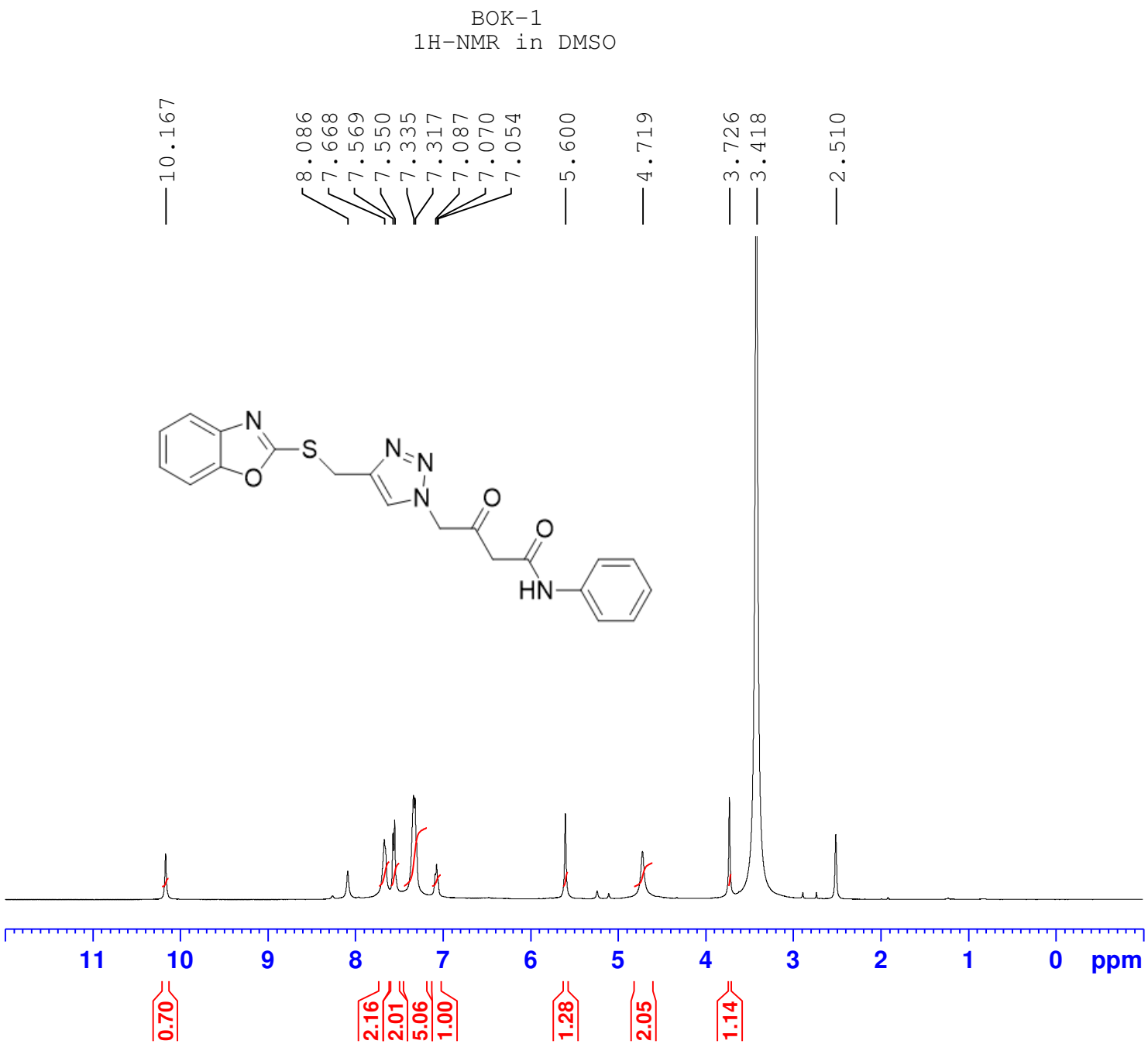
COMPOUND 3a (BOK-1) SPECTRAL DATA



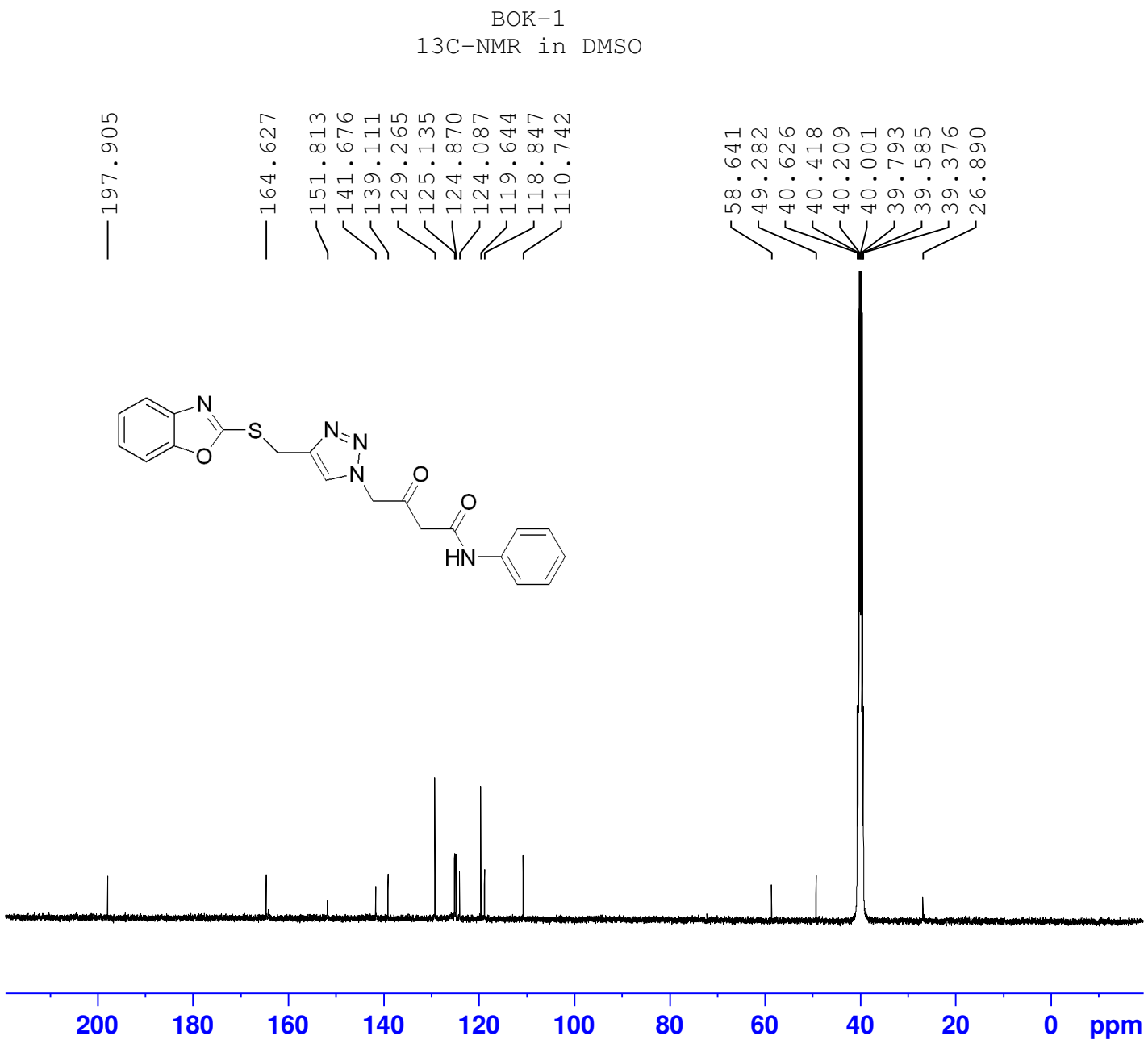
BRUKER

```
Current Data Parameters
NAME      23000786-BO-AN
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230801
Time                8.21 h
INSTRUM            spect
PROBHD   Z108618_0984 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                 100.18
DW                 62.400 usec
DE                 17.09 usec
TE                 297.2 K
D1            1.00000000 sec
TD0                    1
SFO1         400.3124719 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         11.28999996 W

F2 - Processing parameters
SI                 65536
SF           400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR spectrum of 4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-phenyl butanamide **3a (BOK-1)**

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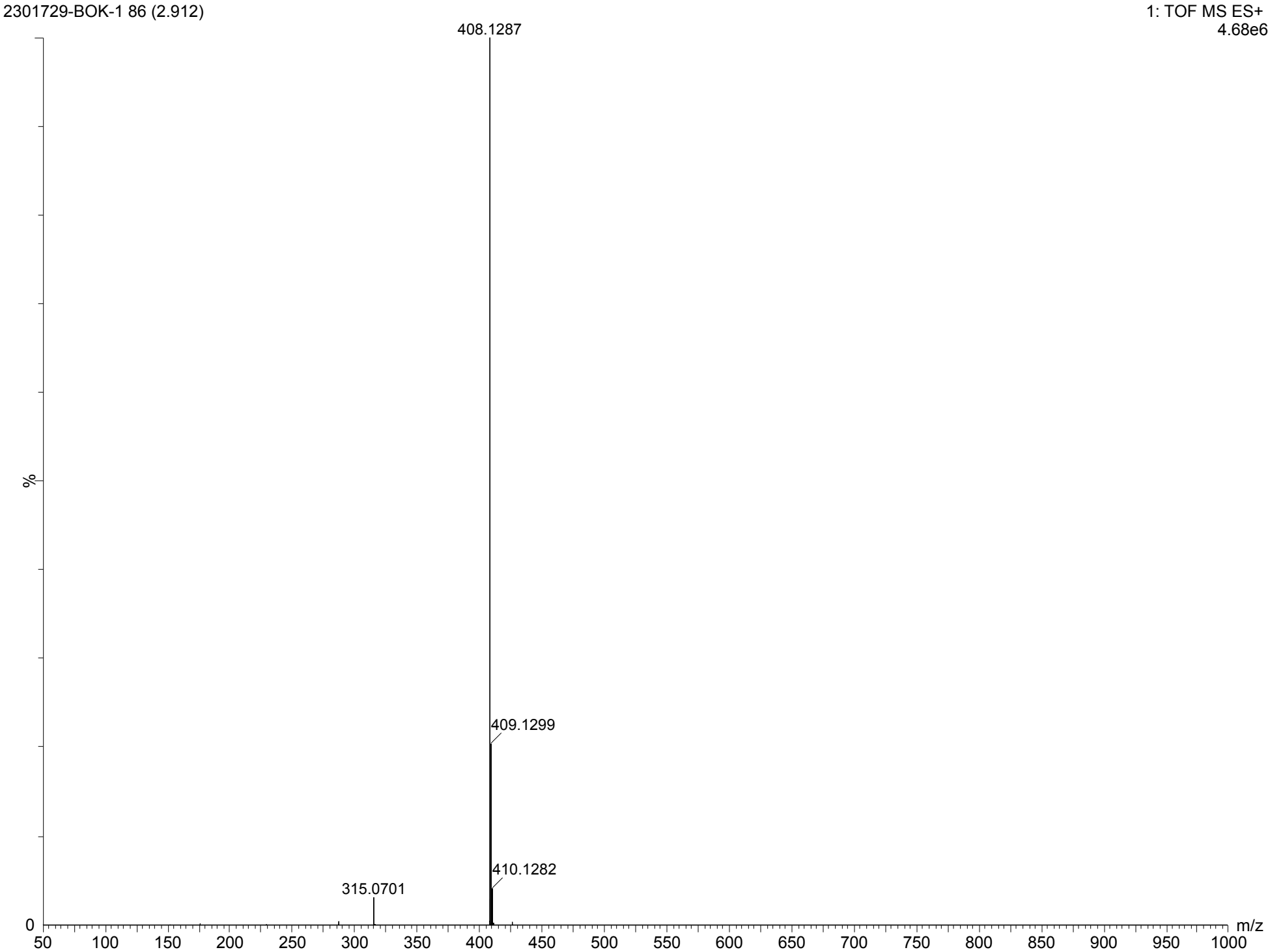
Current Data Parameters
NAME      23000786-BO-AN
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230801
Time               9.03 h
INSTRUM           spect
PROBHD   Z108618_0984 (
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                1024
DS                   4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            1.3631488 sec
RG                2050
DW              20.800 usec
DE               6.50 usec
TE              298.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        100.6680954 MHz
NUC1               13C
P0               3.33 usec
P1              10.00 usec
PLW1        51.02600098 W
SFO2        400.3116012 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2            90.00 usec
PLW2        11.28999996 W
PLW12        0.27318001 W
PLW13        0.13741000 W

F2 - Processing parameters
SI                32768
SF          100.6580296 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

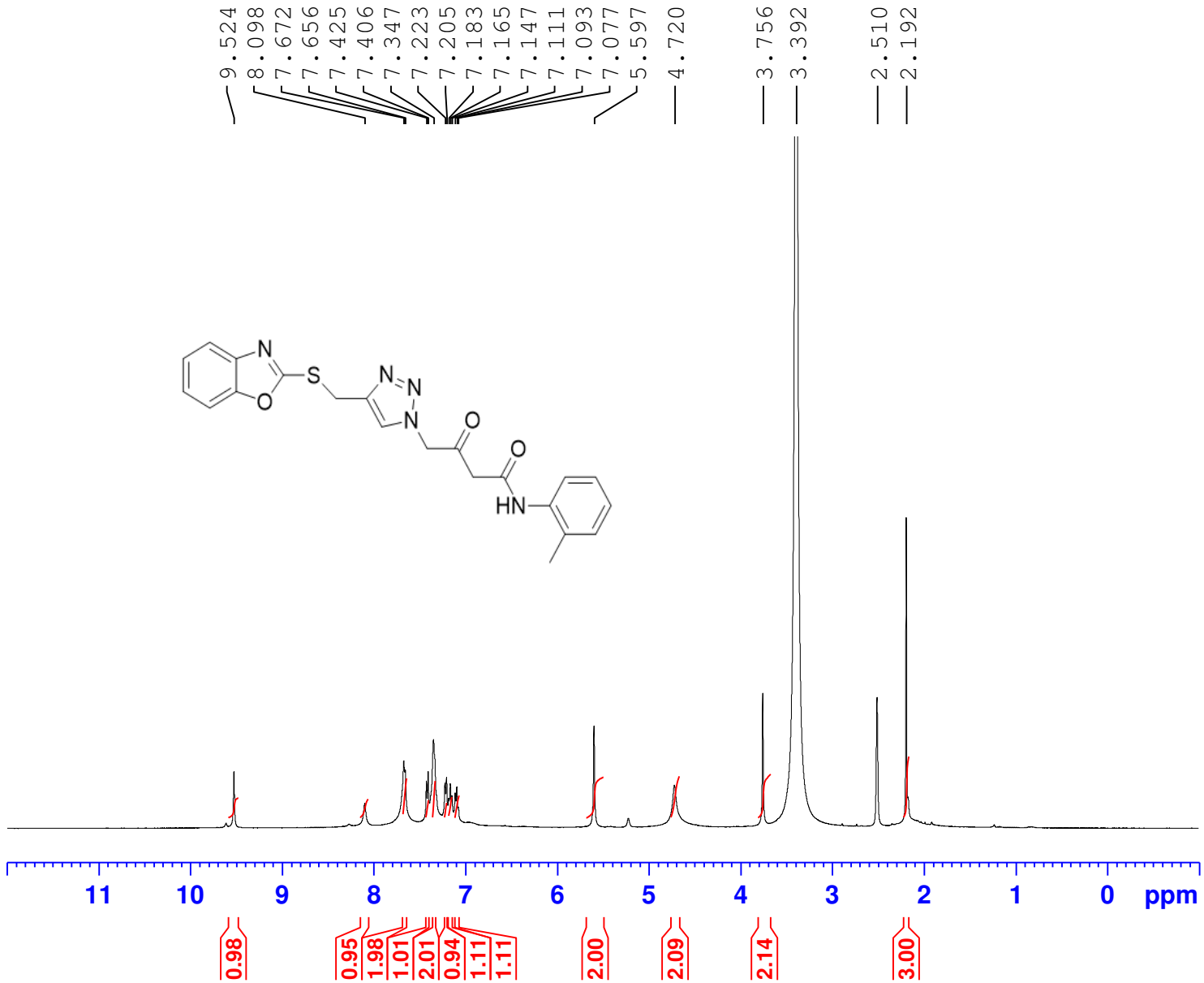
^{13}C NMR spectrum of 4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-phenyl butanamide **3a (BOK-1)**



Mass spectrum of 4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-phenyl butanamide **3a (BOK-1)**

COMPOUND 3b (BOK-2) SPECTRAL DATA

BOK-2
1H-NMR in DMSO

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Current Data Parameters
NAME      23000780-BO-2CH3
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230803
Time               10.03 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                 32.13
DW                62.400 usec
DE                17.09 usec
TE                300.4 K
D1           1.00000000 sec
TD0                    1
SFO1         400.3124719 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         11.28999996 W

F2 - Processing parameters
SI                 65536
SF           400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```
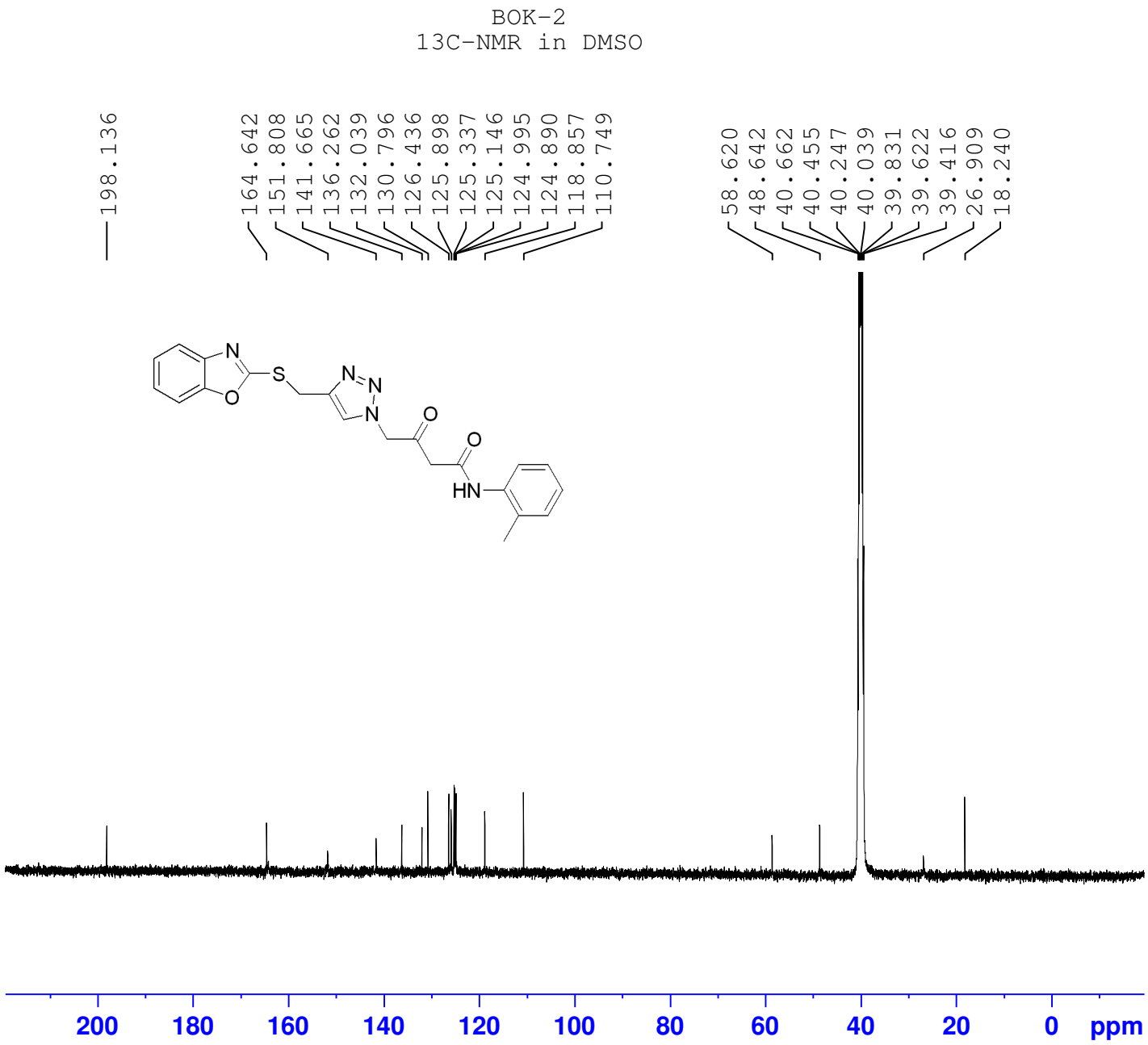

[1]H NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-(o-tolyl) butanamide 3b (BOK-2).



BRUKER

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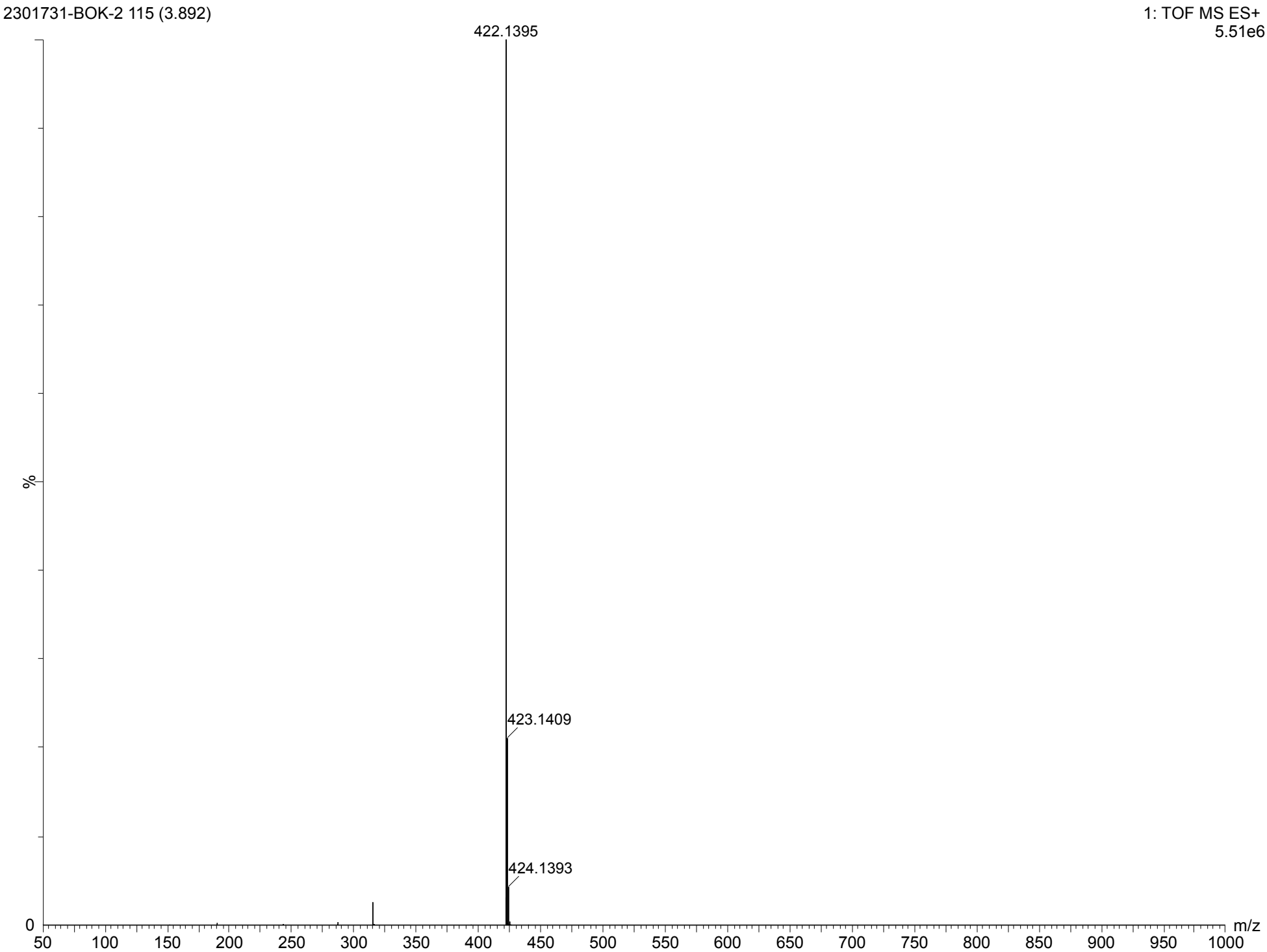
Current Data Parameters
NAME      23000780-BO-2CH3
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230801
Time                  5.07 h
INSTRUM              spect
PROBHD    Z108618_0984 (
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               1.3631488 sec
RG                   2050
DW                 20.800 usec
DE                  6.50 usec
TE                 298.1 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1          100.6680954 MHz
NUC1                 13C
P0                  3.33 usec
P1                 10.00 usec
PLW1          51.02600098 W
SFO2          400.3116012 MHz
NUC2                 1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2          11.28999996 W
PLW12          0.27318001 W
PLW13          0.13741000 W

F2 - Processing parameters
SI                   32768
SF            100.6580296 MHz
WDW                  EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

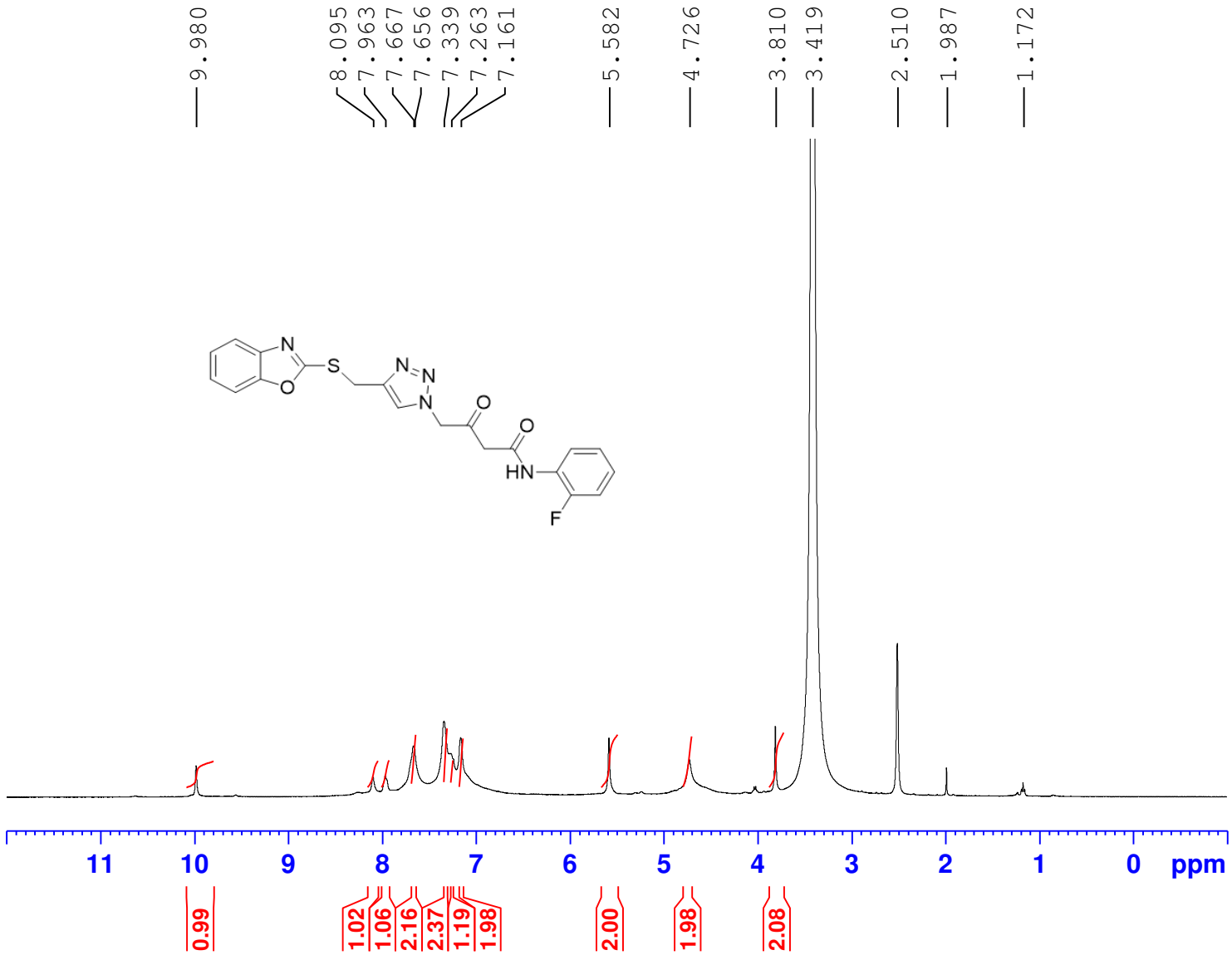
^{13}C NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-(o-tolyl) butanamide 3b (BOK-2).



Mass spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-(o-tolyl) butanamide 3b (BOK-2).

COMPOUND 3c (BOK-3) SPECTRAL DATA

BOK-3
1H-NMR in DMSO

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Current Data Parameters
NAME      23000784-BO-2F
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230801
Time                7.30 h
INSTRUM            spect
PROBHD   Z108618_0984 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                 114.18
DW                 62.400 usec
DE                 17.09 usec
TE                 297.2 K
D1            1.00000000 sec
TD0                    1
SFO1         400.3124719 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         11.28999996 W

F2 - Processing parameters
SI                 65536
SF           400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```
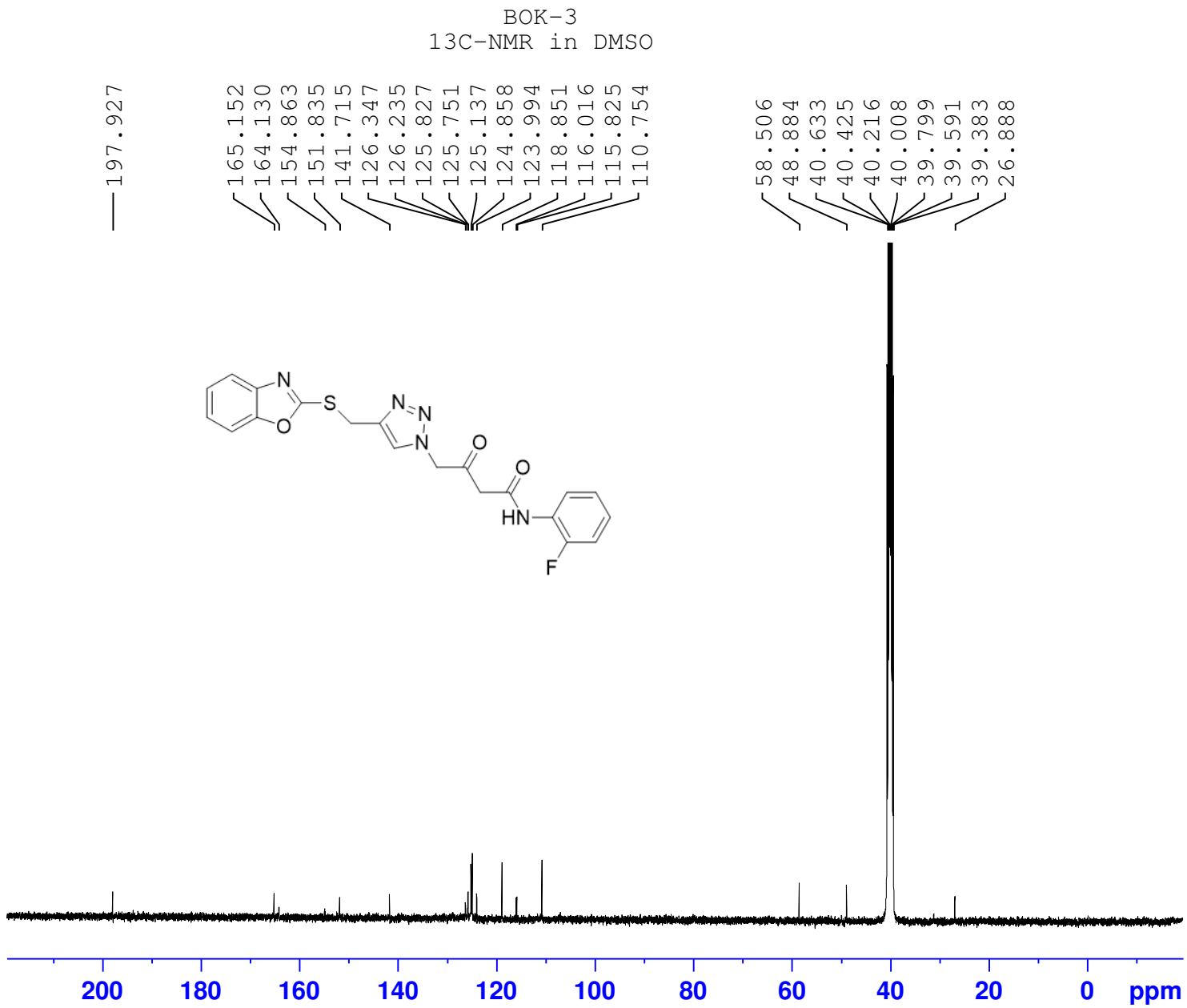
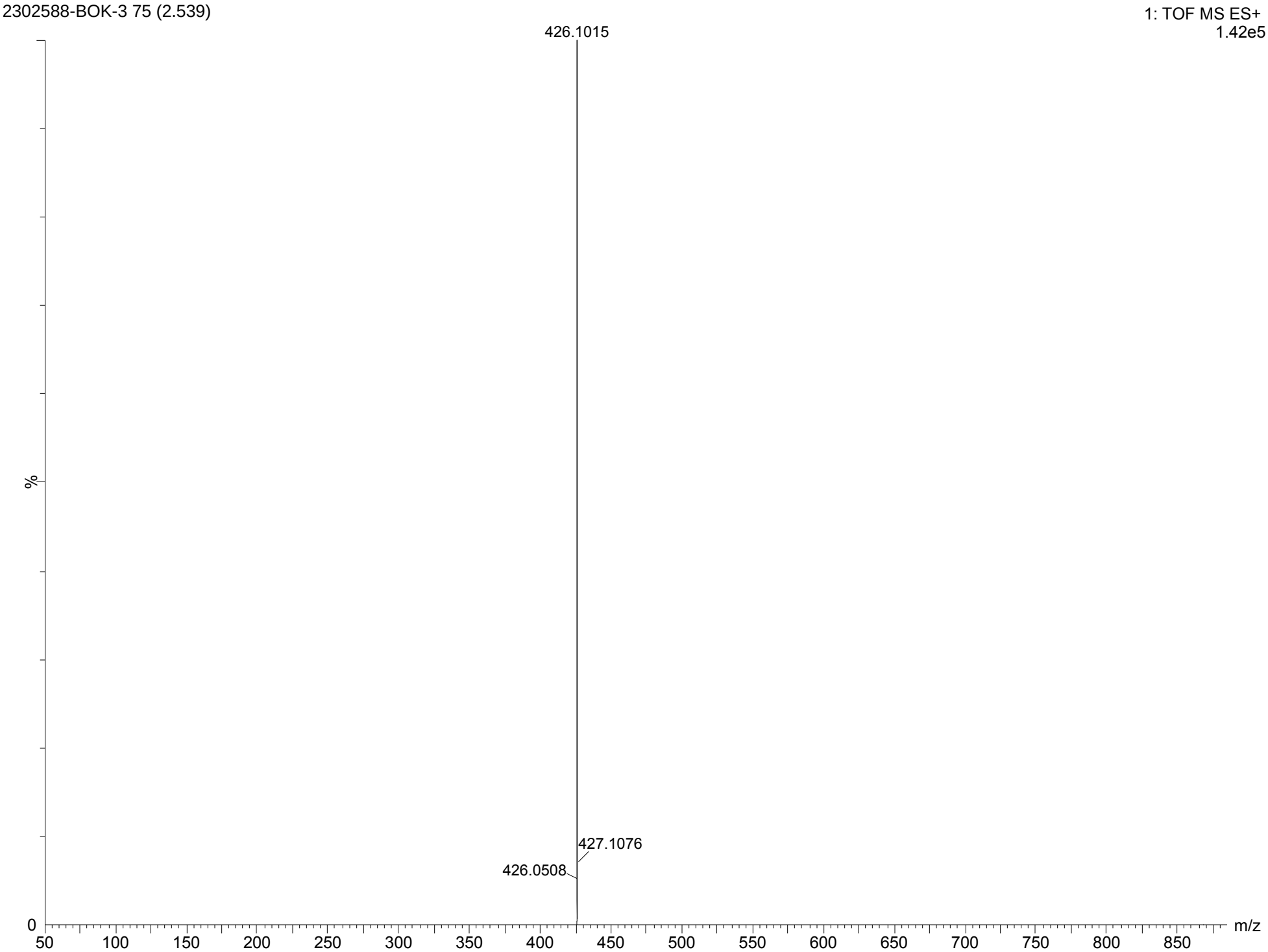

[1]H NMR spectrum of4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(2-fluorophenyl)-3-oxobutanamide **3c (BOK-3)**.



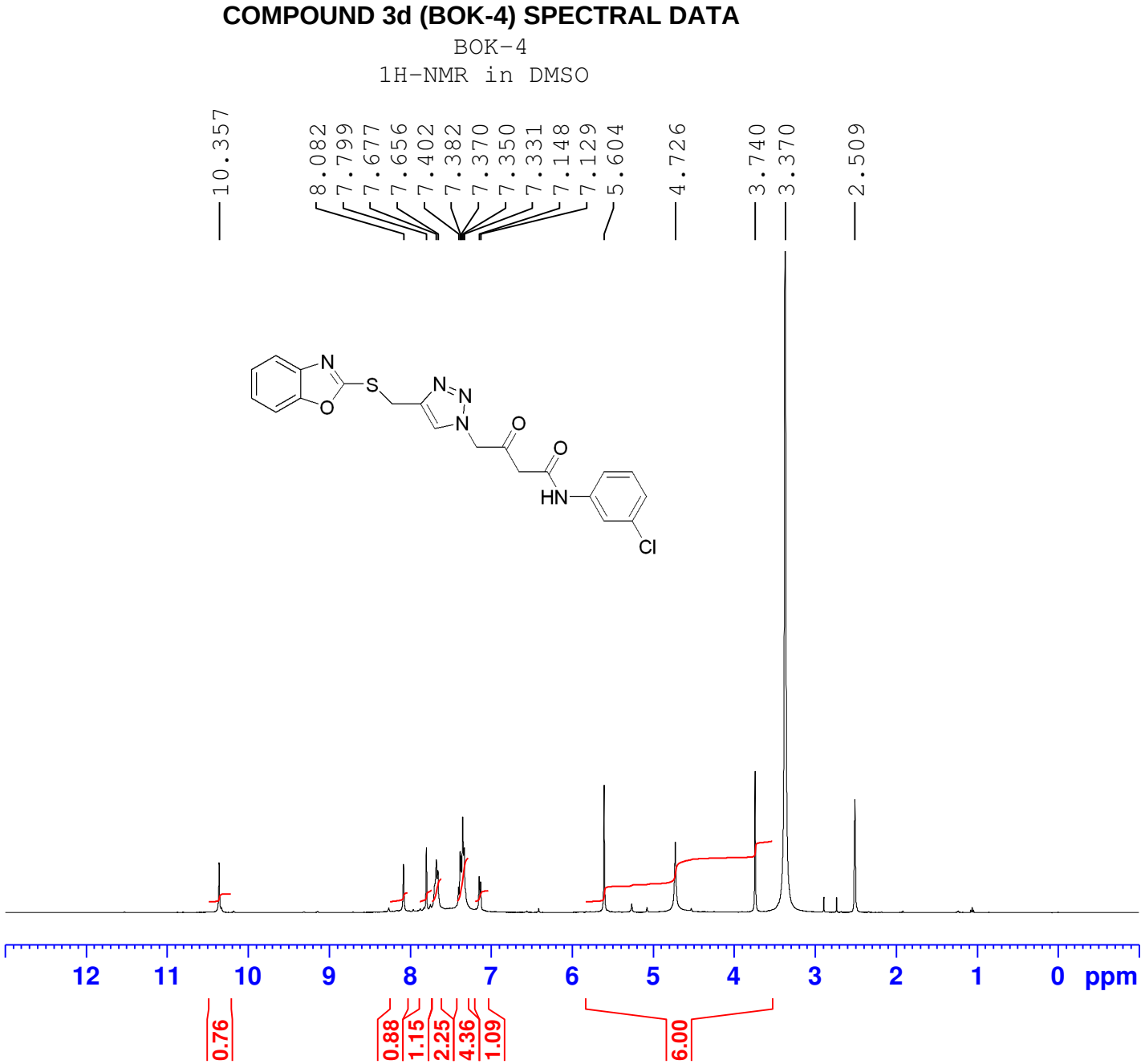
^{13}C NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(2-fluorophenyl)-3-oxobutanamide **3**c **(BOK-3)**.

```
Current Data Parameters
NAME      23000847-BO-2F
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230817
Time              21.11 h
INSTRUM             spect
PROBHD   Z108618_0984 (
PULPROG           zgpg30
TD                65536
SOLVENT            DMSO
NS                 3000
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                202.84
DW                20.800 usec
DE                 6.50 usec
TE                298.1 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6680954 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         51.02600098 W
SFO2         400.3116012 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         11.28999996 W
PLW12         0.27318001 W
PLW13         0.13741000 W

F2 - Processing parameters
SI                 32768
SF           100.6580296 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



Mass spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(2-fluorophenyl)-3-oxobutanamide **3c (BOK-3)**.

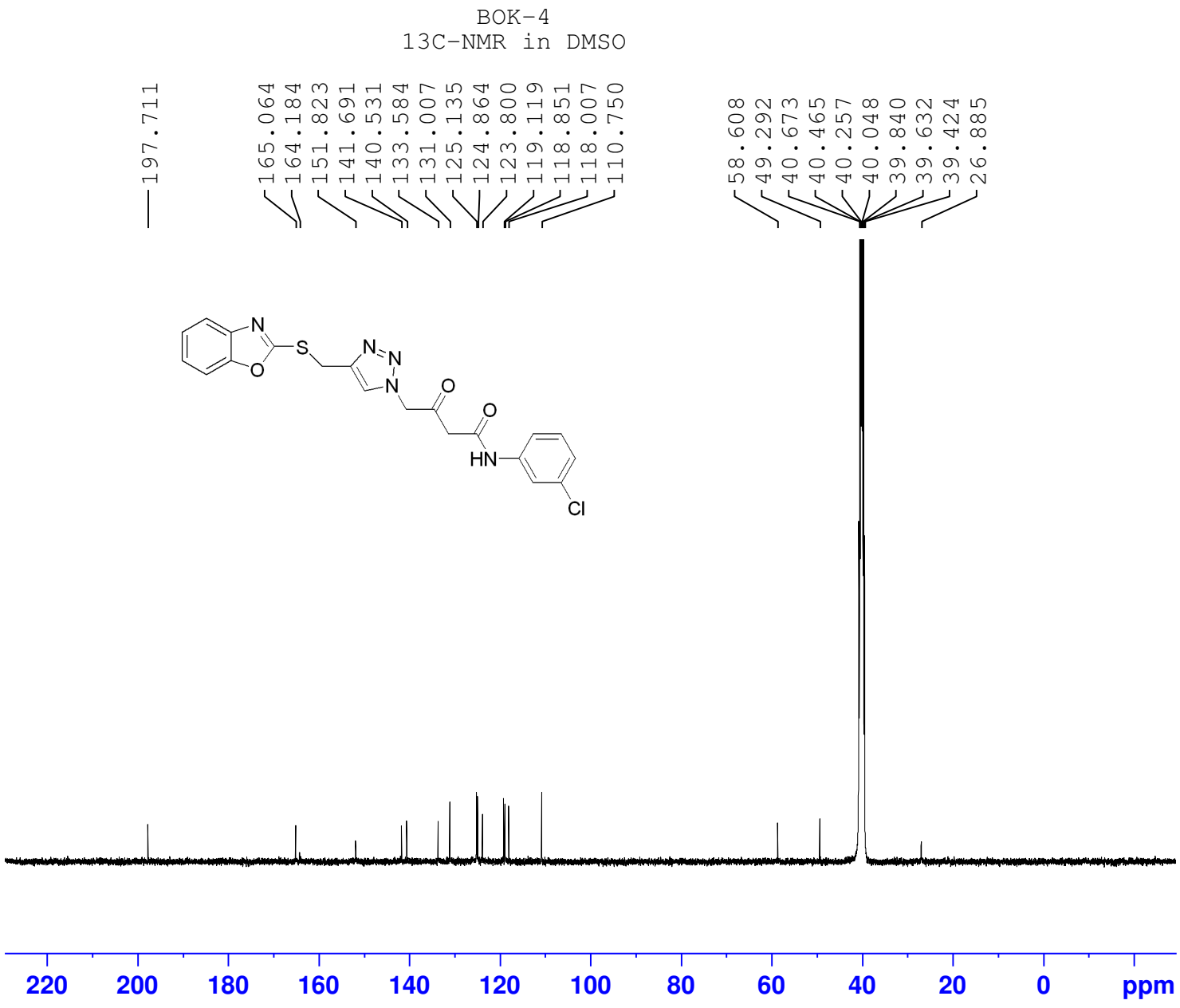
COMPOUND 3d (BOK-4) SPECTRAL DATA



Chromatogen Analytical Solutions

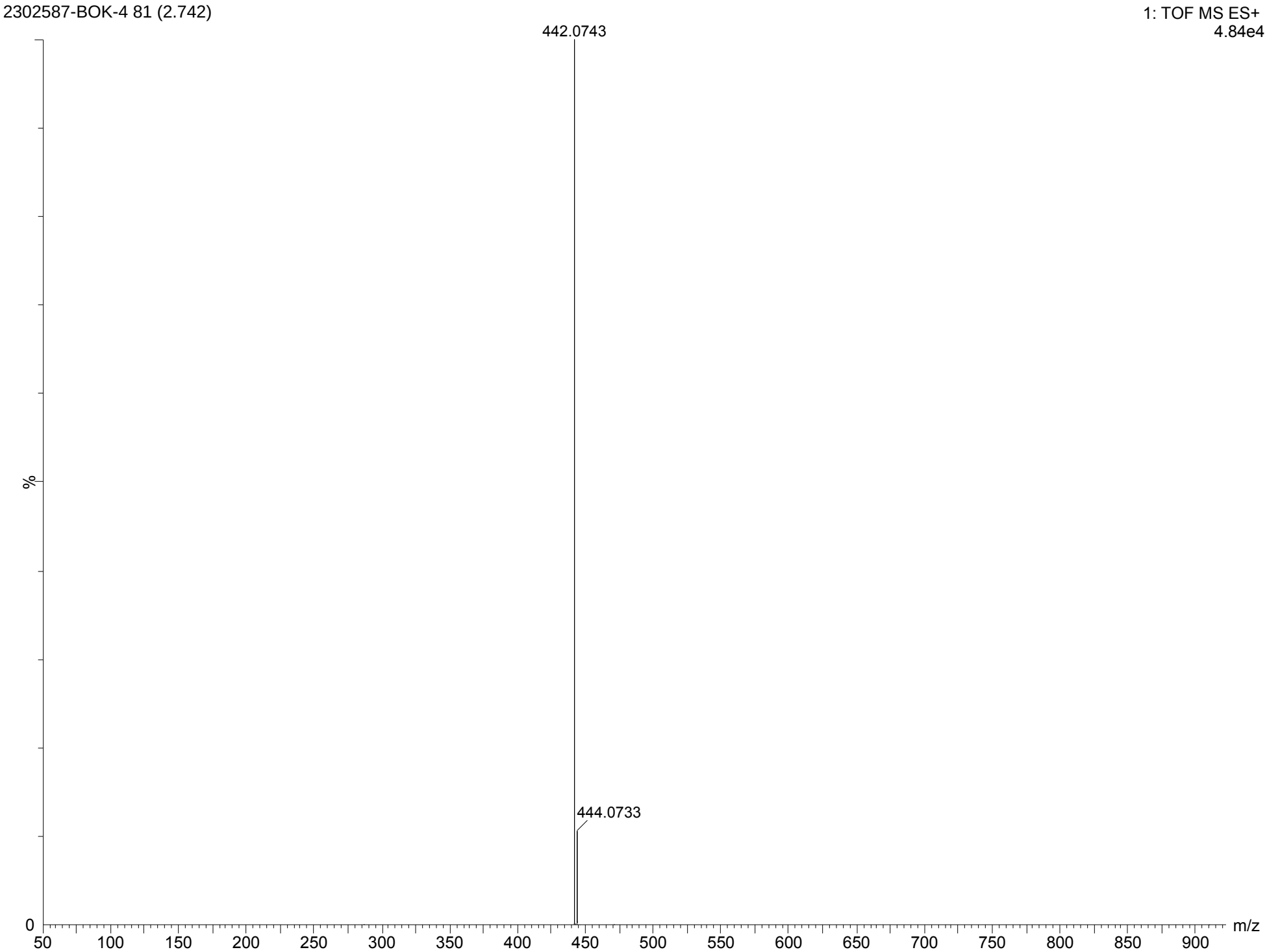
```
Current Data Parameters
NAME      23000836-BO-3Cl
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230814
Time              17.56 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                 160.67
DW                 62.400 usec
DE                 17.09 usec
TE                 297.8 K
D1            1.00000000 sec
TD0                    1
SFO1         400.3124719 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         11.28999996 W

F2 - Processing parameters
SI                 65536
SF          400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(3-chlorophenyl)-3-oxobutanamide **3d (BOK-4)**



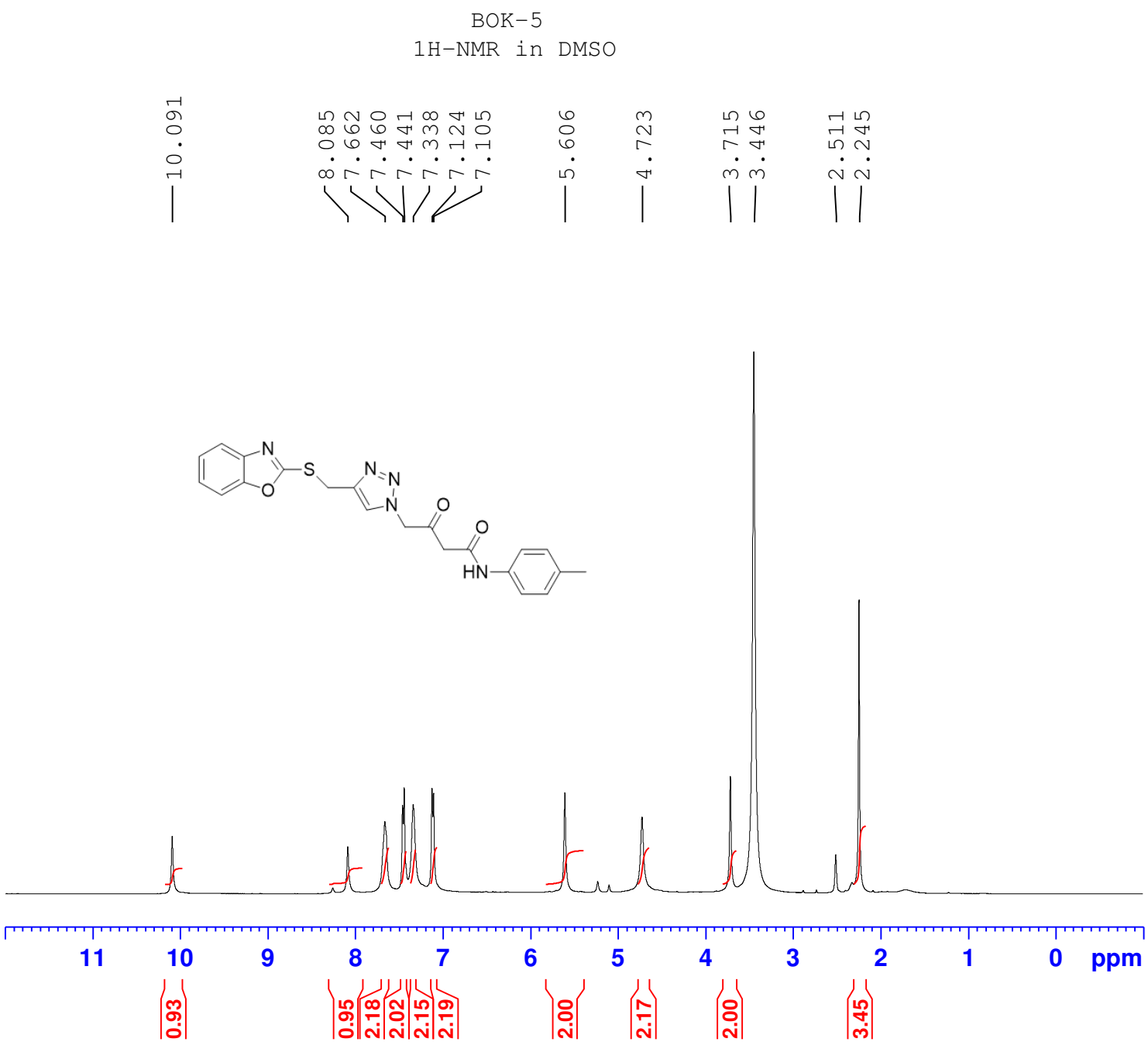
^{13}C NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(3-chlorophenyl)-3-oxobutanamide **3**d **(BOK**-4**)**.

```
Current Data Parameters
NAME      23000836-BO-3Cl
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230816
Time               11.22 h
INSTRUM             spect
PROBHD   Z108618_0984 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  2048
DS                     4
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ            1.2582912 sec
RG               202.84
DW               19.200 usec
DE                6.50 usec
TE                298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        100.6680954 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1        51.02600098 W
SFO2        400.3116012 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2        11.28999996 W
PLW12        0.27318001 W
PLW13        0.13741000 W

F2 - Processing parameters
SI                 32768
SF          100.6580296 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



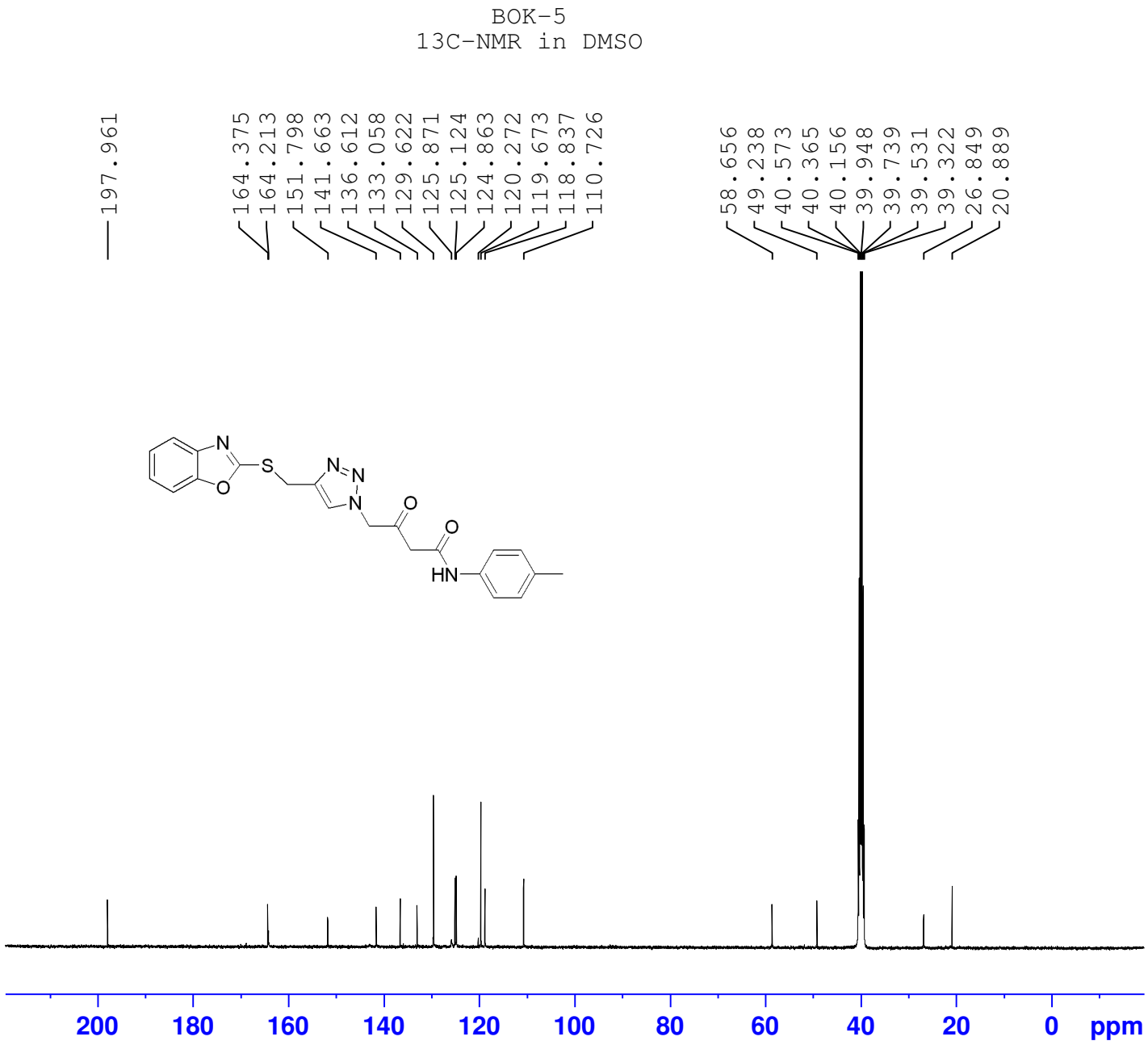
Mass spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(3-chlorophenyl)-3-oxobutanamide **3d (BOK-4)**

COMPOUND 3e (BOK-5) SPECTRAL DATA



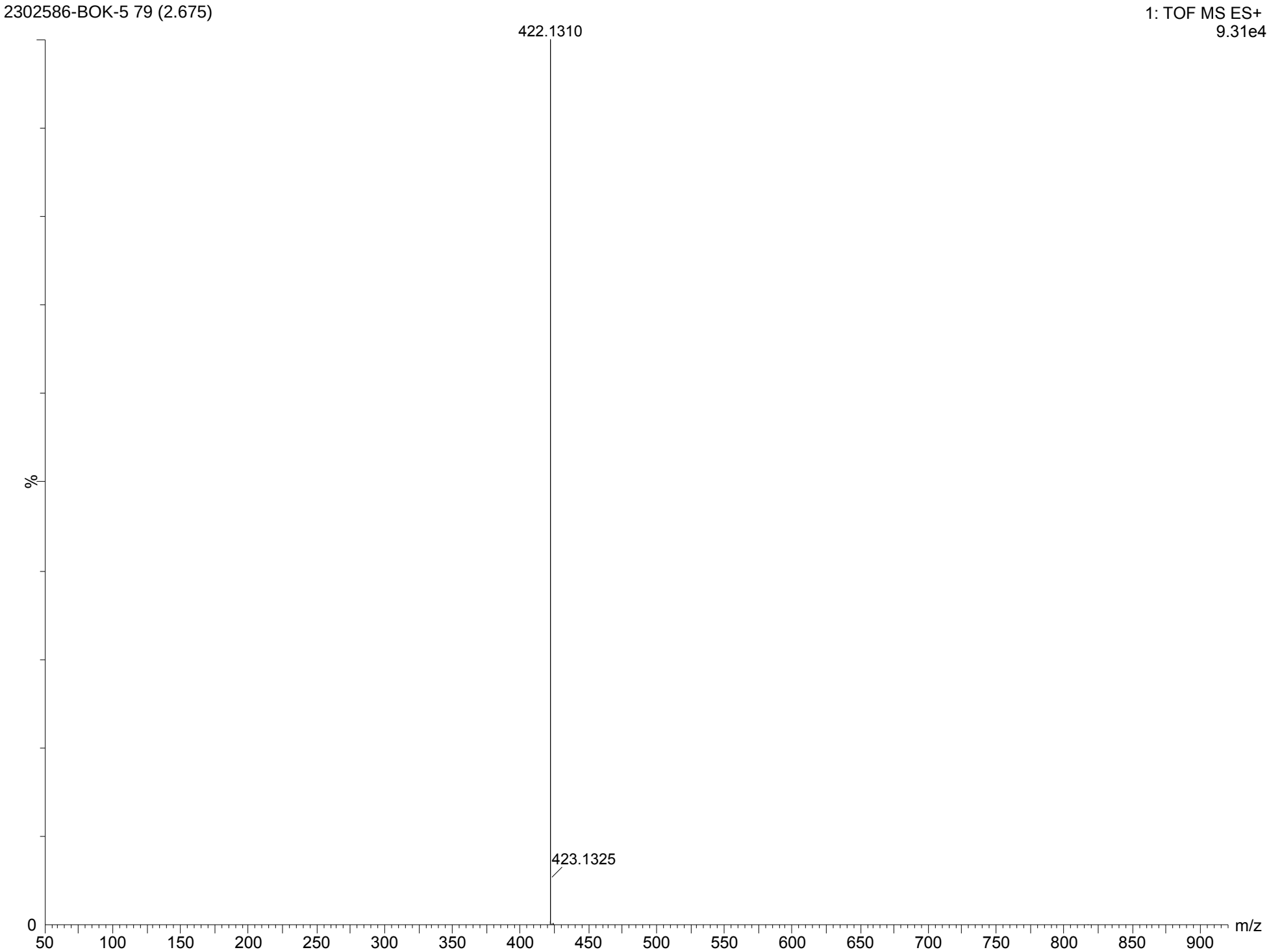

```
Current Data Parameters
NAME      23000781-BO-4CH3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230801
Time                5.11 h
INSTRUM            spect
PROBHD    Z108618_0984 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                 65.15
DW                62.400 usec
DE                17.09 usec
TE                297.0 K
D1           1.00000000 sec
TD0                    1
SFO1         400.3124719 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         11.28999996 W

F2 - Processing parameters
SI                 65536
SF           400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-(p-tolyl) butanamide **3e (BOK-5).**



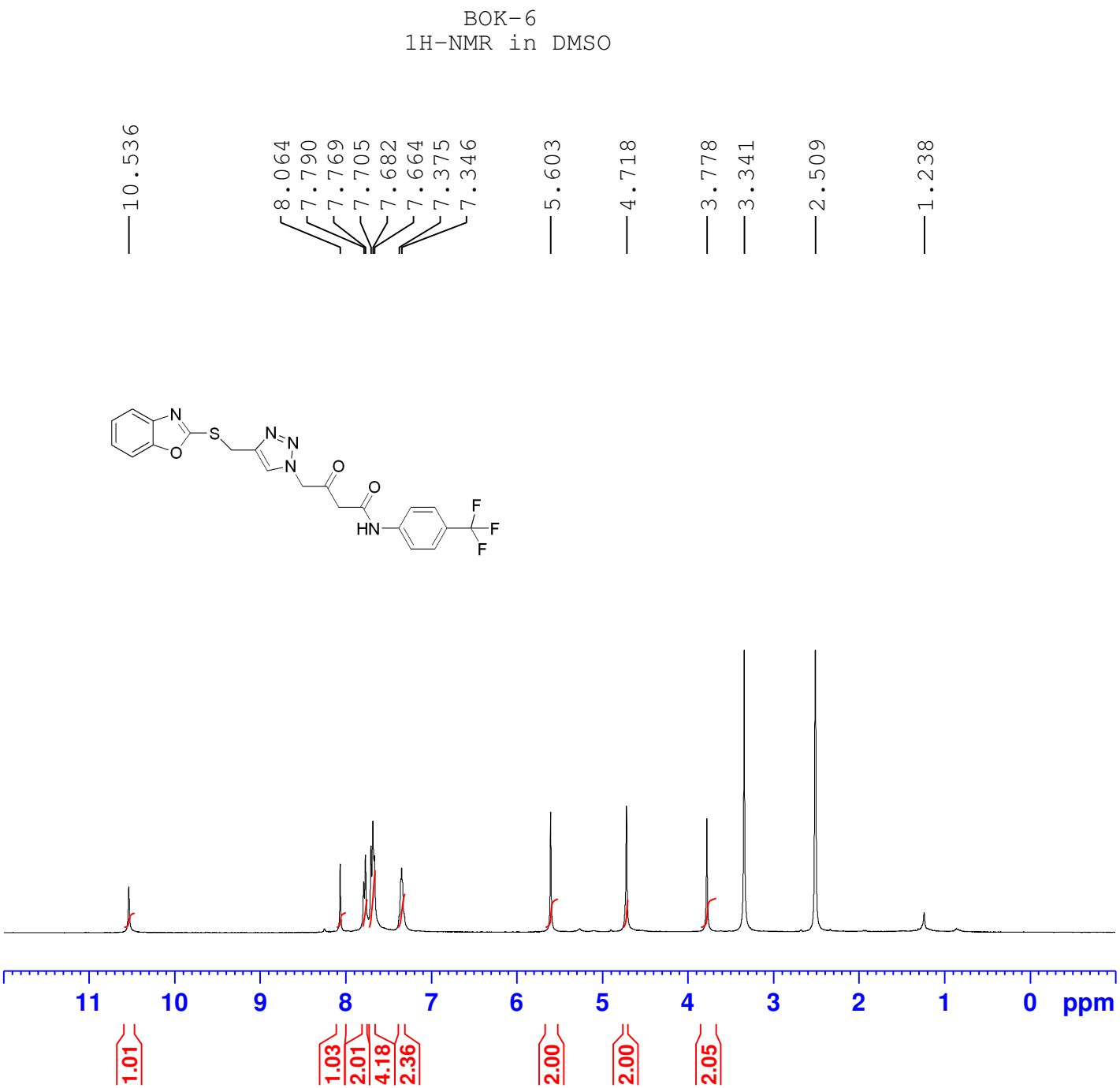

```
Current Data Parameters
NAME      23000781-BO-4CH3
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230801
Time                  5.53 h
INSTRUM              spect
PROBHD    Z108618_0984 (
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                1.3631488 sec
RG                    2050
DW                  20.800 usec
DE                   6.50 usec
TE                  297.9 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           100.6680954 MHz
NUC1                   13C
P0                   3.33 usec
P1                  10.00 usec
PLW1           51.02600098 W
SFO2           400.3116012 MHz
NUC2                   1H
CPDPRG[2           waltz65
PCPD2                90.00 usec
PLW2           11.28999996 W
PLW12           0.27318001 W
PLW13           0.13741000 W

F2 - Processing parameters
SI                   32768
SF             100.6580296 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

^{13}C NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-(p-tolyl) butanamide **3e (BOK-5).**



Mass spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-(p-tolyl) butanamide**3e (BOK-5).**

COMPOUND 3f (BOK-6) SPECTRAL DATA

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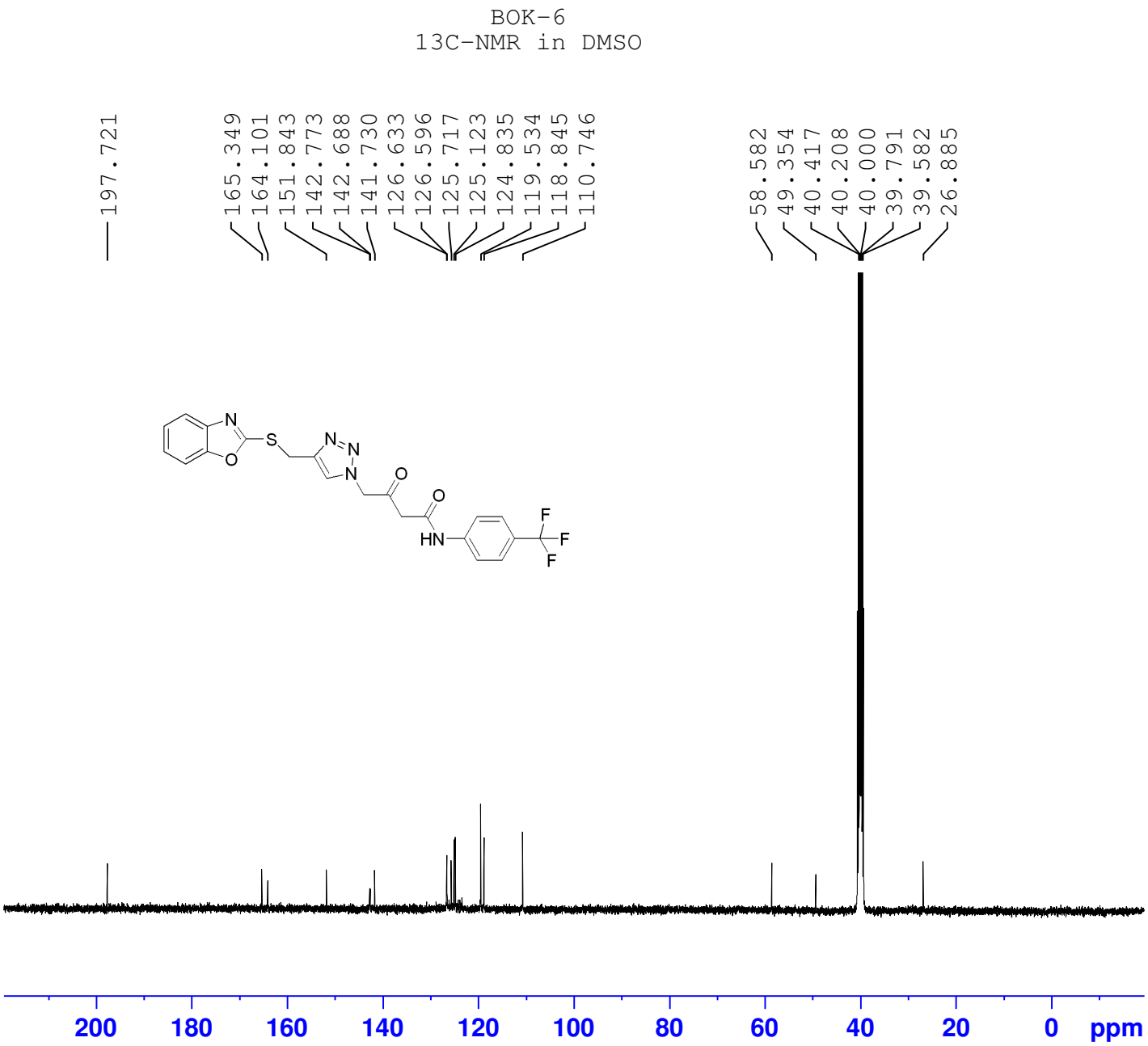
Current Data Parameters
NAME      23000350-BO-CF3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230403
Time              16.06 h
INSTRUM            spect
PROBHD   Z108618_0984 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                 255.12
DW                 62.400 usec
DE                 17.09 usec
TE                 297.3 K
D1            1.00000000 sec
TD0                    1
SFO1         400.3124719 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         11.28999996 W

F2 - Processing parameters
SI                 65536
SF           400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-(4-(trifluoromethyl) phenyl)butanamide **3f (BOK-6).**

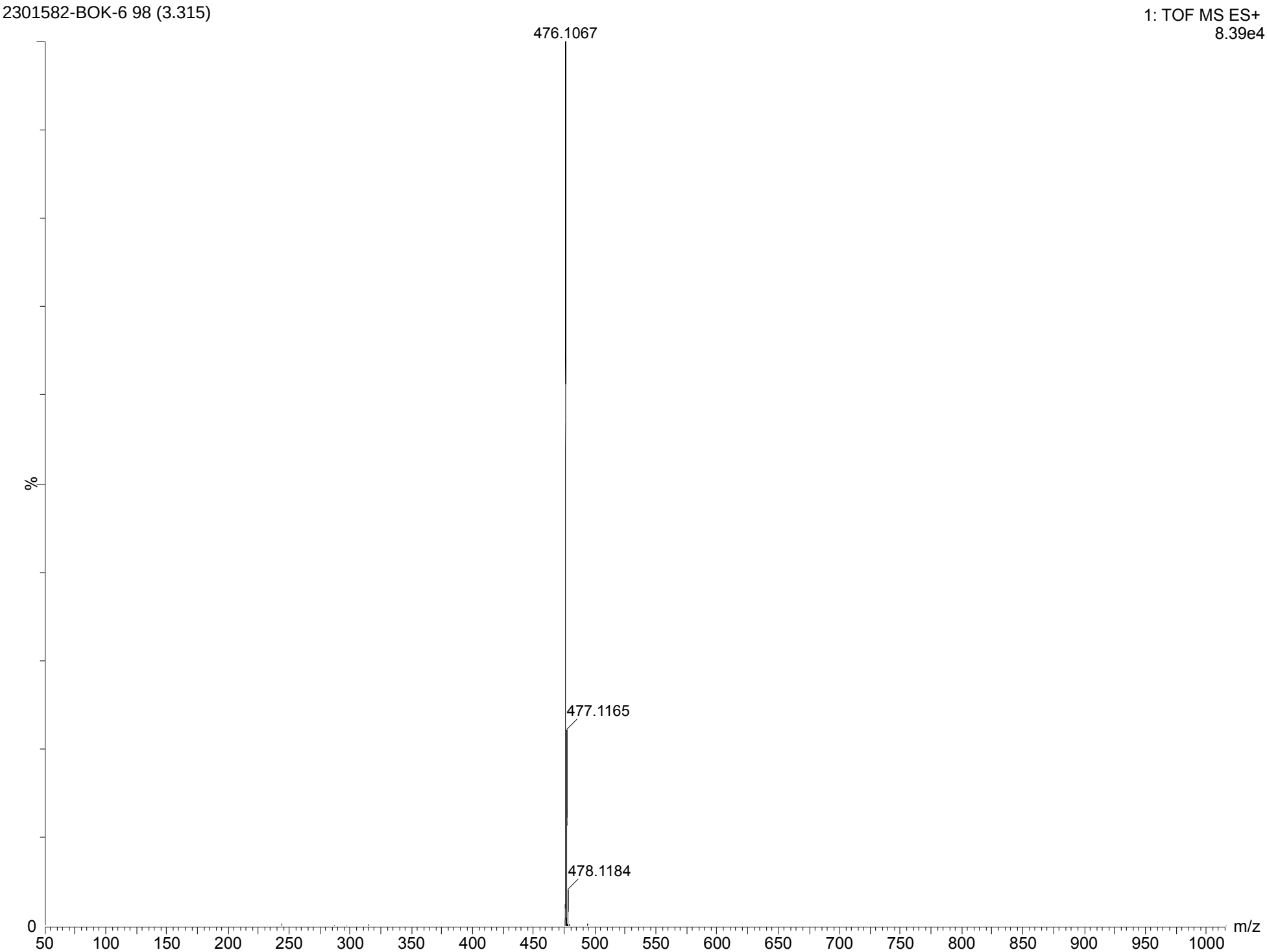


Current Data Parameters
NAME 23000439-BO-4CF3
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230430
Time 16.16 h
INSTRUM spect
PROBHD Z108618_0984 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 202.84
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6680954 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 51.02600098 W
SFO2 400.3116012 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 11.28999996 W
PLW12 0.27318001 W
PLW13 0.13741000 W

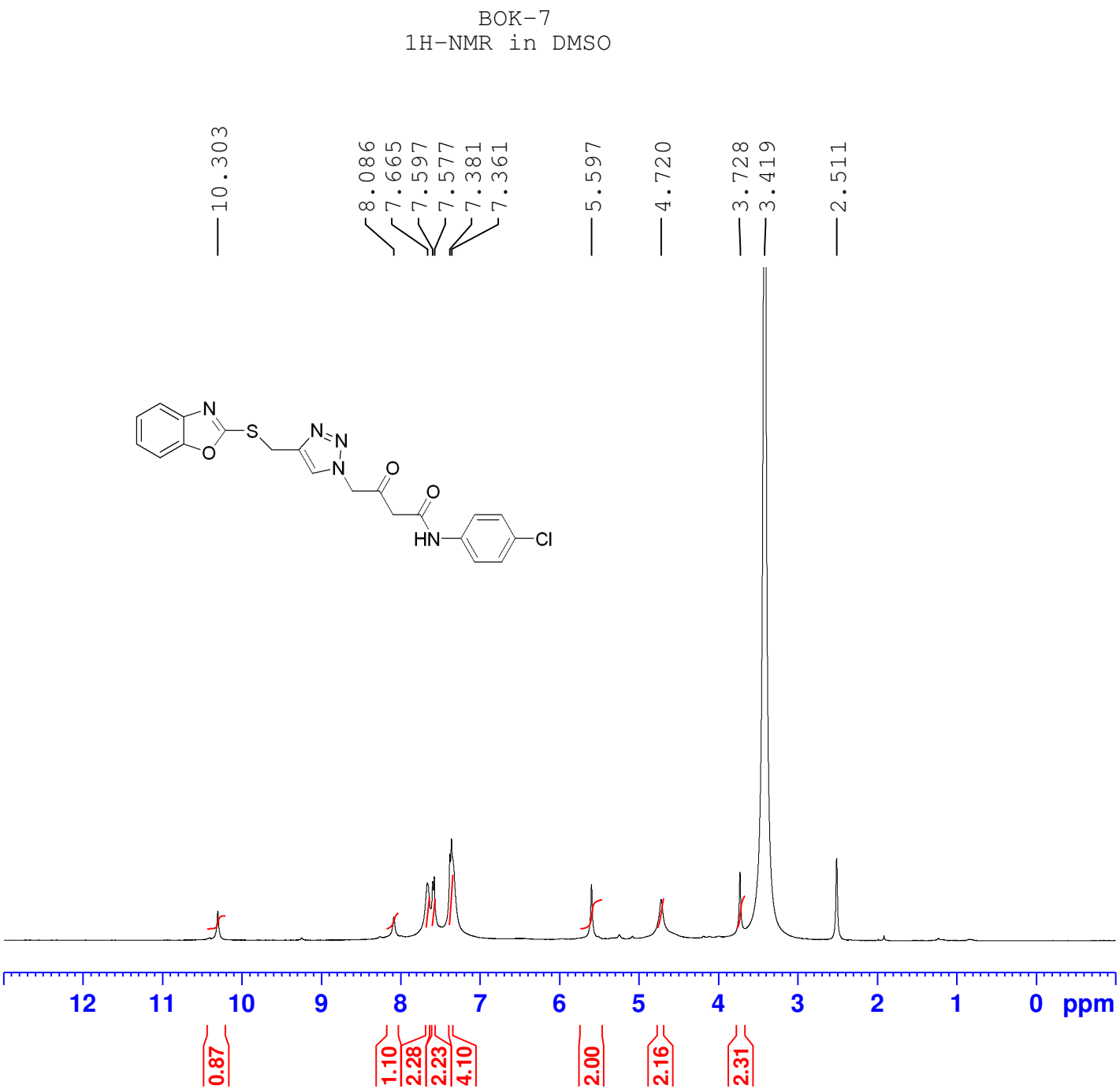
F2 - Processing parameters
SI 32768
SF 100.6580296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-(4-(trifluoromethyl) phenyl)butanamide **3f (BOK-6)**.



Mass spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-3-oxo-N-(4-(trifluoromethyl) phenyl)butanamide **3f (BOK-6)**.

COMPOUND 3g (BOK-7) SPECTRAL DATA

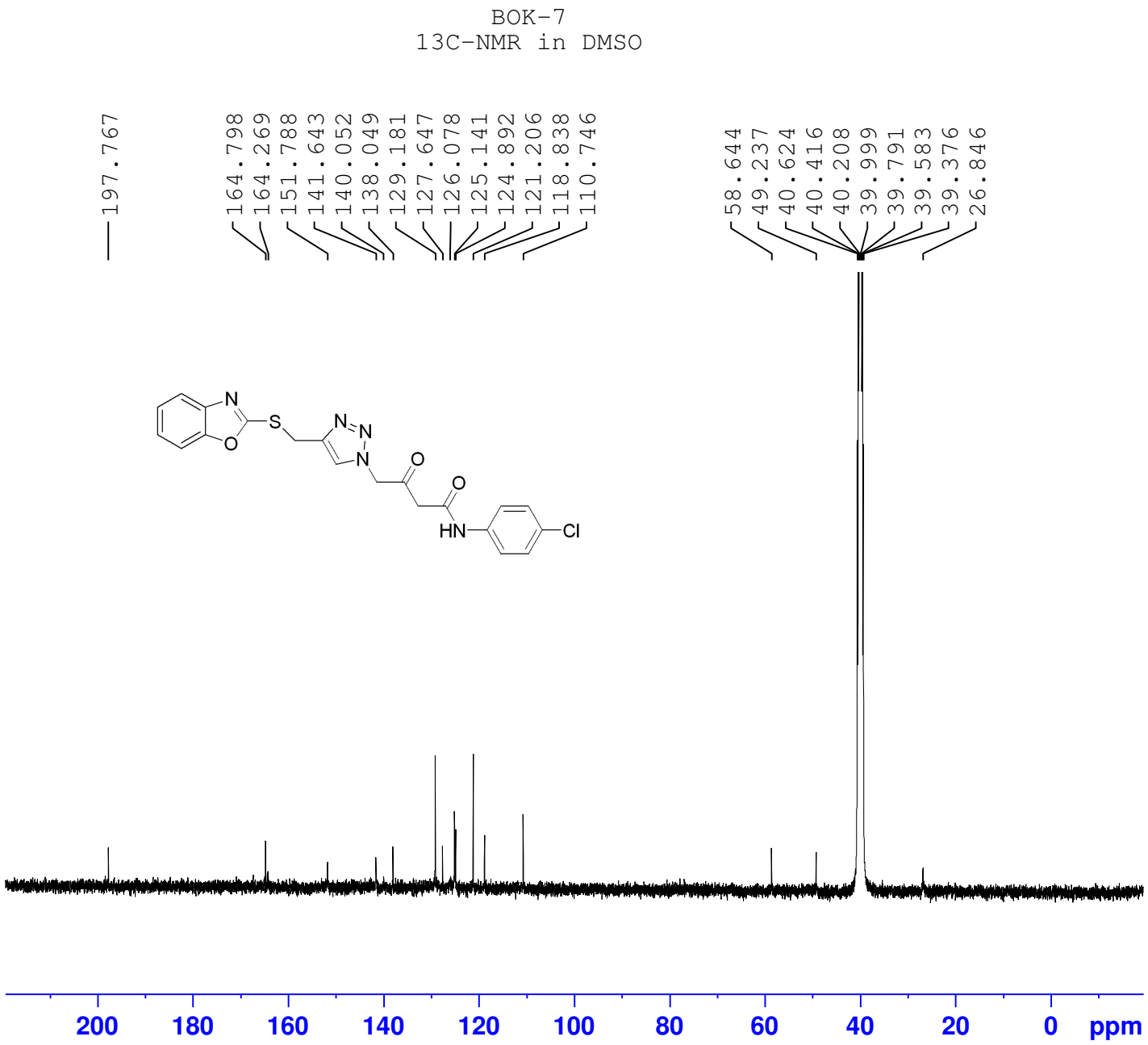



```
Current Data Parameters
NAME      23000783-BO-4CL
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20230801
Time                6.44 h
INSTRUM            spect
PROBHD    Z108618_0984 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                 114.18
DW                 62.400 usec
DE                 17.09 usec
TE                 297.2 K
D1              1.00000000 sec
TD0                    1
SFO1          400.3124719 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1          11.28999996 W

F2 - Processing parameters
SI                 65536
SF            400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

^{1}H NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-chlorophenyl)-3-oxo butanamide **3g (BOK-7).**

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Current Data Parameters
NAME      23000783-BO-4CL
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230801
Time               7.26 h
INSTRUM           spect
PROBHD   Z108618_0984 (
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                1024
DS                   4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            1.3631488 sec
RG                2050
DW              20.800 usec
DE               6.50 usec
TE              298.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        100.6680954 MHz
NUC1               13C
P0               3.33 usec
P1              10.00 usec
PLW1        51.02600098 W
SFO2        400.3116012 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2            90.00 usec
PLW2        11.28999996 W
PLW12        0.27318001 W
PLW13        0.13741000 W

F2 - Processing parameters
SI                32768
SF          100.6580296 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```
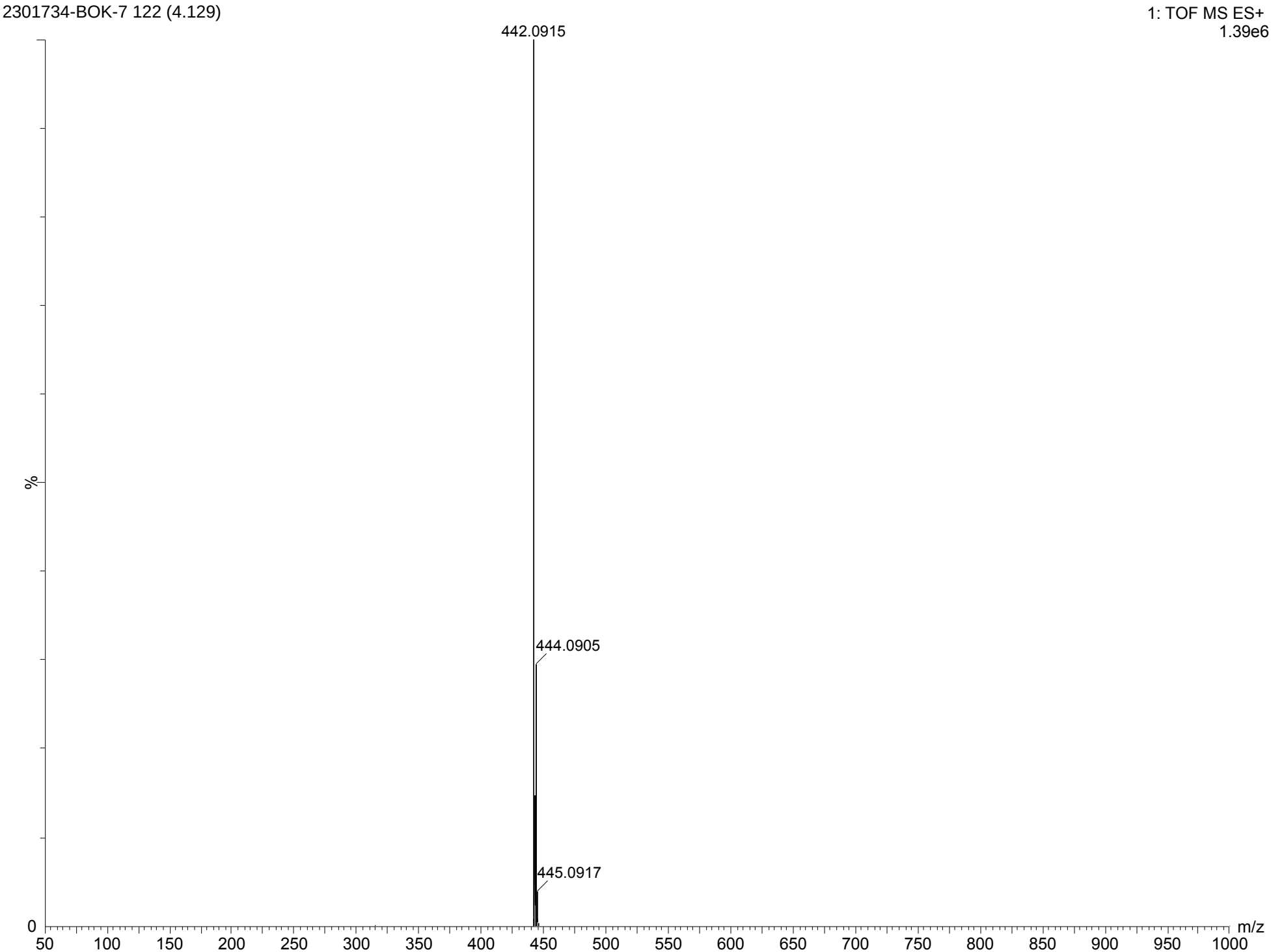
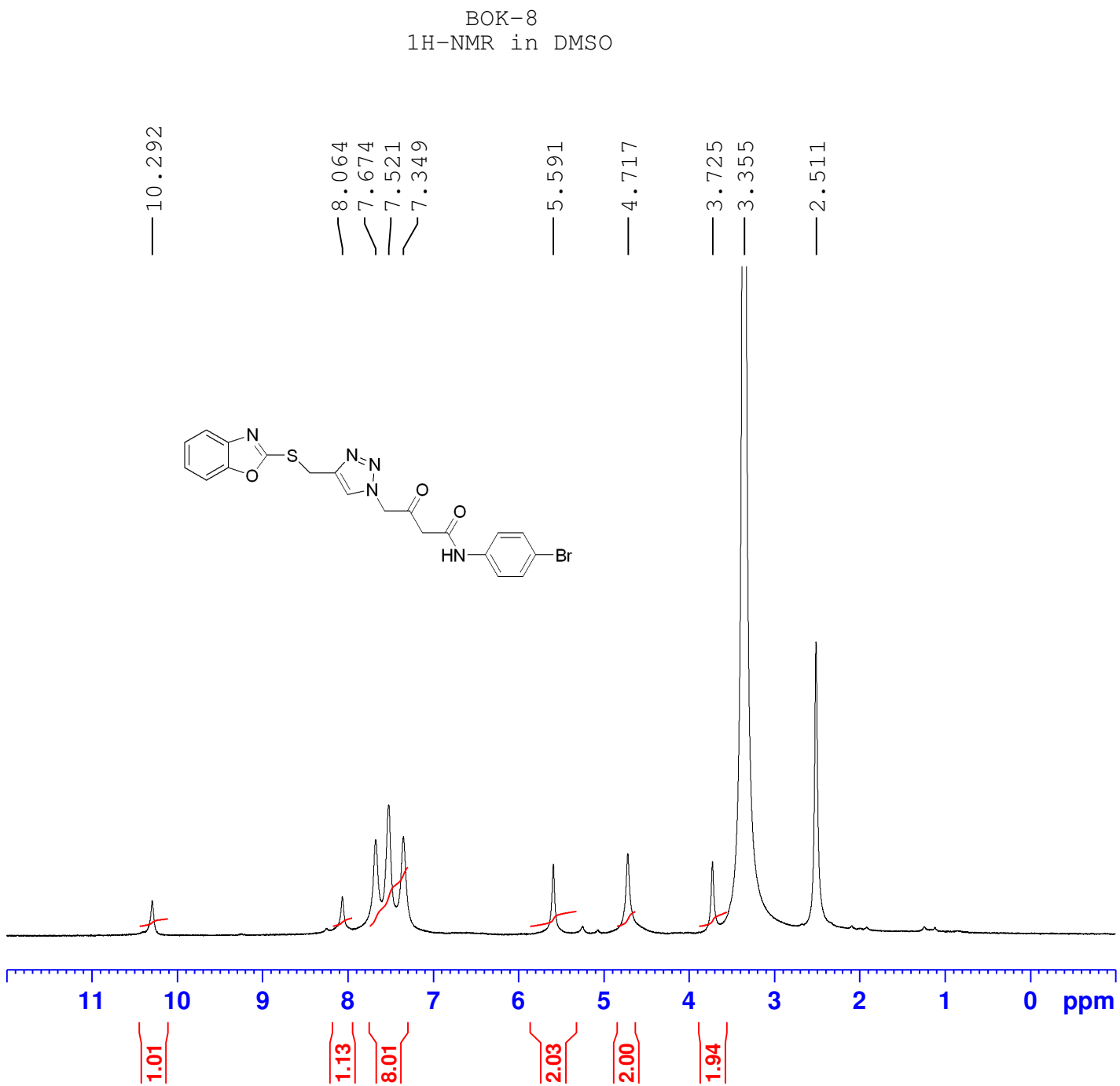

^{13}C NMR spectrum of4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-chlorophenyl)-3-oxo butanamide **3g (BOK-7)**.



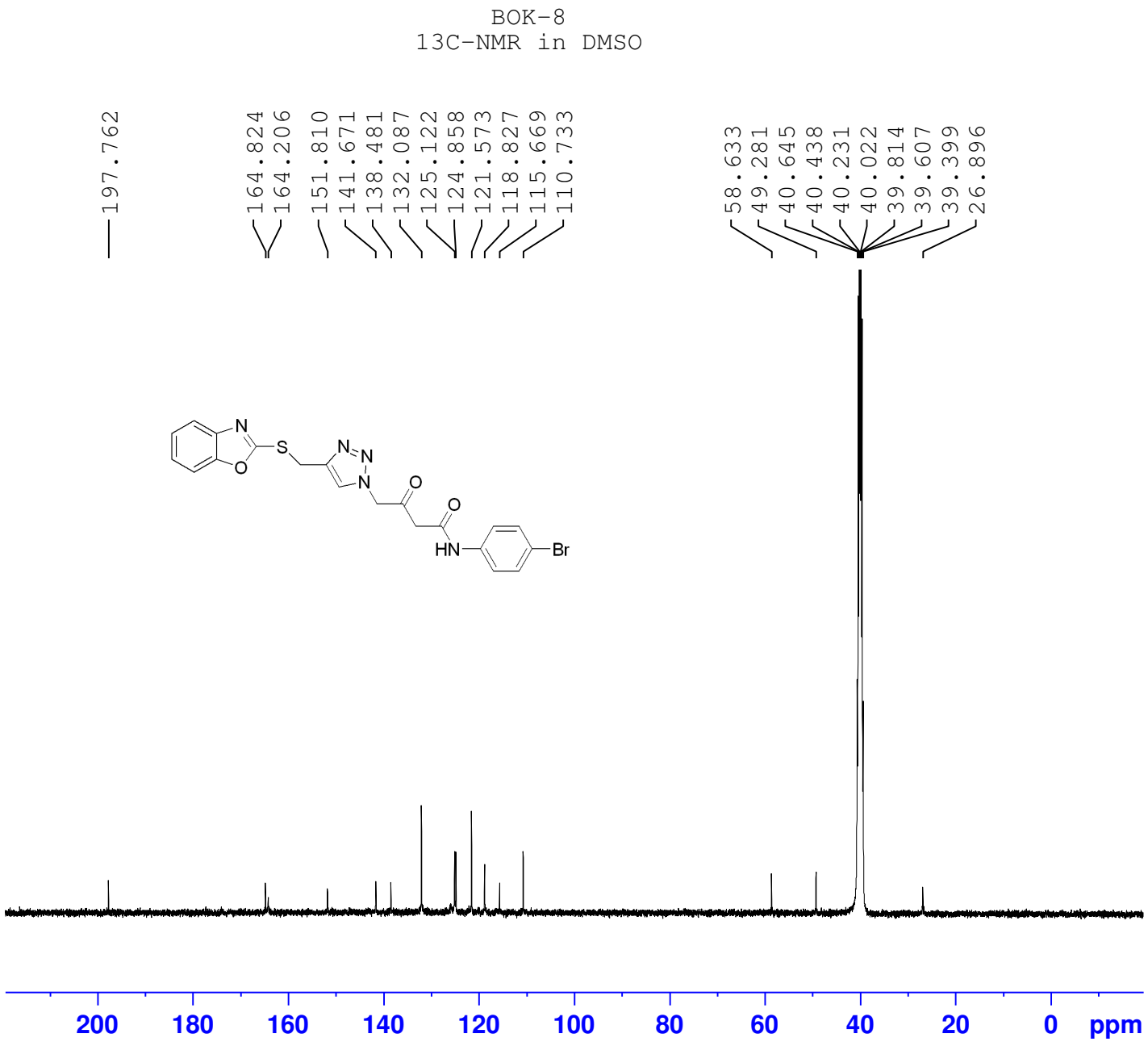
Mass spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-chlorophenyl)-3-oxo butanamide **3g (BOK-7)**.

COMPOUND 3h (BOK-8) SPECTRAL DATA



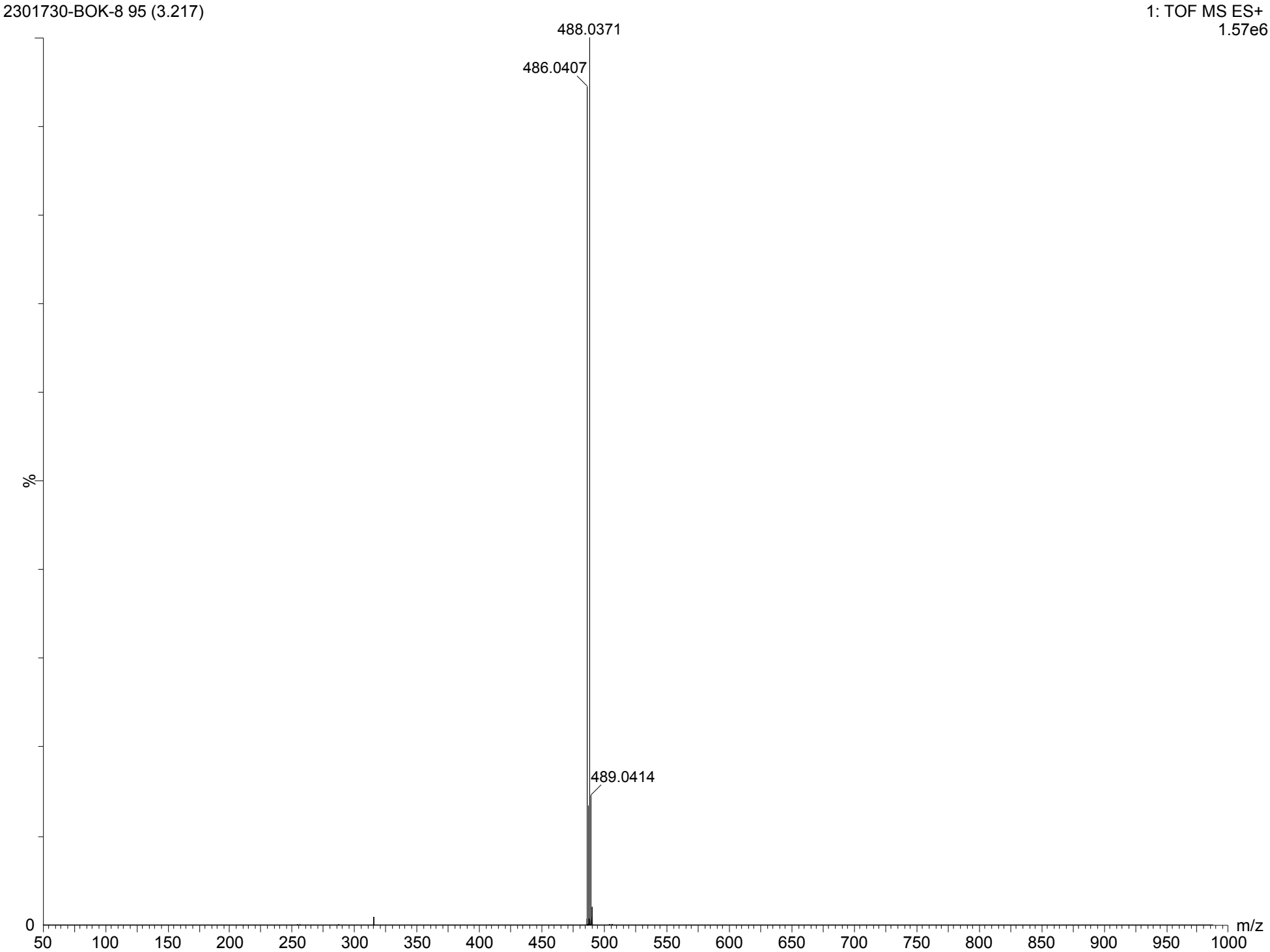

```
Current Data Parameters
NAME      23000509-BO-4Br
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230520
Time              10.36 h
INSTRUM            spect
PROBHD   Z108618_0984 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    32
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                 32.13
DW                62.400 usec
DE                17.09 usec
TE                297.8 K
D1             1.00000000 sec
TD0                    1
SFO1         400.3124719 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         11.28999996 W

F2 - Processing parameters
SI                 65536
SF          400.3100000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

^{1}H NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-bromophenyl)-3-oxo butanamide **3h (BOK-8)**.



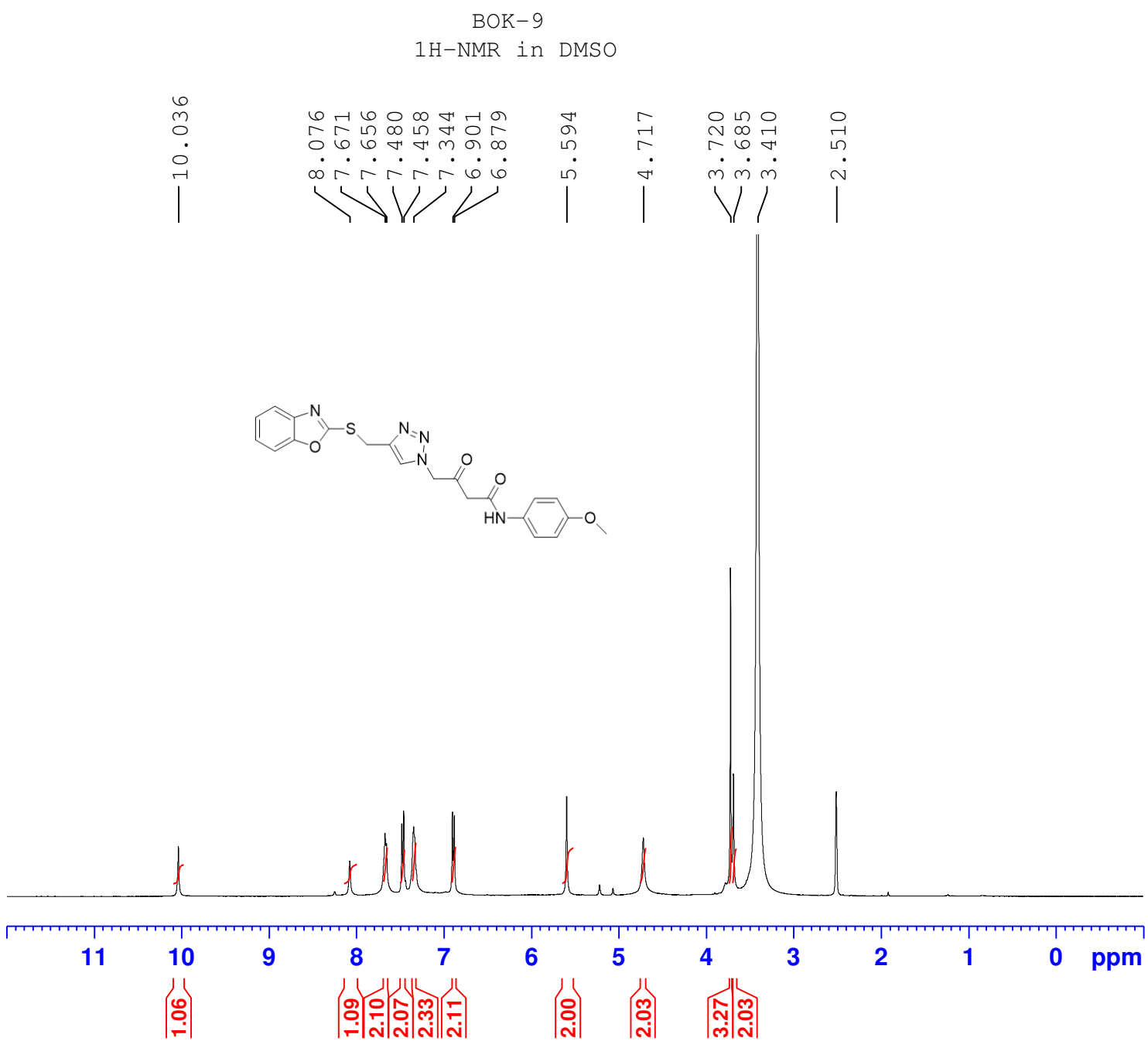
^{13}C NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-bromophenyl)-3-oxo butanamide **3h (BOK-8)**.

```
Current Data Parameters
NAME      23000509-BO-4Br
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230522
Time               14.40 h
INSTRUM            spect
PROBHD   Z108618_0984 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ             1.2582912 sec
RG                202.84
DW                19.200 usec
DE                 6.50 usec
TE                298.8 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6680954 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         51.02600098 W
SFO2        400.3116012 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         11.28999996 W
PLW12         0.27318001 W
PLW13         0.13741000 W

F2 - Processing parameters
SI                32768
SF          100.6580296 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```



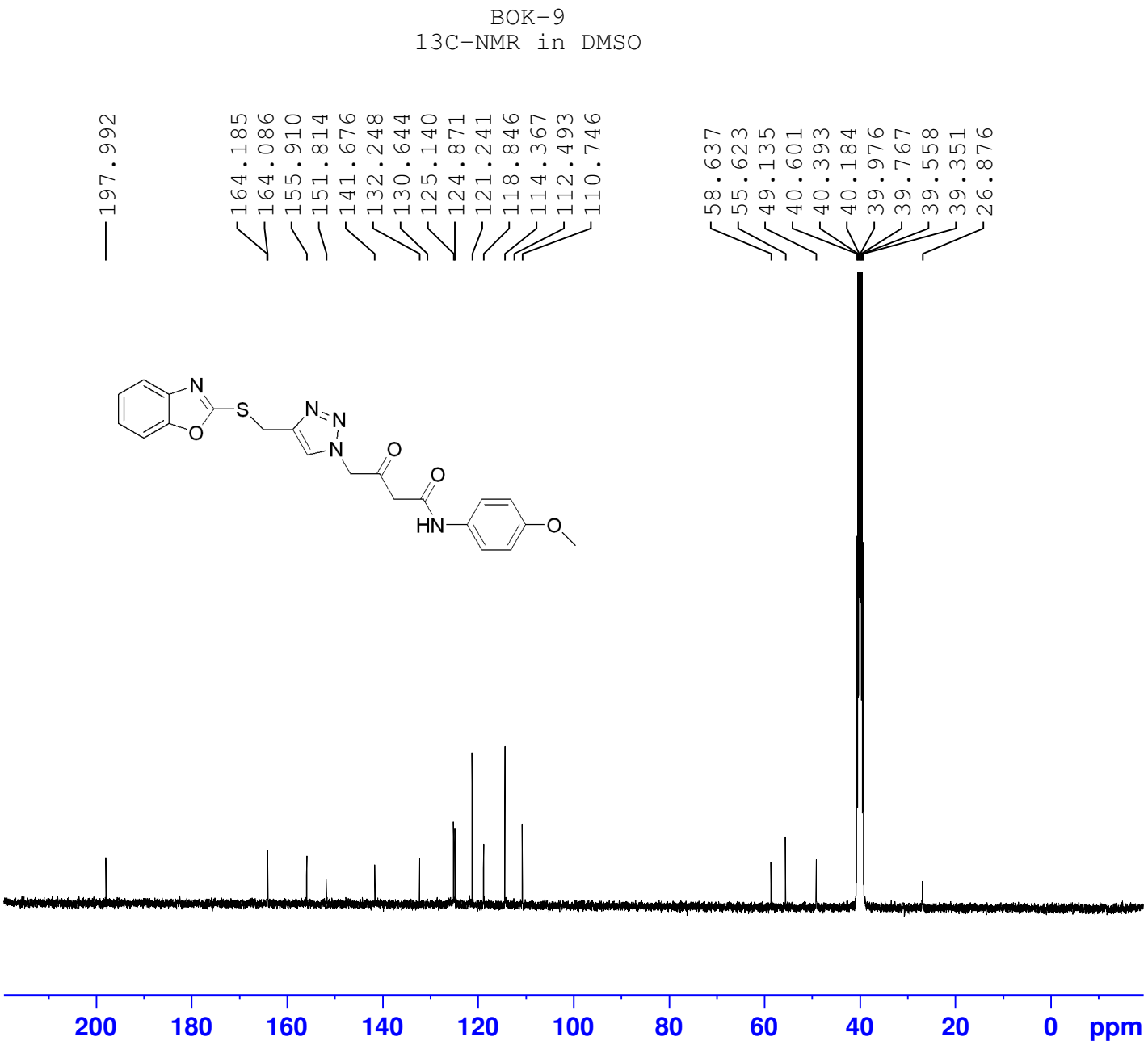
Mass spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-bromophenyl)-3-oxo butanamide **3h (BOK-8)**.

COMPOUND 3i (BOK-9) SPECTRAL DATA



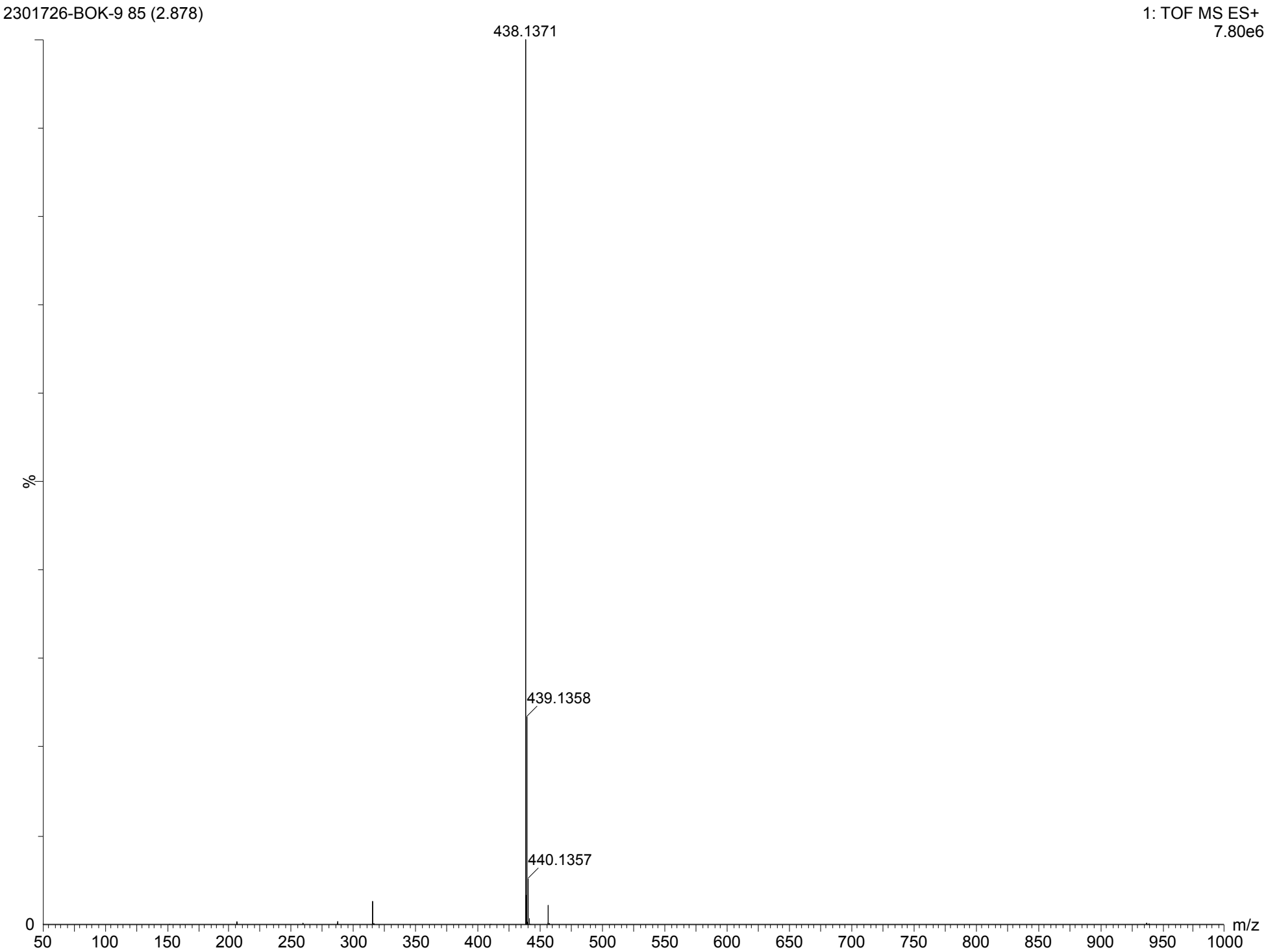

```
Current Data Parameters
NAME      23000782-BO-4OCH3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230801
Time                 5.57 h
INSTRUM              spect
PROBHD    Z108618_0984 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  114.18
DW                  62.400 usec
DE                  17.09 usec
TE                  296.9 K
D1            1.00000000 sec
TD0                     1
SFO1         400.3124719 MHz
NUC1                   1H
P0                  4.67 usec
P1                 14.00 usec
PLW1         11.28999996 W

F2 - Processing parameters
SI                  65536
SF           400.3100000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

^{1}H NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-methoxyphenyl)-3-oxo butanamide **3i (BOK-9)**.




```
Current Data Parameters
NAME      23000782-BO-4OCH3
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230801
Time                 6.40 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                297.9 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6680954 MHz
NUC1                 13C
P0                  3.33 usec
P1                 10.00 usec
PLW1          51.02600098 W
SFO2          400.3116012 MHz
NUC2                 1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2          11.28999996 W
PLW12          0.27318001 W
PLW13          0.13741000 W

F2 - Processing parameters
SI                  32768
SF            100.6580296 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

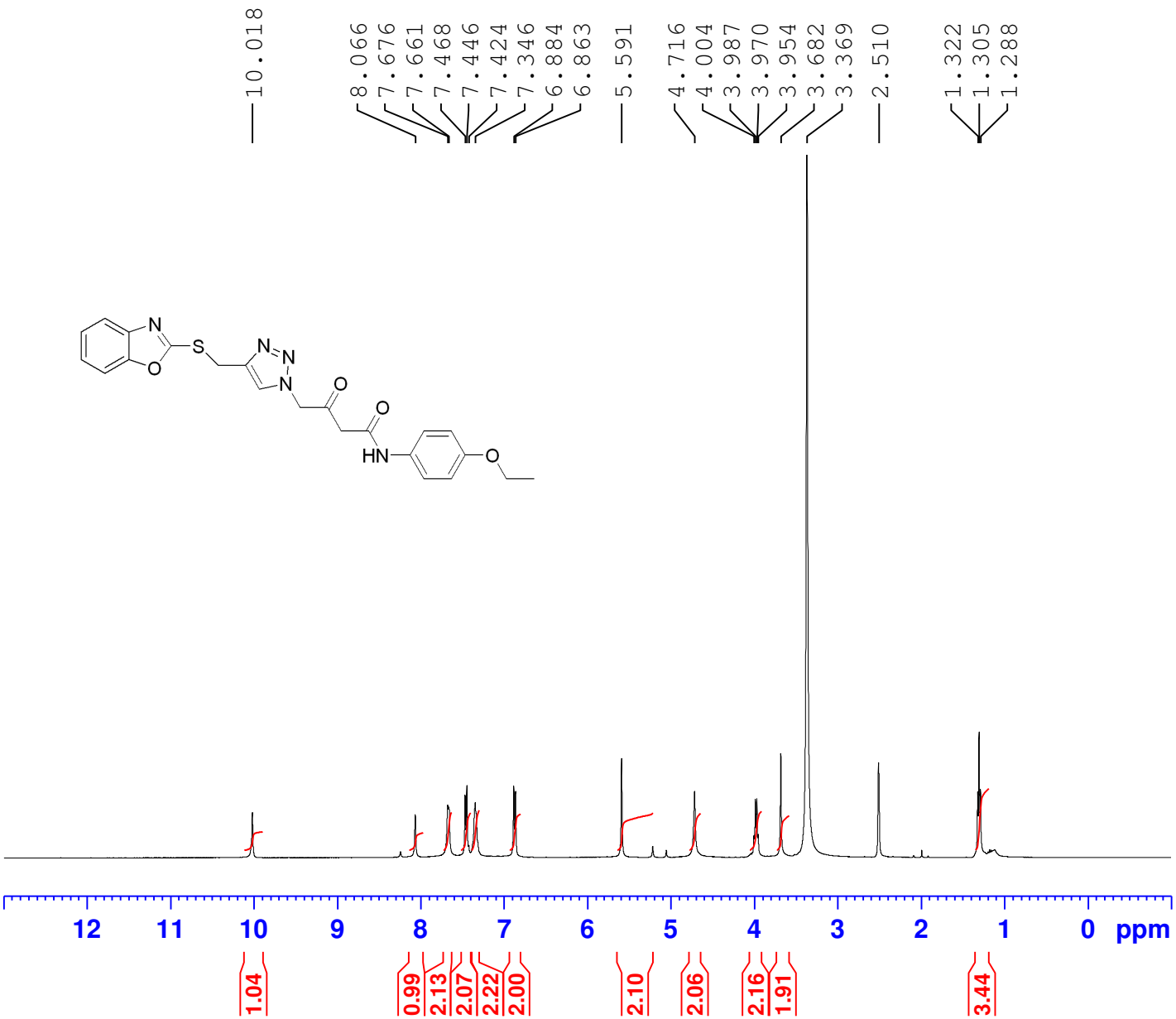
^{13}C NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-methoxyphenyl)-3-oxo butanamide **3i (BOK-9)**.



Mass spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-methoxyphenyl)-3-oxo butanamide **3i (BOK-9)**.

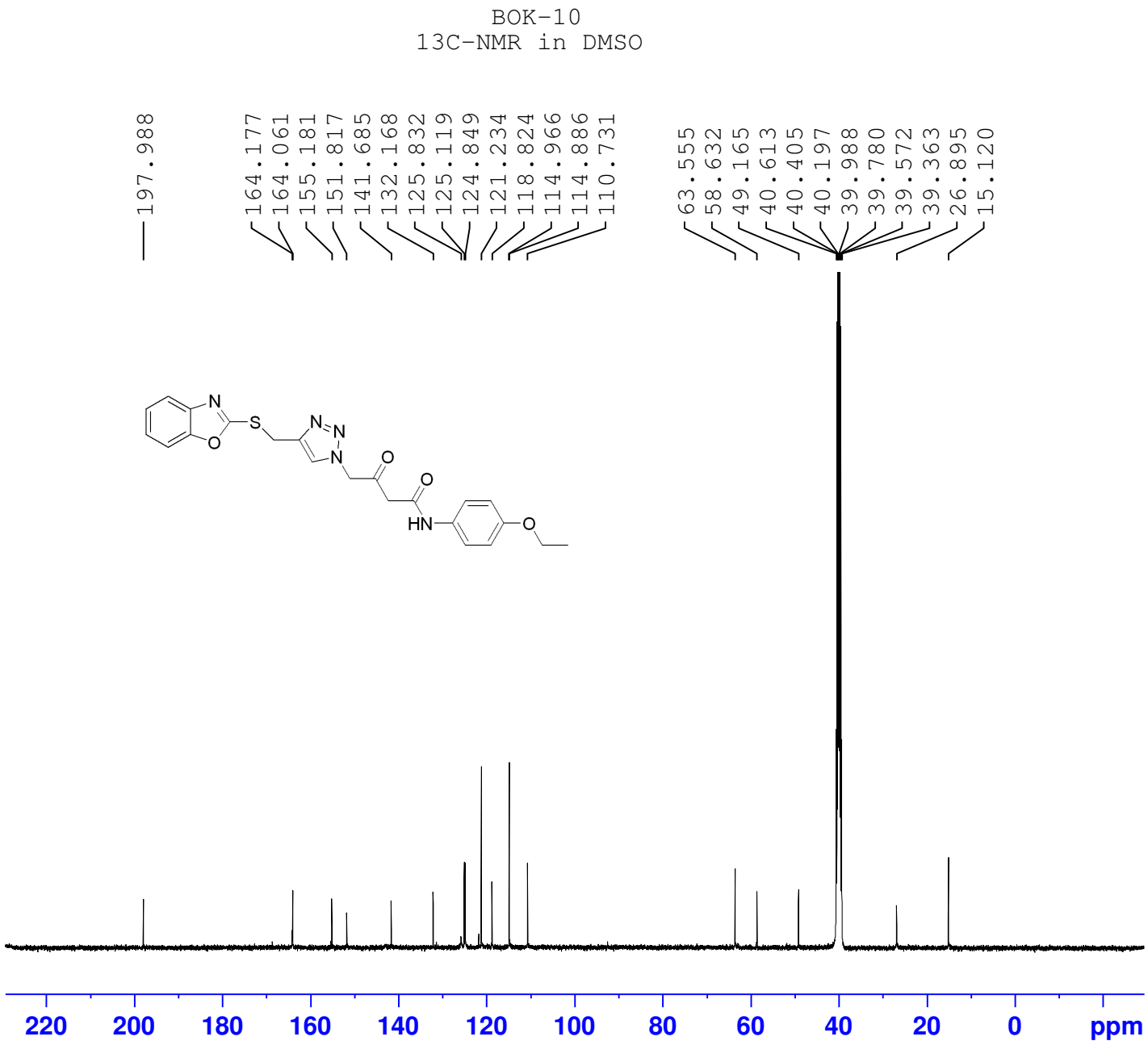
COMPOUND 3j (BOK-10) SPECTRAL DATA

BOK-10
1H-NMR in DMSO



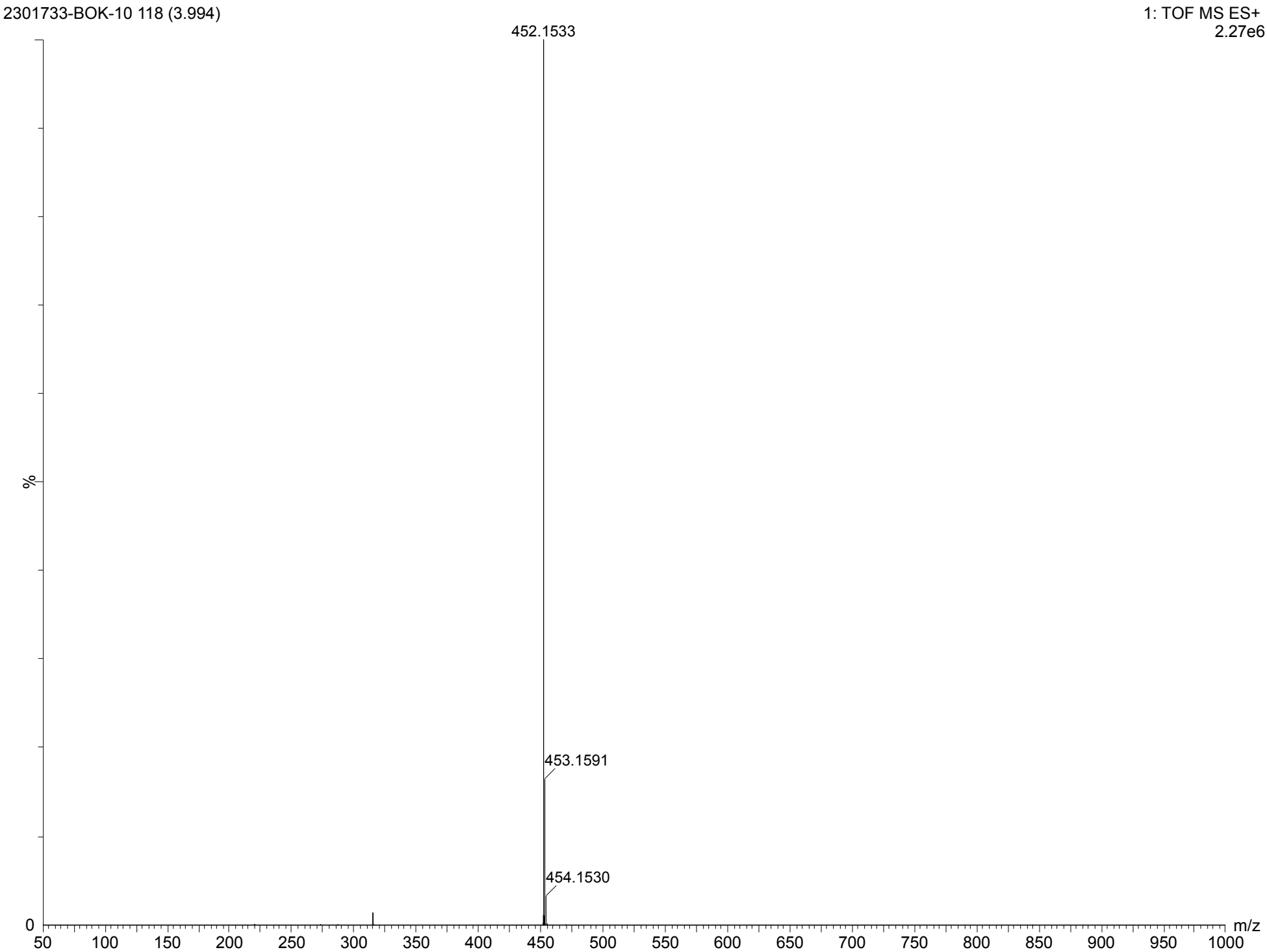

```
Current Data Parameters
NAME      23000512-Bo-4EO
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20230520
Time               10.54 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     32
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  32.13
DW                 62.400 usec
DE                 17.09 usec
TE                 297.5 K
D1              1.00000000 sec
TD0                     1
SFO1          400.3124719 MHz
NUC1                   1H
P0                  4.67 usec
P1                 14.00 usec
PLW1          11.28999996 W

F2 - Processing parameters
SI                  65536
SF            400.3100000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

[1]H NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-ethoxyphenyl)-3-oxo butanamide **3j (BOK-10)**




```
Current Data Parameters
NAME      23000512-Bo-4EO
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230522
Time              10.24 h
INSTRUM             spect
PROBHD   Z108618_0984 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ             1.2582912 sec
RG                202.84
DW                19.200 usec
DE                 6.50 usec
TE                298.8 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6680954 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         51.02600098 W
SFO2         400.3116012 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         11.28999996 W
PLW12         0.27318001 W
PLW13         0.13741000 W

F2 - Processing parameters
SI                32768
SF           100.6580296 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

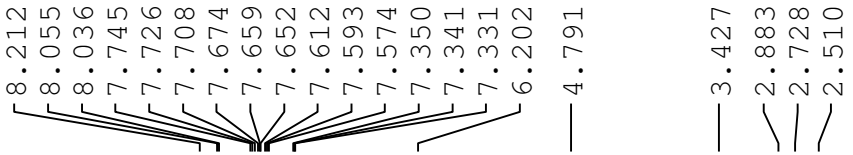
^{13}C NMR spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-ethoxyphenyl)-3-oxo butanamide **3j (BOK-10)**.

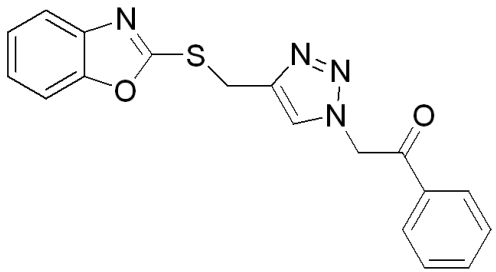


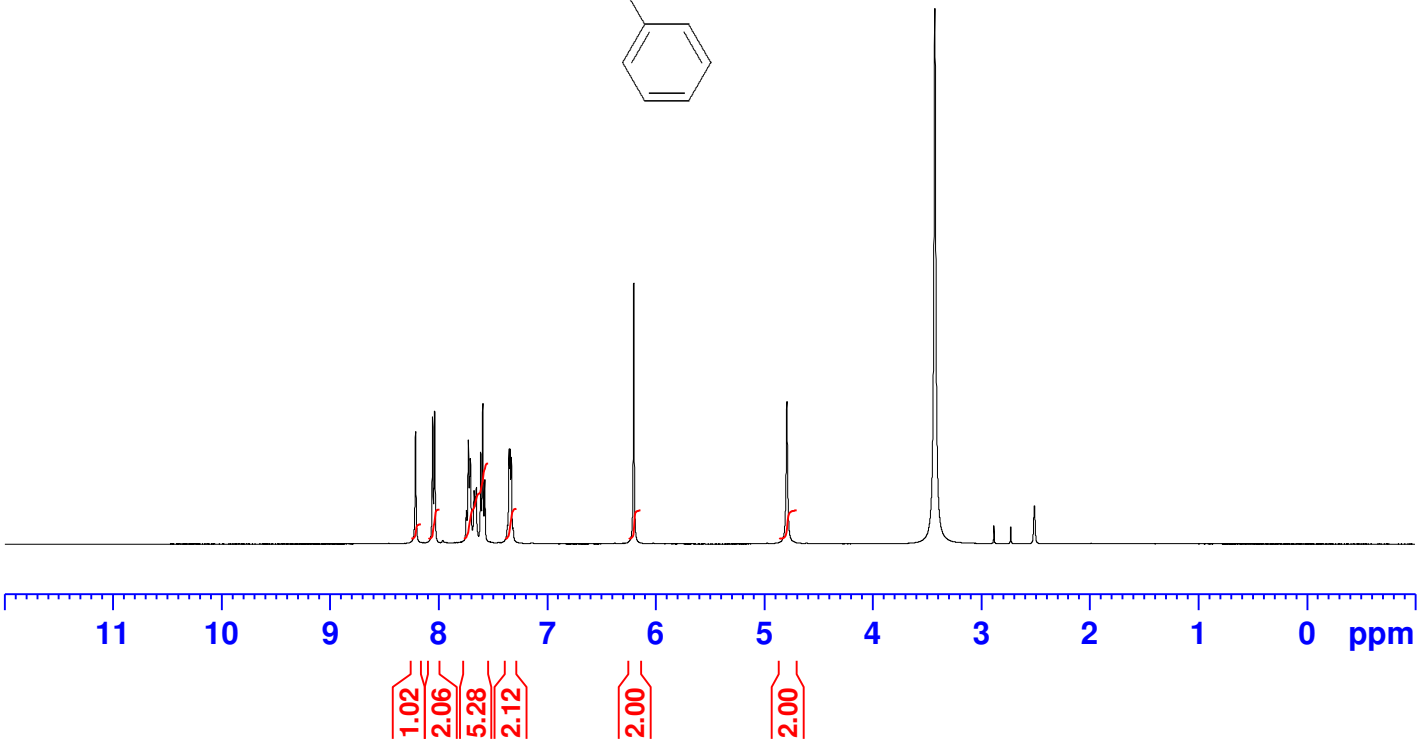
Mass spectrum of 4-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-ethoxyphenyl)-3-oxo butanamide **3j (BOK-10)**.

COMPOUND 3k (BOP-1) SPECTRAL DATA

BOP-1
1H-NMR in DMSO





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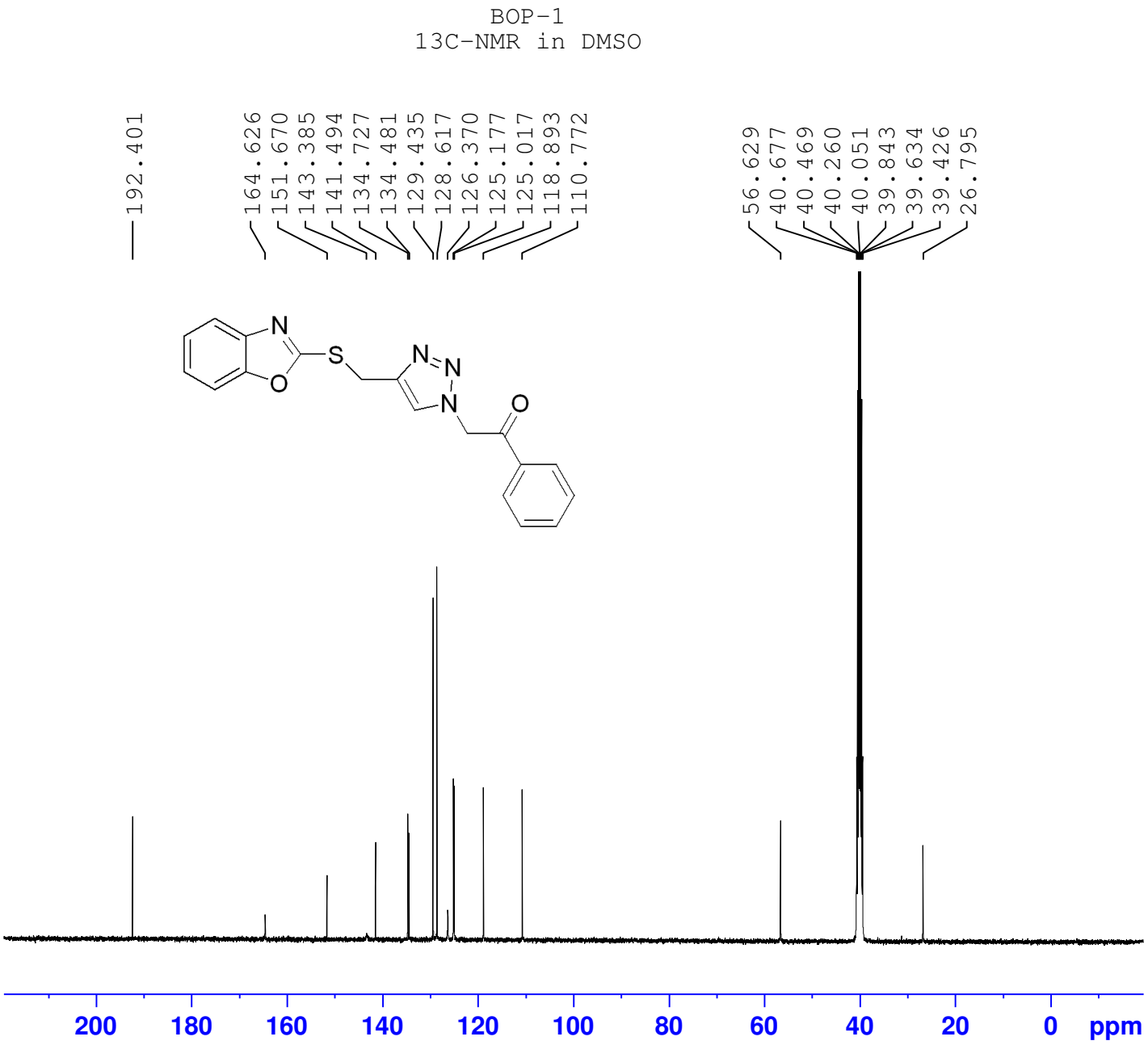
Current Data Parameters
NAME      23000787-Ph-BO
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230801
Time                9.19 h
INSTRUM            spect
PROBHD   Z108618_0984 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                 80.45
DW                62.400 usec
DE                17.09 usec
TE                297.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.3124719 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         11.28999996 W

F2 - Processing parameters
SI                 65536
SF           400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

[1]H NMR spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-phenylethan-1-one 3k (BOP-1).

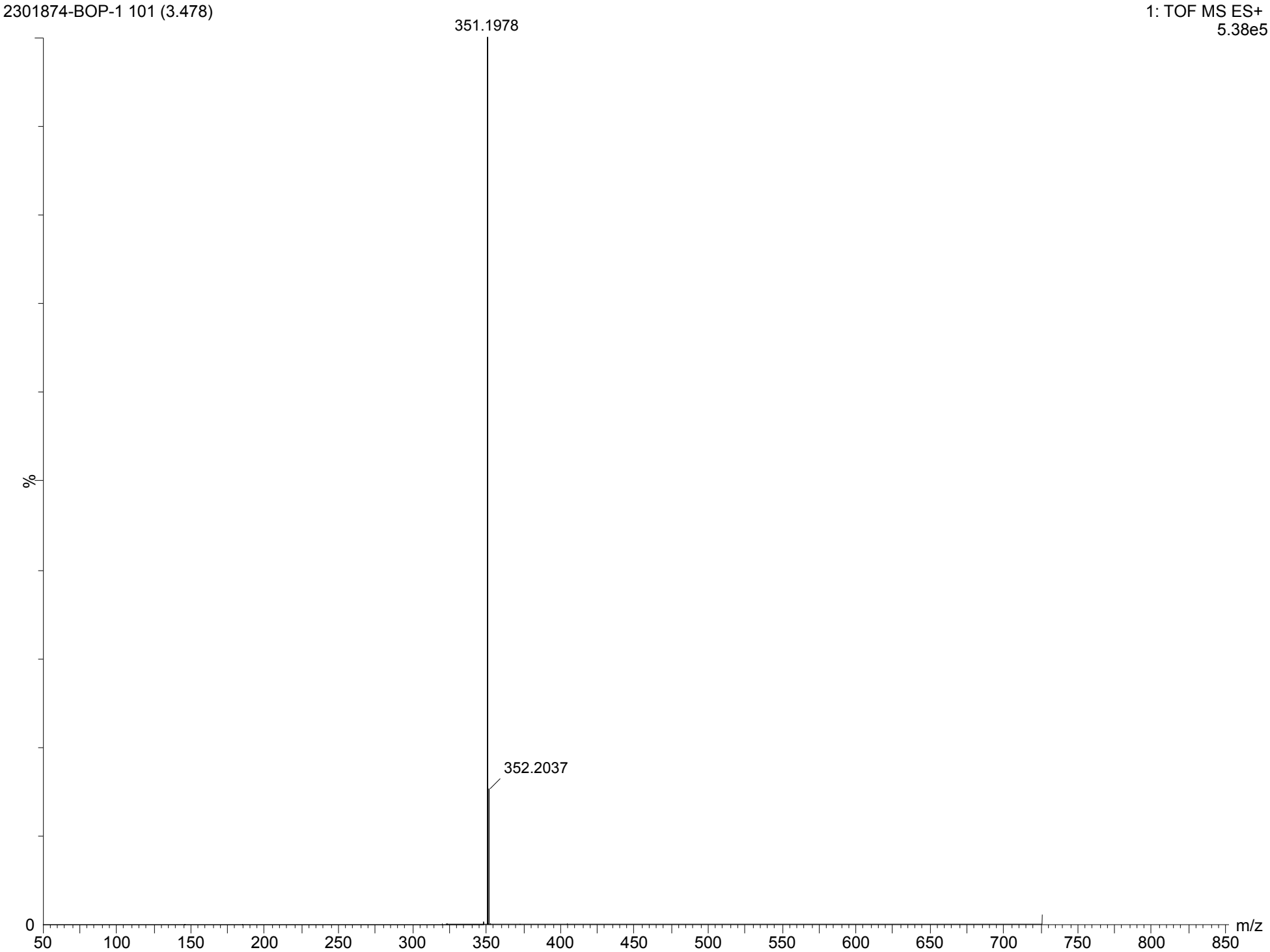



```
Current Data Parameters
NAME      23000787-Ph-BO
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230801
Time              10.02 h
INSTRUM            spect
PROBHD   Z108618_0984 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.50 usec
TE               297.2 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6680954 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1         51.02600098 W
SFO2        400.3116012 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            90.00 usec
PLW2         11.28999996 W
PLW12         0.27318001 W
PLW13         0.13741000 W

F2 - Processing parameters
SI                 32768
SF          100.6580296 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

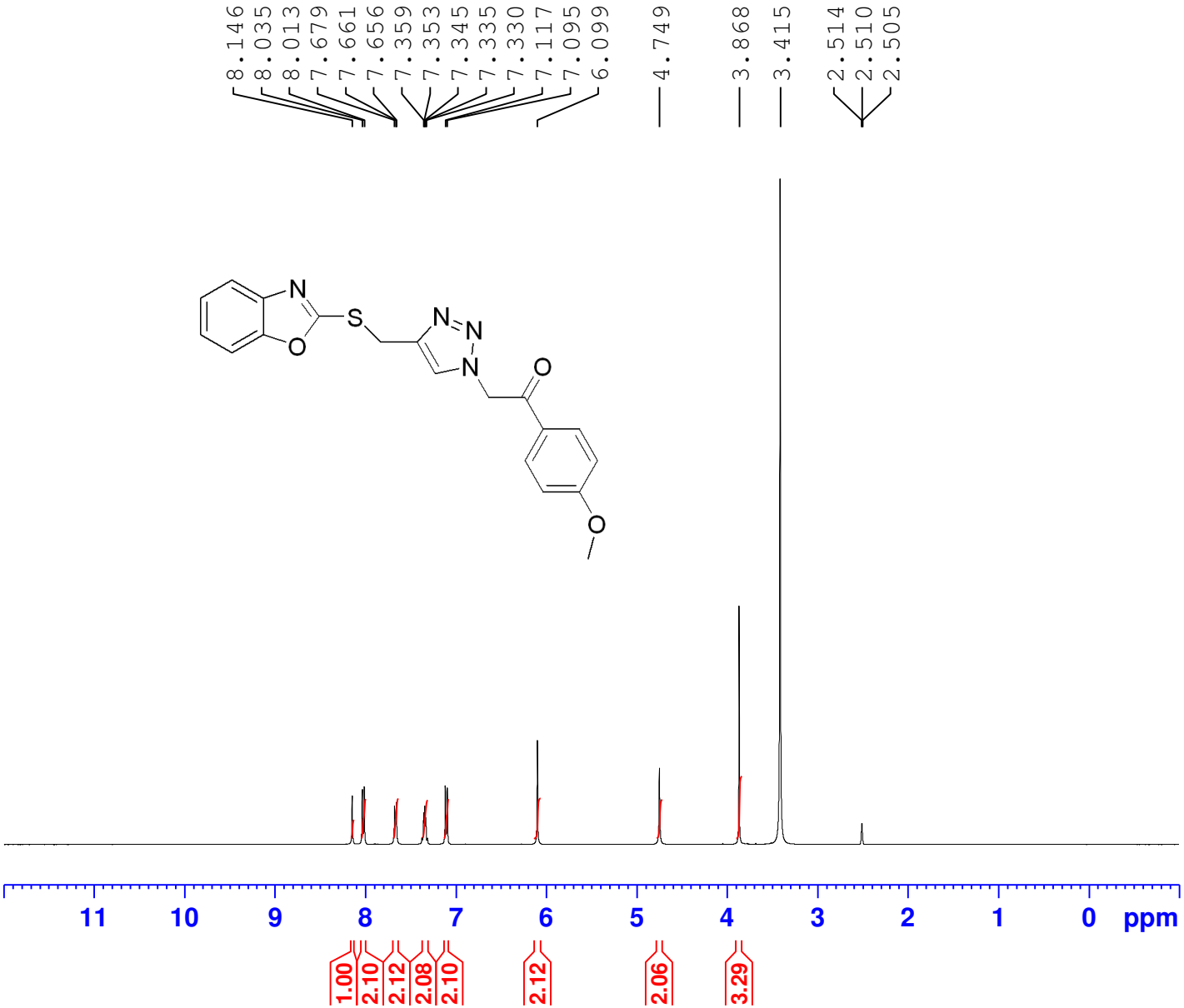
^{13}C NMR spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-phenylethan-1-one **3k (BOP-1).**



Mass spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-phenylethan-1-one **3k (BOP-1)**.

COMPOUND 3l (BOP-2) SPECTRAL DATA

BOP-2
1H-NMR in DMSO

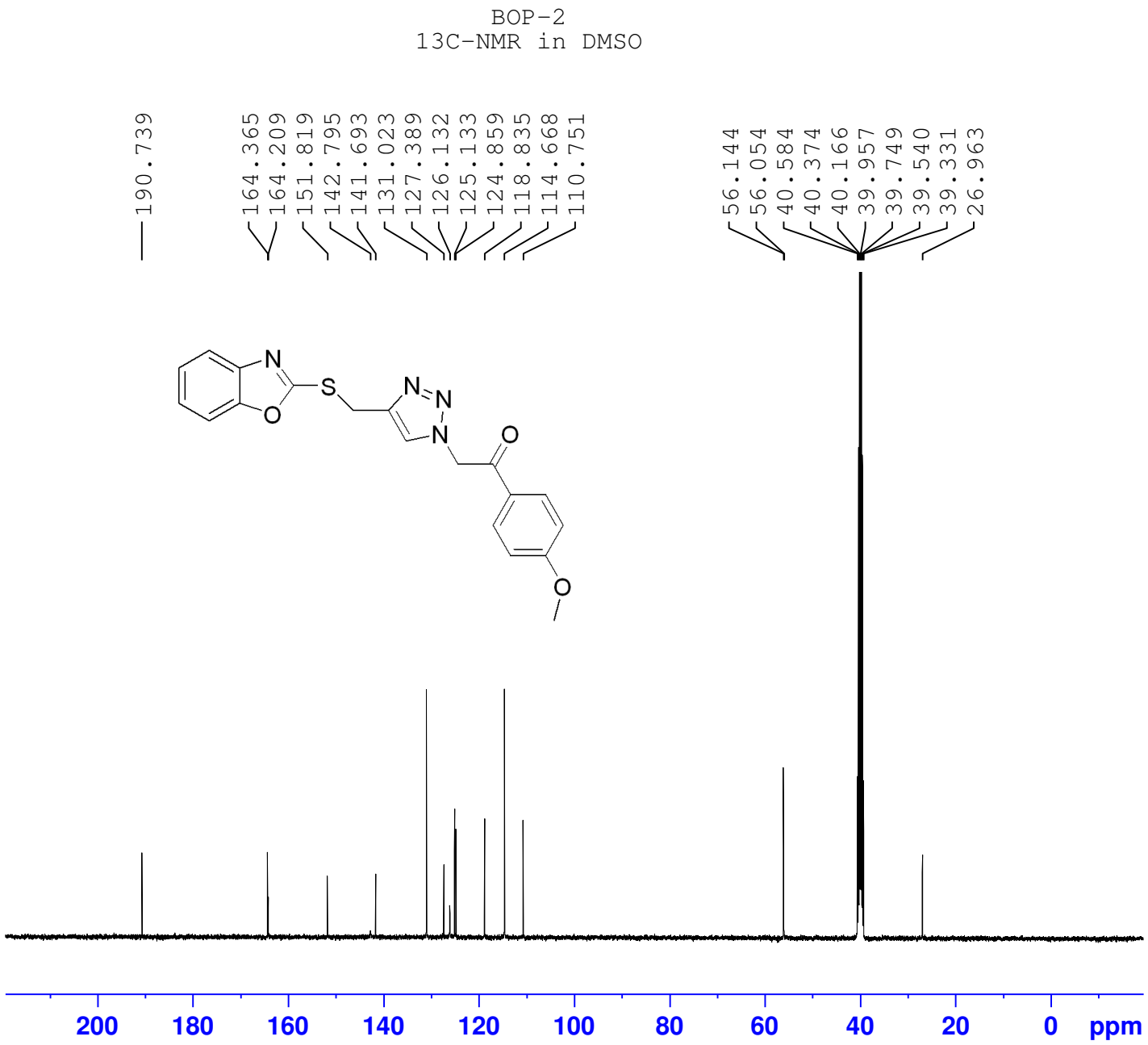



```
Current Data Parameters
NAME      23000789-4OCH3-PhBO
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20230801
Time                10.32 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  89.93
DW                 62.400 usec
DE                 17.09 usec
TE                 297.2 K
D1              1.00000000 sec
TD0                     1
SFO1          400.3124719 MHz
NUC1                   1H
P0                  4.67 usec
P1                 14.00 usec
PLW1          11.28999996 W

F2 - Processing parameters
SI                  65536
SF            400.3100000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

[1]H NMR spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(4-methoxyphenyl)ethan-1-one **3l (BOP-2)**

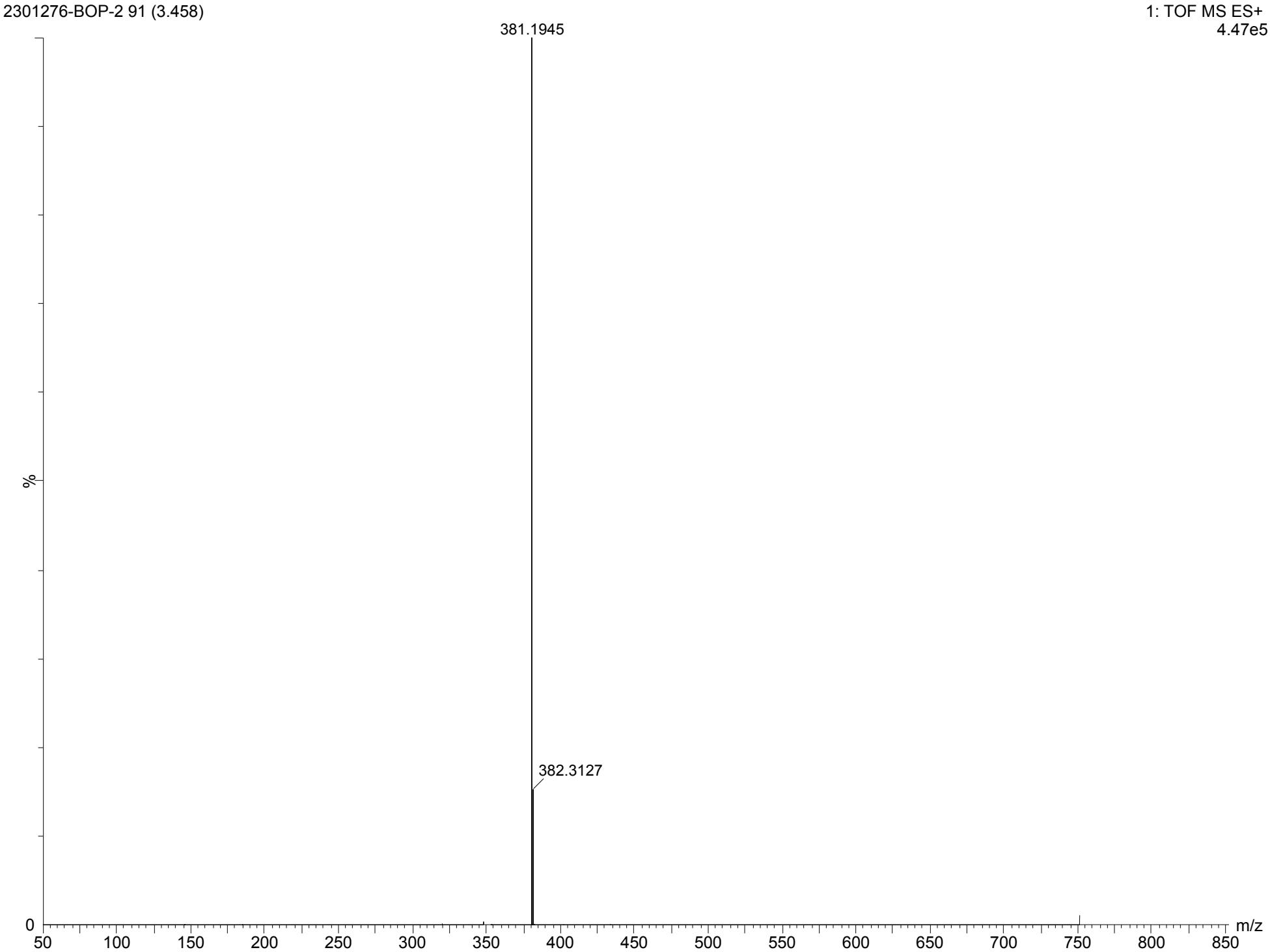



```
Current Data Parameters
NAME      23000789-4OCH3-PhBO
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_            20230801
Time                11.16 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                298.5 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6680954 MHz
NUC1                 13C
P0                  3.33 usec
P1                 10.00 usec
PLW1          51.02600098 W
SFO2          400.3116012 MHz
NUC2                 1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2          11.28999996 W
PLW12          0.27318001 W
PLW13          0.13741000 W

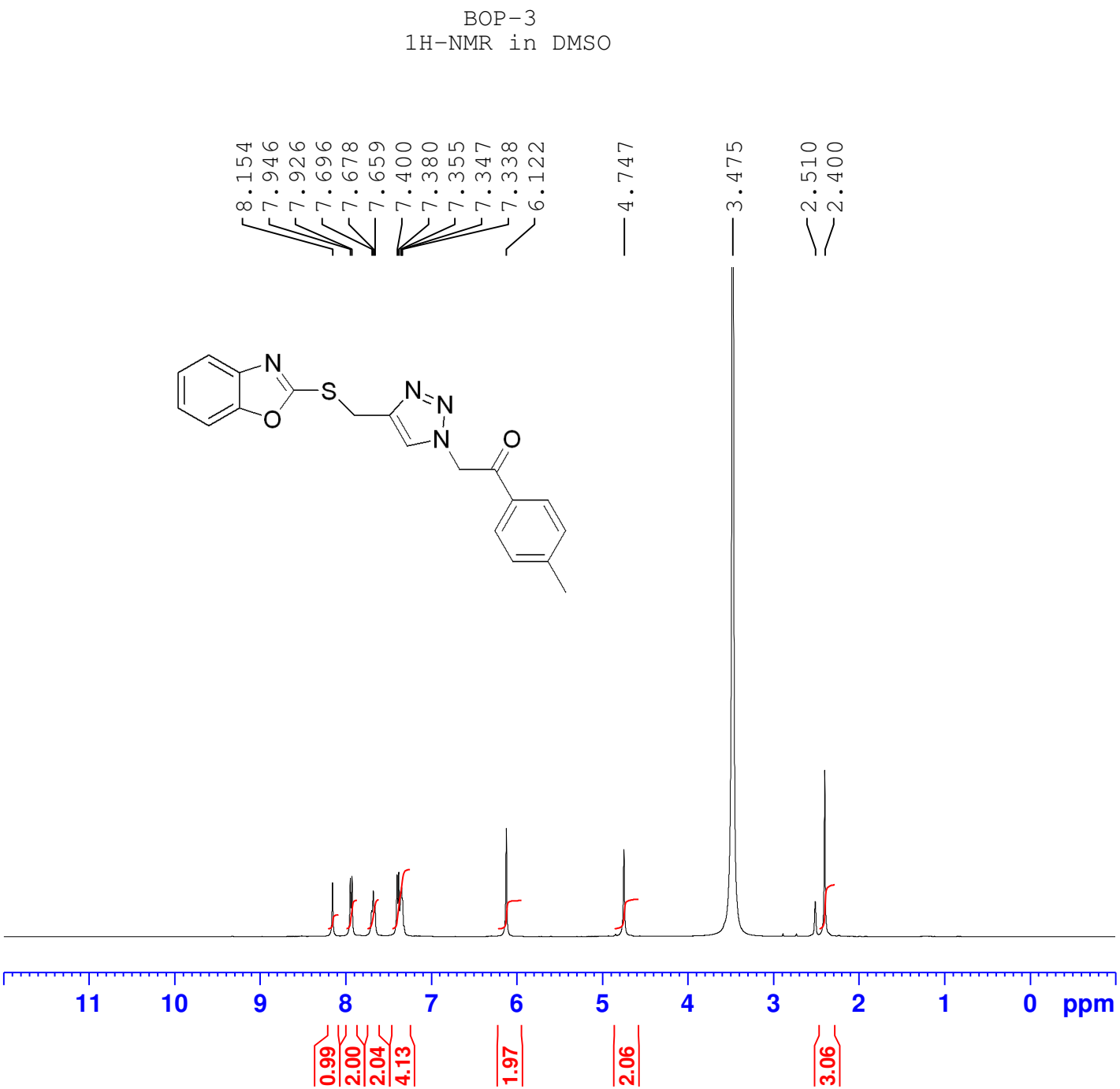
F2 - Processing parameters
SI                 32768
SF            100.6580296 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

^{13}C NMR spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(4-methoxyphenyl)ethan-1-one **3l (BOP-2)**



Mass spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(4-methoxyphenyl)ethan-1-one **3l (BOP-2).**

COMPOUND 3m (BOP-3) SPECTRAL DATA

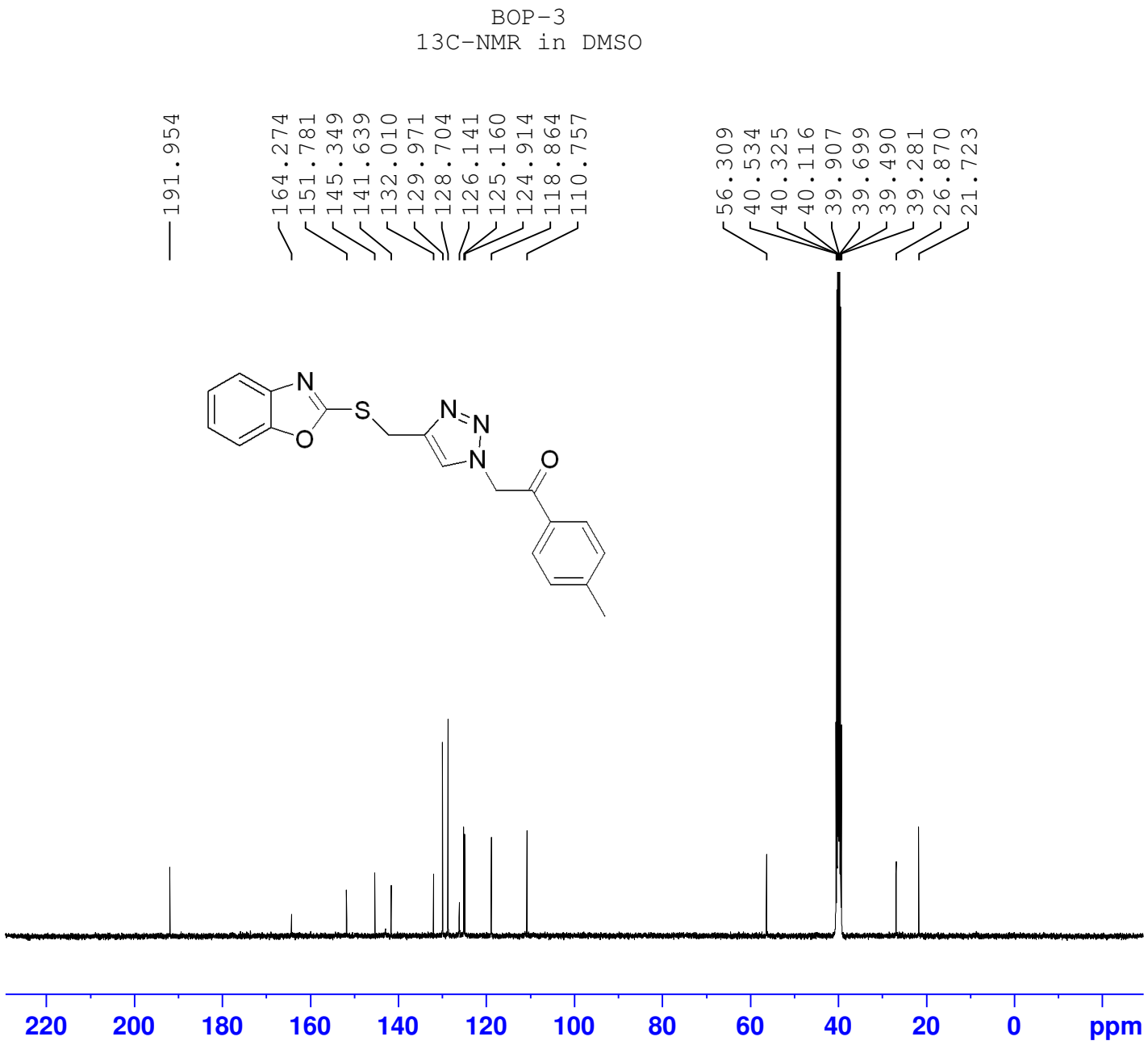



```
Current Data Parameters
NAME      23000622-4CH3-PhBo
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20230628
Time                11.27 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     32
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                  32.13
DW                62.400 usec
DE                17.09 usec
TE                297.5 K
D1             1.00000000 sec
TD0                     1
SFO1          400.3124719 MHz
NUC1                   1H
P0                 4.67 usec
P1                14.00 usec
PLW1          11.28999996 W

F2 - Processing parameters
SI                  65536
SF            400.3100000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

^{1}H NMR spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(p-tolyl)ethan-1-one **3m (BOP-3).**

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Current Data Parameters
NAME      23000622-4CH3-PhBo
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20230628
Time              12.11 h
INSTRUM             spect
PROBHD   Z108618_0984 (
PULPROG           zgpg30
TD                65536
SOLVENT             DMSO
NS                  1128
DS                     4
SWH           26041.666 Hz
FIDRES         0.794729 Hz
AQ             1.2582912 sec
RG                202.84
DW                19.200 usec
DE                 6.50 usec
TE                298.6 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1        100.6680954 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         51.02600098 W
SFO2        400.3116012 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         11.28999996 W
PLW12         0.27318001 W
PLW13         0.13741000 W

F2 - Processing parameters
SI                 32768
SF          100.6580296 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```
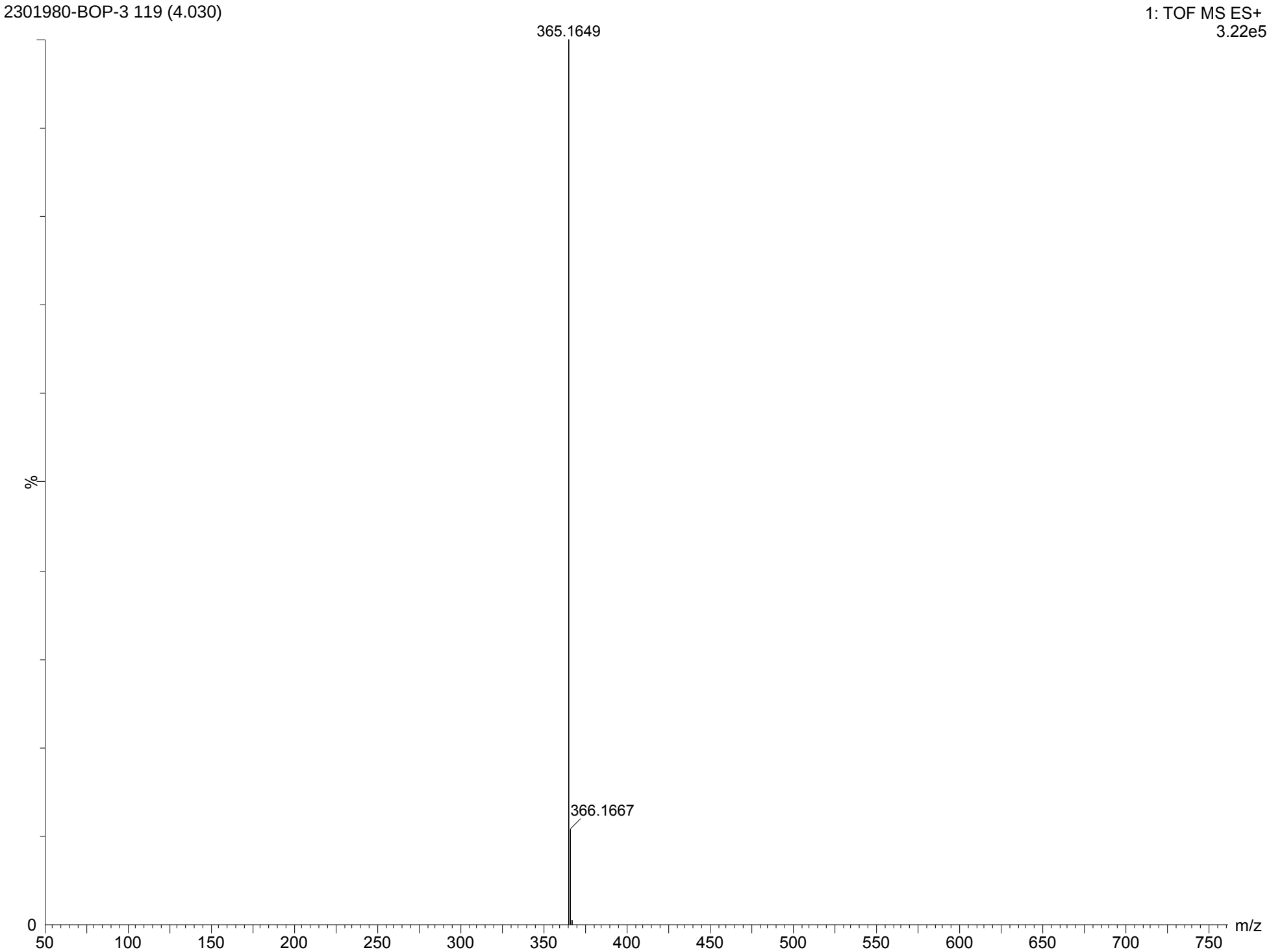
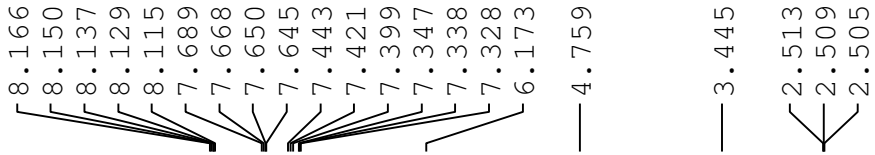

^{13}C NMR spectrum of2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(p-tolyl)ethan-1-one **3m (BOP-3).**

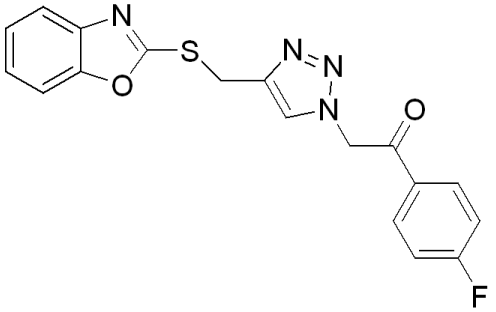


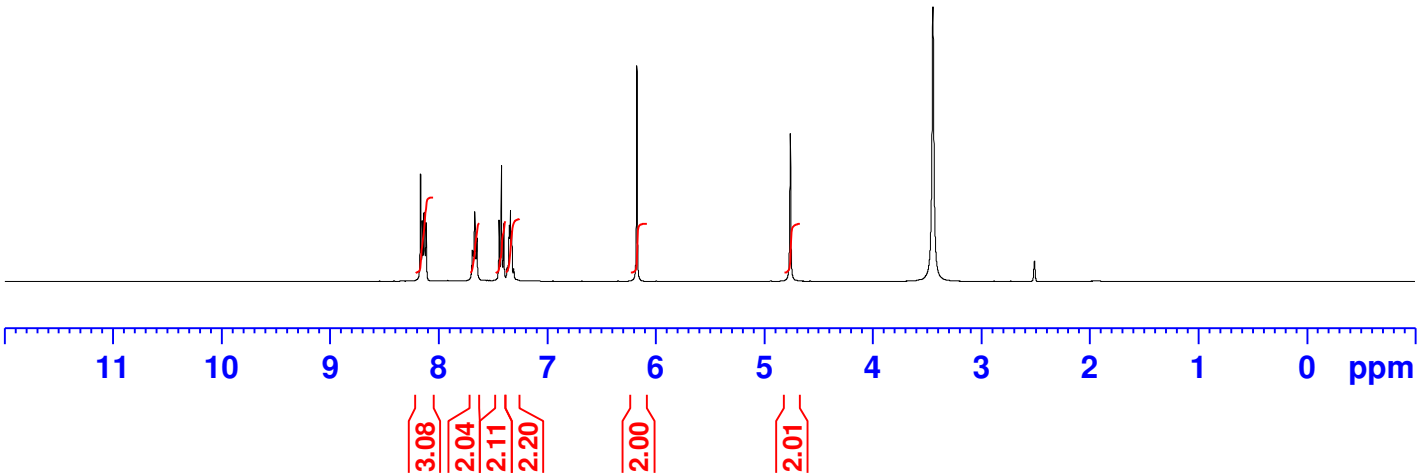
Mass spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(p-tolyl)ethan-1-one **3m (BOP-3)**

COMPOUND 3n (BOP-4) SPECTRAL DATA

BOP-4
1H-NMR in DMSO





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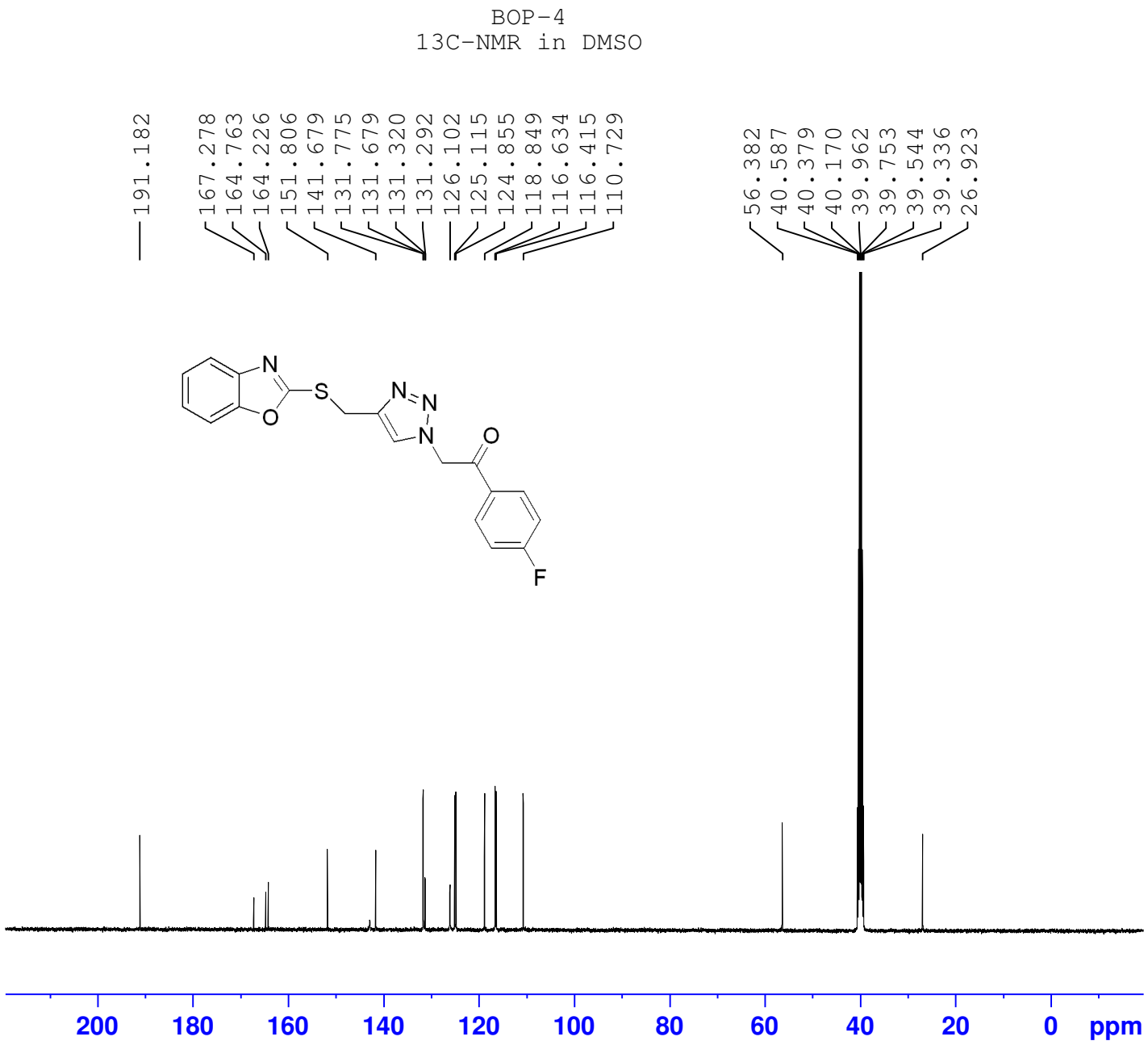
Current Data Parameters
NAME      23000788-4F-Ph-BO
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230801
Time                10.06 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES            0.244532 Hz
AQ                4.0894465 sec
RG                    73.11
DW                  62.400 usec
DE                  17.09 usec
TE                  297.2 K
D1              1.00000000 sec
TD0                     1
SFO1           400.3124719 MHz
NUC1                   1H
P0                   4.67 usec
P1                  14.00 usec
PLW1           11.28999996 W

F2 - Processing parameters
SI                  65536
SF             400.3100000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

^{1}H NMR spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(4-fluorophenyl)ethan-1-one **3n (BOP-4).**

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Current Data Parameters
NAME      23000788-4F-Ph-BO
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230801
Time                10.28 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   512
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                298.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        100.6680954 MHz
NUC1                 13C
P0                 3.33 usec
P1                10.00 usec
PLW1         51.02600098 W
SFO2         400.3116012 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         11.28999996 W
PLW12         0.27318001 W
PLW13         0.13741000 W

F2 - Processing parameters
SI                 32768
SF          100.6580296 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```
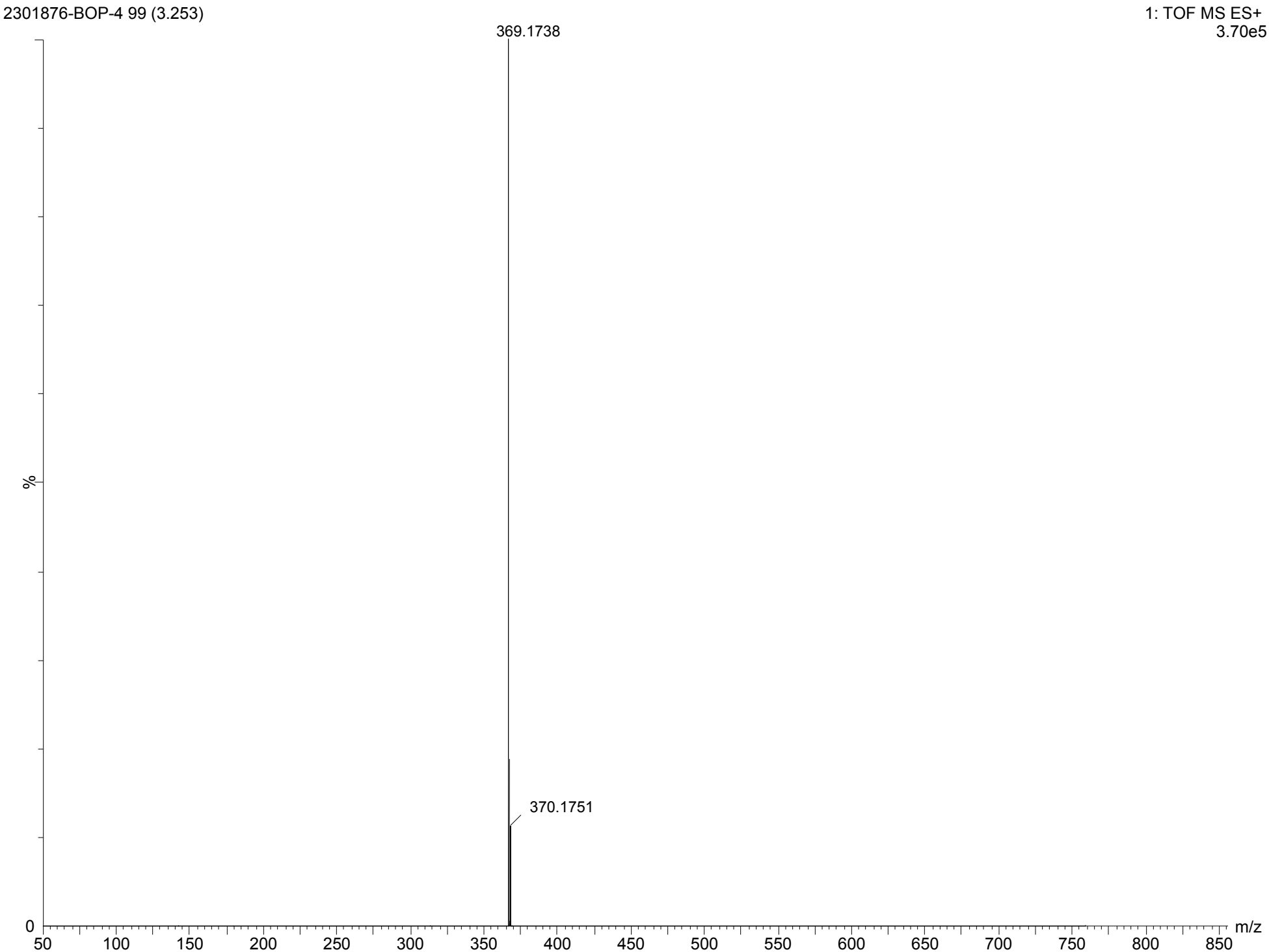
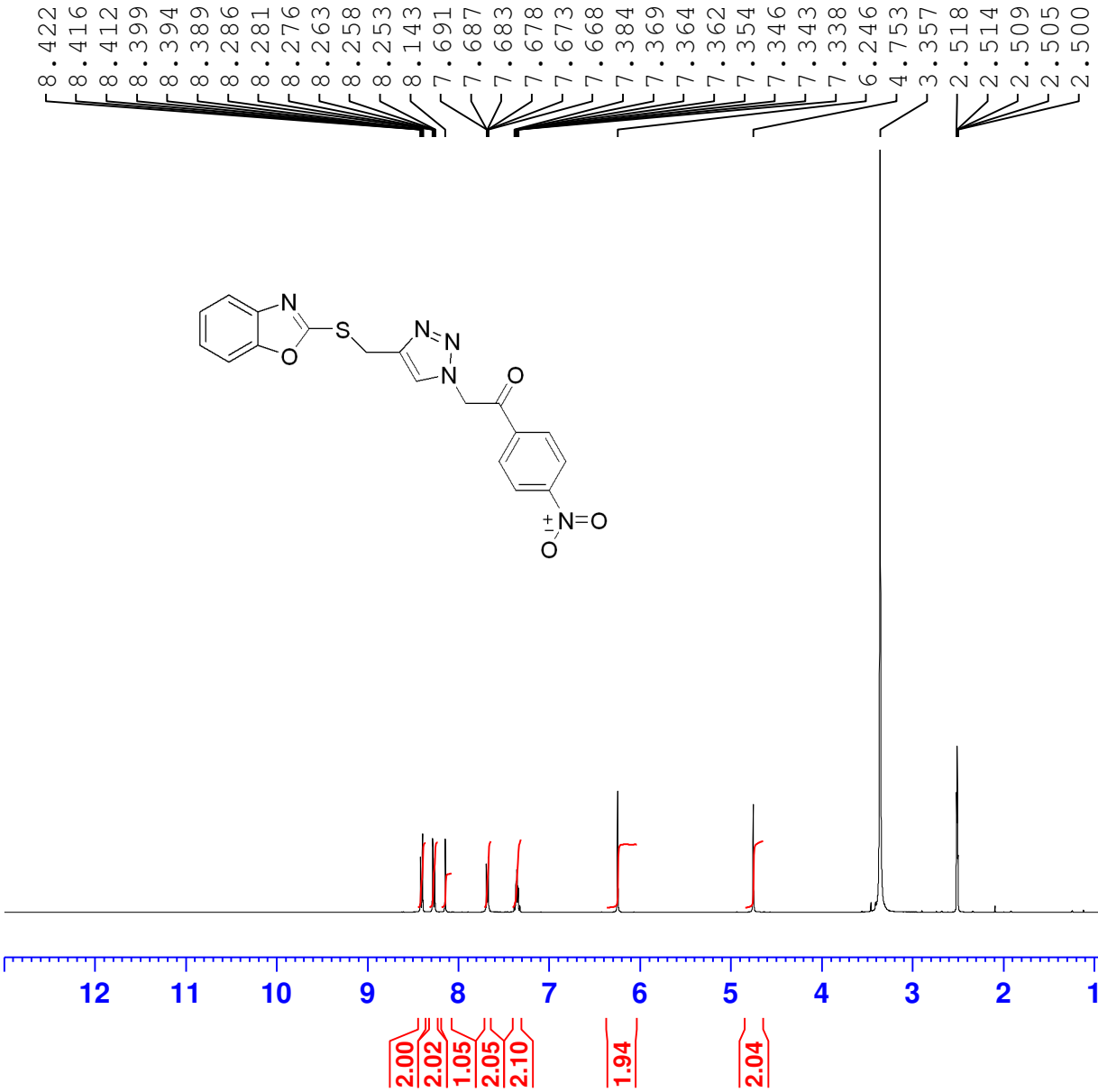

^{13}C NMR spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(4-fluorophenyl)ethan-1-one **3n (BOP-4)**.



Mass spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(4-fluorophenyl)ethan-1-one **3n (BOP-4)**.

COMPOUND 3o (BOP-5) SPECTRAL DATA

BOP-5
1H-NMR in DMSO

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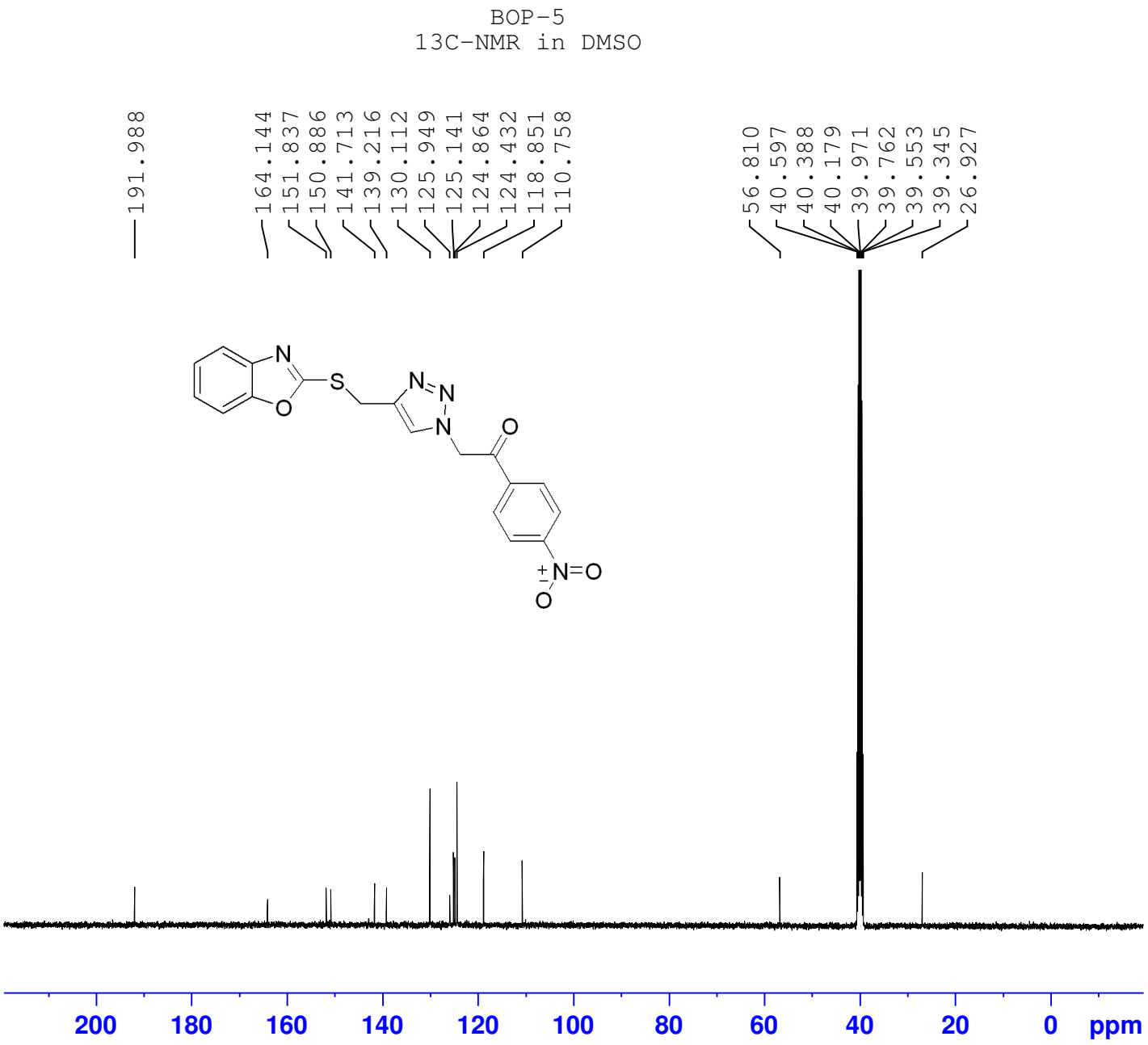
Current Data Parameters
NAME      23000514-4No2-PhBO
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20230520
Time                 11.02 h
INSTRUM              spect
PROBHD    Z108618_0984 (
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      32
DS                       2
SWH               8012.820 Hz
FIDRES               0.244532 Hz
AQ                4.0894465 sec
RG                    32.13
DW                  62.400 usec
DE                  17.09 usec
TE                  297.5 K
D1             1.00000000 sec
TD0                      1
SFO1          400.3124719 MHz
NUC1                   1H
P0                   4.67 usec
P1                  14.00 usec
PLW1          11.28999996 W

F2 - Processing parameters
SI                   65536
SF            400.3100000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

^{1}H NMR spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(4-nitrophenyl)ethan-1-one **3o (BOP-5).**

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Current Data Parameters
NAME      23000514-4No2-PhBO
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_            20230522
Time                12.42 h
INSTRUM             spect
PROBHD    Z108618_0984 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   512
DS                     4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               1.3631488 sec
RG                 202.84
DW                 20.800 usec
DE                  6.50 usec
TE                 297.6 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1           100.6680954 MHz
NUC1                  13C
P0                  3.33 usec
P1                 10.00 usec
PLW1           51.02600098 W
SFO2           400.3116012 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2           11.28999996 W
PLW12           0.27318001 W
PLW13           0.13741000 W

F2 - Processing parameters
SI                 32768
SF             100.6580296 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```
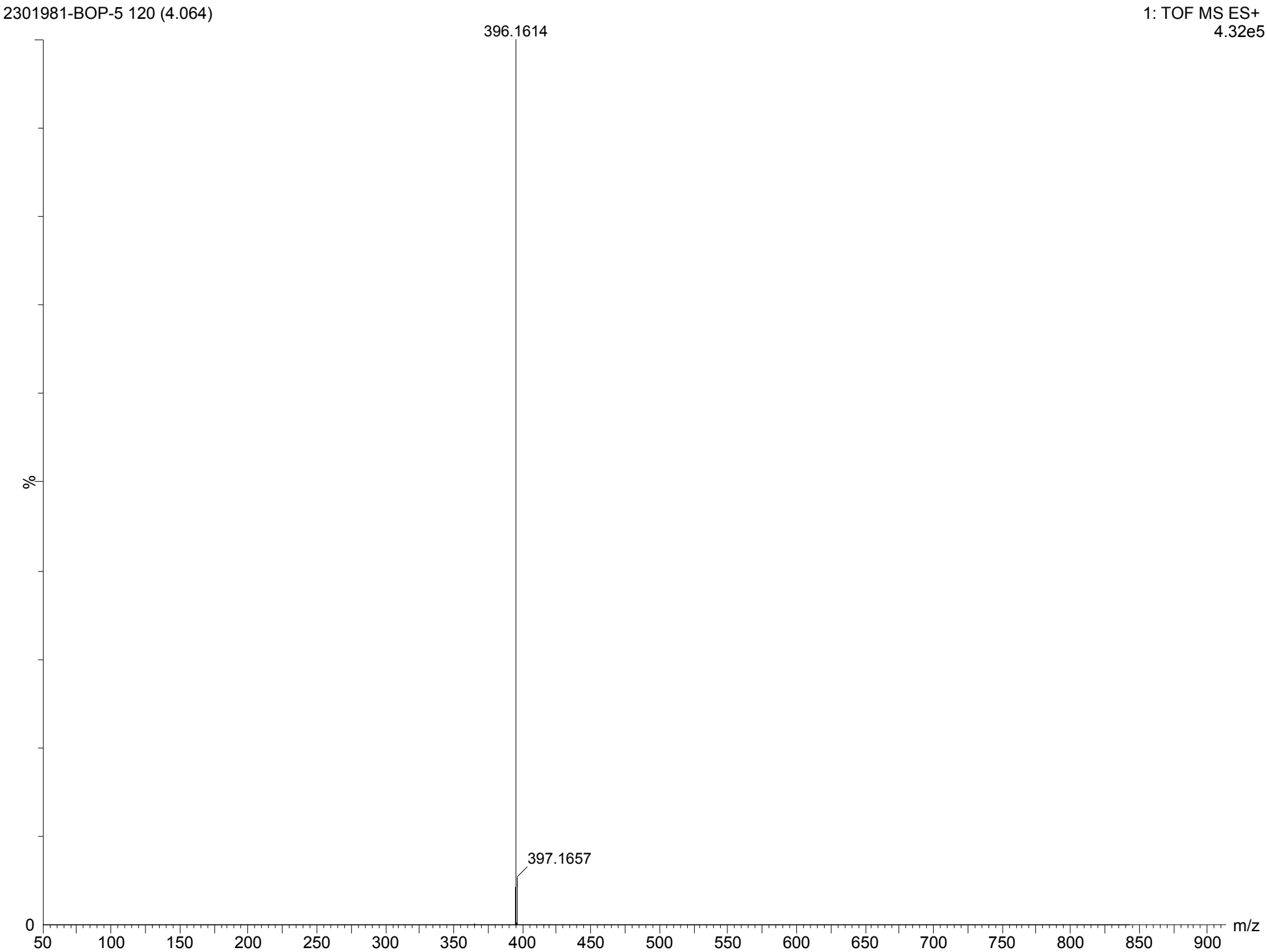

^{13}C NMR spectrum of2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(4-nitrophenyl)ethan-1-one **3o (BOP-5).**



Mass spectrum of 2-(4-((benzo[d]oxazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-1-(4-nitrophenyl)ethan-1-one **3o (BOP-5).**

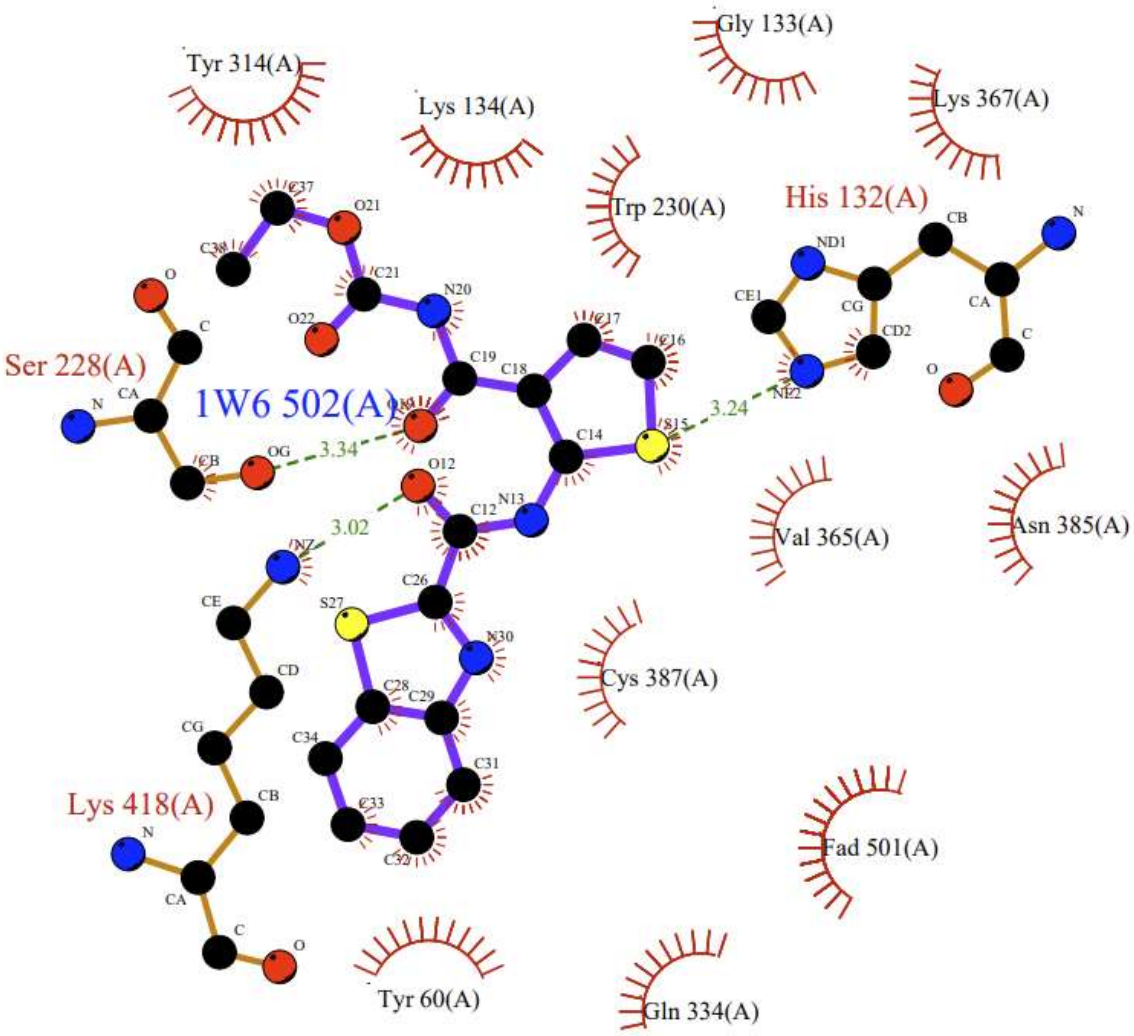


Fig. S46. DprE1 protein binding sheet for TCA-1

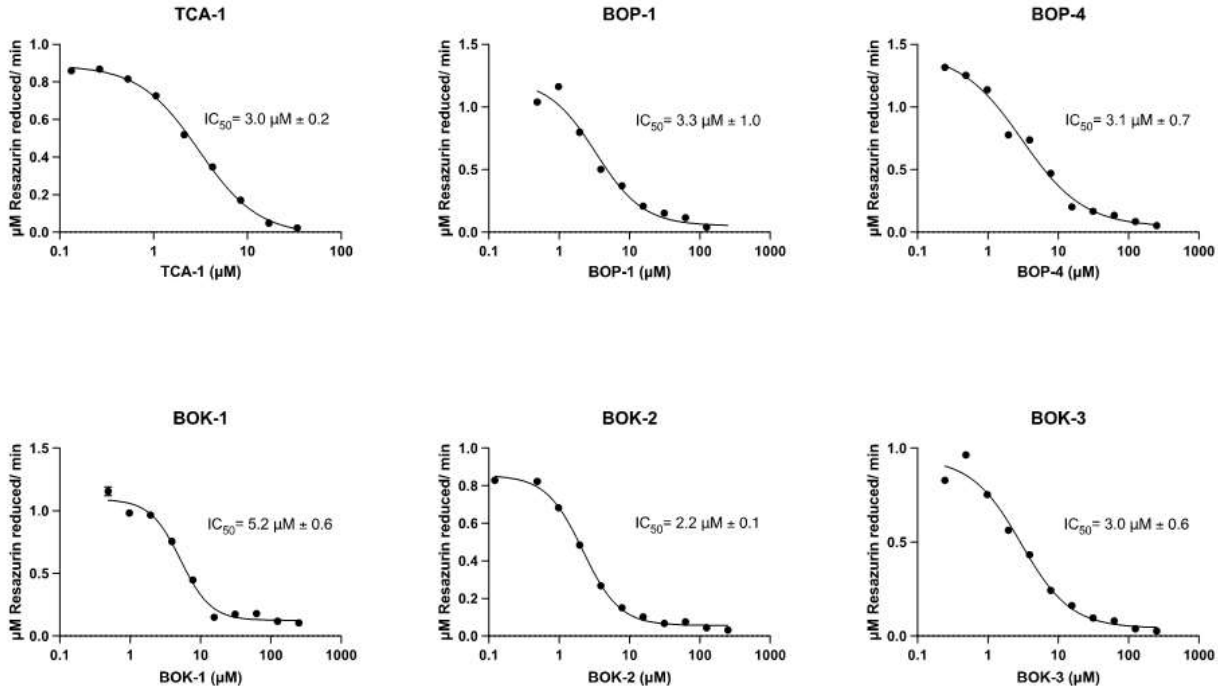


Fig. S47. Concentration response graph of DprE1 inhibition fluorometric assay

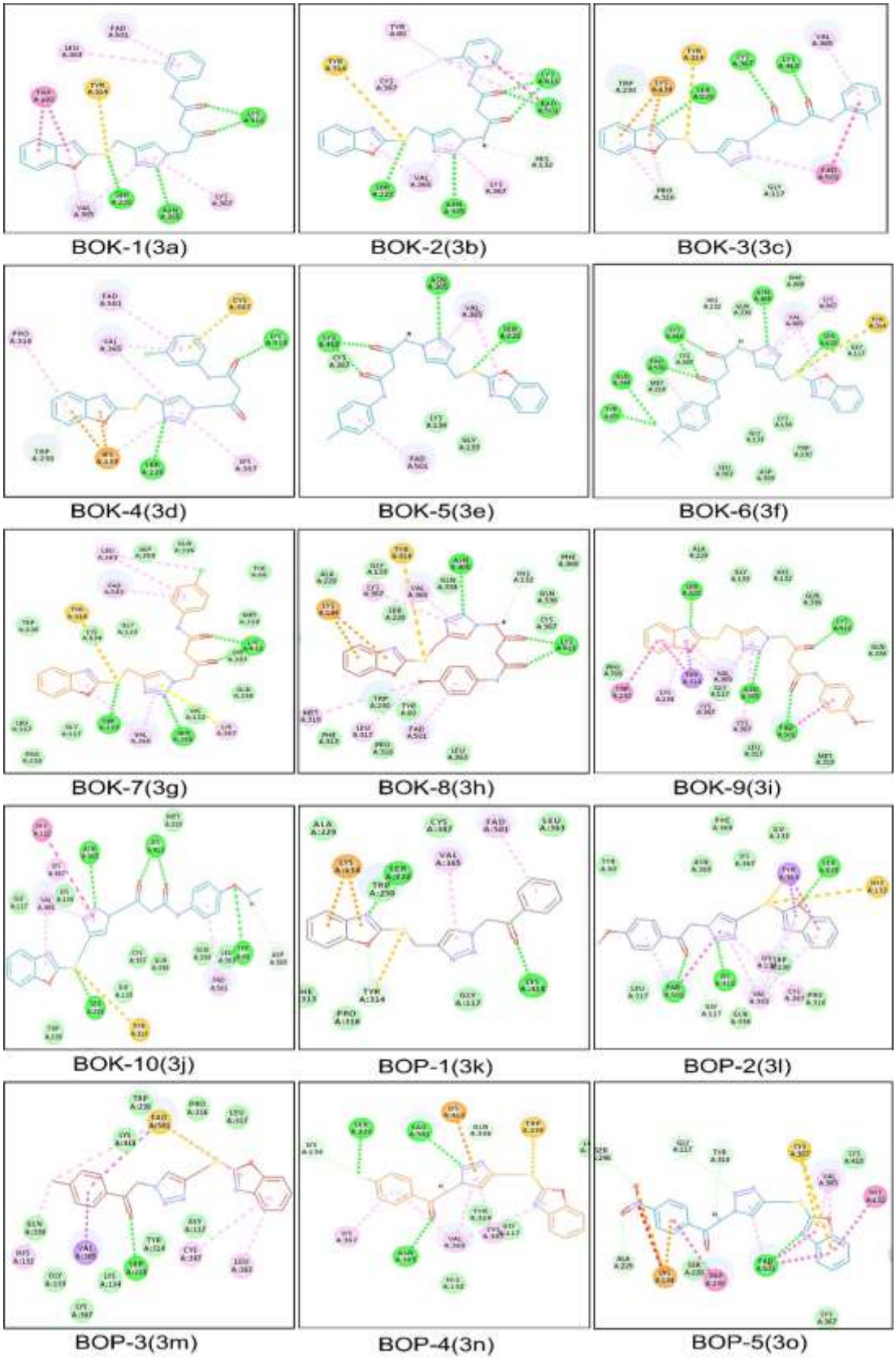


Fig. S48. 2D molecular docking interaction images of the compounds

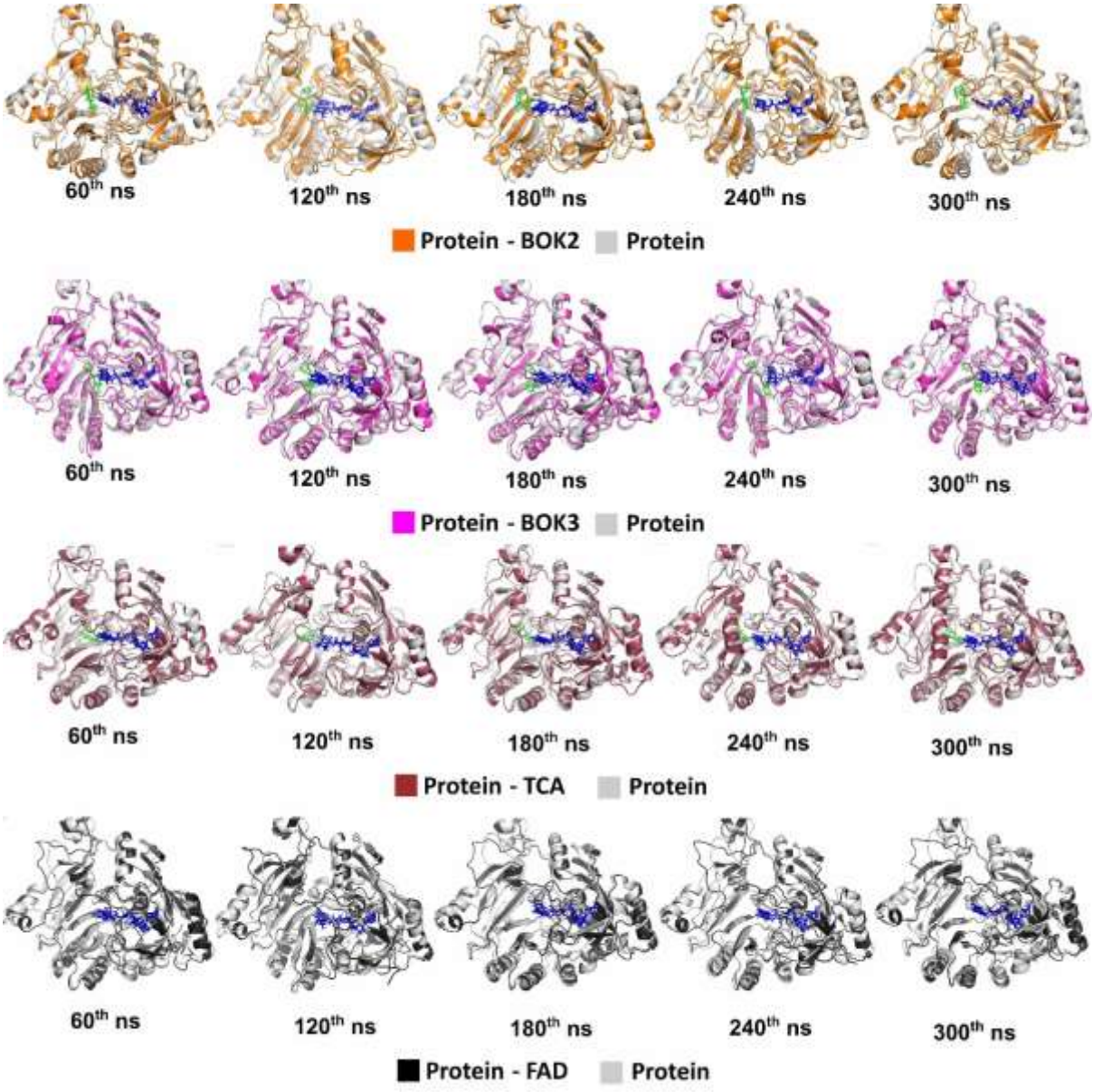


Fig. S49 MD trajectory analysis of superimposed structures of ligand-free protein and ligand-bound protein at different time intervals.

Table. S1. Molecular Docking Scores for Synthesised Compounds with Different substitutions.

S.No.	Compound Code	Substitution	Position of substitution	(-) CDocker Energy	(-) CDocker interaction energy
1.	BOK-4	Chloro	meta	34.54	52.72
2.	BOK-5	Methyl	para	37.58	51.58
3.	BOK-6	TrimethylFluoro	para	37.49	54.15
4.	BOK-7	Chloro	para	36.89	52.36
5.	BOK-8	Bromo	para	35.30	56.69
6.	BOK-9	Methoxy	para	33.81	52.73
7.	BOK-10	Ethoxy	para	36.97	53.26
8.	BOP-2	Methoxy	para	23.74	44.71
9.	BOP-3	Methyl	para	25.71	43.67
10.	BOP-5	Nitro	para	22.28	45.95

Table. S2 Assessment of ADMET Characteristics and Drug-likeness in Newly Synthesised

S.No.	Ligand	MW	RB	HBA	HBD	MR	TPSA	ilogP	ESOL LogS	BBB	log Kp	LV	BS	PAINS alerts
1.	BOK-1	407.45	9	6	1	108.71	128.21	2.07	-4.37	No	-6.44	0	0.55	0
2.	BOK-2	421.47	9	6	1	113.67	128.21	2.7	-4.67	No	-6.26	0	0.55	0
3.	BOK-3	425.44	9	7	1	108.66	128.21	2.54	-4.53	No	-6.47	0	0.55	0
4.	BOK-4	441.89	9	6	1	113.72	128.21	2.11	-4.96	No	-6.33	0	0.55	0
5.	BOK-5	421.47	9	6	1	113.67	128.21	2.32	-4.67	No	-6.06	0	0.55	0
6.	BOK-6	475.44	10	9	1	113.71	128.21	2.34	-5.22	No	-6.60	0	0.55	0
7.	BOK-7	441.89	9	6	1	113.72	128.21	2.28	-4.96	No	-6.33	0	0.55	0
8.	BOK-8	486.34	9	6	1	116.41	128.21	3.20	-5.27	No	-6.39	0	0.55	0
9.	BOK-9	437.47	10	7	1	115.20	137.44	3.29	-4.44	No	-5.84	0	0.55	0
10.	BOK-10	451.50	11	7	1	120.01	137.44	2.88	-4.68	No	-7.27	0	0.55	0
11.	BOP-1	350.39	6	5	1	94.77	99.11	2.74	-4.36	No	-6.01	0	0.55	0
12.	BOP-2	380.42	7	6	0	101.27	108.34	3.08	-4.42	No	-5.34	0	0.55	0
13.	BOP-3	364.42	6	5	0	99.74	99.11	3.02	-4.65	No	-5.56	0	0.55	0
14.	BOP-4	368.38	6	6	1	94.73	99.11	2.7	-4.51	No	-6.05	0	0.55	0
15.	BOP-5	395.39	7	7	0	103.60	144.93	2.31	-4.41	No	-5.76	0	0.55	0
16.	TCA-1	375.42	8	5	2	96	153.87	1.81	-4.54	No	-5.79	0	0.55	0

Compounds[a] in comparison to a literature-reported molecule (TCA-1).

[a]MW = molecular weight, RB = Rotatable bonds, HBA = Hydrogen bond Acceptor, HBD = Hydrogen bond donor, MR = Molecular Refractivity, TPSA = topological polar surface area, ilogP = Octanol-water partition coefficient, ESOL logS = Aqueous Solubility, BBB = blood brain barrier, log kP = Skin Permeation, LV = Lipinski's violation, BS = Bioavailability Score, and PAINS alerts = Pan-Assay Interference.