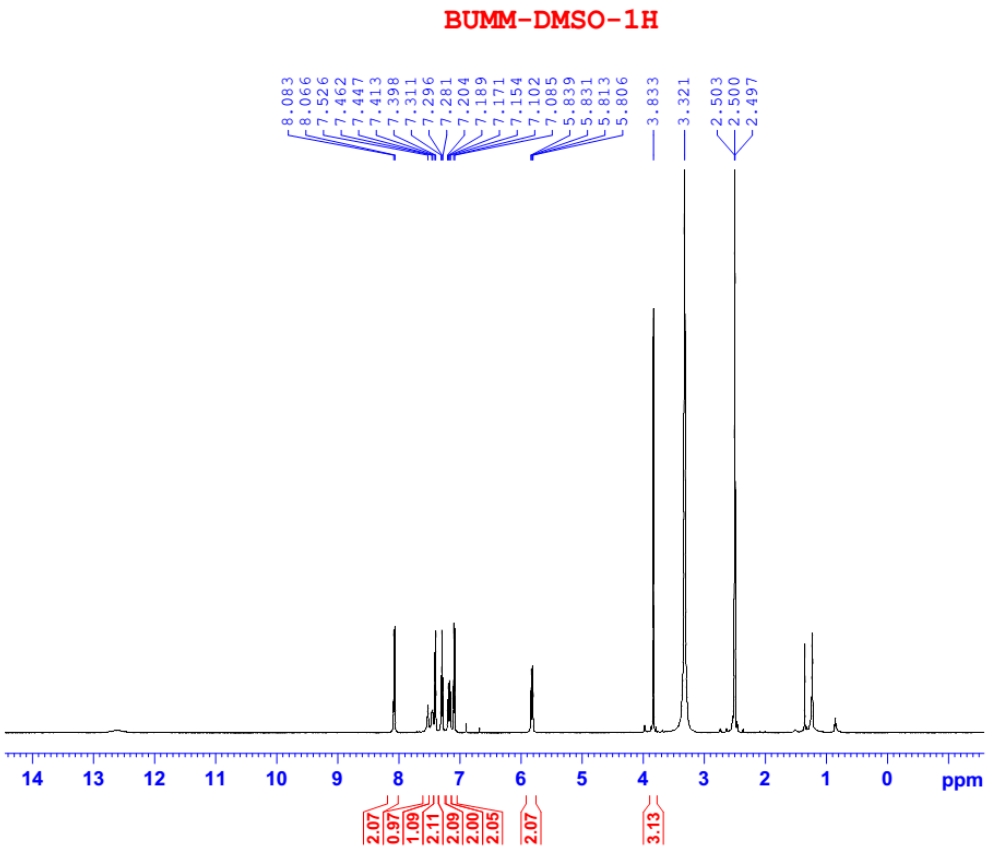
Spectrum from BC4H-ESI.wiff2 (sample 1) - BC4H-ESI, -TOF MS (70 - 1500) from 0.153 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)

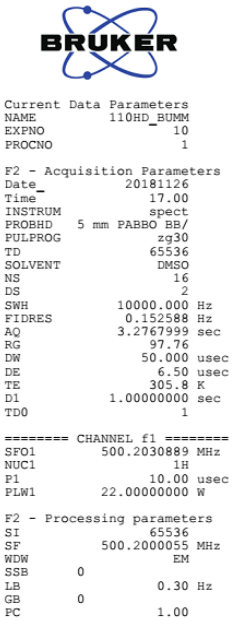


Molecular formula prediction

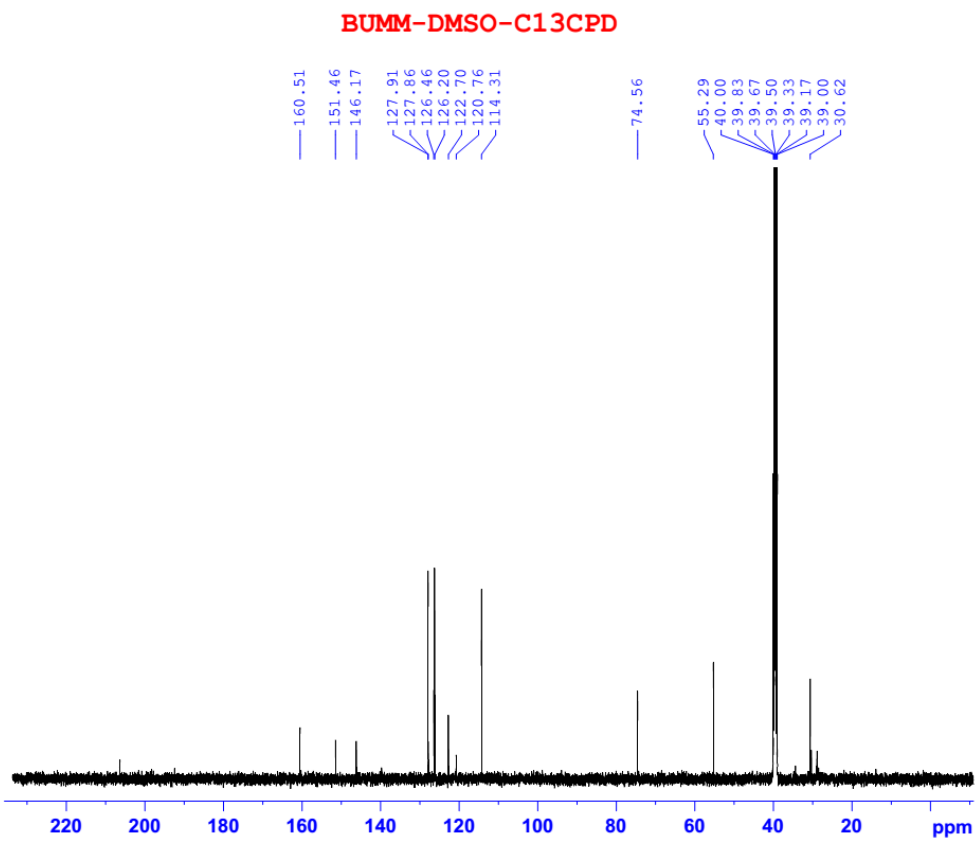
[2-(4-Methoxy-phenyl)-1H-benzoimidazol-5-yl]-phenyl-methanol (**50**):

^{1}H – NMR





^{13}C – NMR



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Current Data Parameters
NAME          110HD_BUMM
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181128
Time               14.33
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                   512
DS                     4
SWH            31250.000 Hz
FIDRES         0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW                16.000 usec
DE                 6.50 usec
TE                304.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          125.7892253 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2          500.2020008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          22.00000000 W
PLW12          0.34375000 W
PLW13          0.22000000 W

F2 - Processing parameters
SI                    32768
SF            125.7754556 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

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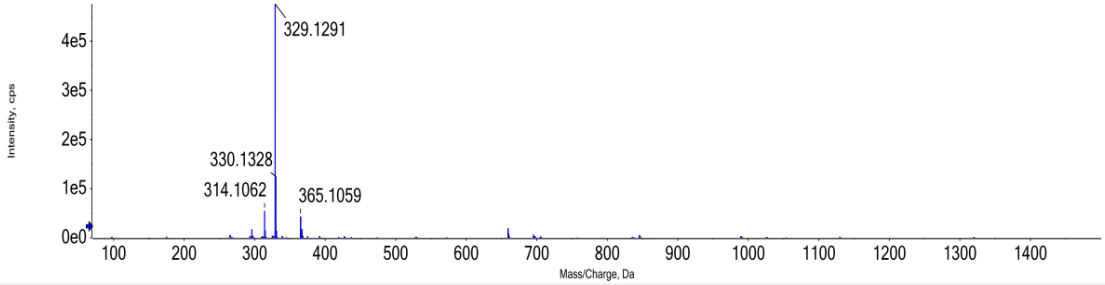
ANALYSIS REPORT

Injection details

Sample name	BUMM	*Vial position*	42
Sample file name	SER. wiff2-CHI	*Inject volume*	5.00
Acquisition date	06/05/2019 1:04:54 PM	*Acquisition method*	**ESI _NEG_SCAN**
Operator	CB21261708	*Instrument name*	$X500_R$ QTOF

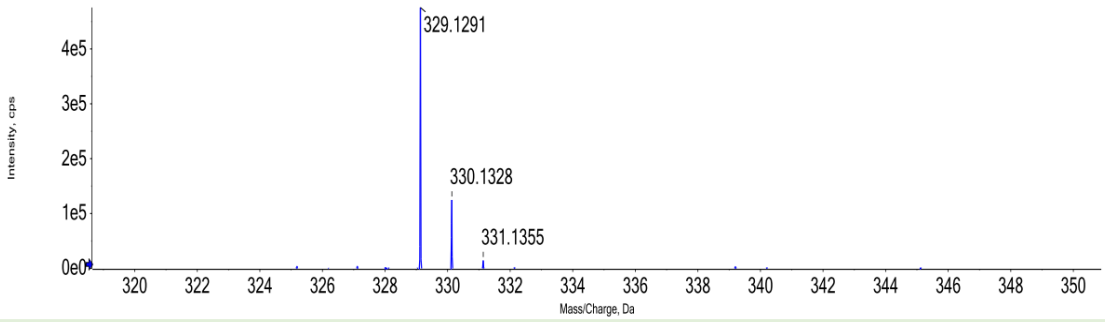
Full mass spectrum

Spectrum from BUMM-ESI.wiff2 (sample 1) - BUMM-ESI, -TOF MS (70 - 1500) from 0.199 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Expanded spectrum

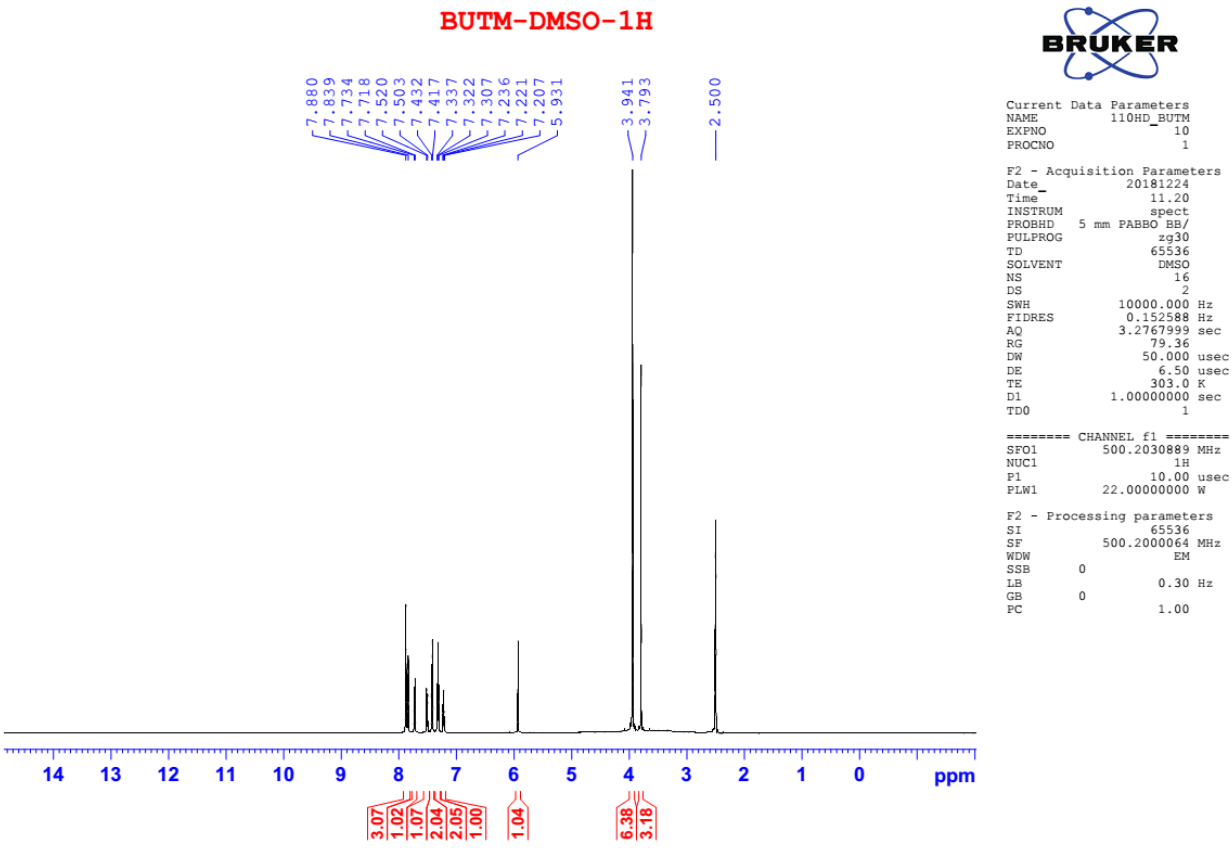
Spectrum from BUMM-ESI.wiff2 (sample 1) - BUMM-ESI, -TOF MS (70 - 1500) from 0.199 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



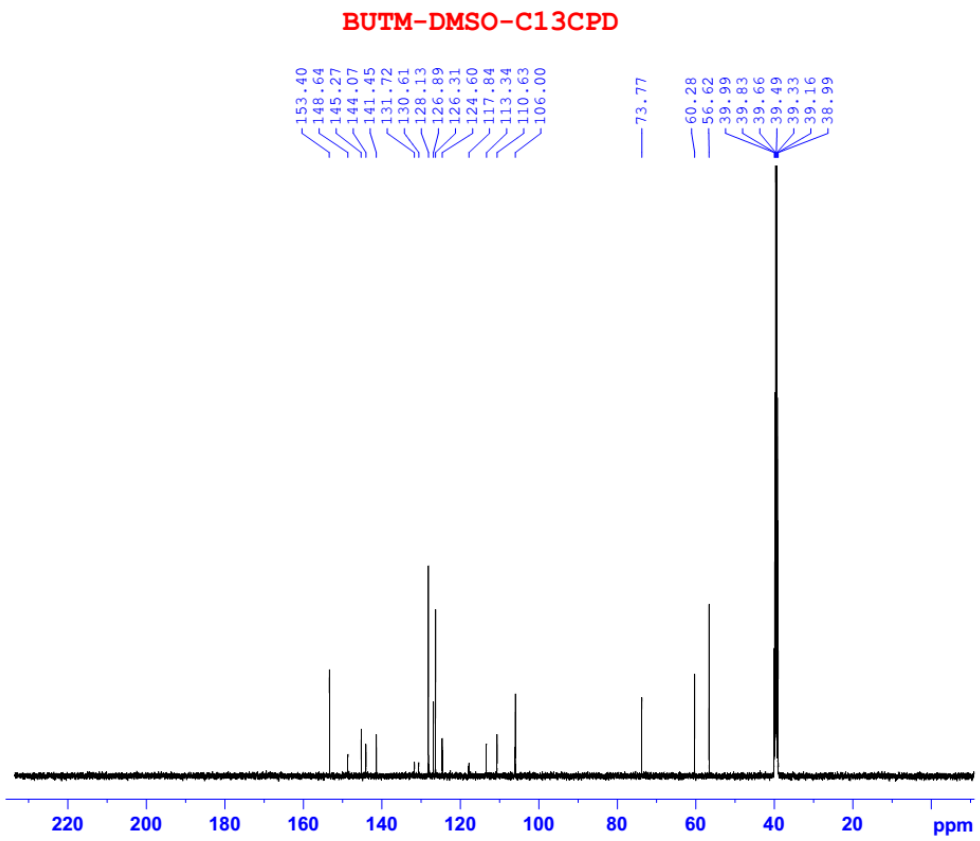
Molecular formula prediction

Phenyl-[2-(3,4,5-trimethoxy-phenyl)-1H-benzoimidazol-5-yl]-methanol (**51**):

^{1}H – NMR



^{13}C – NMR



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```
Current Data Parameters
NAME            110HD_BUTM
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20181226
Time                 23.26
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT               DMSO
NS                      256
DS                        4
SWH               31250.000 Hz
FIDRES            0.476837 Hz
AQ                1.0485760 sec
RG                   198.57
DW                  16.000 usec
DE                   6.50 usec
TE                  305.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            125.7892253 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           88.00000000 W

======== CHANNEL f2 ========
SFO2            500.2020008 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                 80.00 usec
PLW2           22.00000000 W
PLW12           0.34375000 W
PLW13           0.22000000 W

F2 - Processing parameters
SI                      32768
SF              125.7753900 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

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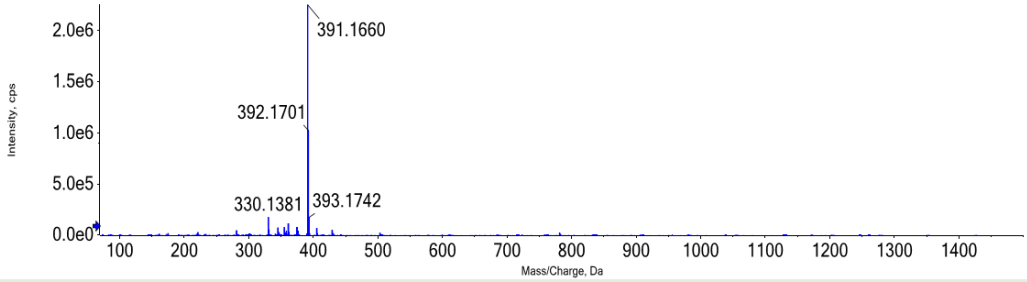
ANALYSIS REPORT

Injection details

Sample name	BUIV	*Vial position*	40
Sample file name	SER. wiff2-CHI	*Inject volume*	5.00
Acquisition date	06/05/2019 1:04:54 PM	*Acquisition method*	**ESI _POS_SCAN**
Operator	CB21261708	*Instrument name*	$X500_R$ QTOF

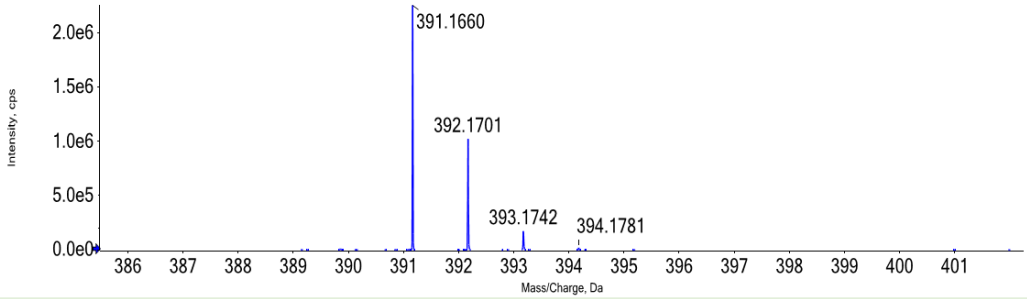
Full mass spectrum

Spectrum from P49-CHI.wiff2 (sample 5) - BUIV-ESI-P49, +TOF MS (70 - 1500) from 0.111 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Expanded spectrum

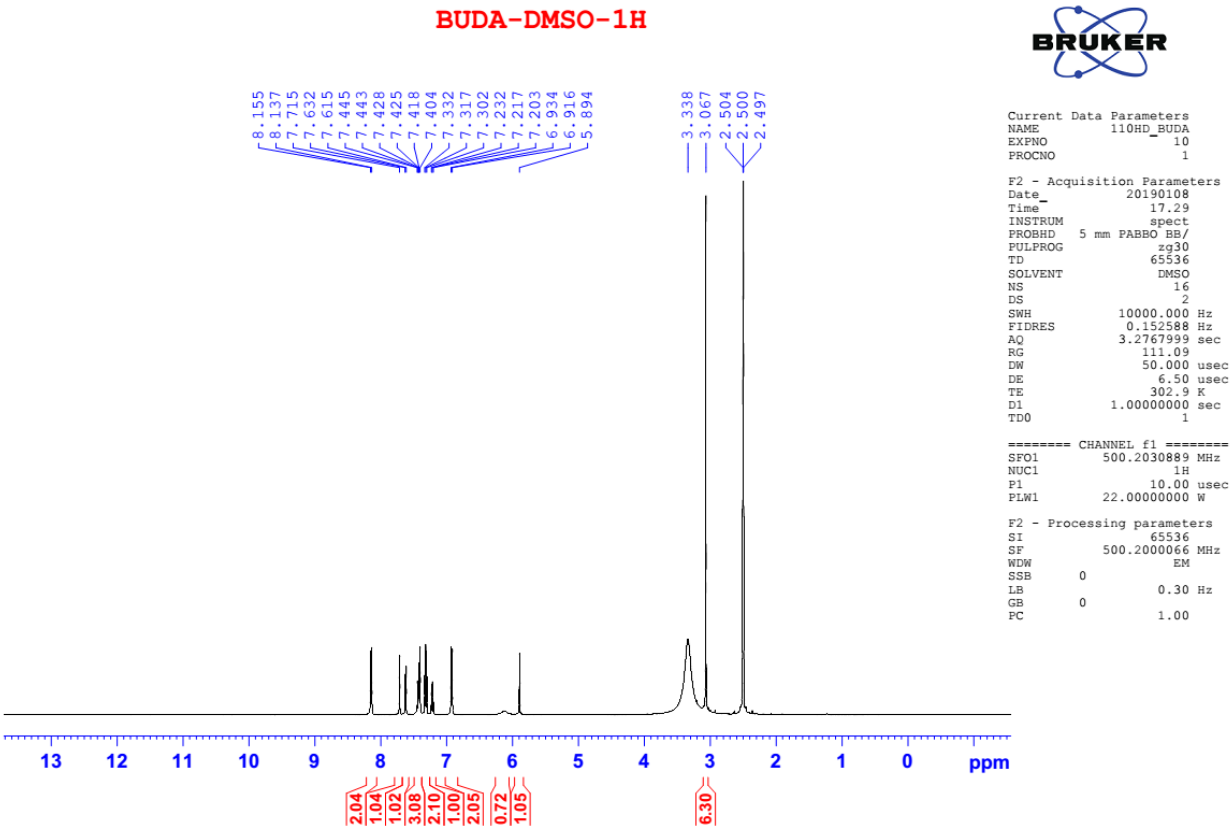
Spectrum from P49-CHI.wiff2 (sample 5) - BUIV-ESI-P49, +TOF MS (70 - 1500) from 0.111 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Molecular formula prediction

[2-(4-Dimethylamino-phenyl)-1H-benzoimidazol-5-yl]-phenyl-methanol (**52**):

^{1}H – NMR

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Current Data Parameters
NAME          110HD_BUDA
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190108
Time              17.29
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               111.09
DW               50.000 usec
DE                6.50 usec
TE               302.9 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                 1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.2000066 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```
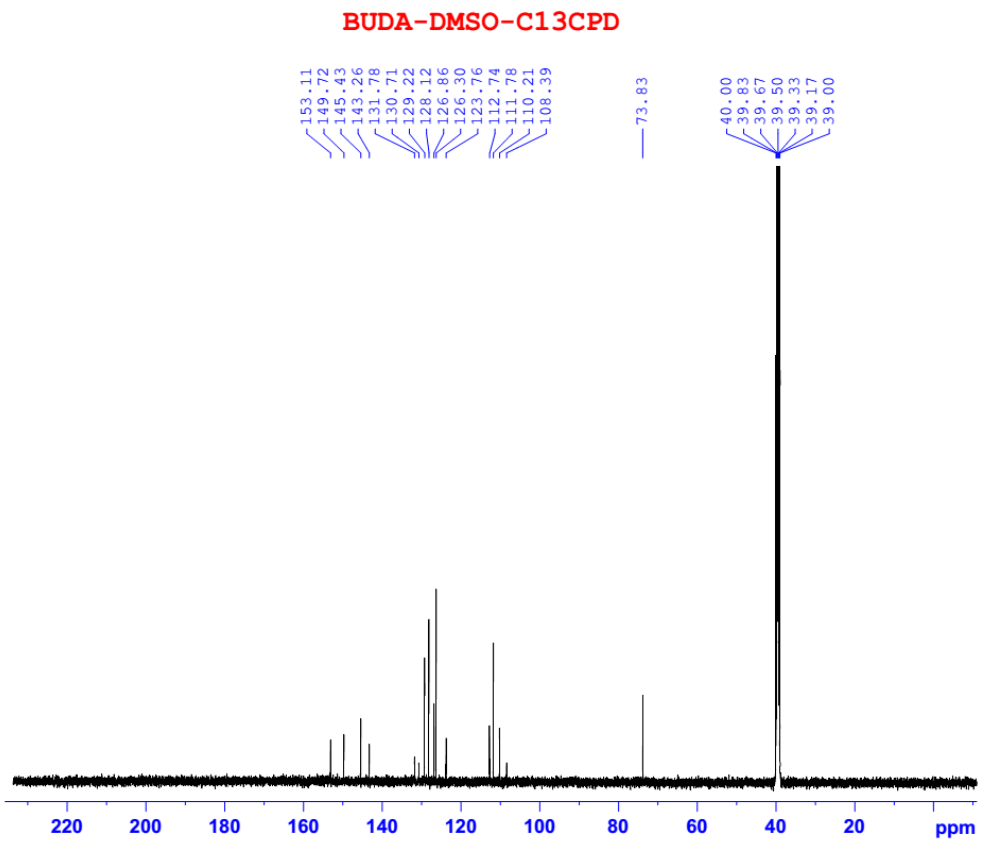

^{13}C – NMR



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```
Current Data Parameters
NAME          110HD_BUDA
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190109
Time              18.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT            DMSO
NS                 2048
DS                    4
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG               198.57
DW               16.000 usec
DE                6.50 usec
TE               303.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7892253 MHz
NUC1                13C
P1                10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                32768
SF           125.7753900 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

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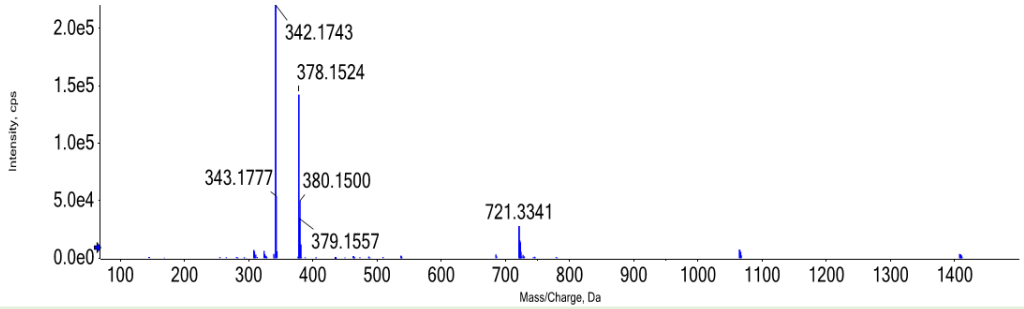
ANALYSIS REPORT

Injection details

Sample name	BUDA	*Vial position*	16
Sample file name	SER. wiff2-CHI	*Inject volume*	5.00
Acquisition date	06/05/2019 1:04:54 PM	*Acquisition method*	**ESI _NEG_SCAN**
Operator	CB21261708	*Instrument name*	X500$_R$ QTOF

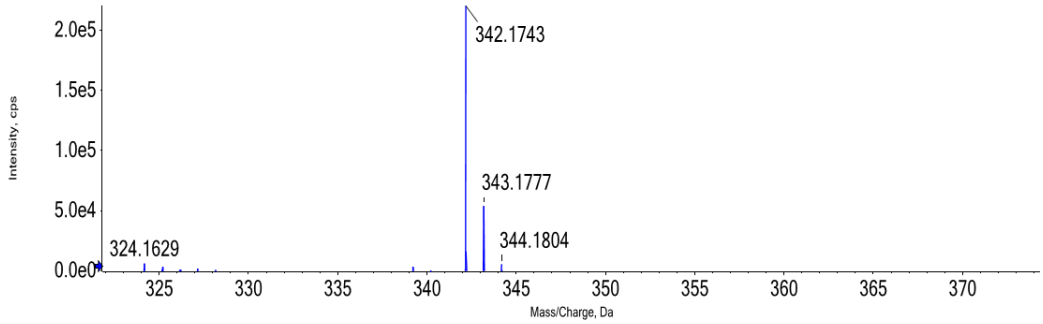
Full mass spectrum

Spectrum from P49-CHI.wiff2 (sample 14) - BUDA-ESI-P49, -TOF MS (70 - 1500) from 0.153 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Expanded spectrum

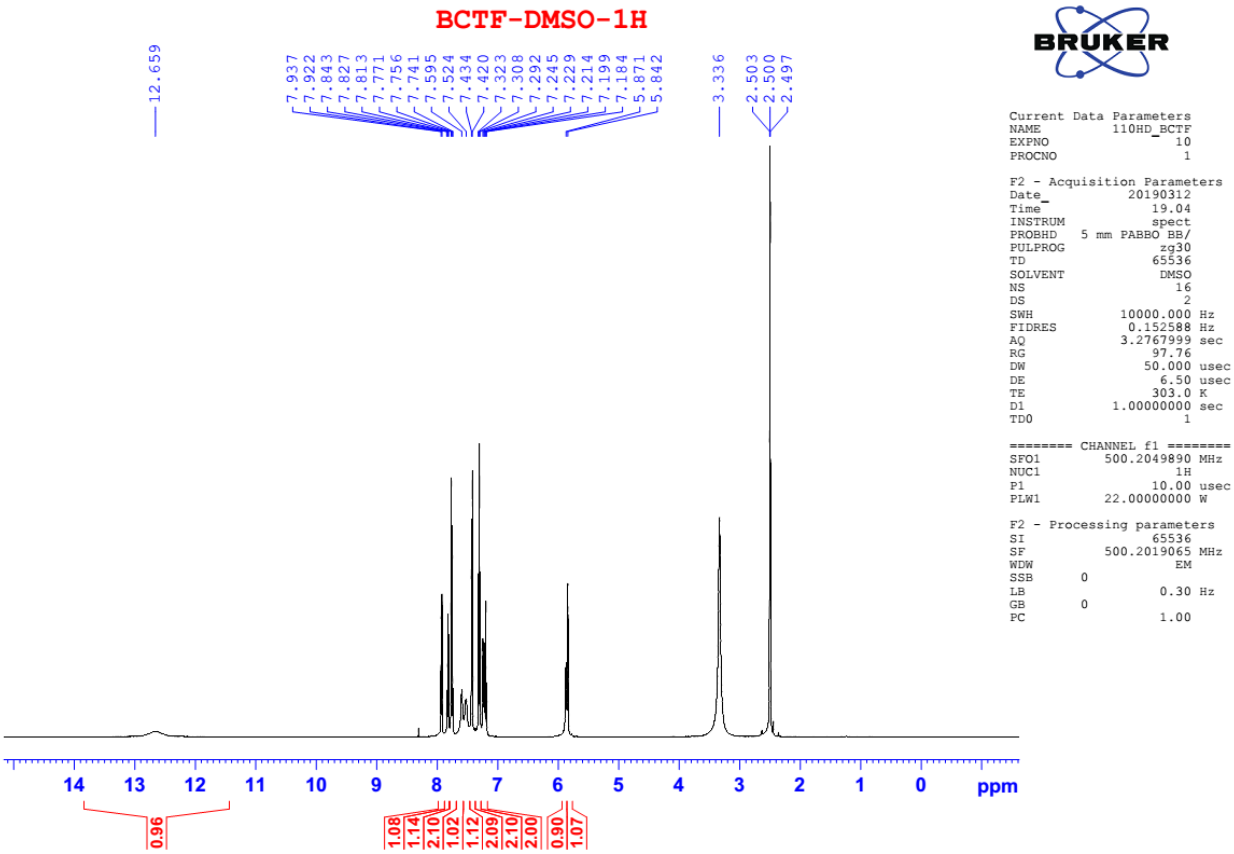
Spectrum from P49-CHI.wiff2 (sample 14) - BUDA-ESI-P49, -TOF MS (70 - 1500) from 0.153 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



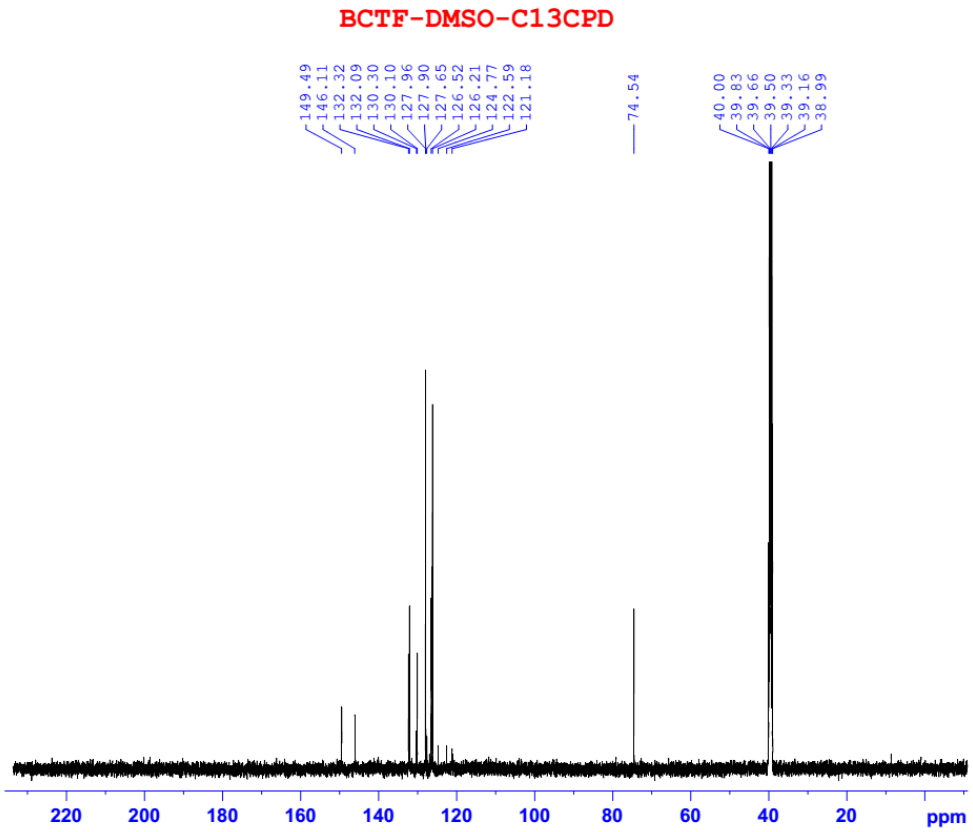
Molecular formula prediction

phenyl(2-(2-(trifluoromethyl)phenyl)-1H-benzo[d]imidazol-5-yl)methanol (**53**):

^{1}H – NMR



^{13}C – NMR



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```
Current Data Parameters
NAME          110HD_BCTF
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190315
Time               15.43
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                    256
DS                      4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW               16.000 usec
DE                6.50 usec
TE                303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        125.7897032 MHz
NUC1                  13C
P1                  10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2039008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2               80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                 32768
SF          125.7759319 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

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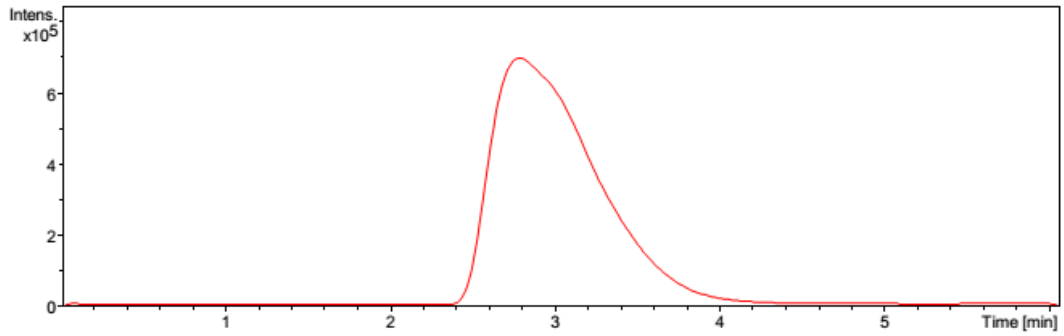
Display Report

Analysis Info

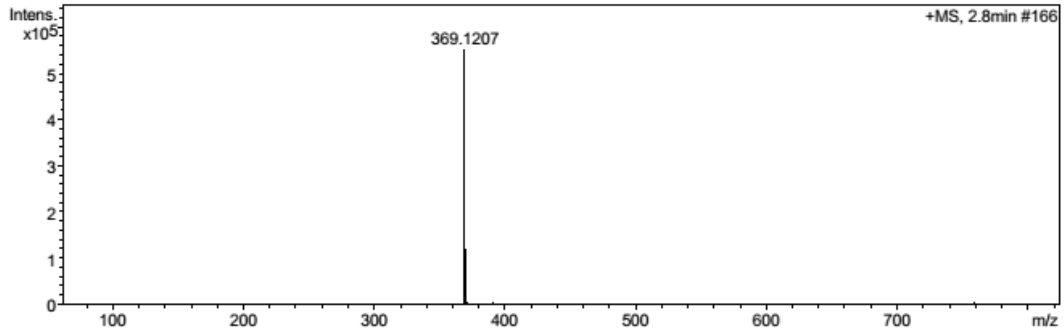
Analysis Name	D:\Data\2019\thang 05\13-05\BCTF_1-B,6_01_1348.d	Acquisition Date	4/19/2019 4:10:26 PM
Method	protein my mass tb.m	Operator	ANH MAI
Sample Name	BCTF	Instrument	micrOTOF-Q 10187
Comment			

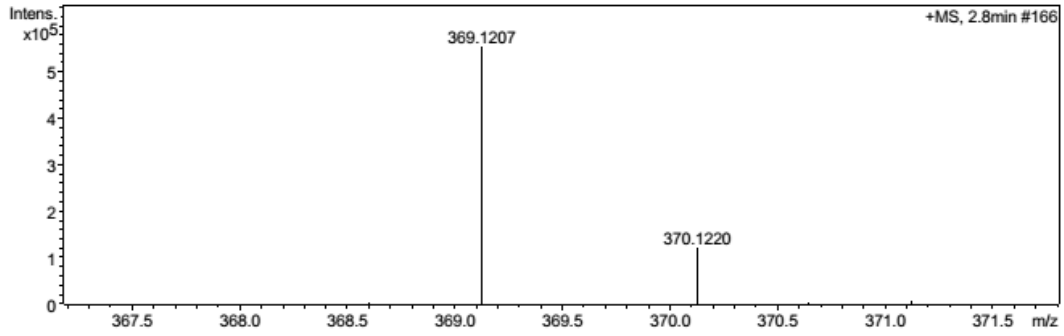
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	900 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



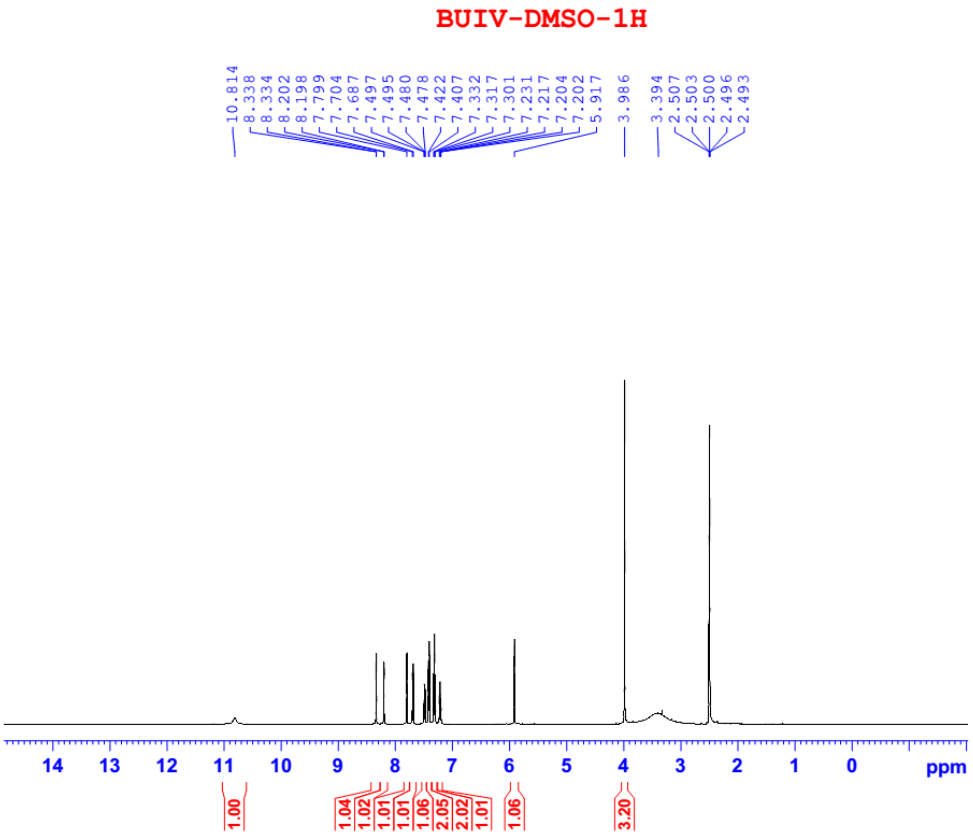
TIC +All MS, Smoothed (2.01,2,GA)





4-[5-(Hydroxy-phenyl-methyl)-1H-benzoimidazol-2-yl]-2-iodo-6-methoxy-phenol (**54**):

^{1}H – NMR




```
Current Data Parameters
NAME          110HD_BUIV
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181224
Time               11.16
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                 89.63
DW                50.000 usec
DE                 6.50 usec
TE                303.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000090 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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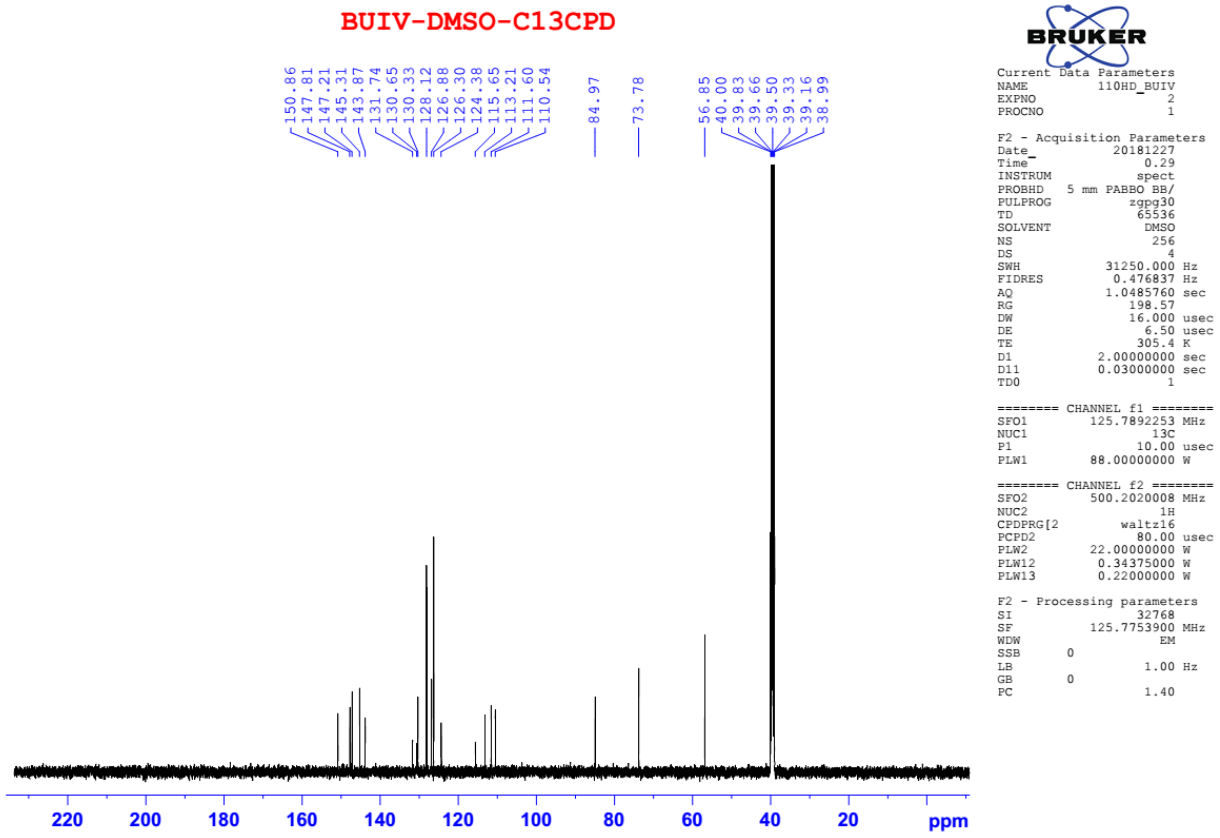
^{13}C – NMR

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Current Data Parameters
NAME          110HD_BUIV
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181227
Time                0.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                   256
DS                     4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ            1.0485760 sec
RG               198.57
DW               16.000 usec
DE                6.50 usec
TE                305.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7892253 MHz
NUC1                  13C
P1                 10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                 32768
SF           125.7753900 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HRMS

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PHARMACEUTICAL CHEMISTRY LABORATORY
01, Mac Dinh Chi St., Dist 1, Ho Chi Minh City, Vietnam. Phone: (84) 907 070 939

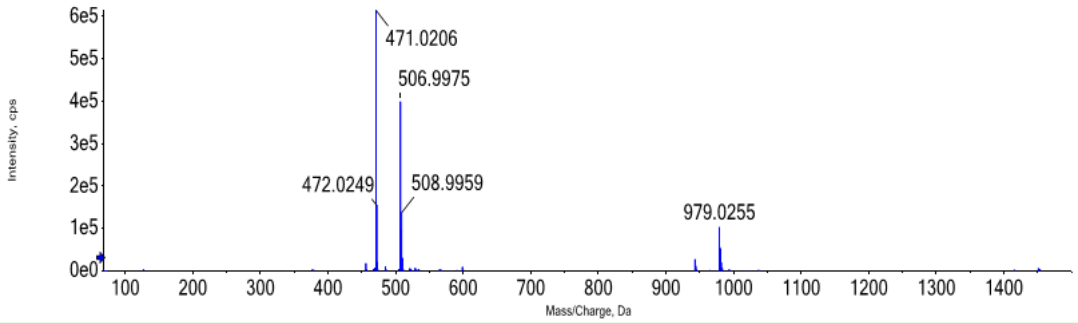
ANALYSIS REPORT

Injection details

Sample name	BUTM	*Vial position*	39
Sample file name	SER. wiff2-CHI	*Inject volume*	5.00
Acquisition date	06/05/2019 1:04:54 PM	*Acquisition method*	**ESI _NEG_SCAN**
Operator	CB21261708	*Instrument name*	X500R QTOF

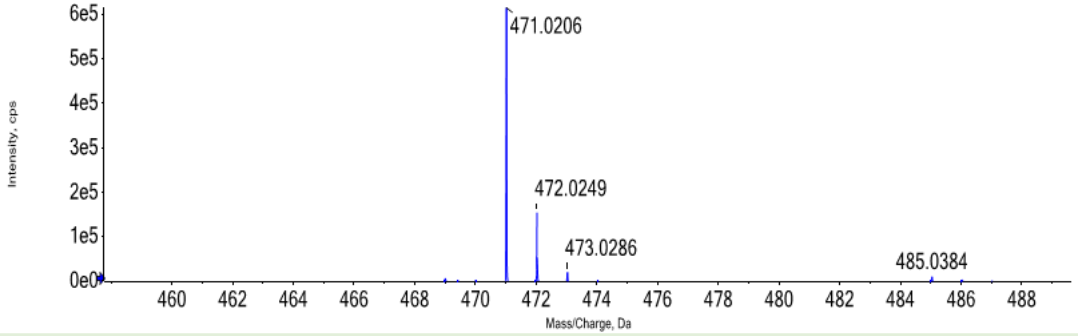
Full mass spectrum

Spectrum from P49-CHI.wiff2 (sample 7) - BUTM-ESI-P49, -TOF MS (70 - 1500) from 0.157 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Expanded spectrum

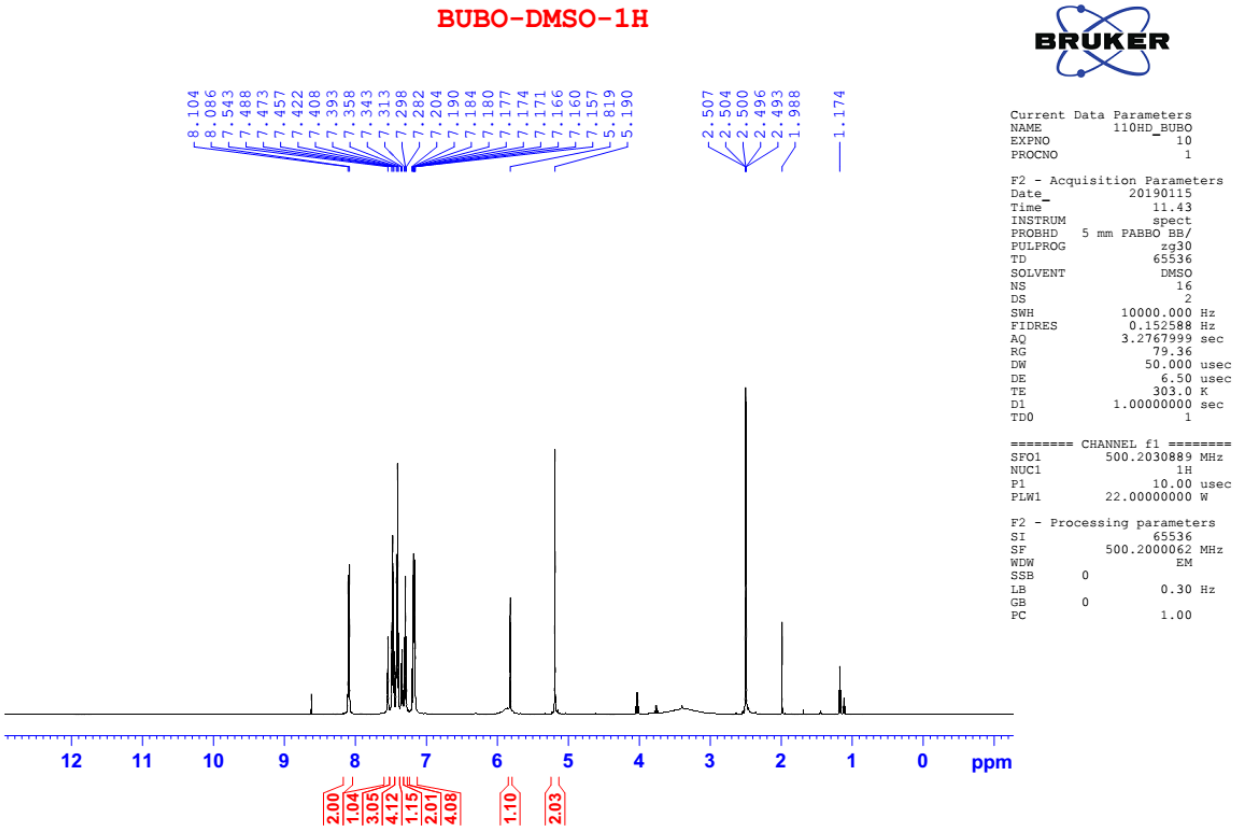
Spectrum from P49-CHI.wiff2 (sample 7) - BUTM-ESI-P49, -TOF MS (70 - 1500) from 0.157 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



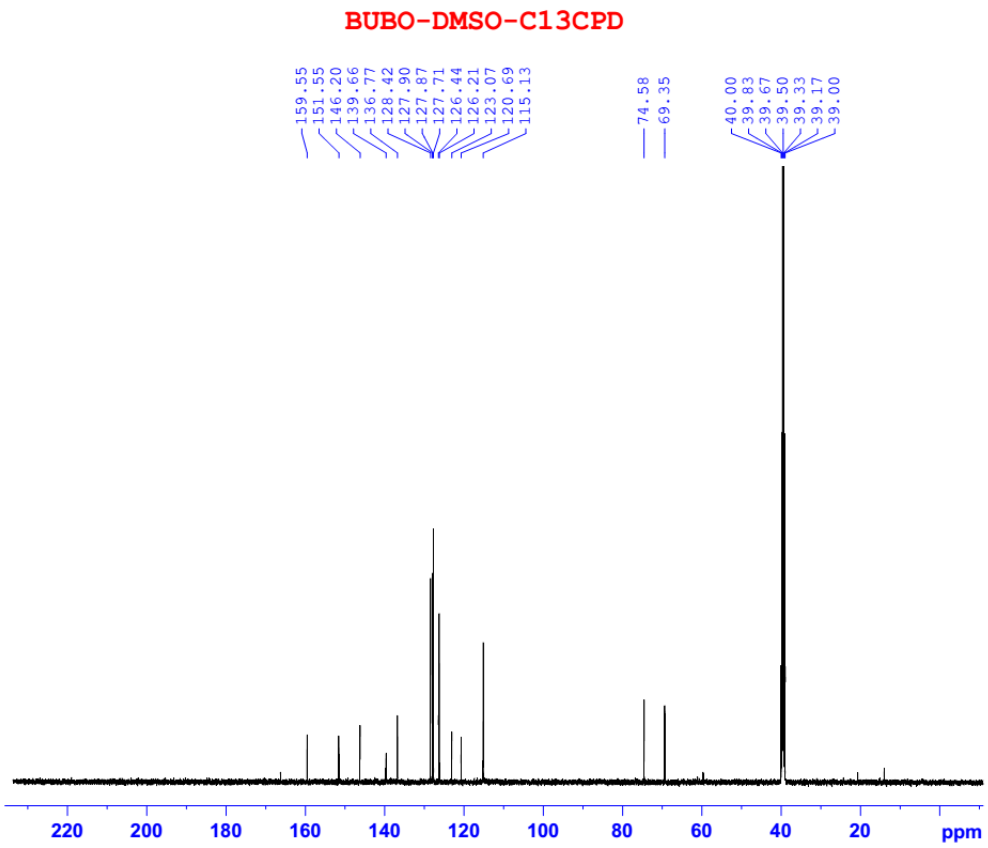
Molecular formula prediction

[2-(4-Benzyloxy-phenyl)-1H-benzoimidazol-5-yl]-phenyl-methanol (**55**):

^{1}H – NMR



^{13}C – NMR



BRUKER

```
Current Data Parameters
NAME          110HD_BUBO
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190117
Time              19.25
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                   256
DS                     4
SWH           31250.000 Hz
FIDRES         0.476837 Hz
AQ             1.0485760 sec
RG                198.57
DW              16.000 usec
DE               6.50 usec
TE               303.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        125.7892253 MHz
NUC1                13C
P1               10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        22.00000000 W
PLW12        0.34375000 W
PLW13        0.22000000 W

F2 - Processing parameters
SI                 32768
SF          125.7754562 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

HRMS

Created with SCIEX OS 1.2

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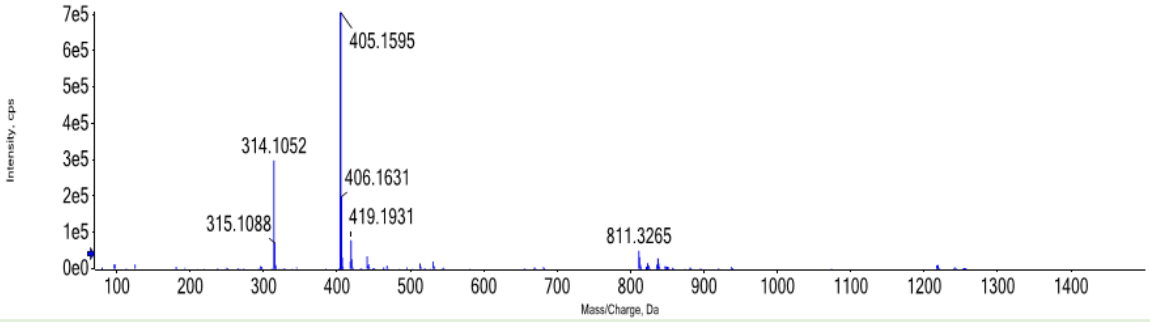
ANALYSIS REPORT

Injection details

Sample name	BUBO	*Vial position*	10
Sample file name	SER. wiff2 – CHI	*Inject volume*	5.00
Acquisition date	23/1/2019 1:04:54 PM	*Acquisition method*	ESI_NEG_SCAN
Operator	CB21261708	*Instrument name*	$X500_R$ QTOF

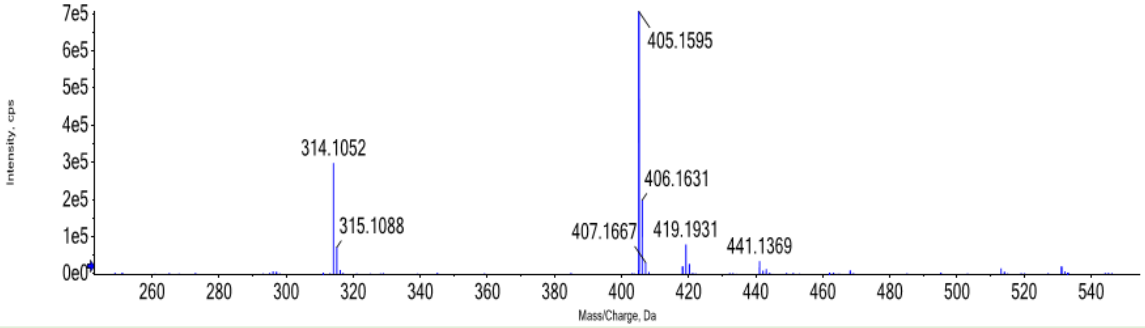
Full mass spectrum

Spectrum from BUBO-ESI.wiff2 (sample 1) - BUBO-ESI, -TOF MS (70 - 1500) from 0.129 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Expanded spectrum

Spectrum from BUBO-ESI.wiff2 (sample 1) - BUBO-ESI, -TOF MS (70 - 1500) from 0.129 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



Molecular formula prediction