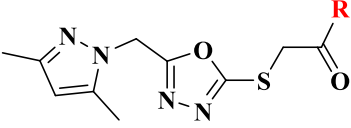


# **SUPPORTING DOCUMENT**

# I. Drug likeness properties of the designed compounds (Lipinski rule of five)

| <div style="text-align: center;">  <p>PO1-PO22</p> </div> |          |                               |                  |               |                  |        |
|--------------------------------------------------------------------------------------------------------------------------------------------|----------|-------------------------------|------------------|---------------|------------------|--------|
| Sl                                                                                                                                         | Cpd code | R group                       | H bond acceptors | H bond donors | Molecular weight | A LogP |
| 1                                                                                                                                          | PO1      | Phenylamino                   | 7                | 1             | 343.403          | 1.778  |
| 2                                                                                                                                          | PO2      | 3-methyl phenylamino          | 7                | 1             | 357.43           | 2.264  |
| 3                                                                                                                                          | PO3      | 4-trifluoromethyl phenylamino | 7                | 1             | 411.401          | 2.721  |
| 4                                                                                                                                          | PO4      | 4-bromo phenylamino           | 7                | 1             | 422.3            | 2.527  |
| 5                                                                                                                                          | PO5      | 3-methoxy phenylamino         | 8                | 1             | 373.429          | 1.762  |
| 6                                                                                                                                          | PO6      | 2-chlorophenylamino           | 7                | 1             | 377.849          | 2.443  |
| 7                                                                                                                                          | PO7      | 4-methyl phenylamino          | 7                | 1             | 357.43           | 2.264  |
| 8                                                                                                                                          | PO8      | 4-nitro phenylamino           | 10               | 1             | 388.401          | 1.673  |
| 9                                                                                                                                          | PO9      | 4-methoxy phenylamino         | 8                | 1             | 373.429          | 1.762  |
| 10                                                                                                                                         | PO10     | 4-chloro phenylamino          | 7                | 1             | 377.849          | 2.443  |
| 11                                                                                                                                         | PO11     | Pyridine-2-amino              | 8                | 1             | 344.392          | 1.167  |
| 12                                                                                                                                         | PO12     | 2-nitro phenylamino           | 10               | 1             | 388.401          | 1.673  |
| 13                                                                                                                                         | PO13     | 4-ethoxy phenylamino          | 8                | 1             | 387.456          | 2.111  |
| 14                                                                                                                                         | PO14     | Cyclohexyl-1-amino            | 7                | 1             | 349.451          | 2.06   |
| 15                                                                                                                                         | PO15     | 4-fluoro phenylamino          | 7                | 1             | 361.394          | 1.984  |
| 16                                                                                                                                         | PO16     | 3-trifluoromethyl phenylamino | 7                | 1             | 411.401          | 2.721  |
| 17                                                                                                                                         | PO17     | Morpholine                    | 8                | 0             | 337.397          | 0.095  |
| 18                                                                                                                                         | PO18     | Phenyl                        | 6                | 0             | 328.389          | 2.398  |
| 19                                                                                                                                         | PO19     | 4-methoxy phenyl              | 7                | 0             | 358.415          | 2.381  |
| 20                                                                                                                                         | PO20     | 4-methyl phenyl               | 6                | 0             | 342.415          | 2.884  |
| 21                                                                                                                                         | PO21     | 4-fluoro phenyl               | 6                | 0             | 346.379          | 2.603  |
| 22                                                                                                                                         | PO22     | 4-nitro phenyl                | 9                | 0             | 373.386          | 2.292  |

## II. Predicted ADMET properties of the designed molecules

| Sl | Cpd code | Solubility | Solubility Level | BBB       | BBB Level | CYP2D6   | CYP2D6 Prediction | HIA level |
|----|----------|------------|------------------|-----------|-----------|----------|-------------------|-----------|
| 1  | PO1      | -3.015     | 3                | -0.899    | 3         | -9.95161 | FALSE             | 0         |
| 2  | PO2      | -3.488     | 3                | -0.748    | 3         | -9.61108 | FALSE             | 0         |
| 3  | PO3      | -4.172     | 2                | -0.607    | 3         | -5.94374 | FALSE             | 0         |
| 4  | PO4      | -3.783     | 3                | -0.667    | 3         | -10.7456 | FALSE             | 0         |
| 5  | PO5      | -3.011     | 3                | -1.045    | 3         | -11.189  | FALSE             | 0         |
| 6  | PO6      | -3.728     | 3                | -0.693    | 3         | -8.06757 | FALSE             | 0         |
| 7  | PO7      | -3.47      | 3                | -0.748    | 3         | -9.01906 | FALSE             | 0         |
| 8  | PO8      | -3.112     | 3                | undefined | 4         | -14.3655 | FALSE             | 0         |
| 9  | PO9      | -2.994     | 3                | -1.045    | 3         | -11.3601 | FALSE             | 0         |
| 10 | PO10     | -3.71      | 3                | -0.693    | 3         | -7.9148  | FALSE             | 0         |
| 11 | PO11     | -2.566     | 3                | -1.266    | 3         | -10.5001 | FALSE             | 0         |
| 12 | PO12     | -3.165     | 3                | undefined | 4         | -12.3571 | FALSE             | 0         |
| 13 | PO13     | -3.163     | 3                | -0.937    | 3         | -12.9087 | FALSE             | 0         |
| 14 | PO14     | -3.261     | 3                | -0.812    | 3         | -5.00917 | FALSE             | 0         |
| 15 | PO15     | -3.309     | 3                | -0.835    | 3         | -8.33709 | FALSE             | 0         |
| 16 | PO16     | -4.208     | 2                | -0.607    | 3         | -5.9661  | FALSE             | 0         |
| 17 | PO17     | -1.377     | 4                | -1.41     | 3         | -10.4416 | FALSE             | 0         |
| 18 | PO18     | -3.387     | 3                | -0.504    | 2         | -4.35879 | FALSE             | 0         |
| 19 | PO19     | -3.303     | 3                | -0.651    | 3         | -6.04798 | FALSE             | 0         |
| 20 | PO20     | -3.852     | 3                | -0.354    | 2         | -3.74701 | FALSE             | 0         |
| 21 | PO21     | -3.607     | 3                | -0.441    | 2         | -1.89197 | FALSE             | 0         |
| 22 | PO22     | -3.348     | 3                | undefined | 4         | -8.044   | FALSE             | 0         |

### III. SPECTRAL DATA OF SYNTHESIZED COMPOUNDS (PO1-PO22)

- $^1\text{H}$  NMR
- $^{13}\text{C}$  NMR
- Mass spectra



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-phenylacetamide (PO1)

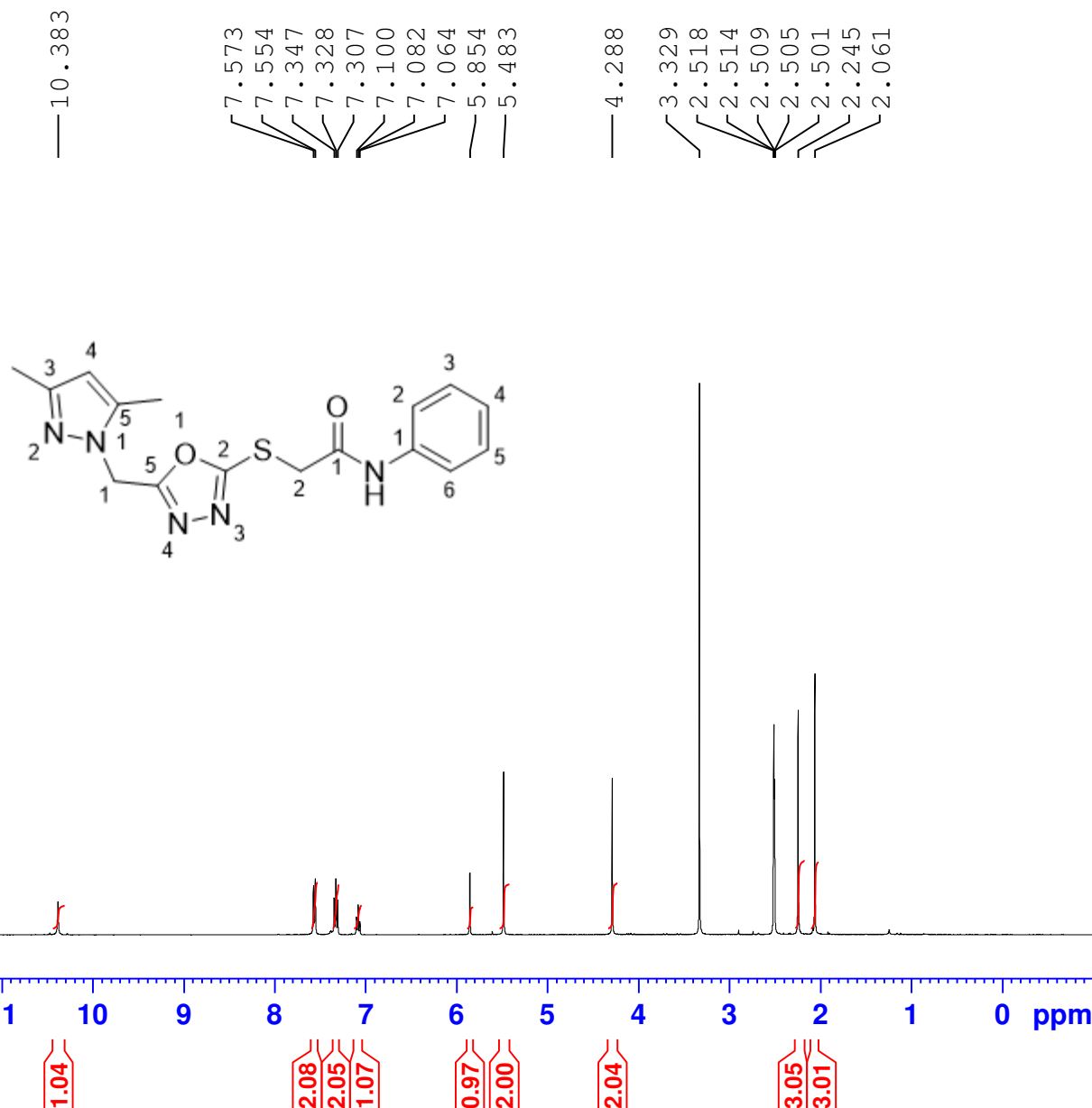
PDA  
1H-NMR in DMSO



Current Data Parameters  
NAME 23000427-PDA  
EXPNO 1  
PROCNO 1

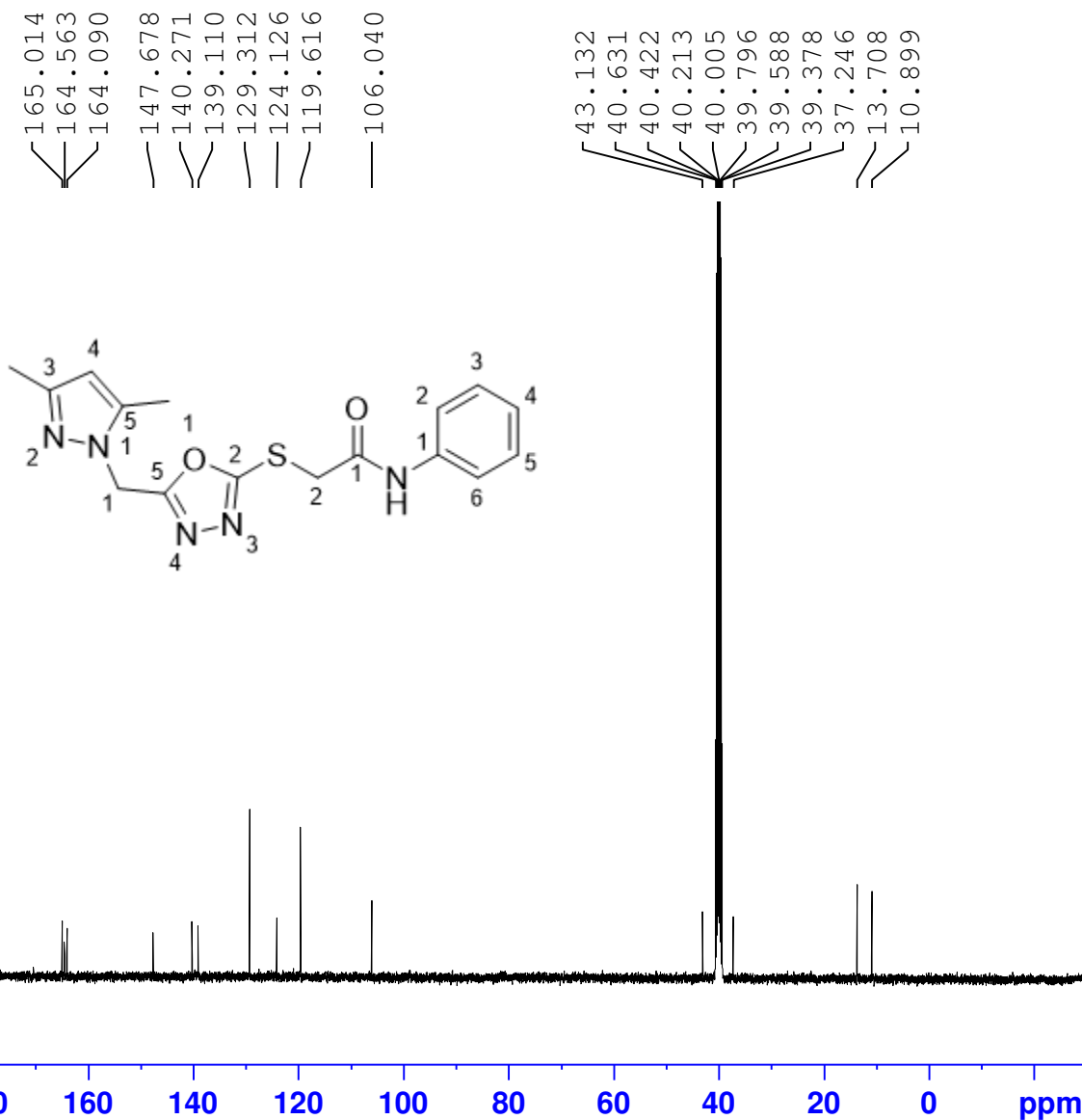
F2 - Acquisition Parameters  
Date\_ 20230426  
Time 14.19 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 32.13  
DW 62.400 usec  
DE 17.09 usec  
TE 297.7 K  
D1 1.00000000 sec  
TD0 1  
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



# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-phenylacetamide (PO1)

PDA  
13C-NMR in DMSO



Current Data Parameters  
NAME 23000427-PDA  
EXPNO 2  
PROCNO 1

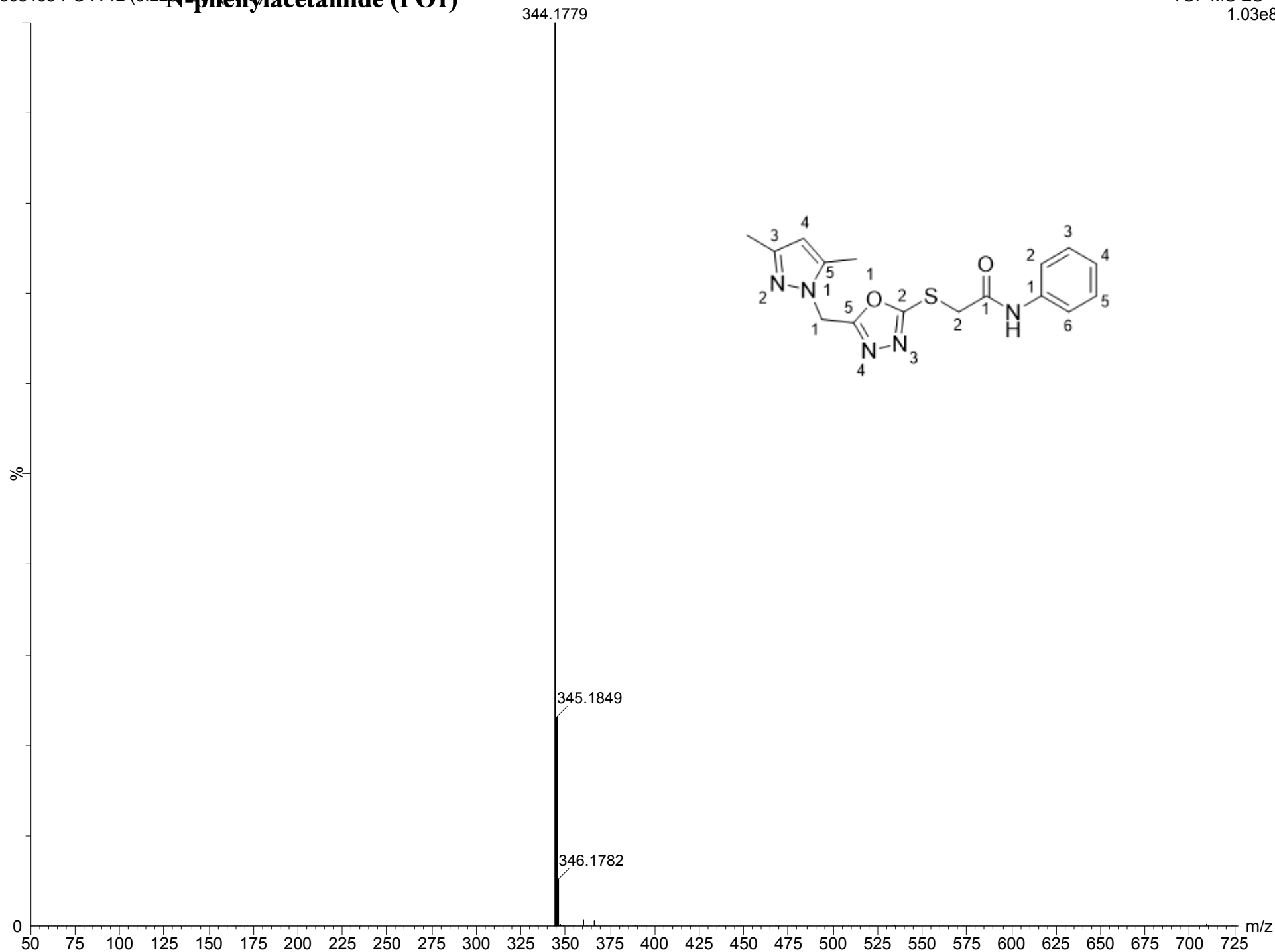
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Time 17.11 h  
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PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1024  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.794729 Hz  
AQ 1.2582912 sec  
RG 202.84  
DW 19.200 usec  
DE 6.50 usec  
TE 298.4 K  
D1 1.00000000 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 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-phenylacetamide (PO1)

2303465-PO-A 12 (0.22 µg, 1:15)

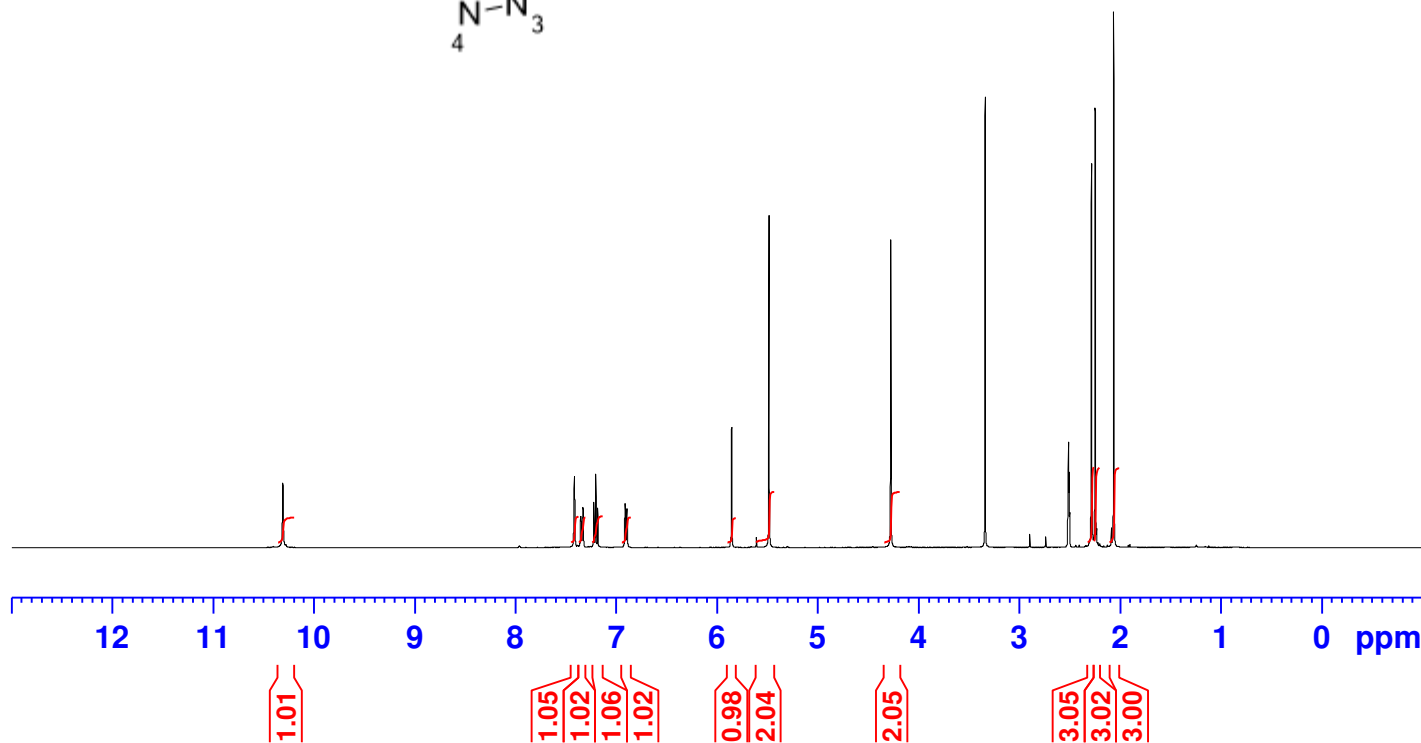
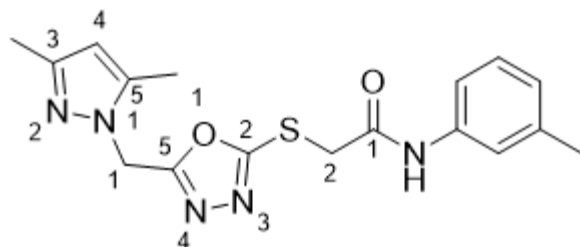
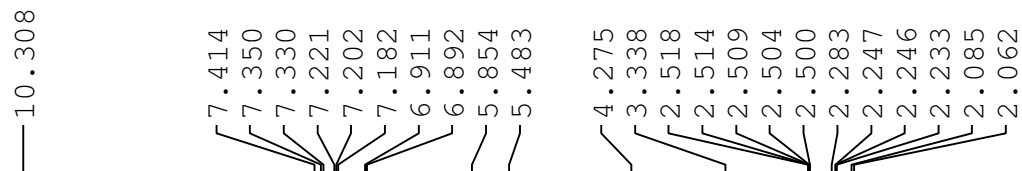
TOF MS ES+  
1.03e8



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(m-tolyl)acetamide (PO2)

PO4T

<sup>1</sup>H-NMR in DMSO



## Current Data Parameters

NAME 23000463-PO4T  
EXPNO 1  
PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20230507  
Time 17.17 h  
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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 297.6 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

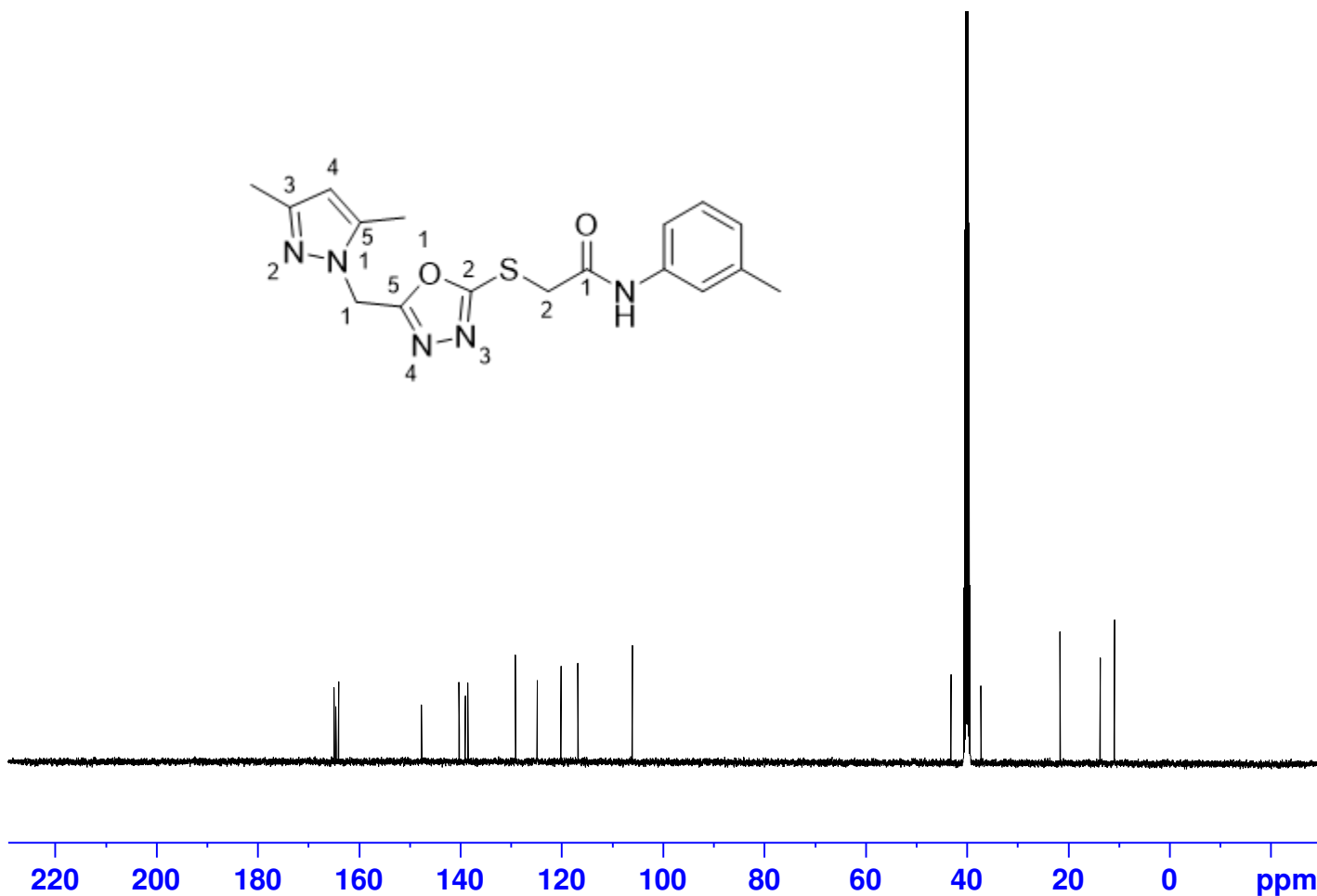
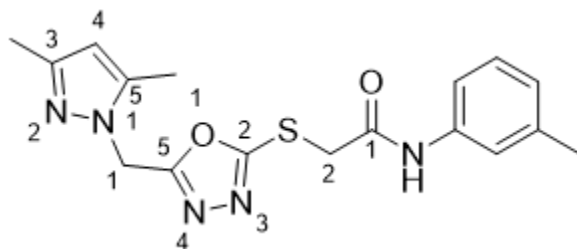
**$^{13}\text{C}$  NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(m-tolyl)acetamide (PO2)**

PO4T  
 $^{13}\text{C}$ -NMR in DMSO



164.934  
164.565  
164.075  
147.681  
140.270  
139.039  
138.525  
129.137  
124.820  
120.132  
116.812  
106.038

43.128  
40.630  
40.421  
40.212  
40.004  
39.795  
39.587  
39.378  
37.250  
21.635  
13.705  
10.898



Current Data Parameters  
NAME 23000463-PO4T  
EXPNO 2  
PROCNO 1

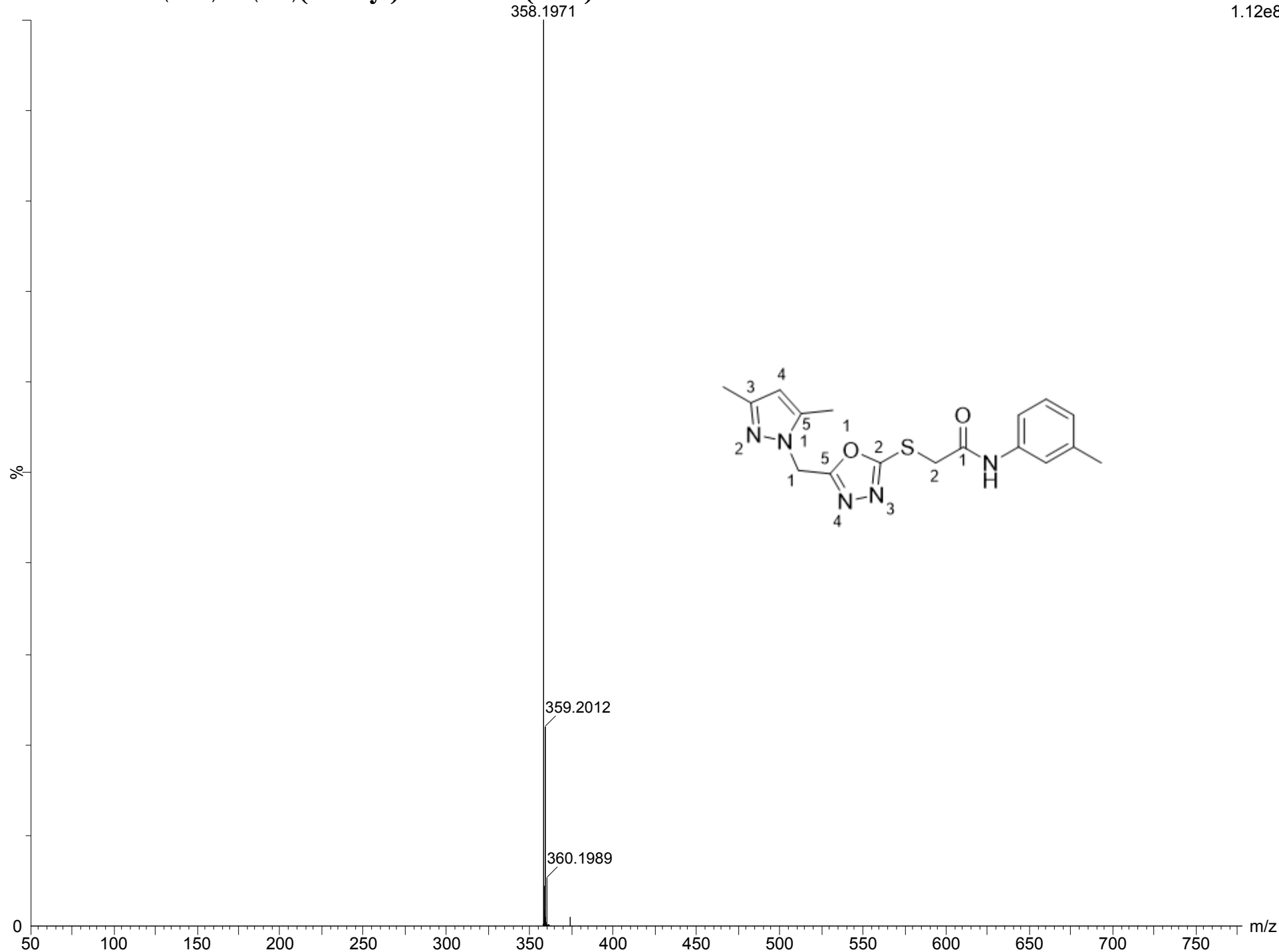
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PULPROG zgpg30  
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SOLVENT DMSO  
NS 1024  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.794729 Hz  
AQ 1.2582912 sec  
RG 202.84  
DW 19.200 usec  
DE 6.50 usec  
TE 298.6 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6680954 MHz  
NUC1  $^{13}\text{C}$   
P0 3.33 usec  
P1 10.00 usec  
PLW1 51.02600098 W  
SFO2 400.3116012 MHz  
NUC2  $^1\text{H}$   
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 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(m-tolyl)acetamide (PO2)

2303472-PO-1CH3 13 (0.237) Cm (5.1e7)

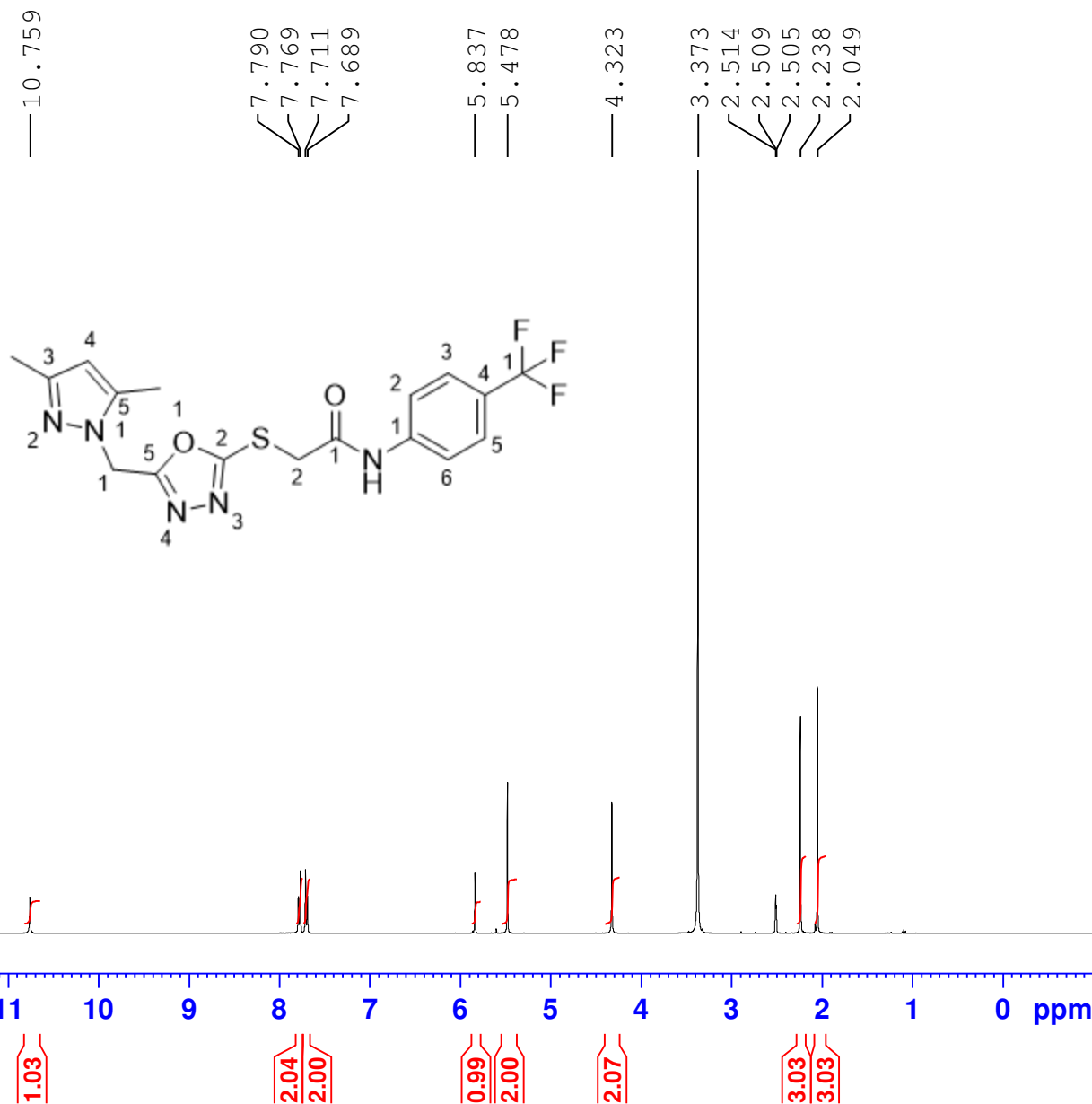
TOF MS ES+  
1.12e8



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-(trifluoromethyl)phenyl)acetamide (PO3)

PO4CF3-new

<sup>1</sup>H-NMR in DMSO



Current Data Parameters  
NAME 23000506-PO4CF3-new  
EXPNO 1  
PROCNO 1

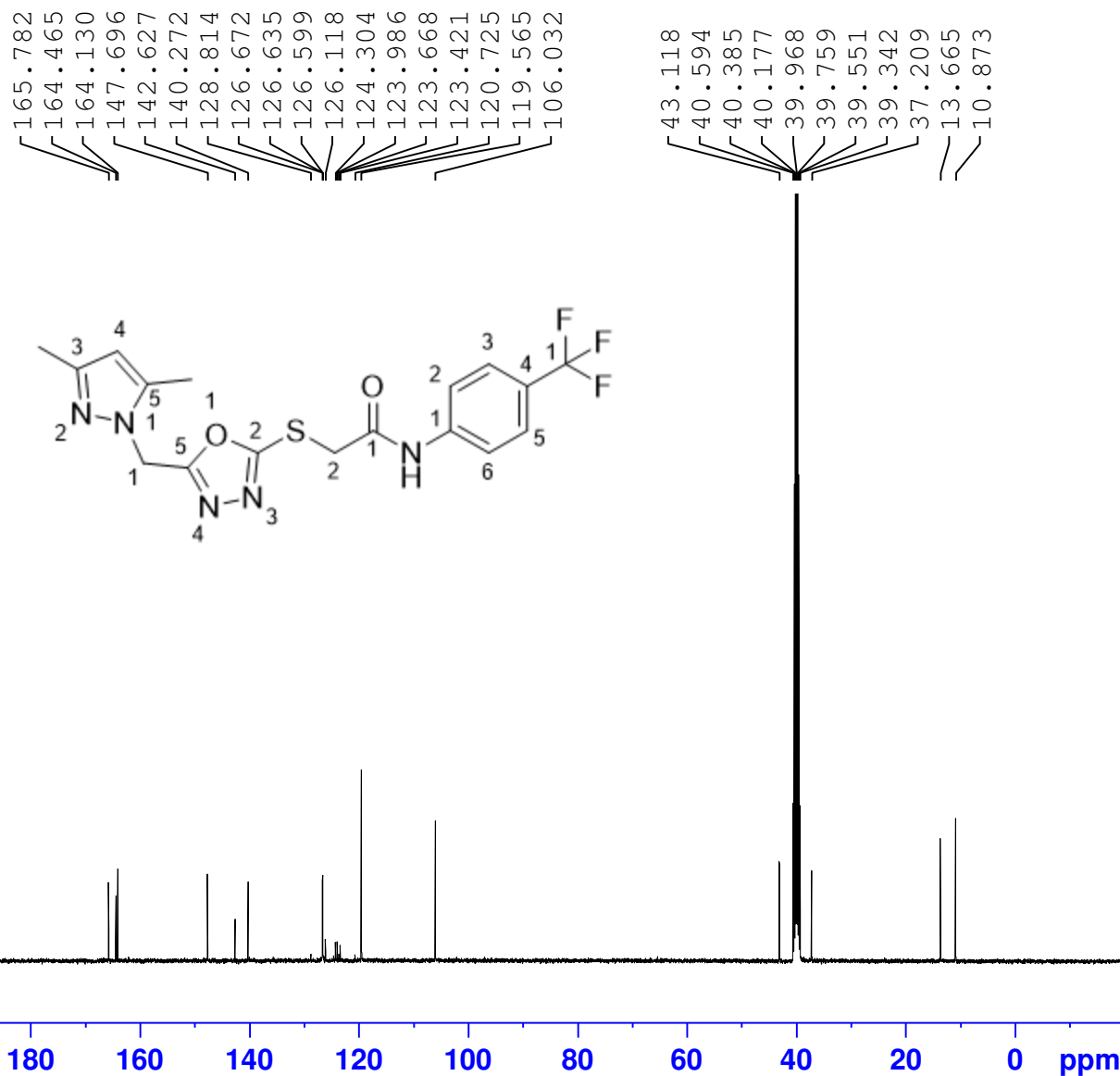
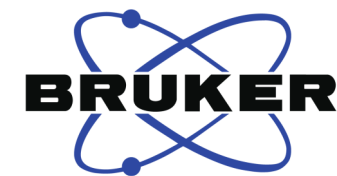
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Time 11.32 h  
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 4  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 32.13  
DW 62.400 usec  
DE 17.09 usec  
TE 297.6 K  
D1 1.00000000 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

# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-(trifluoromethyl)phenyl)acetamide (PO3)

PO4CF3-new

<sup>13</sup>C-NMR in DMSO



Current Data Parameters  
 NAME 23000506-PO4CF3-new  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230520  
 Time 10.24 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 298.5 K  
 D1 1.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6680954 MHz  
 NUC1 <sup>13</sup>C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 51.02600098 W  
 SFO2 400.3116012 MHz  
 NUC2 <sup>1</sup>H  
 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 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-(trifluoromethyl)phenyl)acetamide (PO3)

2303473-PO-4CF3 13 (0.237) Cm (8:16)

**N-(4-(trifluoromethyl)phenyl)acetamide (PO3)**

TOF MS ES+  
1.06e8

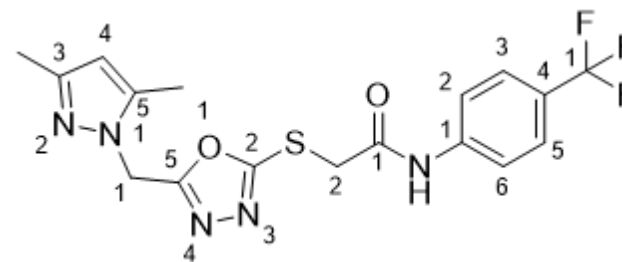
412.1798

413.1861

414.1811

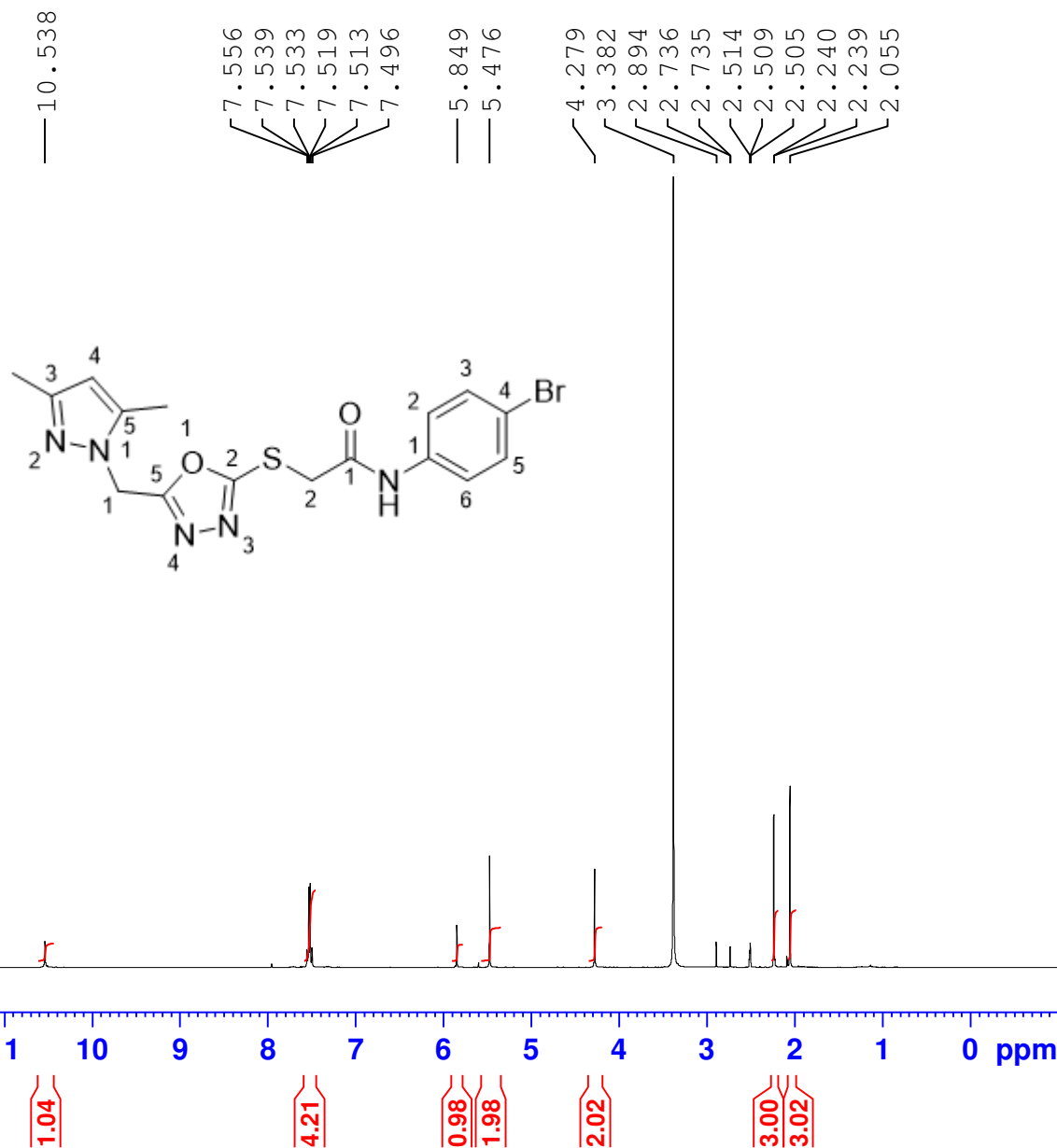
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m/z



**<sup>1</sup>H NMR of N-(4-bromophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO4)**

PO4Br  
1H-NMR in DMSO



Current Data Parameters  
NAME 23000476-PO4Br  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230509  
Time 17.36 h  
INSTRUM spect  
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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 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

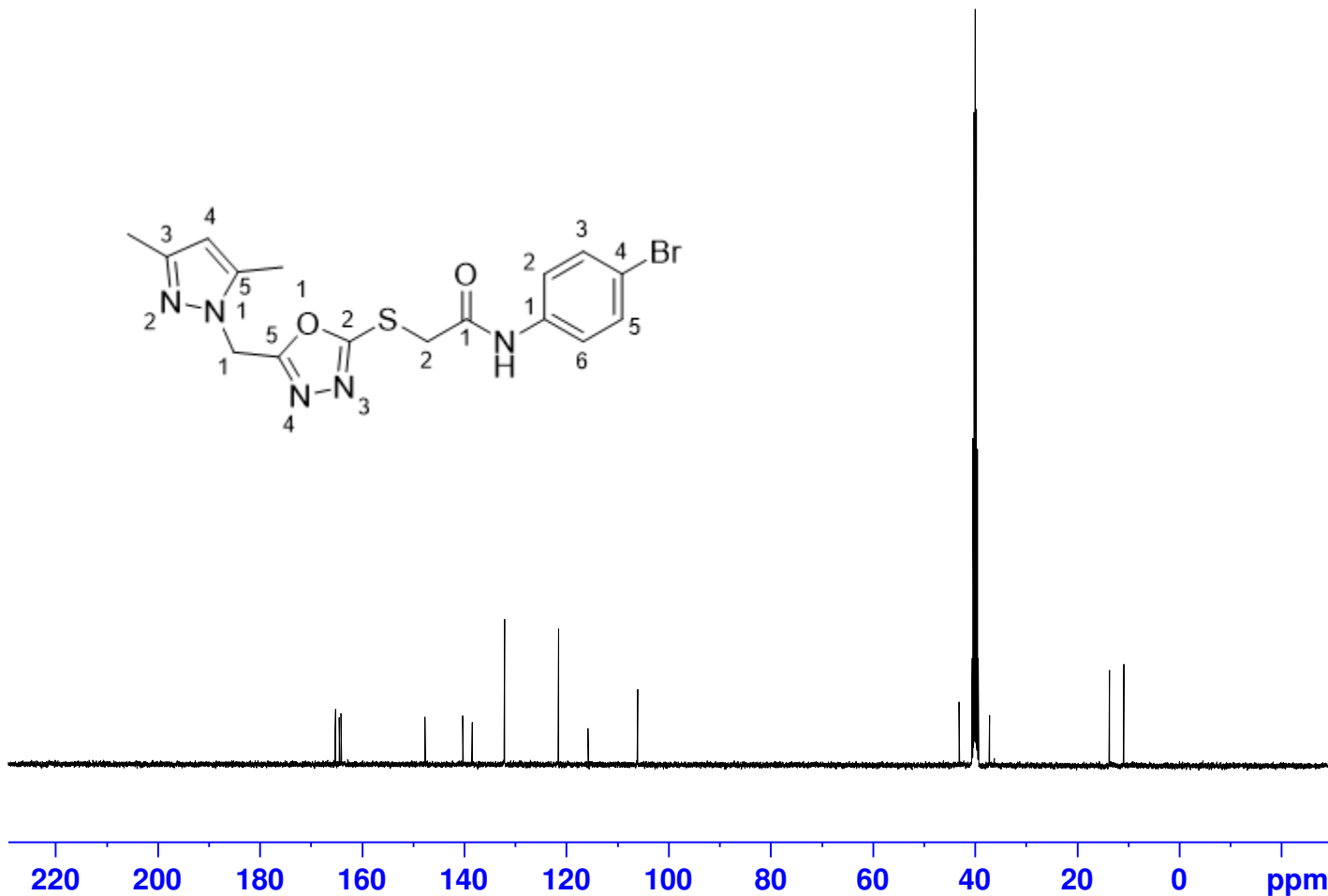
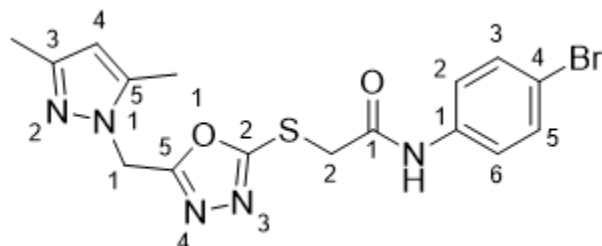
# <sup>13</sup>C NMR of N-(4-bromophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO4)

PO4Br  
<sup>13</sup>C-NMR in DMSO



165.260  
 164.501  
 164.105  
 147.701  
 140.284  
 138.457  
 132.143  
 121.565  
 115.748  
 106.049

43.116  
 40.589  
 40.380  
 40.172  
 39.963  
 39.754  
 39.545  
 39.337  
 37.177  
 13.692  
 10.889



Current Data Parameters  
 NAME 23000476-PO4Br  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230509  
 Time 17.56 h  
 INSTRUM spect  
 PROBHD Z108618\_0984 (   
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 512  
 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 298.5 K  
 D1 1.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6680954 MHz  
 NUC1 <sup>13</sup>C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 51.02600098 W  
 SFO2 400.3116012 MHz  
 NUC2 <sup>1</sup>H  
 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 N-(4-bromophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO4)

2303470-PO-4Br 13 (0.237) Cm (6:17)

TOF MS ES+  
4.60e7

424.1042

422.1085

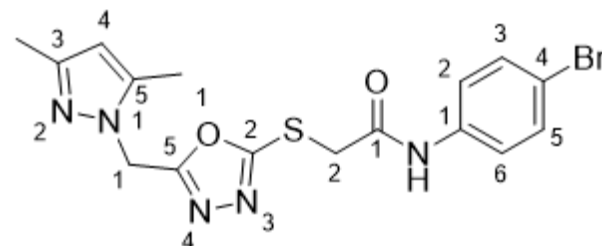
425.1080

426.1046

%

0

m/z



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3-methoxyphenyl)acetamide (PO5)

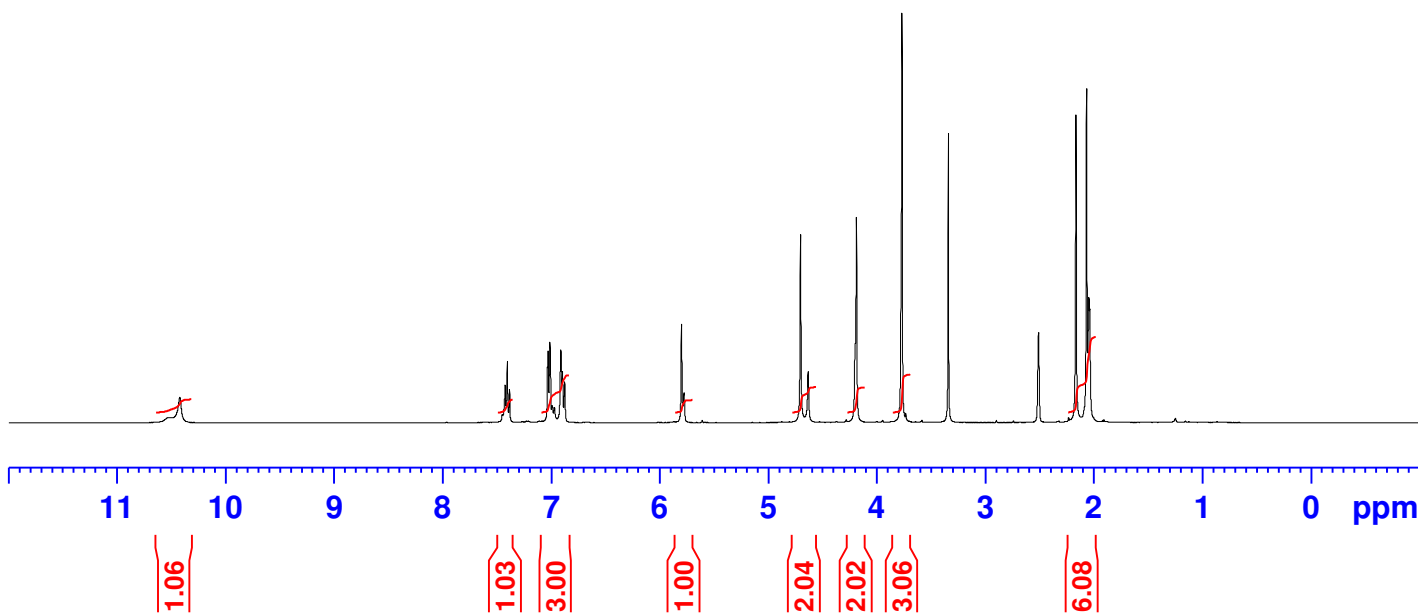
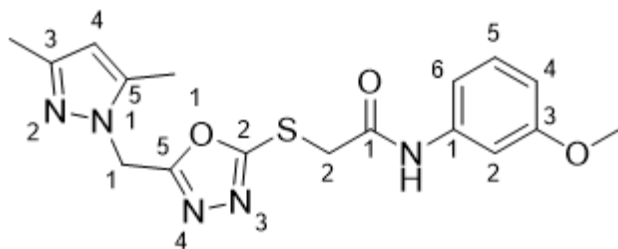
PO3MO

<sup>1</sup>H-NMR in DMSO



—10.422

7.423  
7.403  
7.383  
7.032  
7.028  
7.012  
7.007  
6.911  
6.896  
6.876  
5.799  
5.775  
4.702  
4.631  
4.187  
3.767  
3.340  
2.513  
2.509  
2.505  
2.164  
2.066  
2.045  
2.037



## Current Data Parameters

NAME 23000458-PO3MO  
EXPNO 1  
PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20230507  
Time 17.00 h  
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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 298.0 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

# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3-methoxyphenyl)acetamide (PO5)

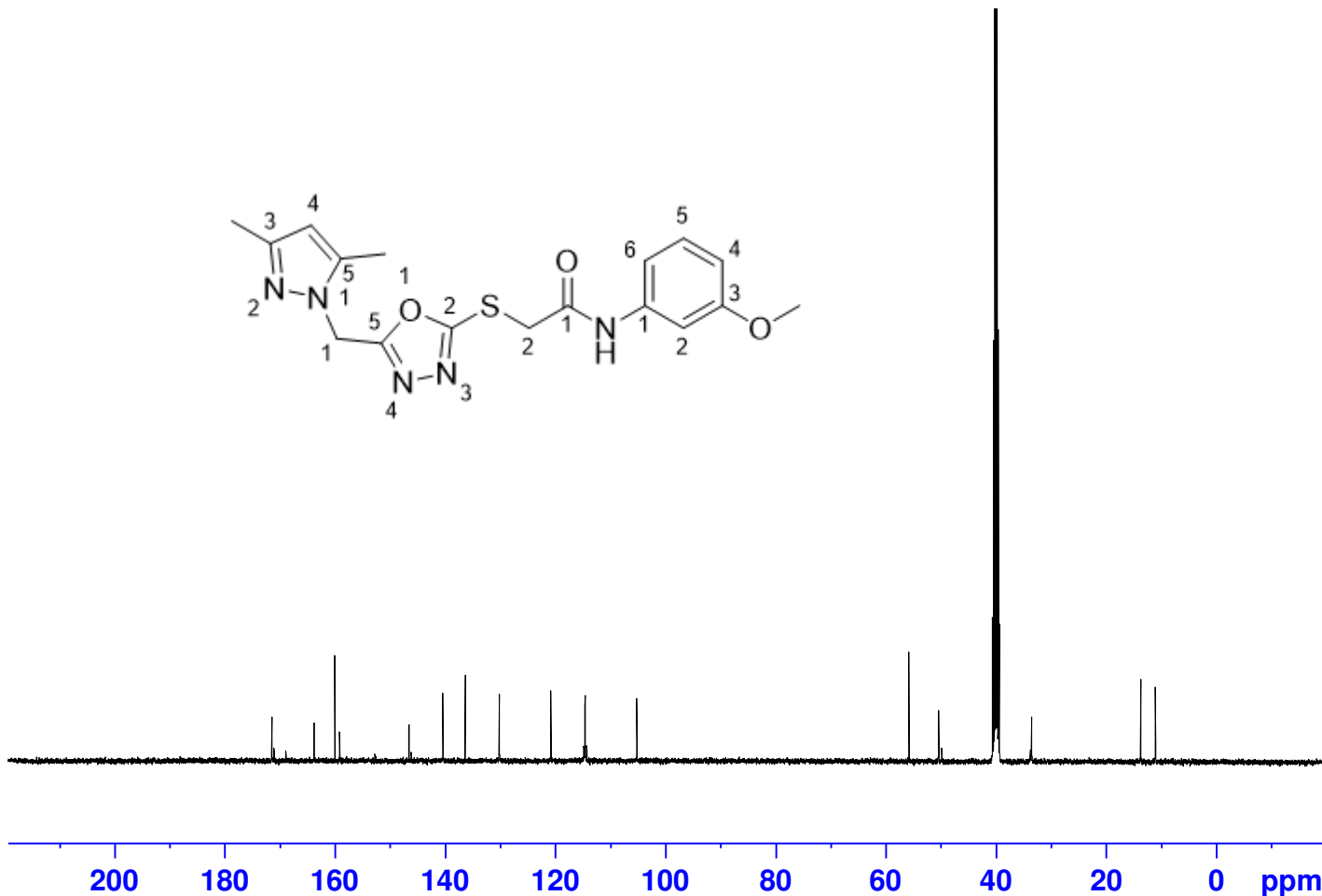
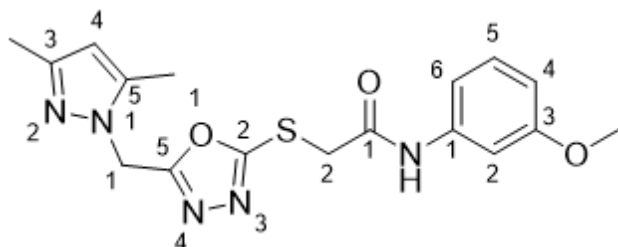
PO3MO

<sup>13</sup>C-NMR in DMSO



171.492  
163.821  
160.064  
159.194  
146.592  
140.445  
136.370  
130.195  
120.841  
114.656  
114.615  
105.259

55.834  
50.424  
40.629  
40.421  
40.212  
40.003  
39.795  
39.586  
39.378  
33.520  
13.719  
11.098  
11.007



Current Data Parameters  
NAME 23000458-PO3MO  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230508  
Time 10.34 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 298.1 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

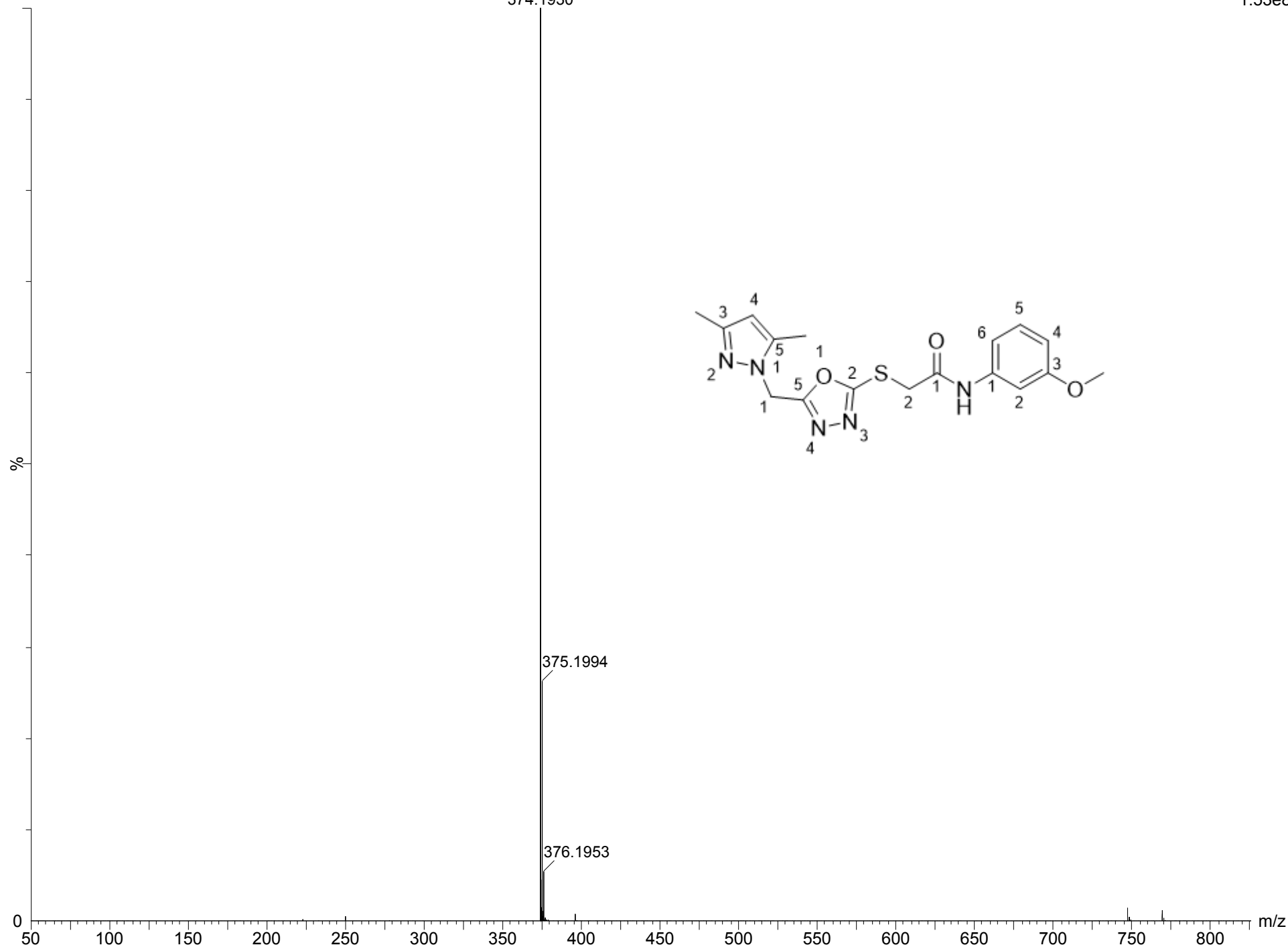
F2 - Processing parameters  
SI 32768  
SF 100.6580296 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3-methoxyphenyl)acetamide (PO5)

2303468-PO-3MO 13 (0.237) Cm (5:19)

**N-(3-methoxyphenyl)acetamide (PO5)**

TOF MS ES+  
1.53e8



# <sup>1</sup>H NMR of N-(2-chlorophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO6)

PO2C1  
1H-NMR in DMSO

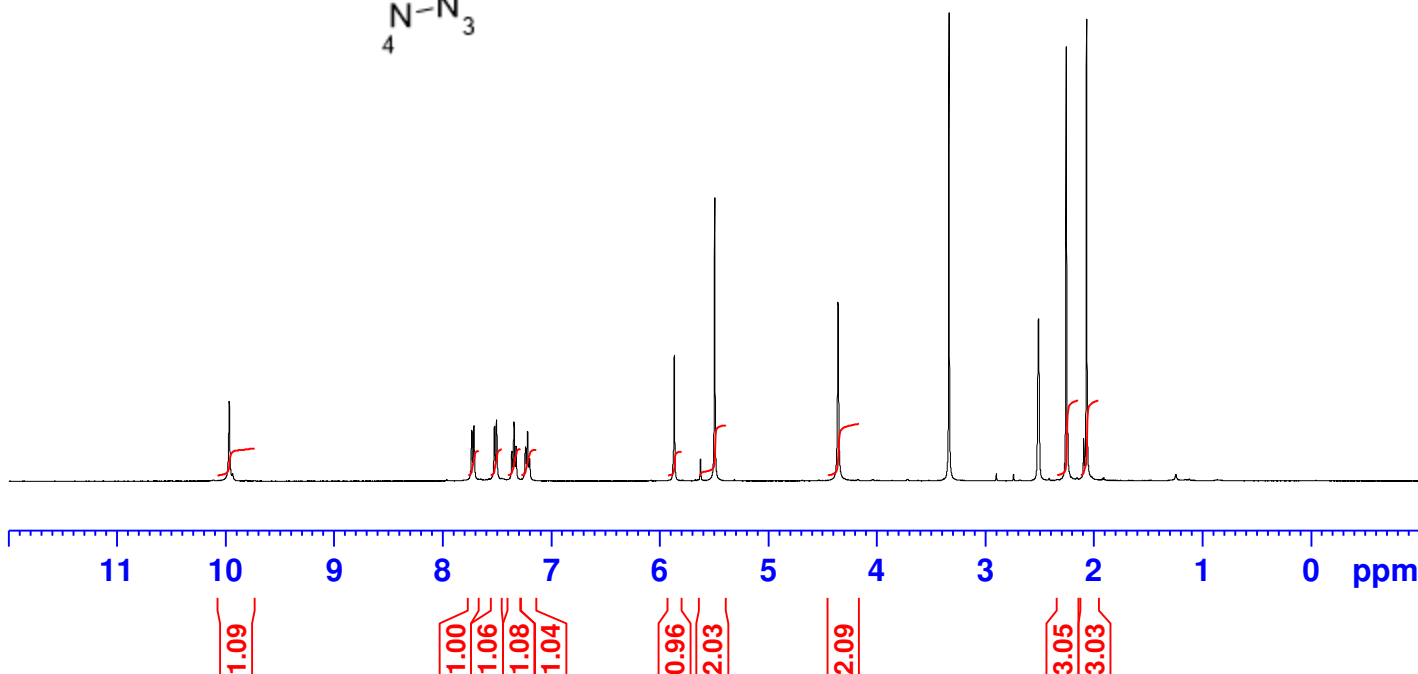
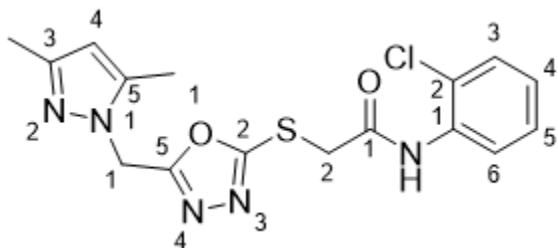


— 9.966  
7.731  
7.711  
7.522  
7.502  
7.361  
7.342  
7.324  
7.236  
7.217  
7.200  
5.865  
5.624  
5.493  
— 4.356  
— 3.334  
2.509  
2.253  
2.240  
2.093  
2.066

Current Data Parameters  
NAME 23000460-PO2C1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230507  
Time 17.07 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 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 400.310000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



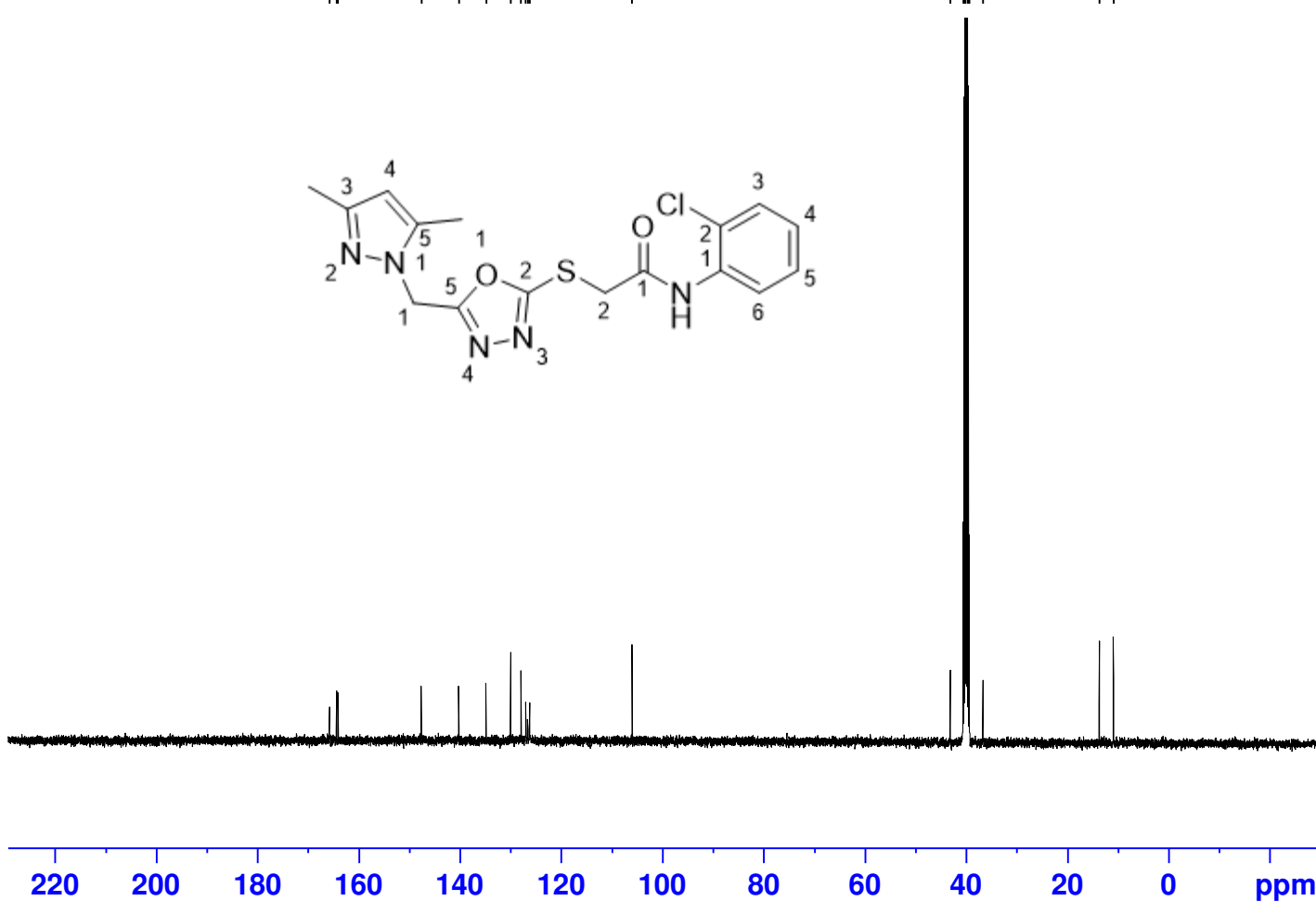
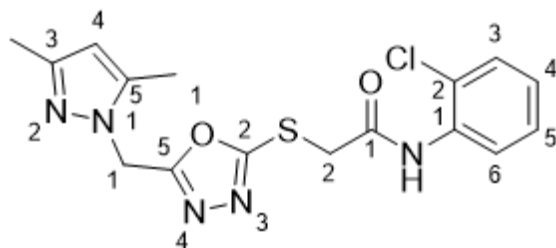


**<sup>13</sup>C NMR of N-(2-chlorophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO6)**

PO2C1  
<sup>13</sup>C-NMR in DMSO



165.801  
 164.430  
 164.142  
 147.677  
 140.277  
 134.894  
 130.030  
 127.979  
 127.062  
 126.664  
 126.238  
 106.050  
 43.155  
 40.631  
 40.423  
 40.214  
 39.796  
 39.588  
 39.379  
 36.691  
 13.715  
 10.912



Current Data Parameters  
 NAME 23000460-PO2C1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230508  
 Time 11.55 h  
 INSTRUM spect  
 PROBHD Z108618\_0984 (   
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 900  
 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 298.1 K  
 D1 1.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6680954 MHz  
 NUC1 <sup>13</sup>C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 51.02600098 W  
 SFO2 400.3116012 MHz  
 NUC2 <sup>1</sup>H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 11.28999996 W  
 PLW12 0.27318001 W  
 PLW13 0.13741000 W

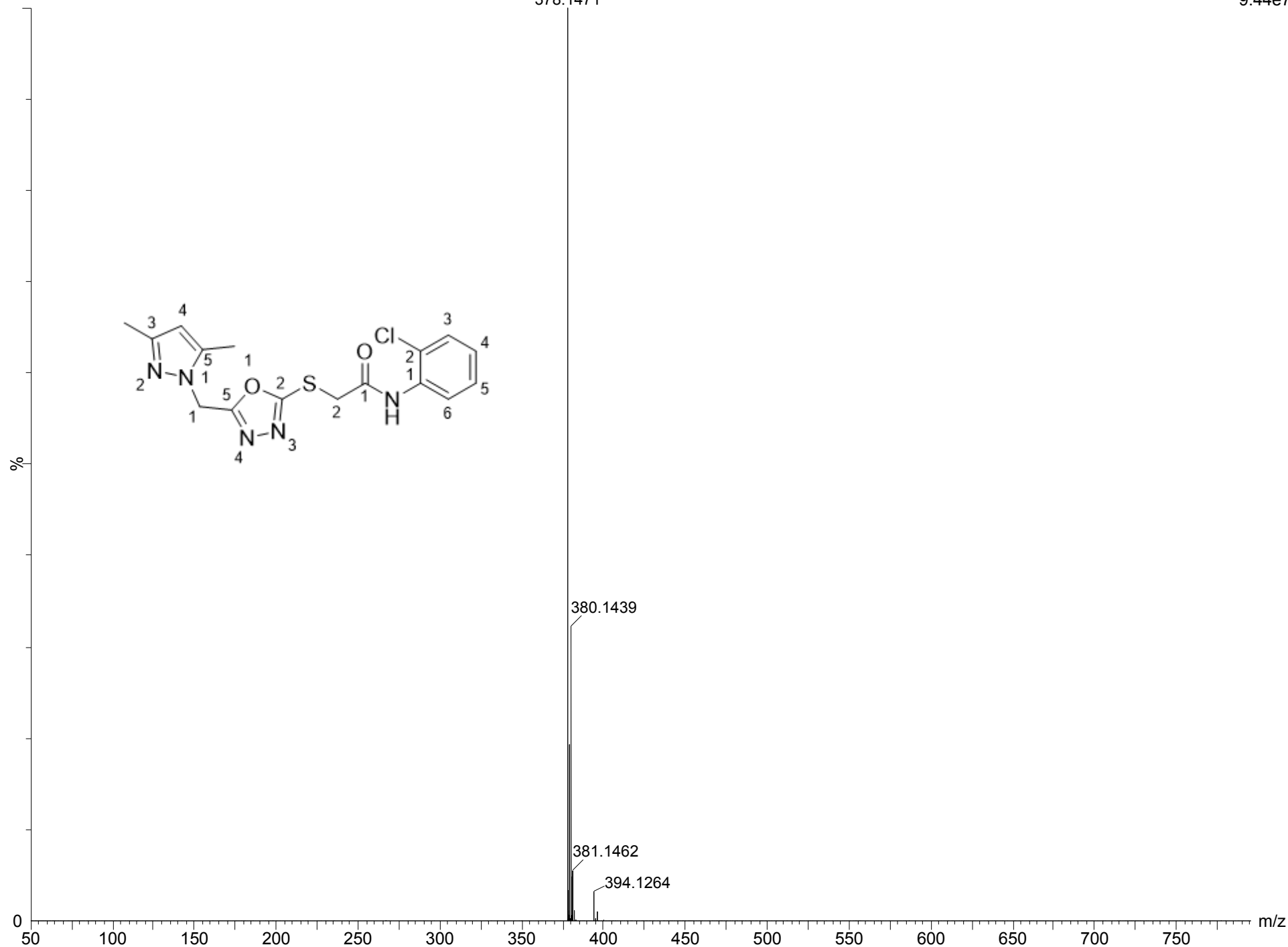
F2 - Processing parameters  
 SI 32768  
 SF 100.6580296 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

# Mass spectrum of N-(2-chlorophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-

2303467-PO-2Cl 12 (0.220) Cm (6:16) **oxadiazol-2-yl)thio)acetamide (PO6)**

TOF MS ES+  
9.44e7

378.1471



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(p-tolyl)acetamide (PO7)

PO4CH3  
1H-NMR in DMSO

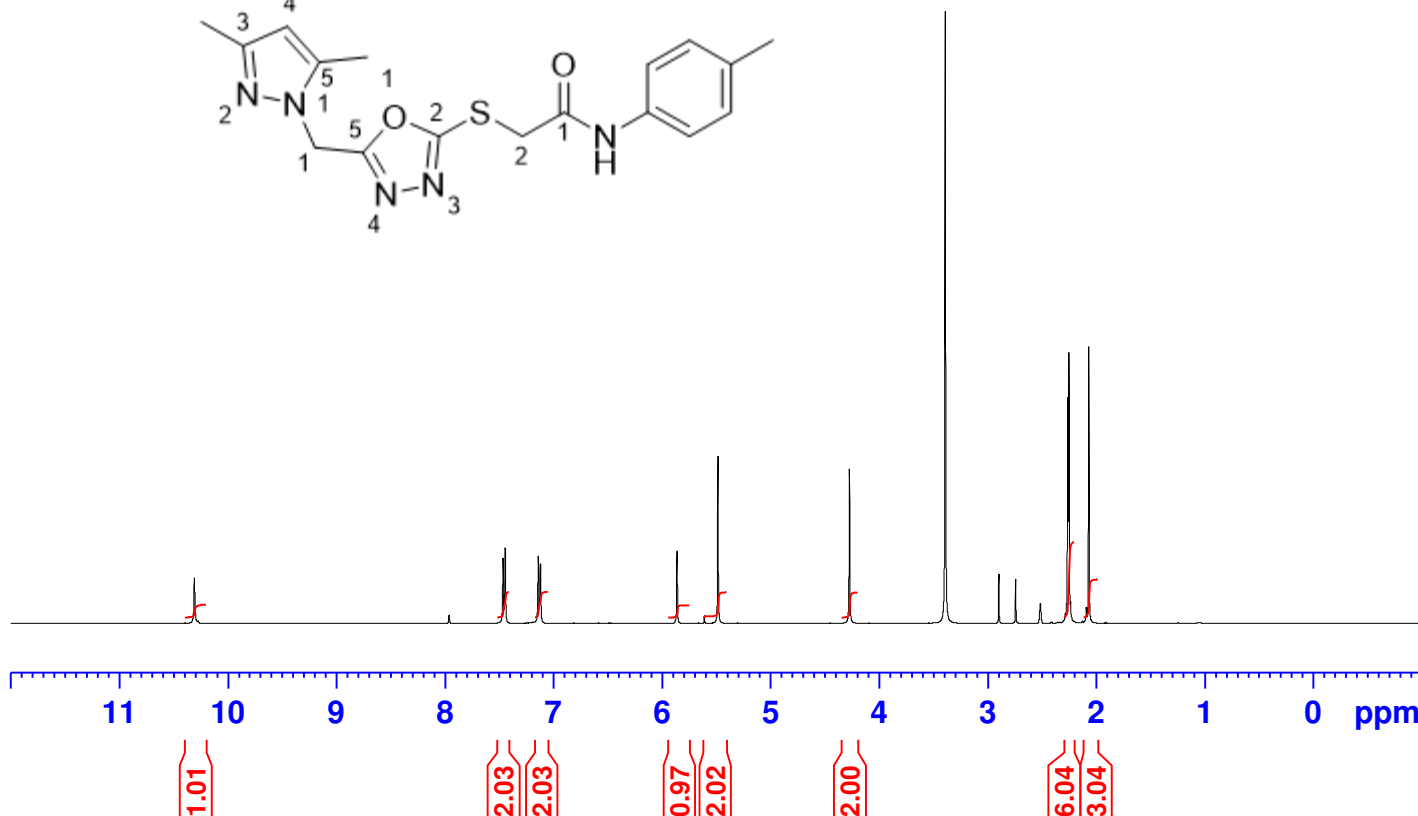
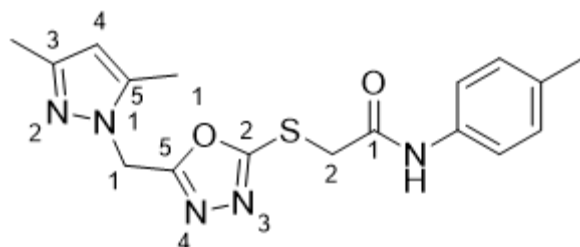


— 10.305

7.462  
7.441  
7.137  
7.116

5.857  
5.480

4.269  
3.386  
2.892  
2.737  
2.514  
2.510  
2.506  
2.257  
2.246  
2.231  
2.087  
2.064



Current Data Parameters  
NAME 23000494-PO4CH3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230513  
Time 15.36 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 298.0 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

# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(p-tolyl)acetamide (PO7)

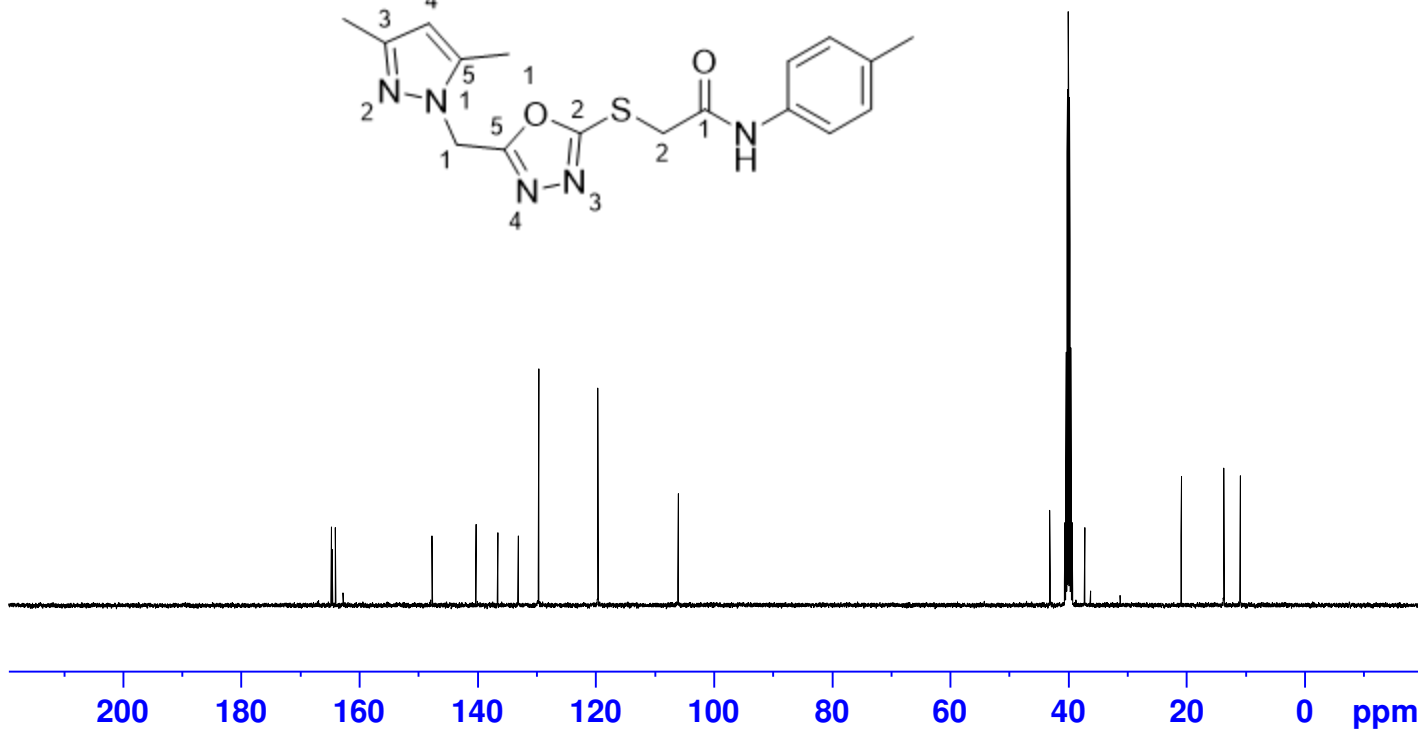
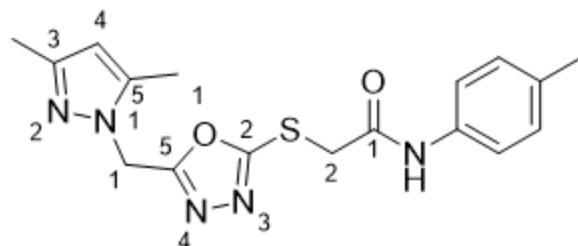
PO4CH3

<sup>13</sup>C-NMR in DMSO



164.757  
164.596  
164.066  
147.710  
140.285  
136.597  
133.115  
129.667  
119.651  
106.056

43.129  
40.601  
40.392  
40.184  
39.975  
39.766  
39.557  
39.349  
37.228  
20.900  
13.692  
10.888



Current Data Parameters  
NAME 23000494-PO4CH3  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230513  
Time 16.41 h  
INSTRUM spect  
PROBHD Z108618\_0984 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 471  
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 299.6 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

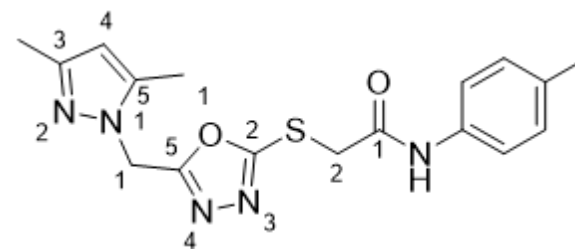
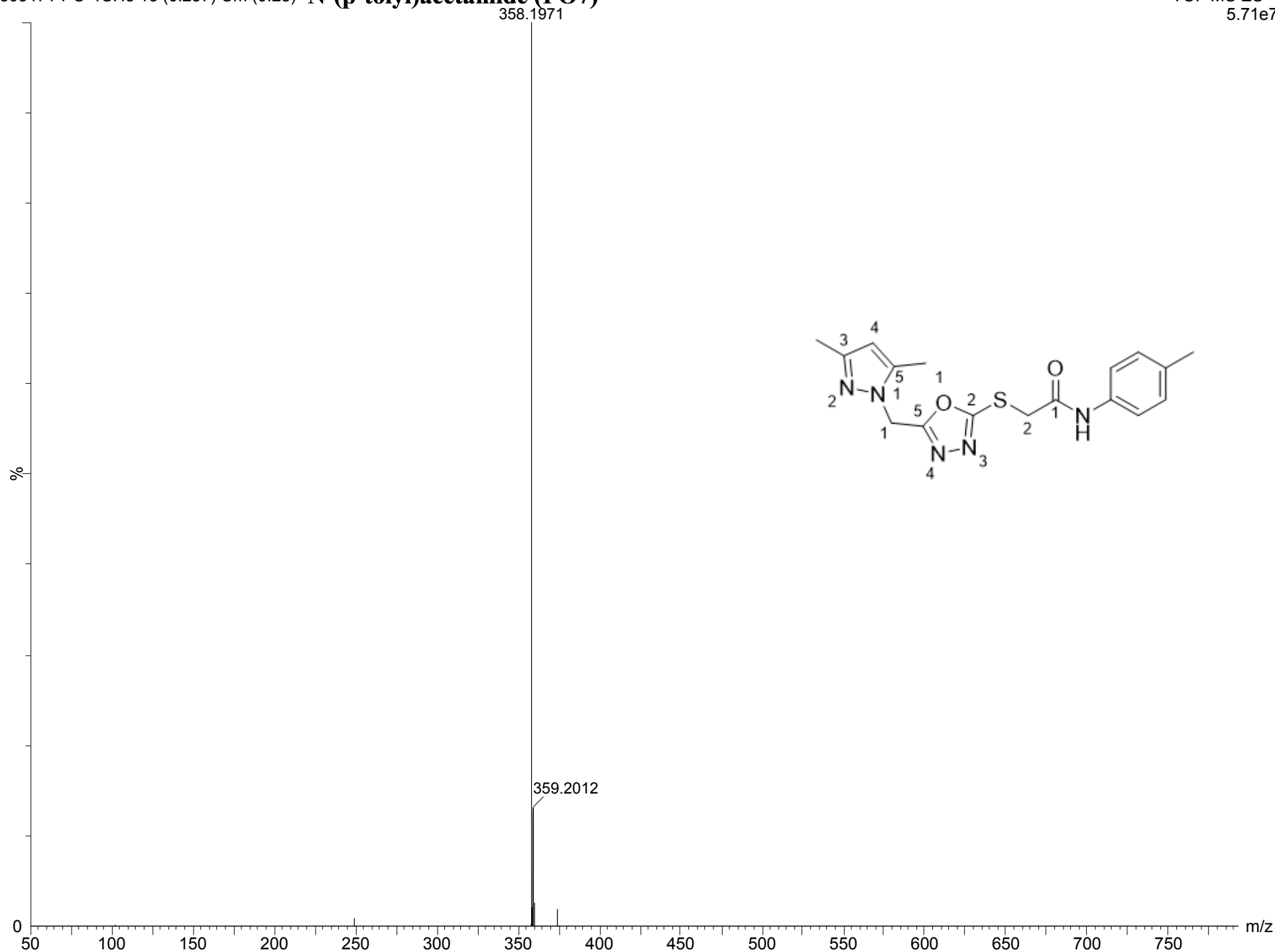
F2 - Processing parameters  
SI 32768  
SF 100.6580296 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(p-tolyl)acetamide (PO7)

2303471-PO-4CH3 13 (0.237) Cm (9:28)

**N-(p-tolyl)acetamide (PO7)**

TOF MS ES+  
5.71e7



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-nitrophenyl)acetamide (PO8)

PO4NO2

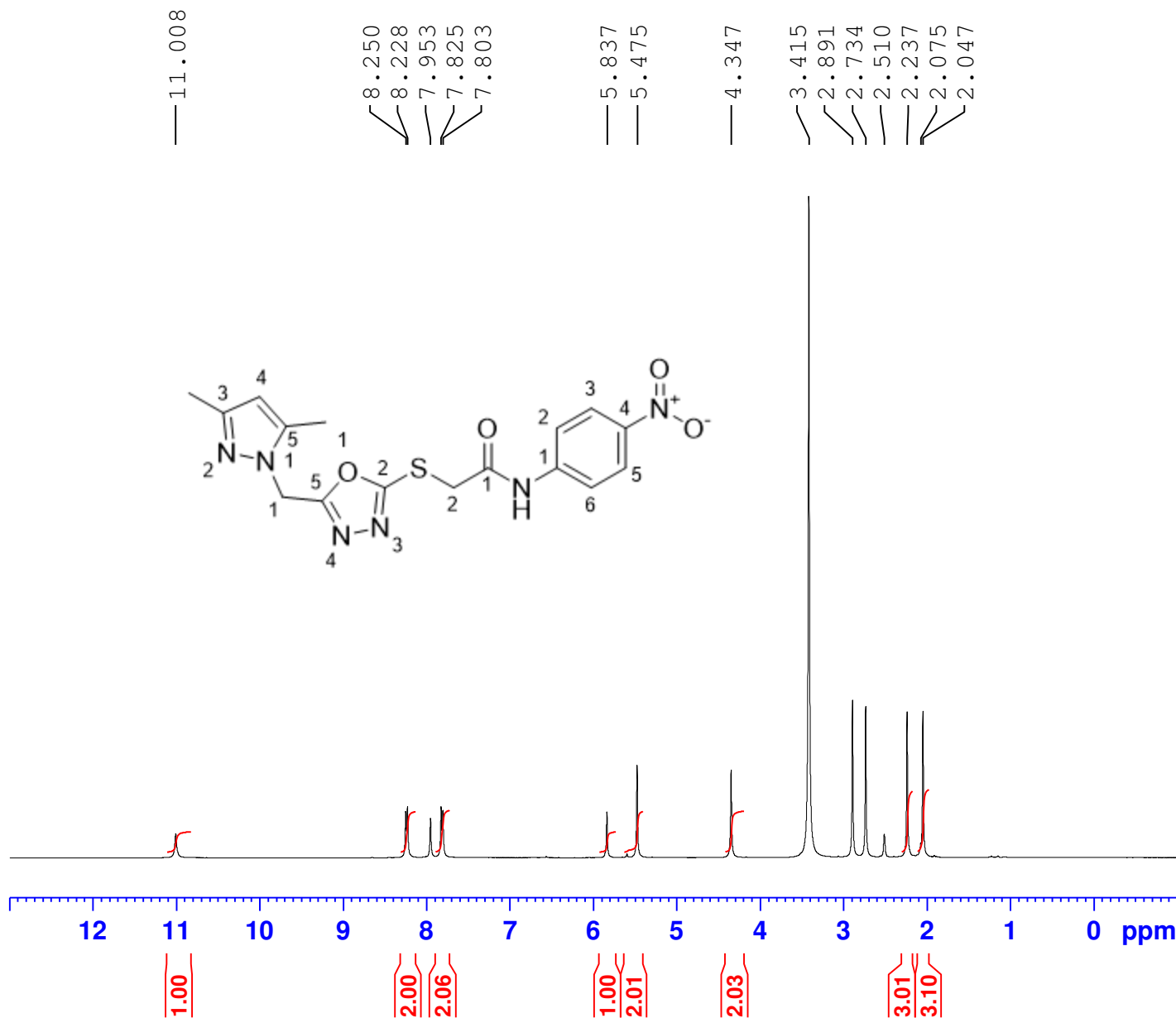
<sup>1</sup>H-NMR in DMSO



Current Data Parameters  
NAME 23000462-PO4NO2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230507  
Time 17.14 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 297.7 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



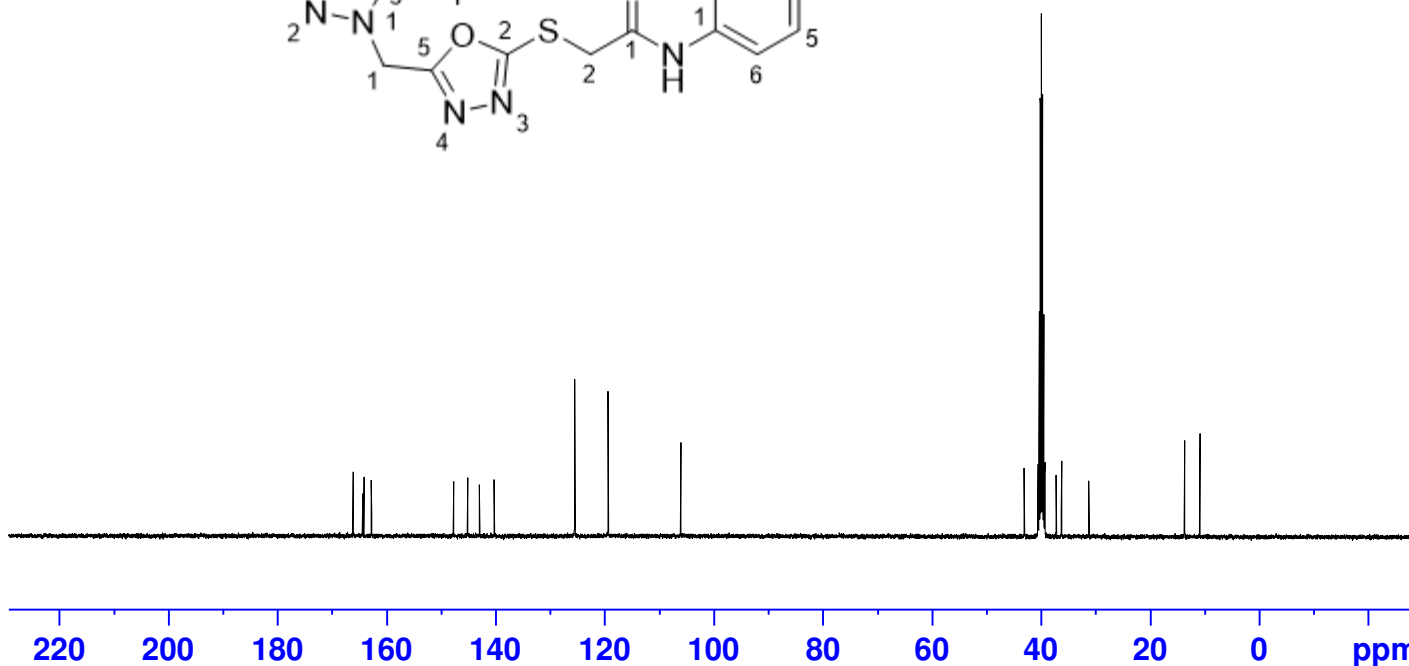
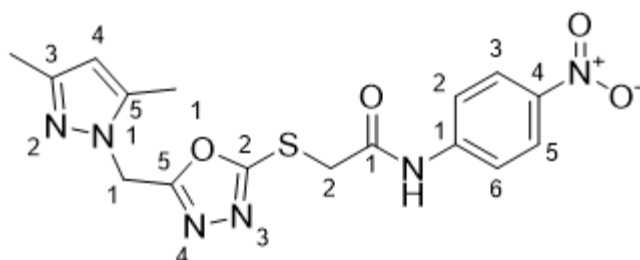
# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-nitrophenyl)acetamide (PO8)

PO4NO2  
13C-NMR in DMSO



166.166  
164.415  
164.155  
162.810  
147.723  
145.150  
142.985  
140.293  
— 125.521  
— 119.408  
— 106.044

43.105  
40.555  
40.347  
40.138  
39.929  
39.721  
39.512  
39.303  
37.250  
36.249  
31.234  
13.660  
10.865



Current Data Parameters  
NAME 23000462-PO4NO2  
EXPNO 2  
PROCNO 1

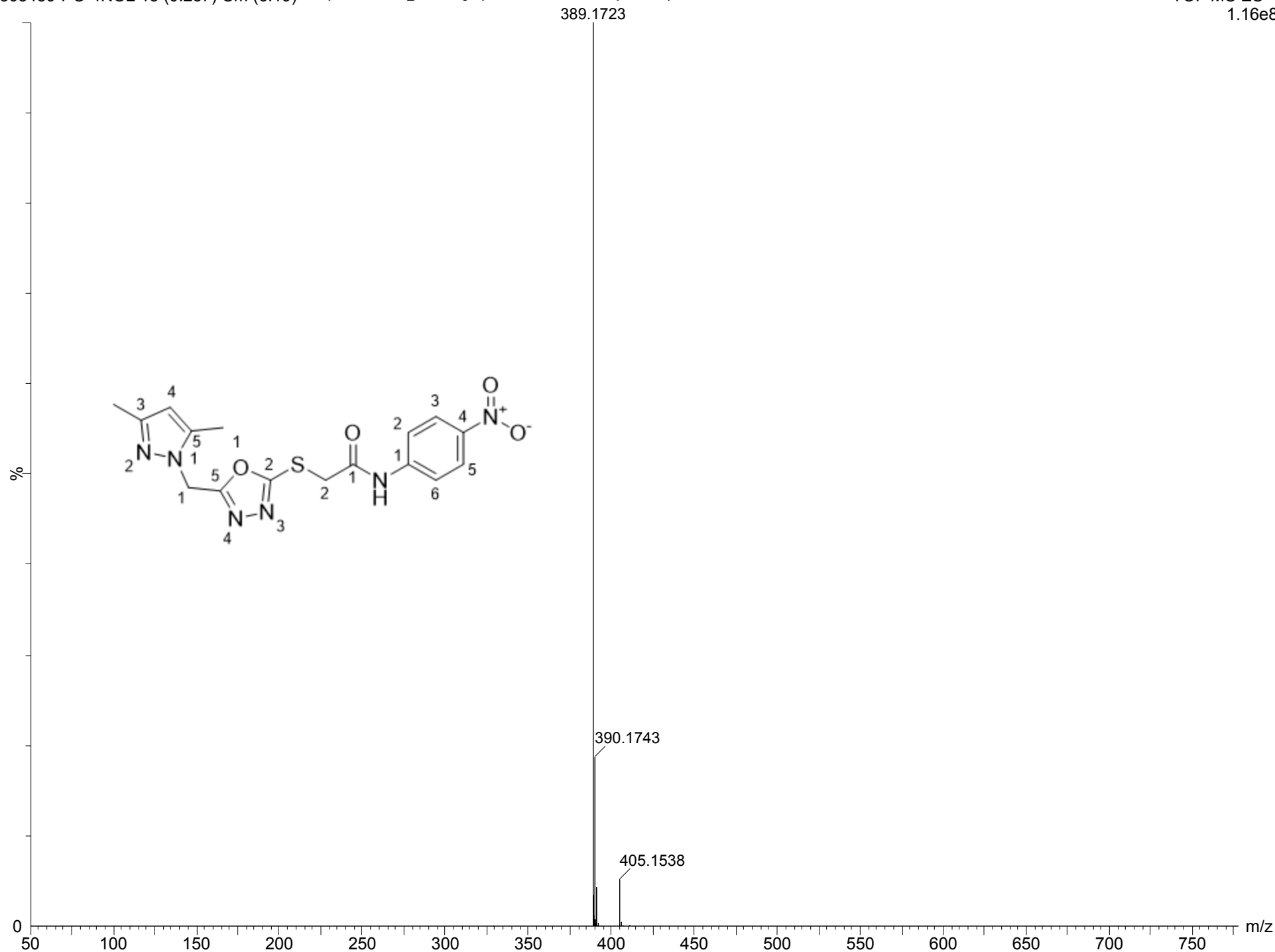
F2 - Acquisition Parameters  
Date\_ 20230508  
Time 12.49 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 600  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.794729 Hz  
AQ 1.2582912 sec  
RG 202.84  
DW 19.200 usec  
DE 6.50 usec  
TE 298.6 K  
D1 1.00000000 sec  
D11 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

Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-nitrophenyl)acetamide (PO8)

2303459-PO-4NO2 13 (0.237) Cm (6:19)

TOF MS ES+  
1.16e8





# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-methoxyphenyl)acetamide (PO9)

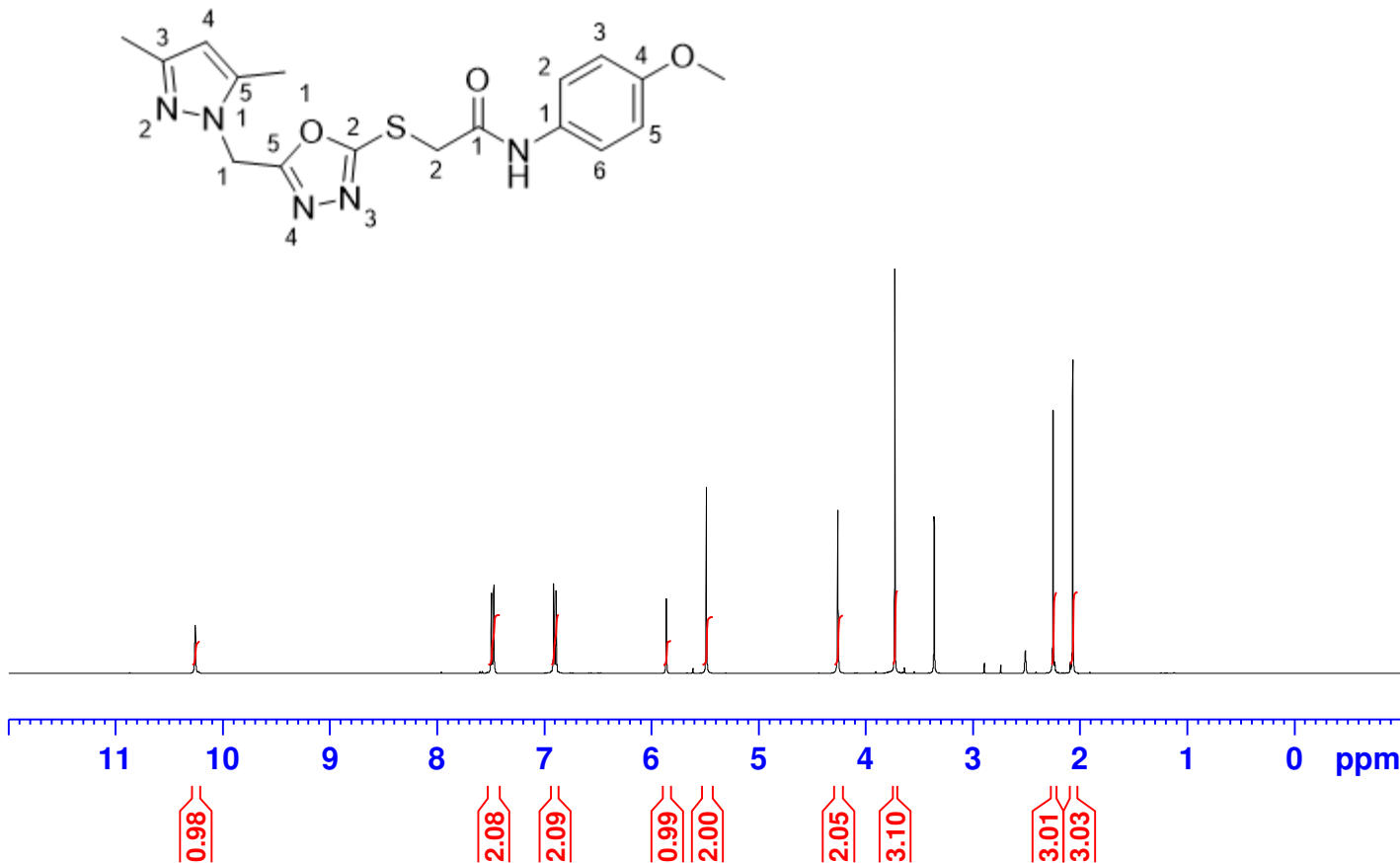
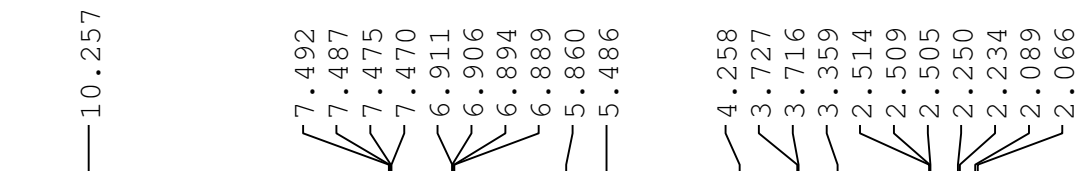
PO4MO  
1H-NMR in DMSO



Current Data Parameters  
NAME 23000459-PO4MO  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230507  
Time 17.04 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
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



# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-methoxyphenyl)acetamide (PO9)

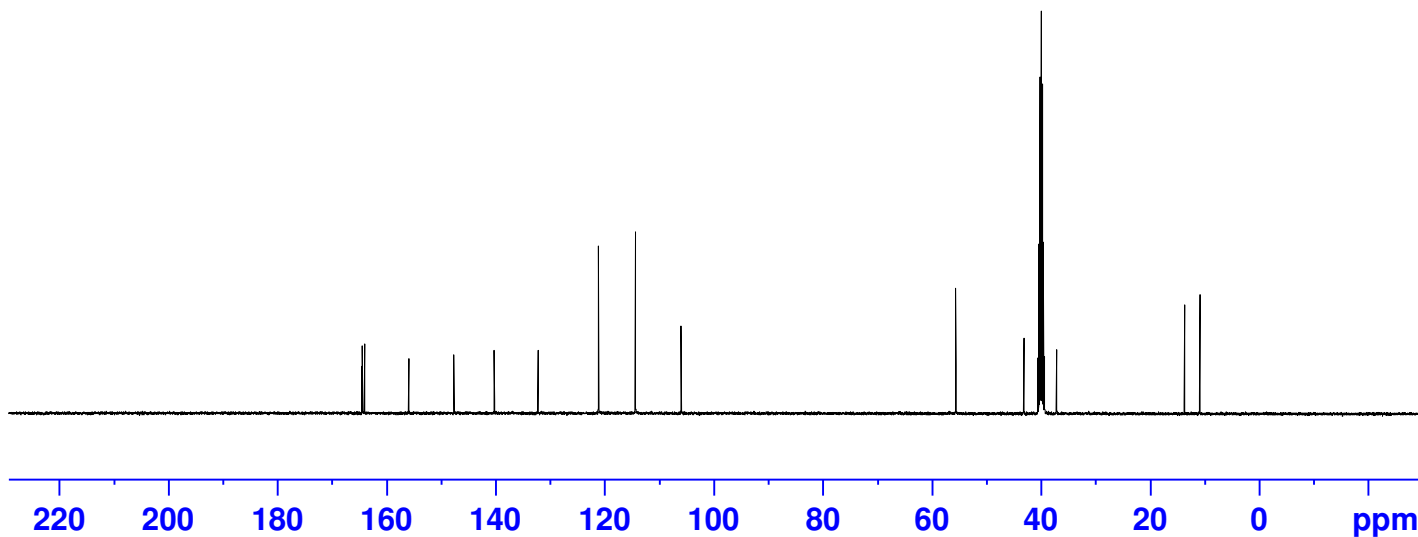
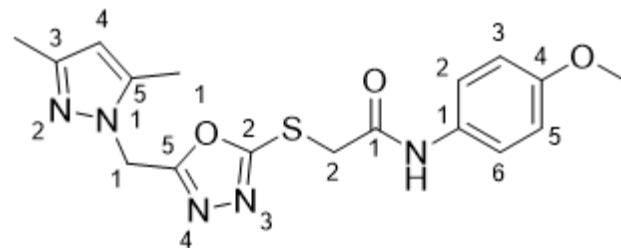
PO4MO

<sup>13</sup>C-NMR in DMSO



164.604  
164.486  
164.067  
155.957  
147.692  
140.277  
132.241  
121.192  
114.411  
106.048

55.633  
43.135  
40.616  
40.408  
40.199  
39.991  
39.782  
39.574  
39.365  
37.160  
13.701  
10.897



Current Data Parameters  
NAME 23000459-PO4MO  
EXPNO 2  
PROCNO 1

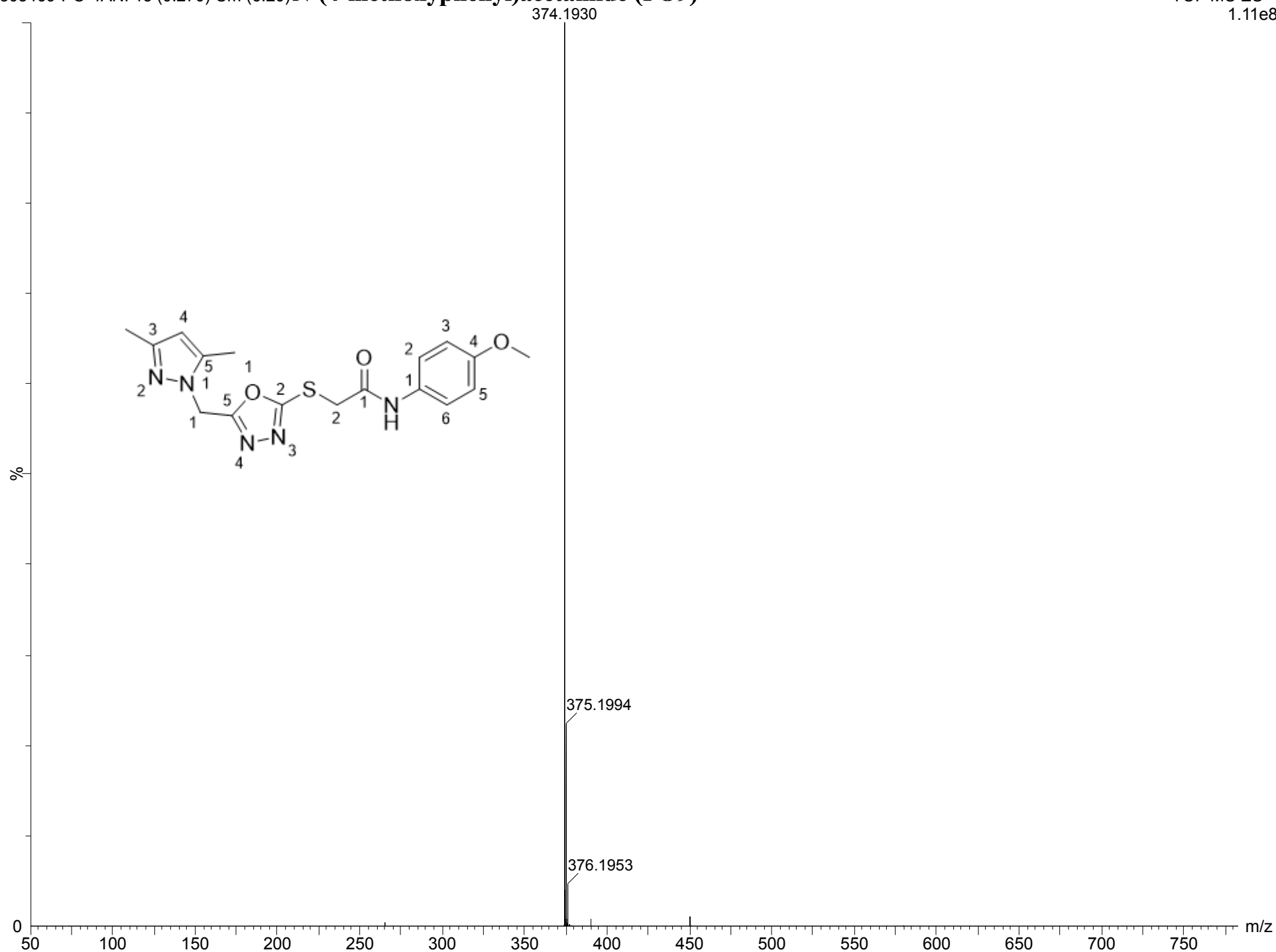
F2 - Acquisition Parameters  
Date\_ 20230508  
Time 11.16 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 600  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.794729 Hz  
AQ 1.2582912 sec  
RG 202.84  
DW 19.200 usec  
DE 6.50 usec  
TE 298.6 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6680954 MHz  
NUC1 <sup>13</sup>C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 51.02600098 W  
SFO2 400.3116012 MHz  
NUC2 <sup>1</sup>H  
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 2-(((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-

2303469-PO-4ANI 15 (0.270) Cm (6:20) **N-(4-methoxyphenyl)acetamide (PO9)**

TOF MS ES+  
1.11e8



# <sup>1</sup>H NMR of N-(4-chlorophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO10)

PO4C1

<sup>1</sup>H-NMR in DMSO



— 10.532

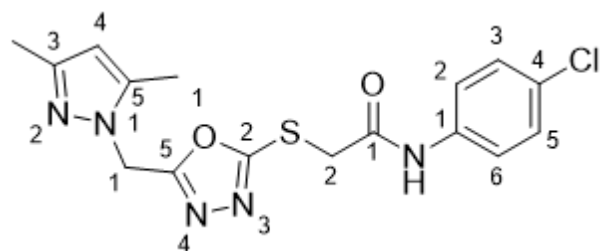
7.607  
7.585  
7.395  
7.373

5.849  
5.478

— 4.283

— 3.372

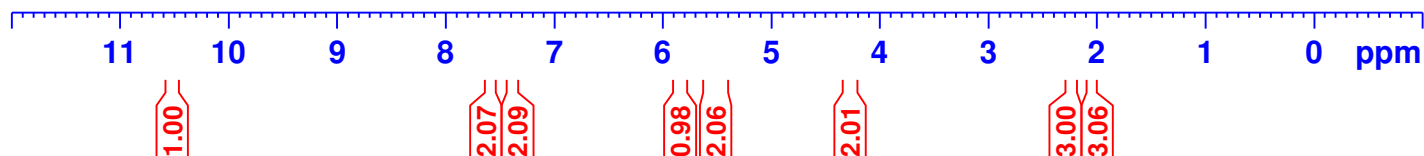
2.509  
2.241  
2.090  
2.082  
2.057



Current Data Parameters  
NAME 23000461-PO4C1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230507  
Time 17.11 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 32.13  
DW 62.400 usec  
DE 17.09 usec  
TE 297.7 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



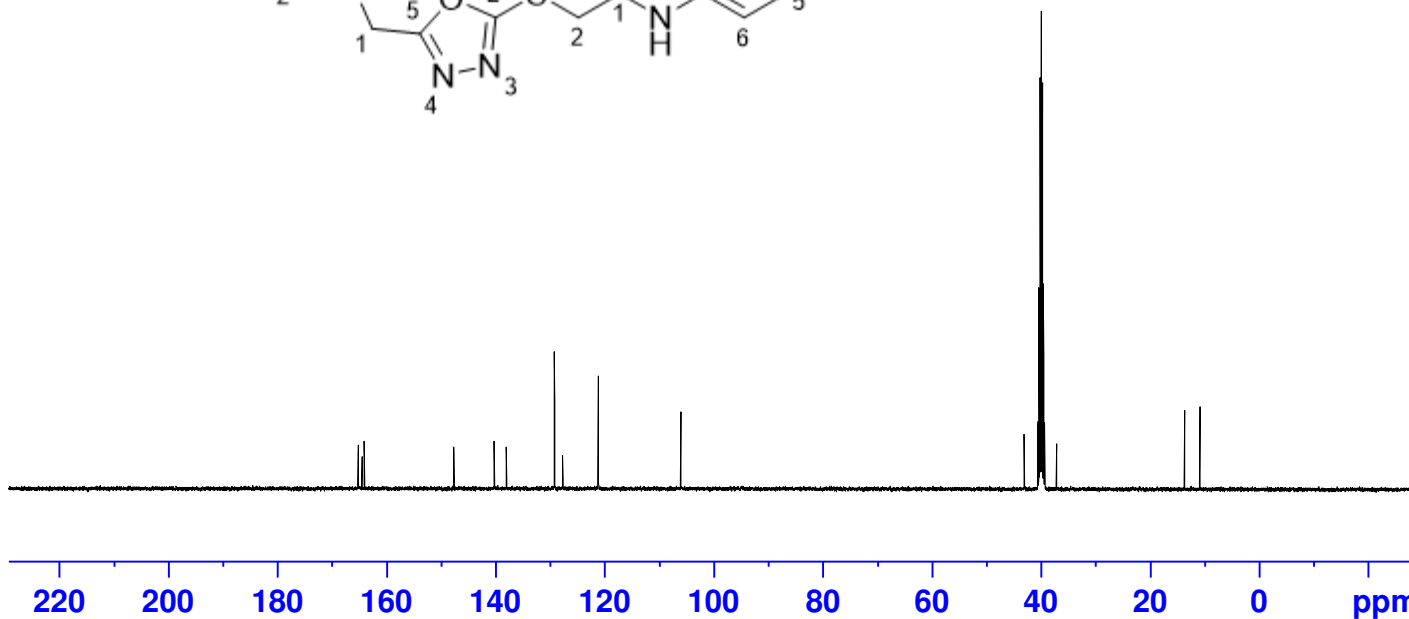
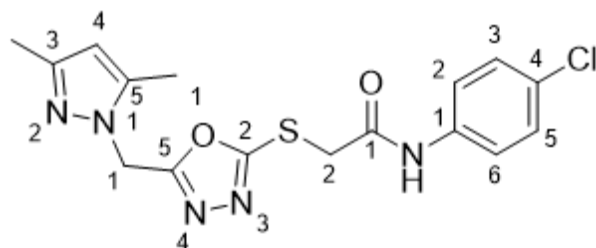
# <sup>13</sup>C NMR of N-(4-chlorophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO10)

PO4C1  
13C-NMR in DMSO



165.234  
164.508  
164.105  
147.699  
140.278  
138.044  
129.232  
127.717  
121.190  
— 106.044

43.120  
40.599  
40.391  
40.182  
39.974  
39.765  
39.556  
39.348  
37.162  
13.692  
10.889



Current Data Parameters  
NAME 23000461-PO4C1  
EXPNO 2  
PROCNO 1

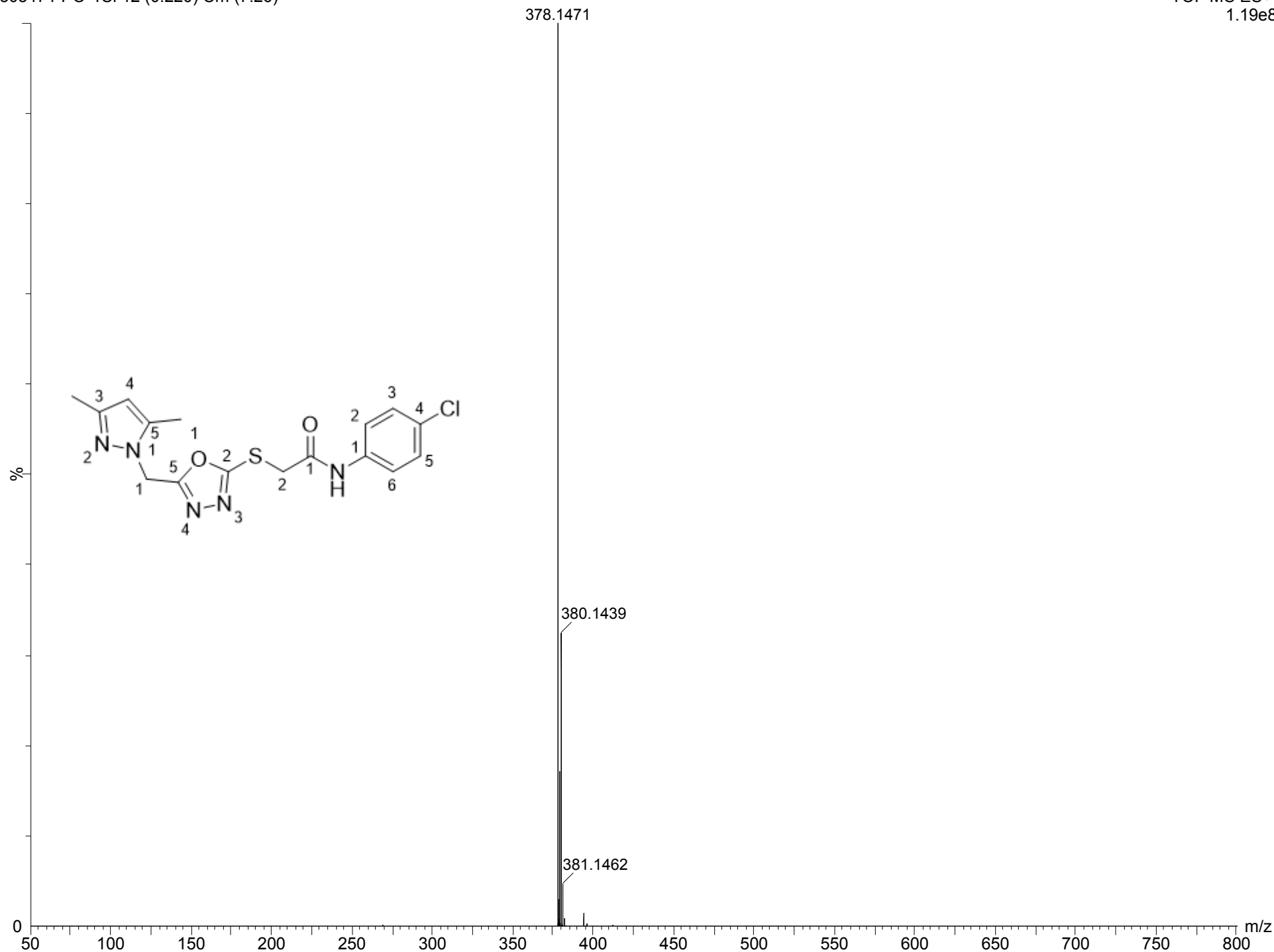
F2 - Acquisition Parameters  
Date\_ 20230508  
Time 12.22 h  
INSTRUM spect  
PROBHD Z108618\_0984 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 600  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.794729 Hz  
AQ 1.2582912 sec  
RG 202.84  
DW 19.200 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
D11 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 N-(4-chlorophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO10)**

2303474-PO-4Cl 12 (0.220) Cm (7:26)

TOF MS ES+  
1.19e8



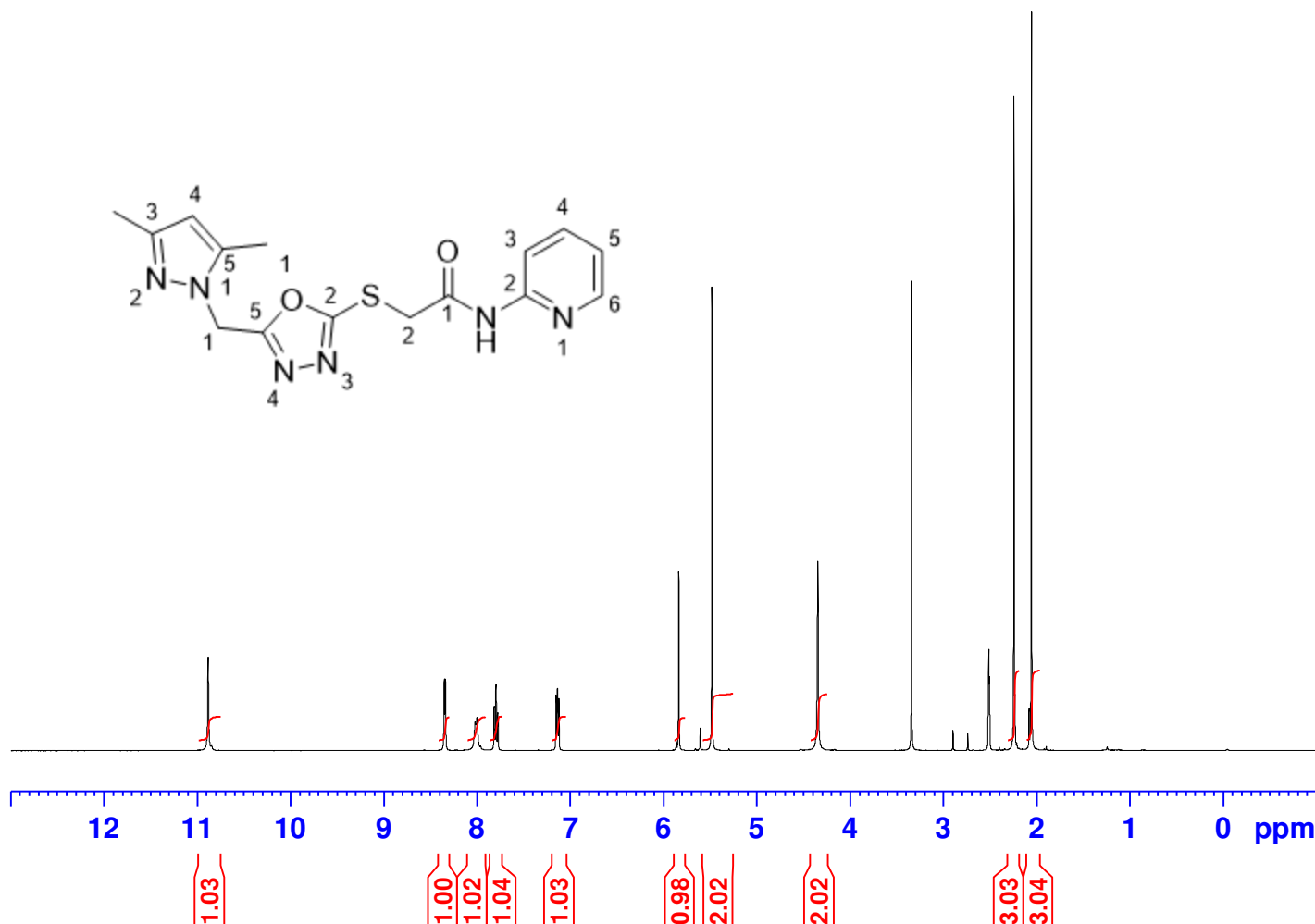
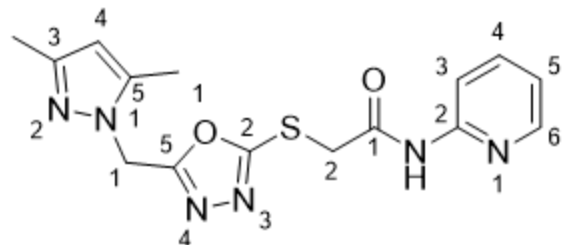
# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(pyridin-2-yl)acetamide (PO11)

PO2AP

<sup>1</sup>H-NMR in DMSO



10.882  
8.351  
8.349  
8.347  
8.341  
8.339  
8.337  
8.019  
8.000  
7.817  
7.813  
7.795  
7.778  
7.773  
7.152  
7.150  
7.140  
7.138  
7.134  
7.132  
7.122  
7.120  
5.835  
5.480  
4.345  
3.339  
2.514  
2.509  
2.505  
2.241  
2.231  
2.054



Current Data Parameters  
NAME 23000441-PO2AP  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230501  
Time 13.46 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 297.6 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

# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(pyridin-2-yl)acetamide (PO11)

PO2AP

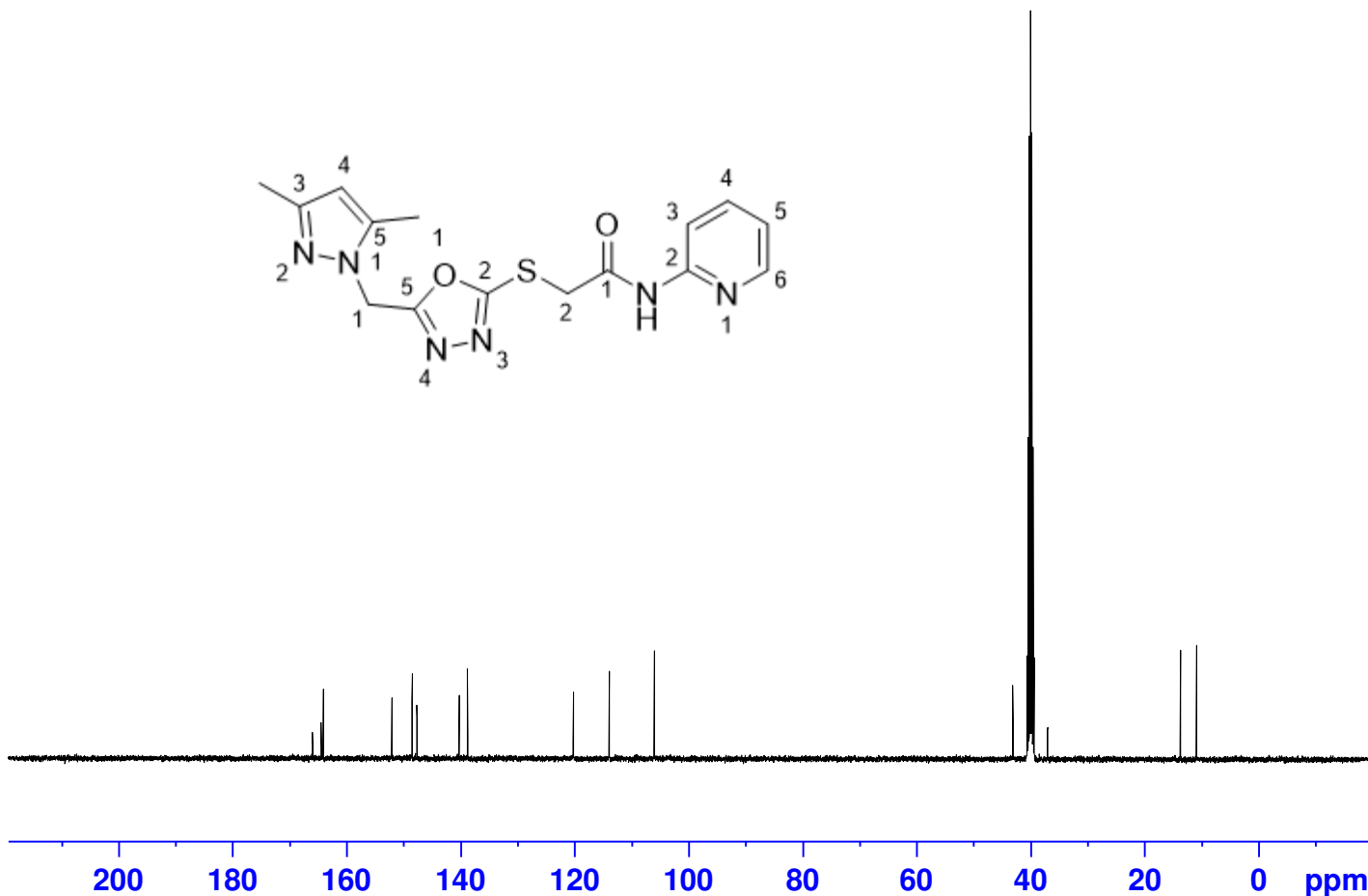
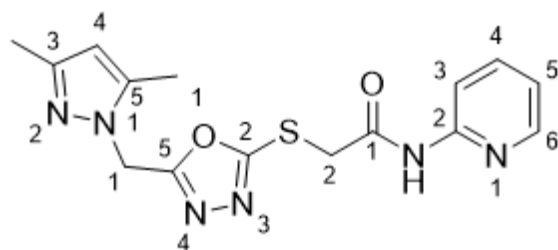
<sup>13</sup>C-NMR in DMSO



166.002  
164.477  
164.116  
152.047  
148.542  
147.680  
140.264  
138.806

— 120.236  
— 113.928  
— 106.016

43.125  
40.627  
40.418  
40.210  
40.001  
39.792  
39.584  
39.375  
37.043  
13.698  
10.887

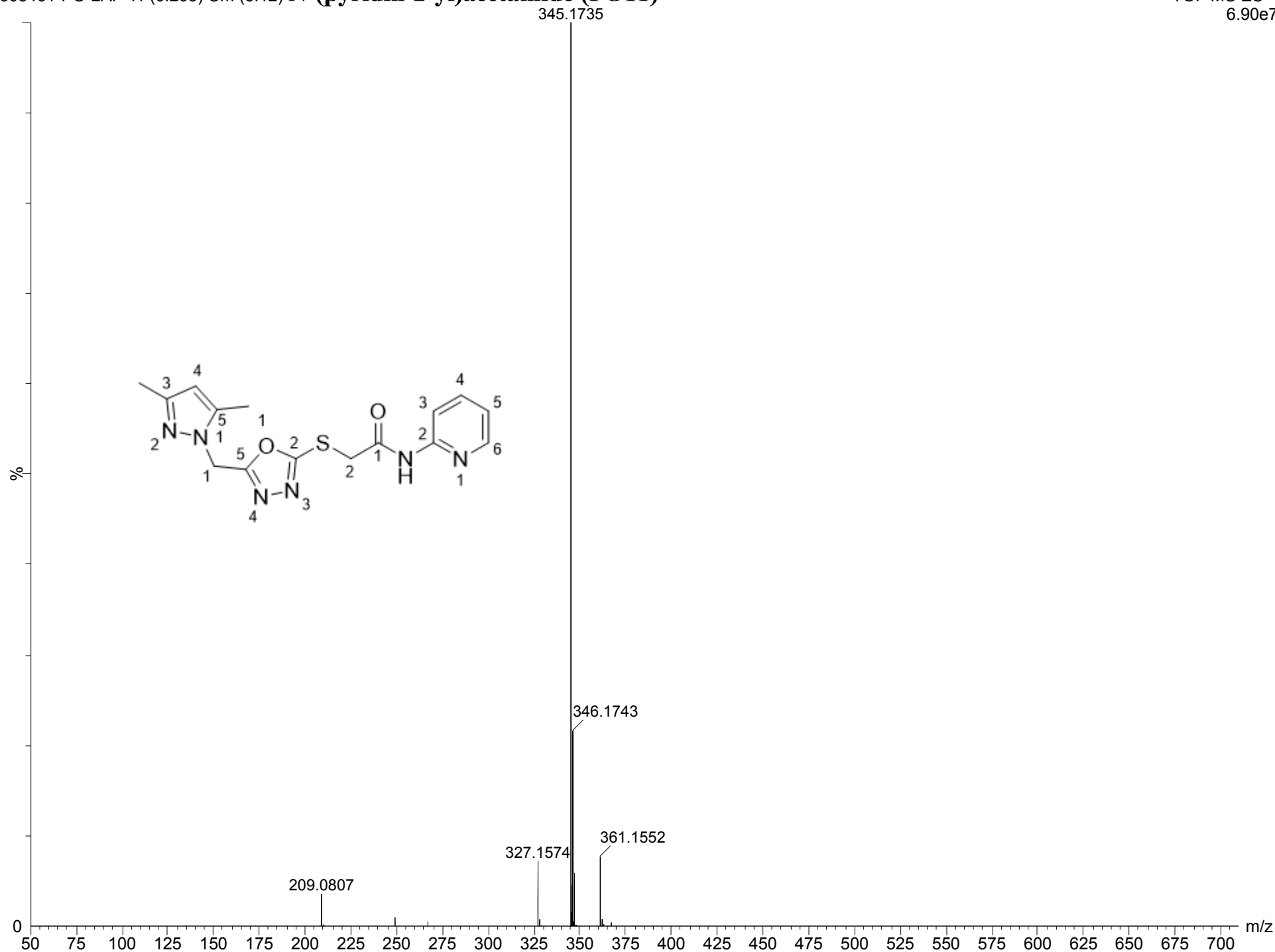


Current Data Parameters  
NAME 23000441-PO2AP  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230501  
Time 14.12 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 601  
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





# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(2-nitrophenyl)acetamide (PO12)

PO2NO2

<sup>1</sup>H-NMR in DMSO



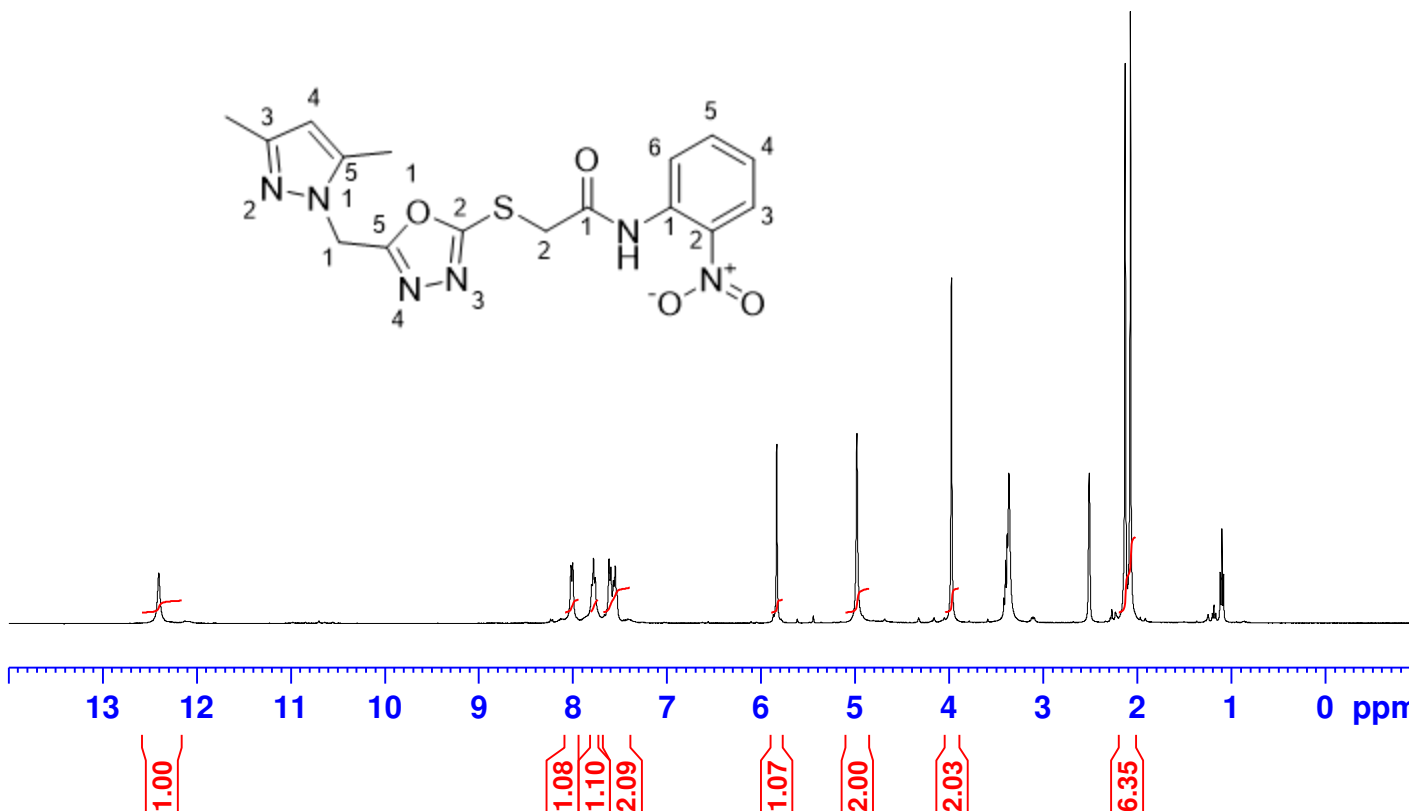
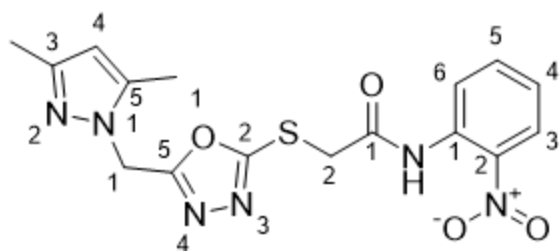
Current Data Parameters  
NAME 23000438-PO2NO2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230430  
Time 13.42 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 299.4 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

—12.403

8.020  
8.001  
7.799  
7.781  
7.763  
7.615  
7.596  
7.569  
7.550  
7.532  
5.832  
— 4.980  
3.974  
3.400  
3.382  
3.364  
2.510  
2.127  
2.072  
1.117  
1.099  
1.082

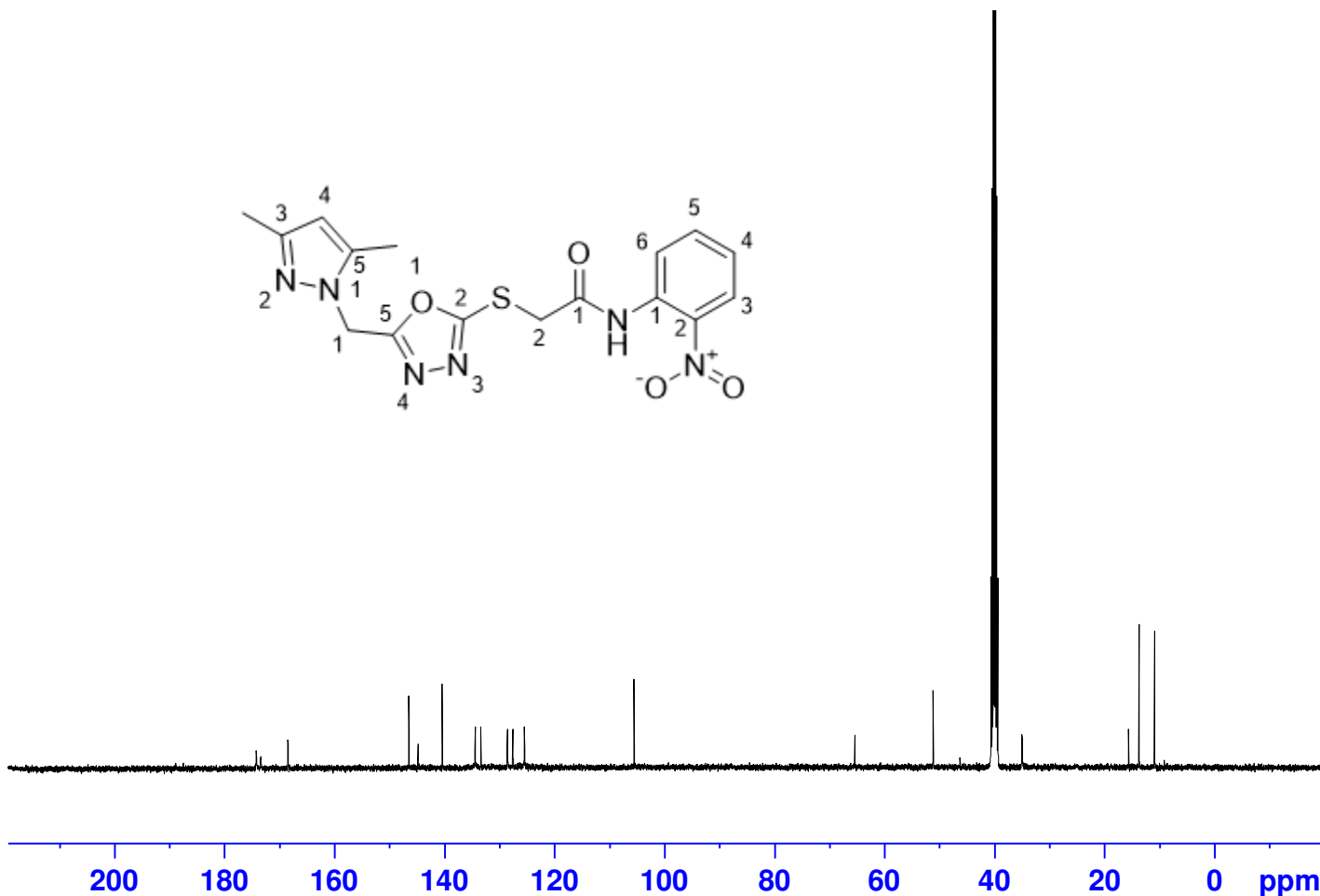
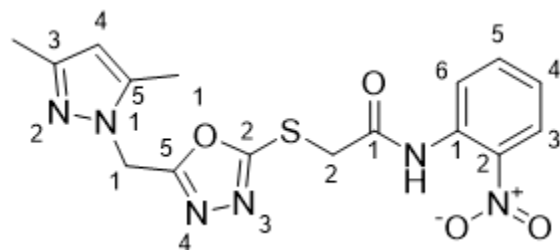


# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(2-nitrophenyl)acetamide (PO12)

PO2NO2  
13C-NMR in DMSO



174.273  
173.420  
168.482  
146.489  
144.804  
140.431  
134.429  
133.413  
128.583  
127.576  
125.498  
105.551  
65.384  
51.168  
34.997  
15.638  
13.698  
10.866



Current Data Parameters  
NAME 23000438-PO2NO2  
EXPNO 2  
PROCNO 1

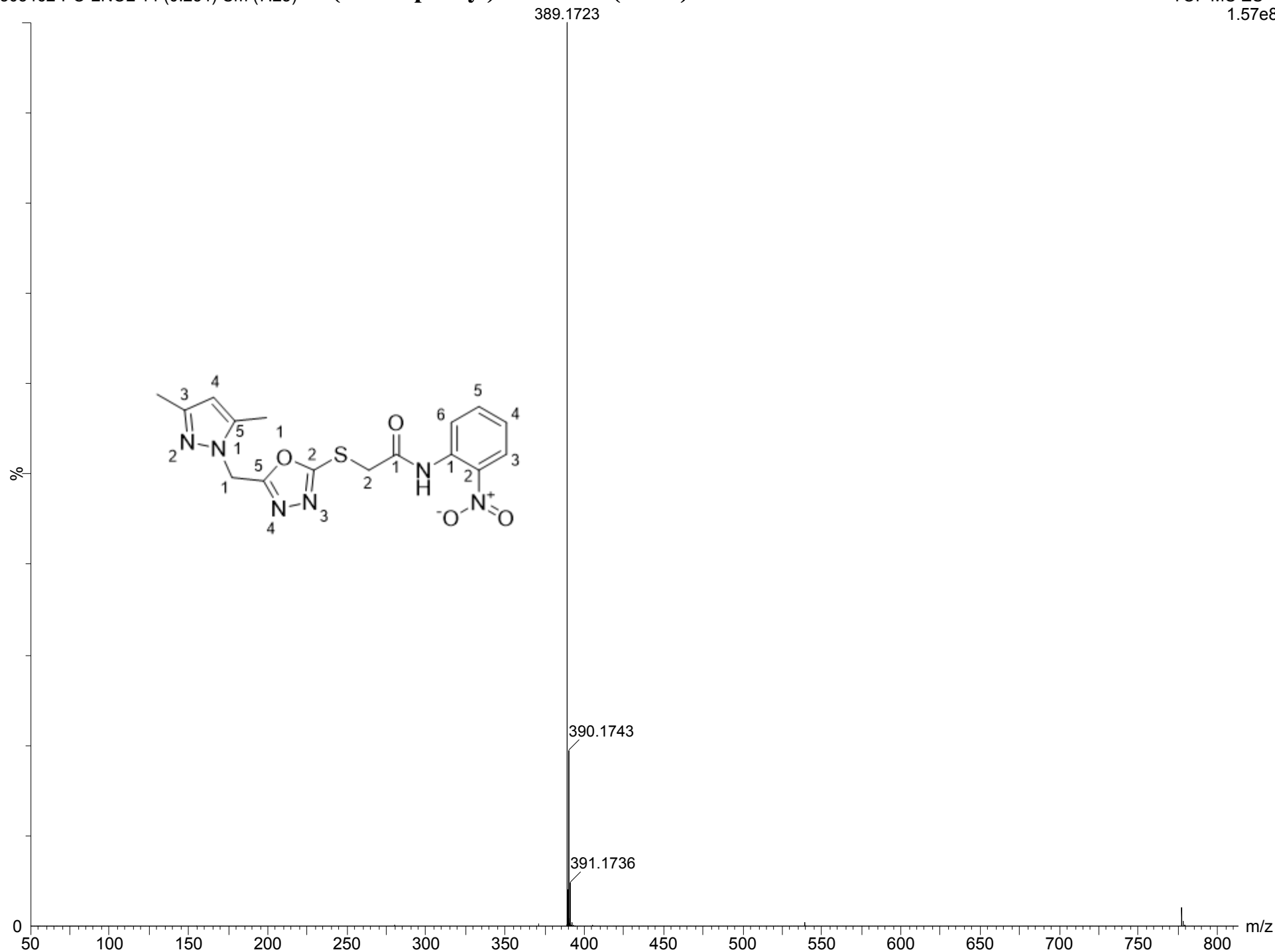
F2 - Acquisition Parameters  
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Time 15.22 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2048  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 202.84  
DW 20.800 usec  
DE 6.50 usec  
TE 298.9 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

Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-  
N-(2-nitrophenyl)acetamide (PO12)

2303462-PO-2NO2 14 (0.254) Cm (7:25)

TOF MS ES+  
1.57e8



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-ethoxyphenyl)acetamide (PO13)

POPP  
1H-NMR in DMSO



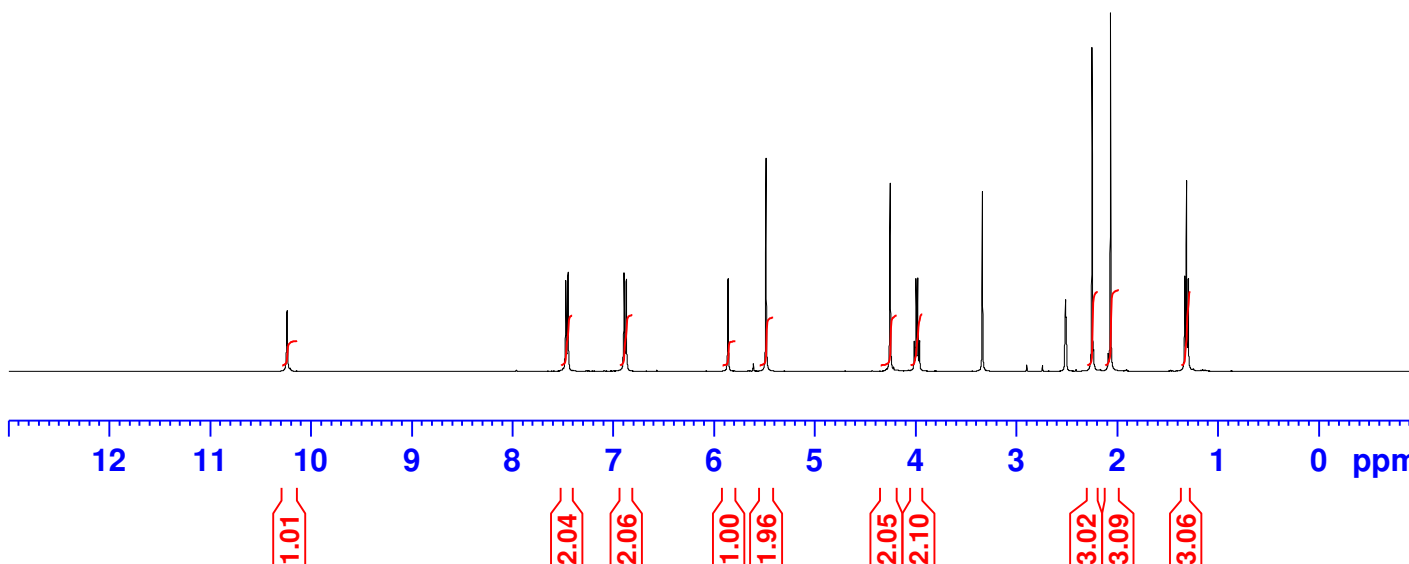
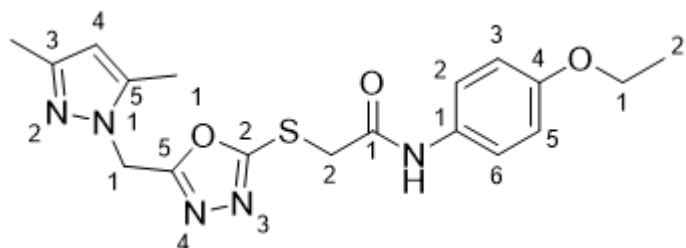
Current Data Parameters  
NAME 23000435-POPP  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230429  
Time 16.17 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 297.9 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

— 10.236

7.470  
7.448  
6.892  
6.870  
5.860  
5.483  
4.251  
4.012  
3.994  
3.977  
3.960  
3.336  
2.514  
2.509  
2.505  
2.248  
2.234  
2.088  
2.065  
1.328  
1.310  
1.293

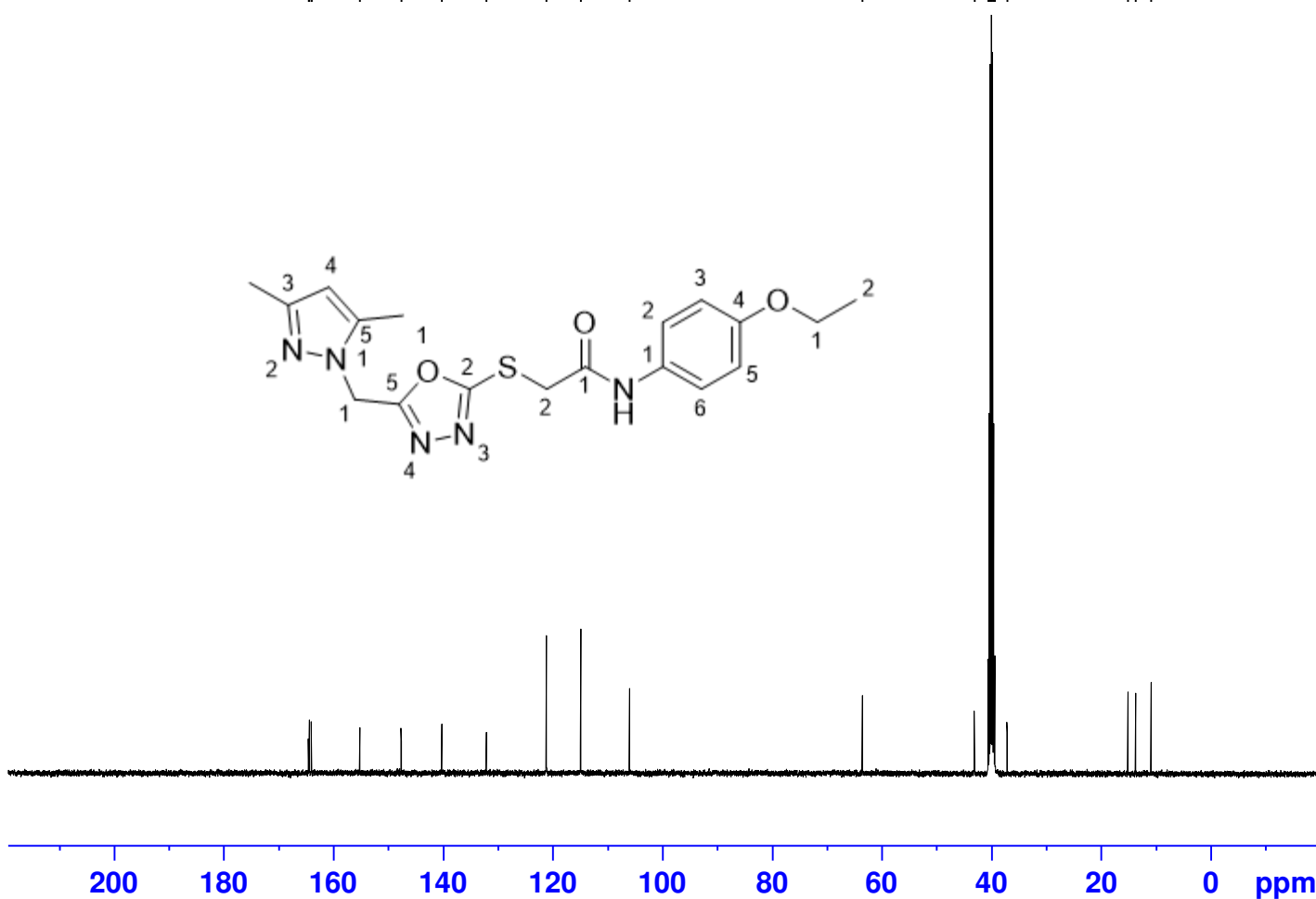
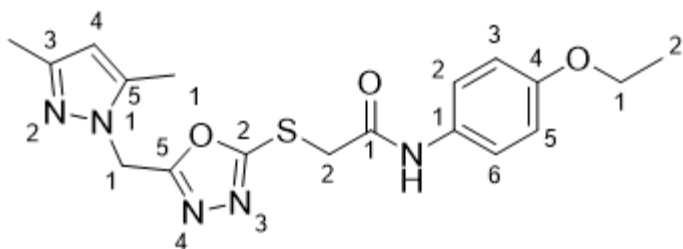


# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-ethoxyphenyl)acetamide (PO13)

POPP  
13C-NMR in DMSO



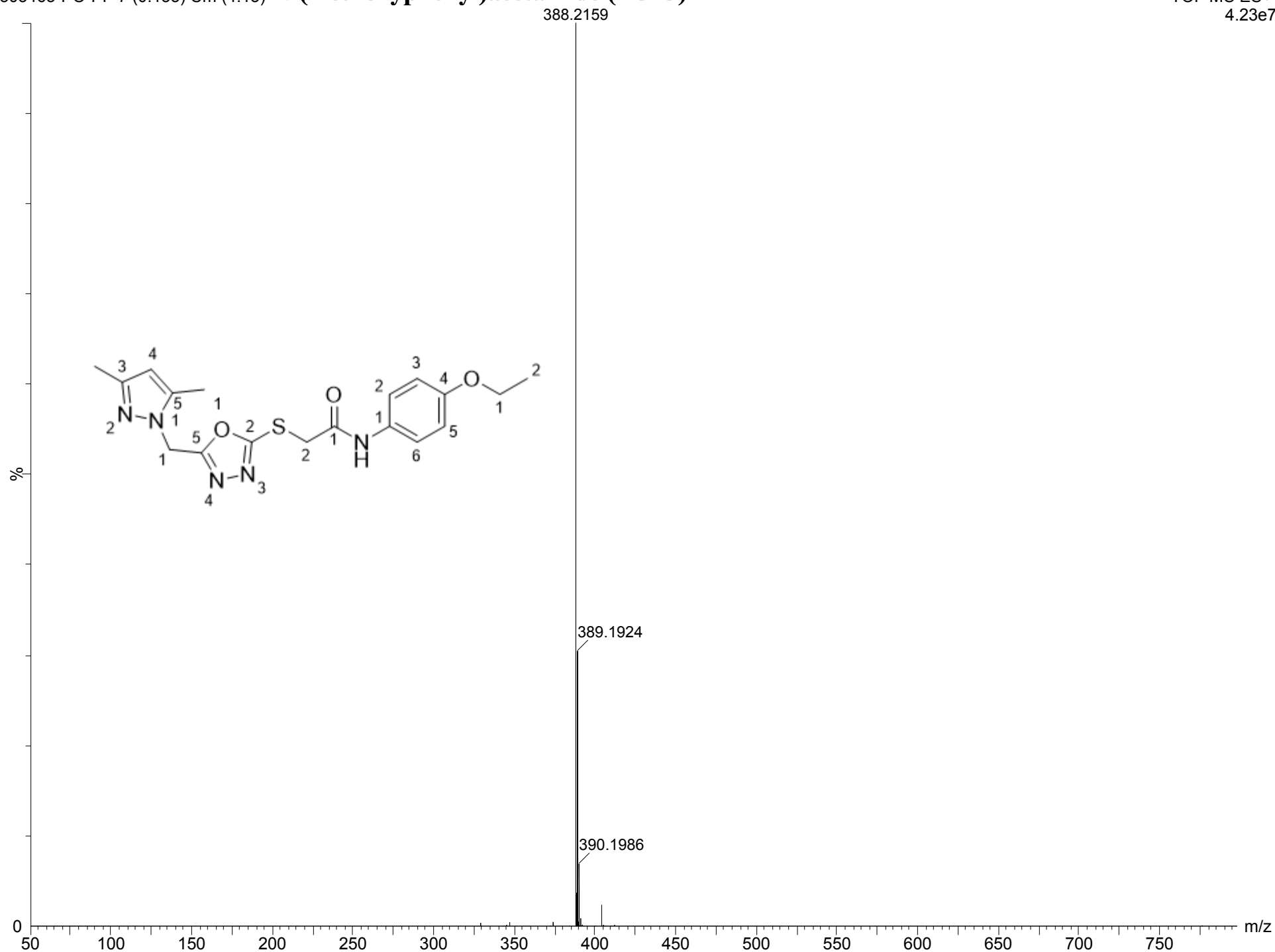
164.593  
164.458  
164.067  
155.217  
147.680  
140.271  
132.140  
121.173  
114.934  
106.044  
63.565  
43.136  
40.632  
40.424  
40.215  
40.007  
39.798  
39.589  
39.381  
37.159  
15.139  
13.709  
10.901



Current Data Parameters  
NAME 23000435-POPP  
EXPNO 2  
PROCNO 1

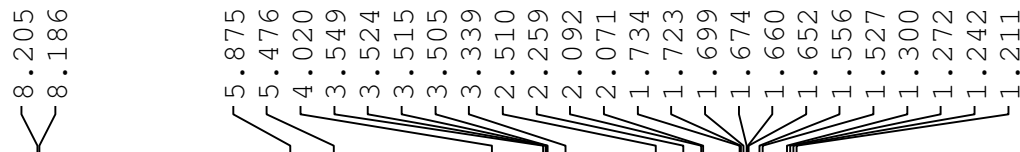
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Time 17.26 h  
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PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 536  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 202.84  
DW 20.800 usec  
DE 6.50 usec  
TE 297.9 K  
D1 1.00000000 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



# <sup>1</sup>H NMR of N-cyclohexyl-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO14)

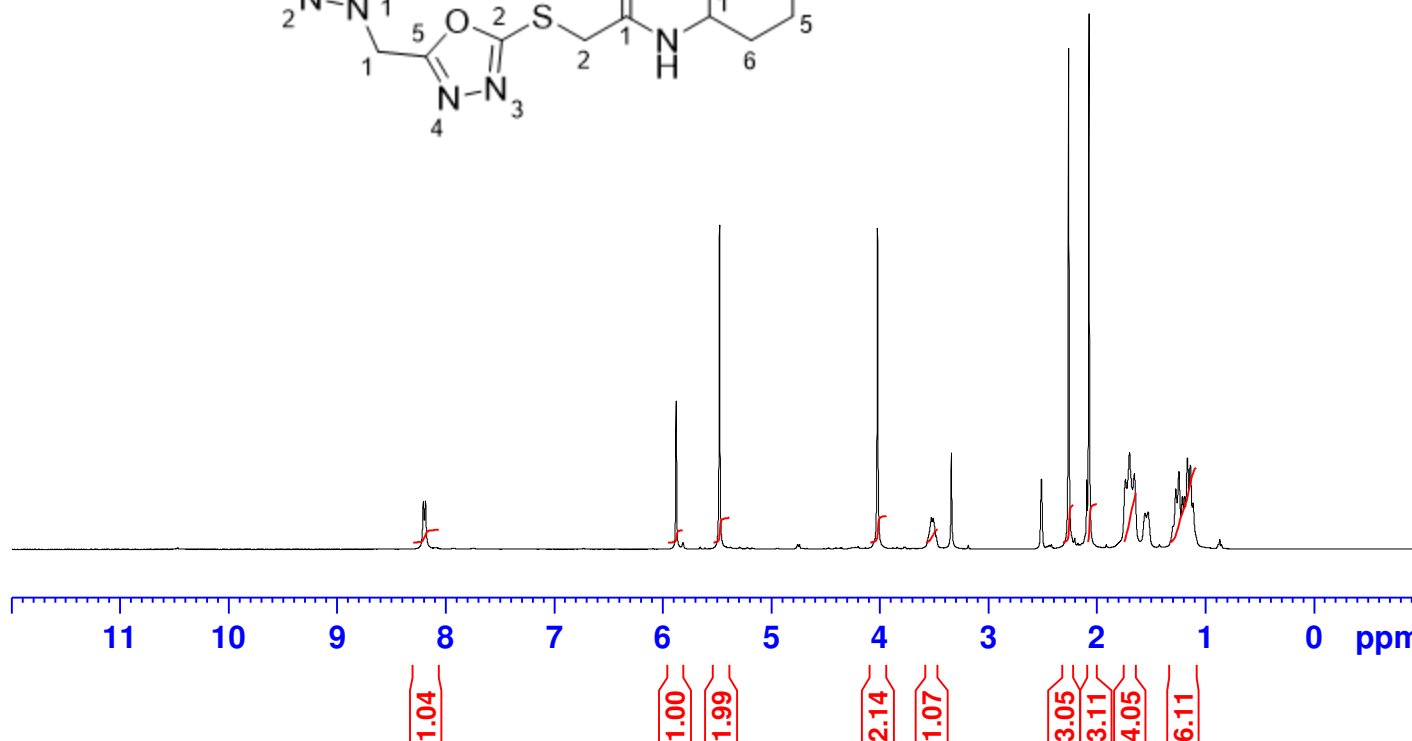
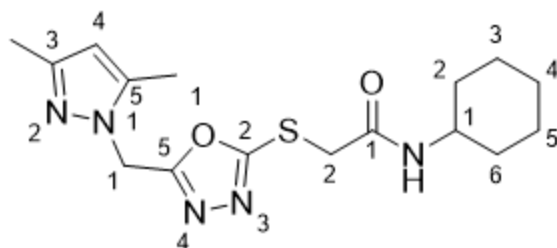
POCyclo  
1H-NMR in DMSO



Current Data Parameters  
NAME 23000433-POCyclo  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230428  
Time 18.52 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 297.9 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

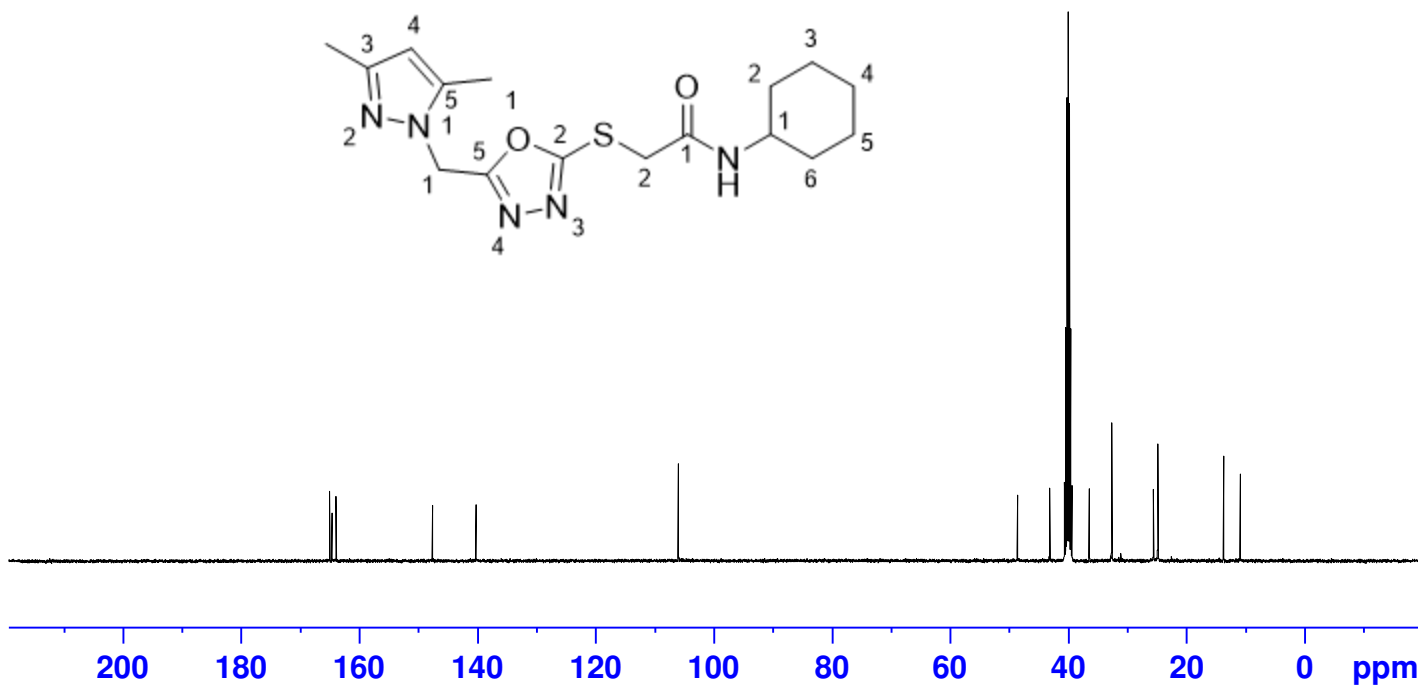
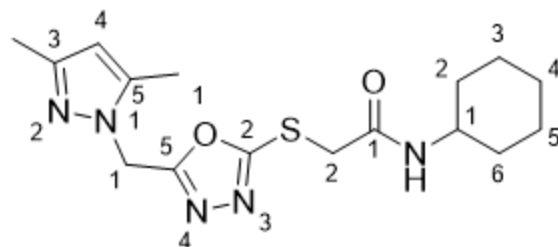
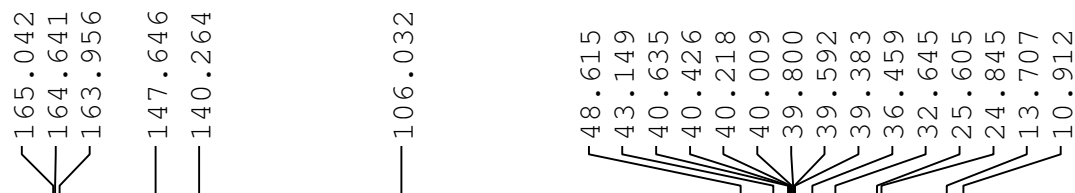
F2 - Processing parameters  
SI 65536  
SF 400.3100000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





# <sup>13</sup>C NMR of N-cyclohexyl-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO14)

POCyclo  
13C-NMR in DMSO



Current Data Parameters  
NAME 23000433-POCyclo  
EXPNO 2  
PROCNO 1

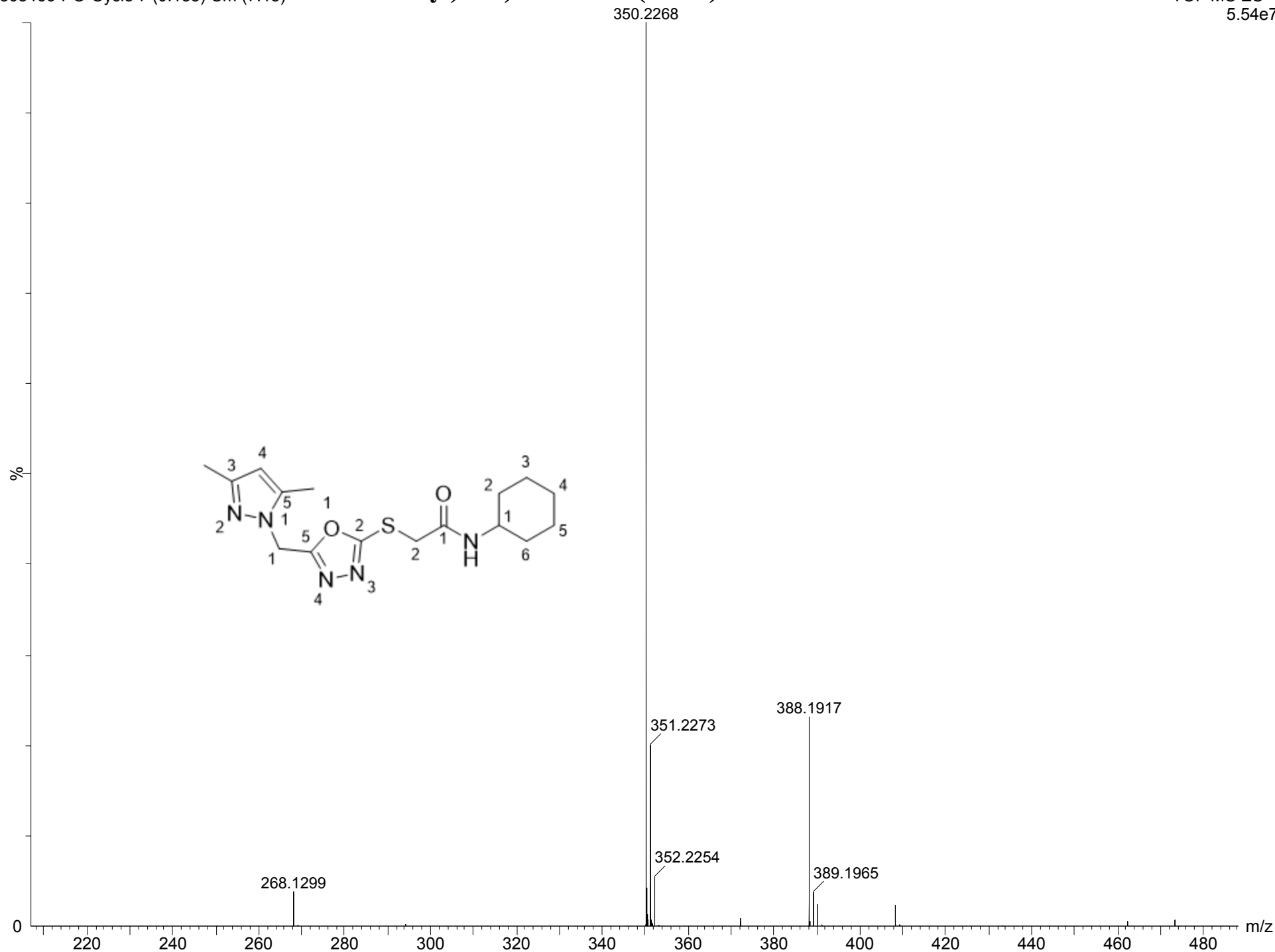
F2 - Acquisition Parameters  
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Time 12.35 h  
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PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 202.84  
DW 20.800 usec  
DE 6.50 usec  
TE 299.1 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 N-cyclohexyl-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO14)

2303466-PO-Cyclo 7 (0.135) Cm (7:15)

TOF MS ES+  
5.54e7



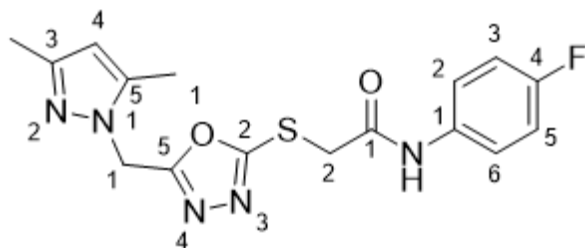
# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-fluorophenyl)acetamide (PO15)

POF  
1H-NMR in DMSO



— 10.455

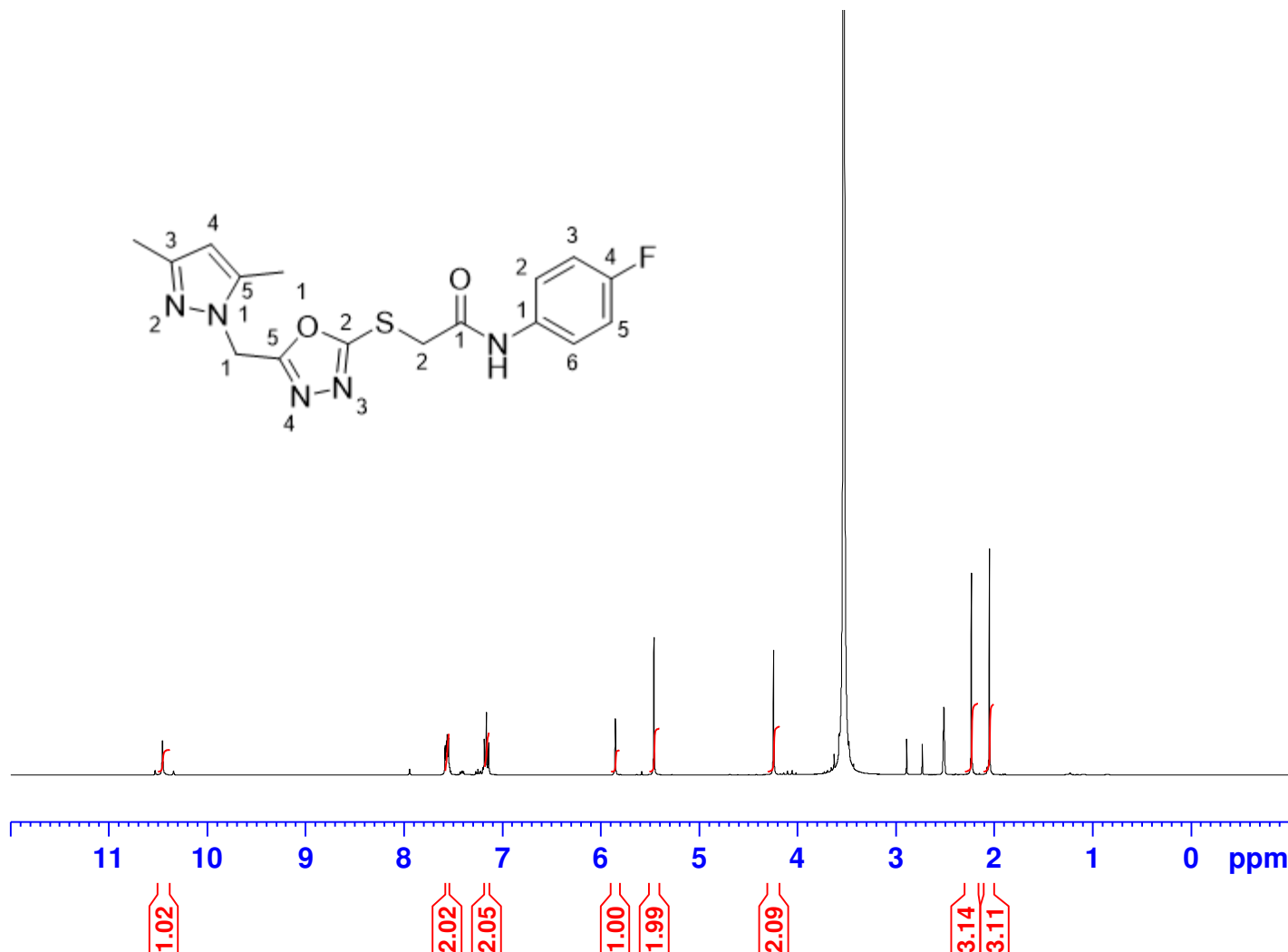
7.581  
7.569  
7.563  
7.559  
7.552  
7.546  
7.183  
7.161  
7.138  
— 5.851  
— 5.458  
4.242  
3.628  
3.576  
3.571  
3.476  
2.889  
2.731  
2.514  
2.510  
2.505  
2.231  
2.047



Current Data Parameters  
NAME 23000429-POF  
EXPNO 1  
PROCNO 1

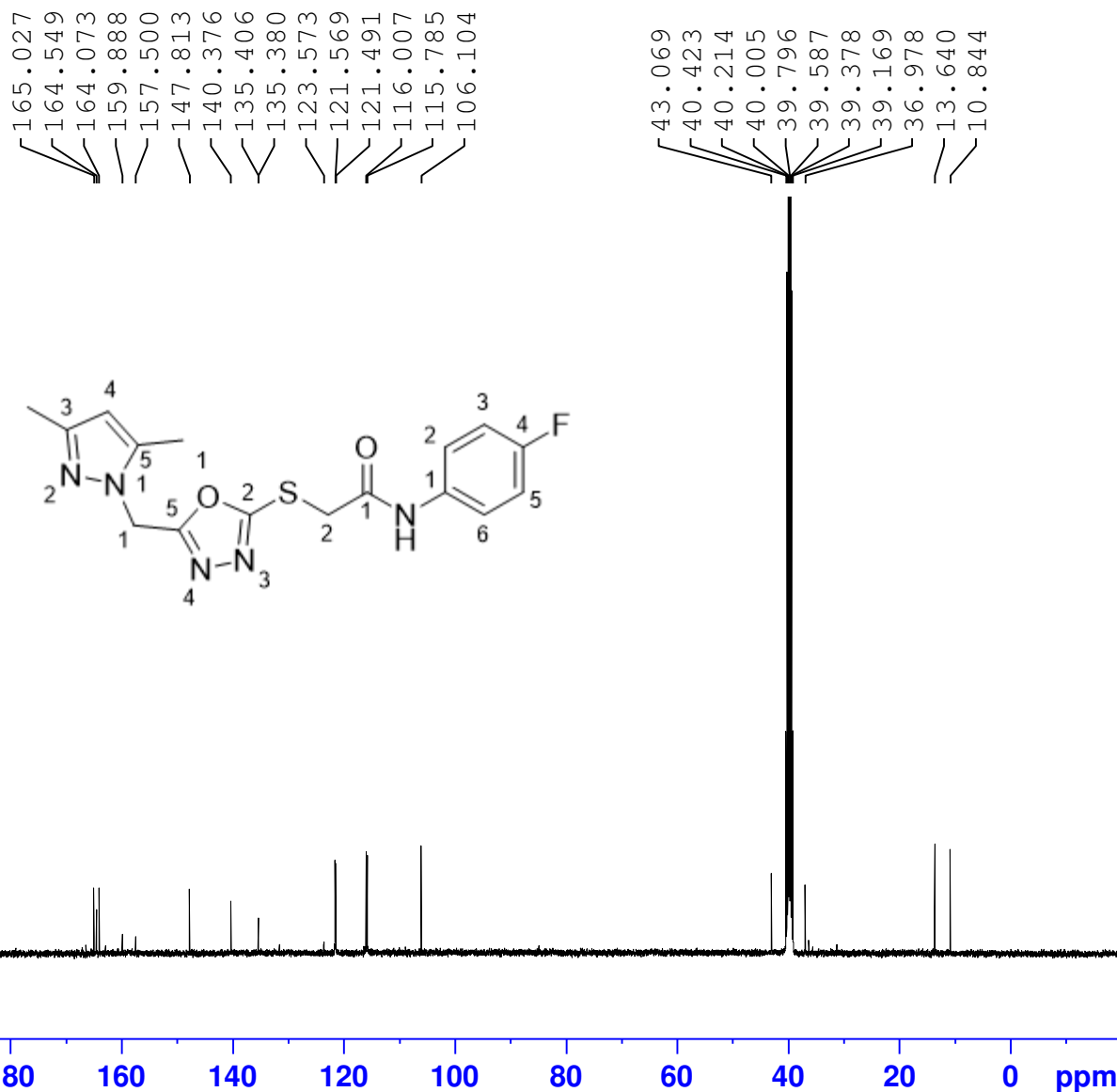
F2 - Acquisition Parameters  
Date\_ 20230427  
Time 14.11 h  
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PROBHD Z108618\_0984 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 32.13  
DW 62.400 usec  
DE 17.09 usec  
TE 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



# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-fluorophenyl)acetamide (PO15)

POF  
13C-NMR in DMSO



Current Data Parameters  
NAME 23000429-POF  
EXPNO 2  
PROCNO 1

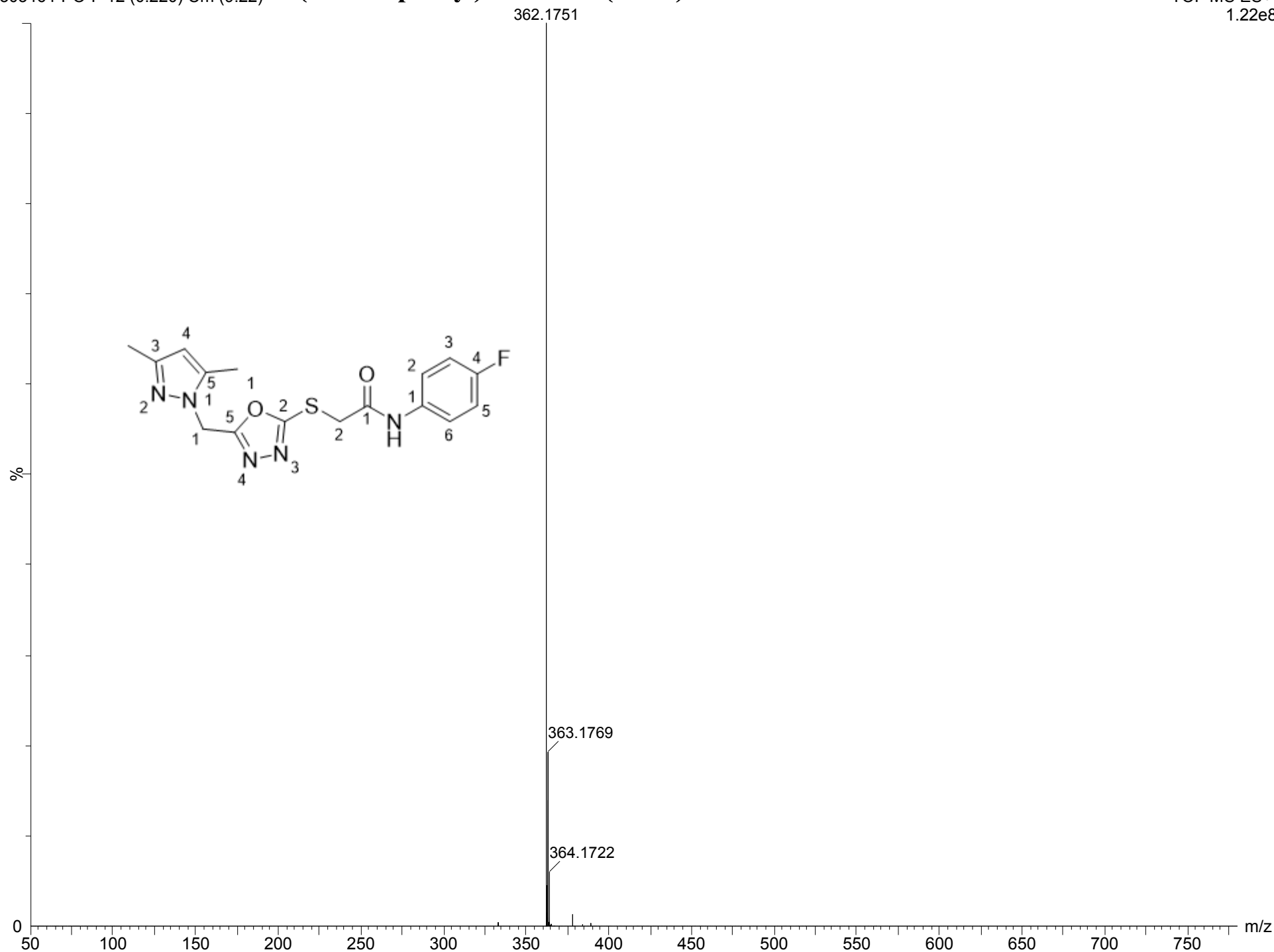
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Date\_ 20230427  
Time 17.18 h  
INSTRUM spect  
PROBHD Z108618\_0984 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1684  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 202.84  
DW 20.800 usec  
DE 6.50 usec  
TE 299.0 K  
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

2303464-PO-F 12 (0.220) Cm (9:22)

**Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-fluorophenyl)acetamide (PO15)**

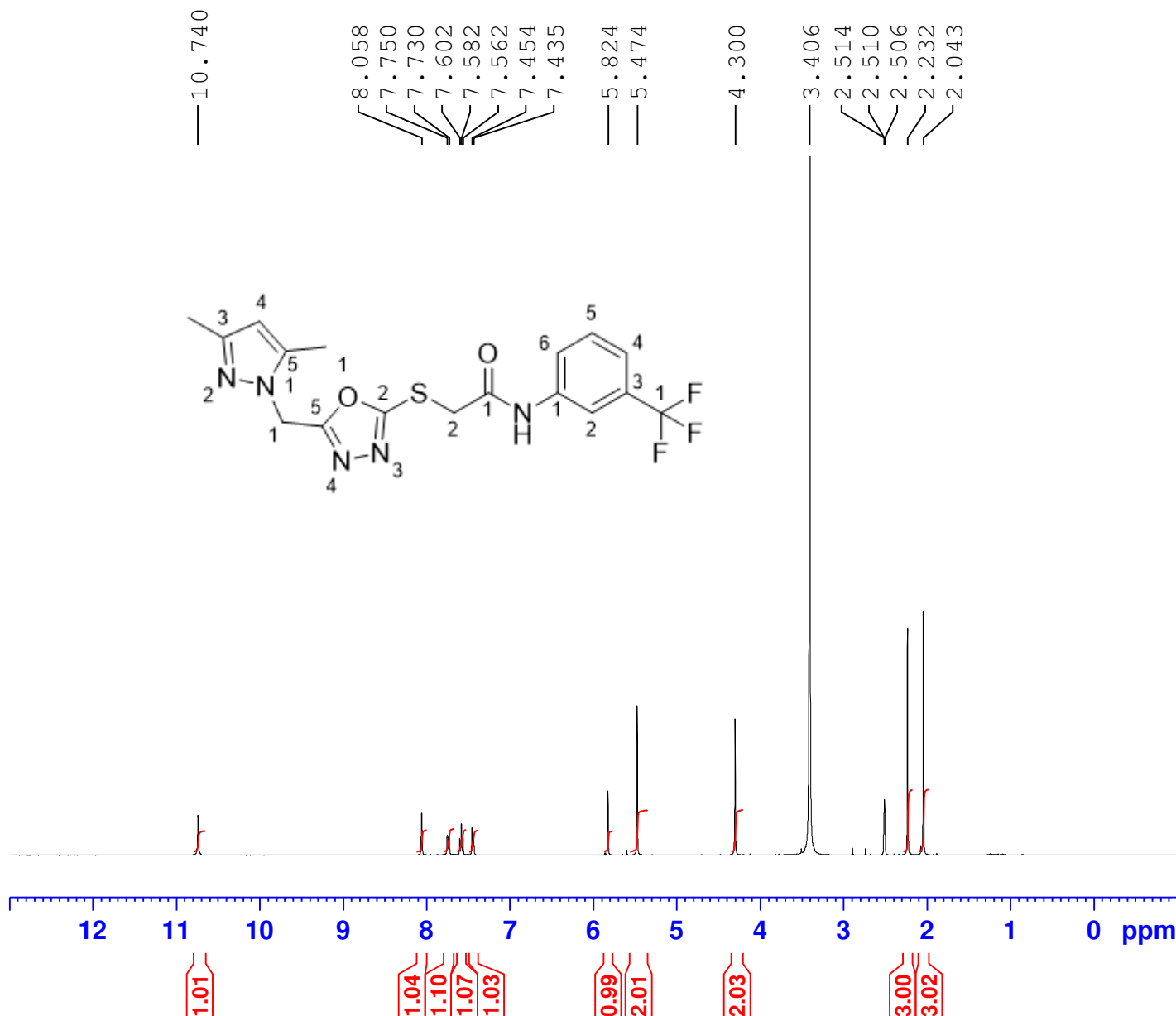
TOF MS ES+  
1.22e8



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3-(trifluoromethyl)phenyl)acetamide (PO16)

POCF3

<sup>1</sup>H-NMR in DMSO



Current Data Parameters  
 NAME 23000428-POCF3  
 EXPNO 1  
 PROCNO 1

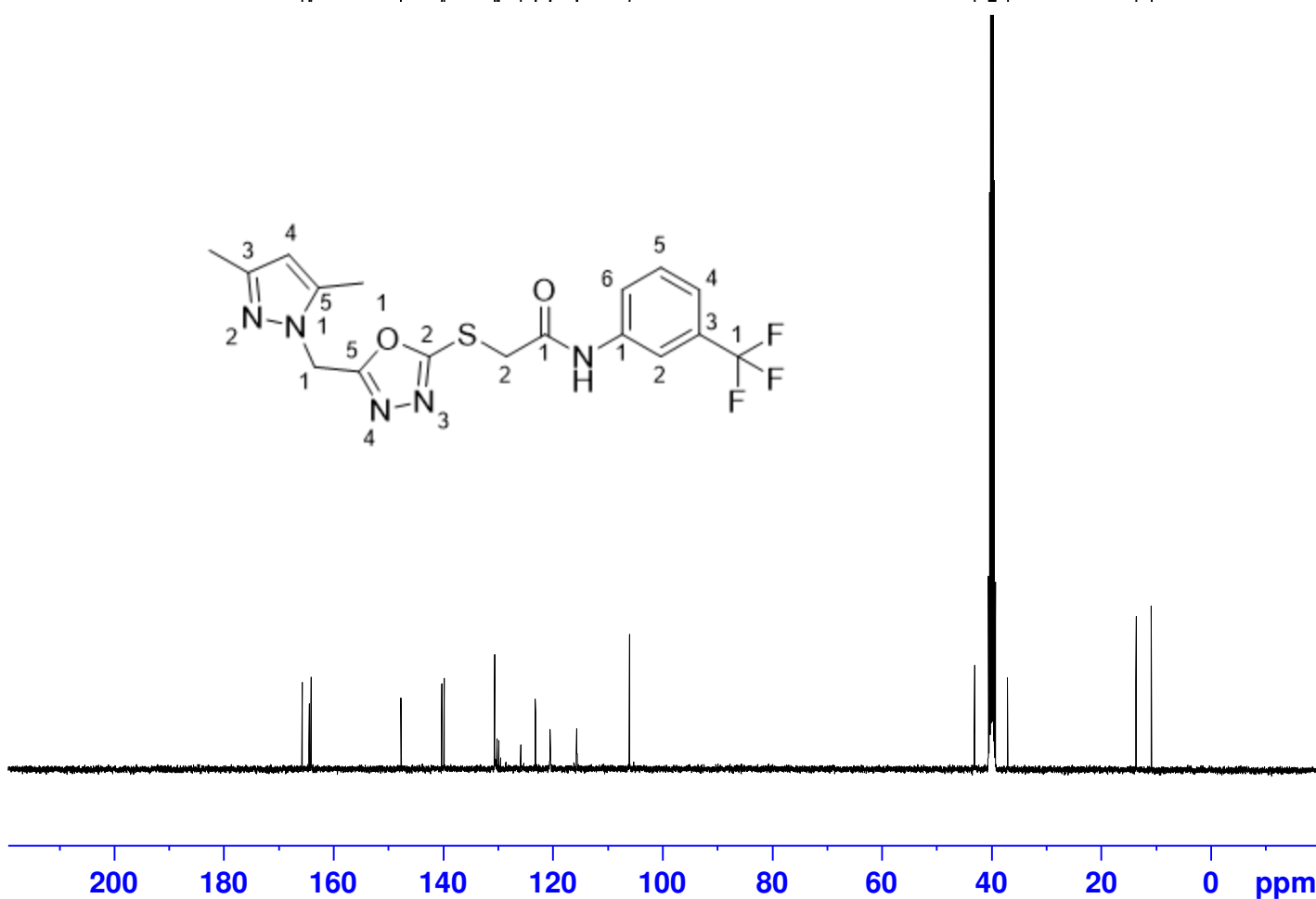
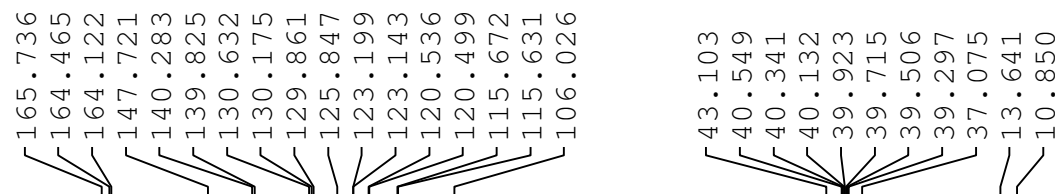
F2 - Acquisition Parameters  
 Date\_ 20230427  
 Time 14.04 h  
 INSTRUM spect  
 PROBHD Z108618\_0984 (   
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 4.0894465 sec  
 RG 32.13  
 DW 62.400 usec  
 DE 17.09 usec  
 TE 297.5 K  
 D1 1.00000000 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

# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3-(trifluoromethyl)phenyl)acetamide (PO16)

POCF3

<sup>13</sup>C-NMR in DMSO



## Current Data Parameters

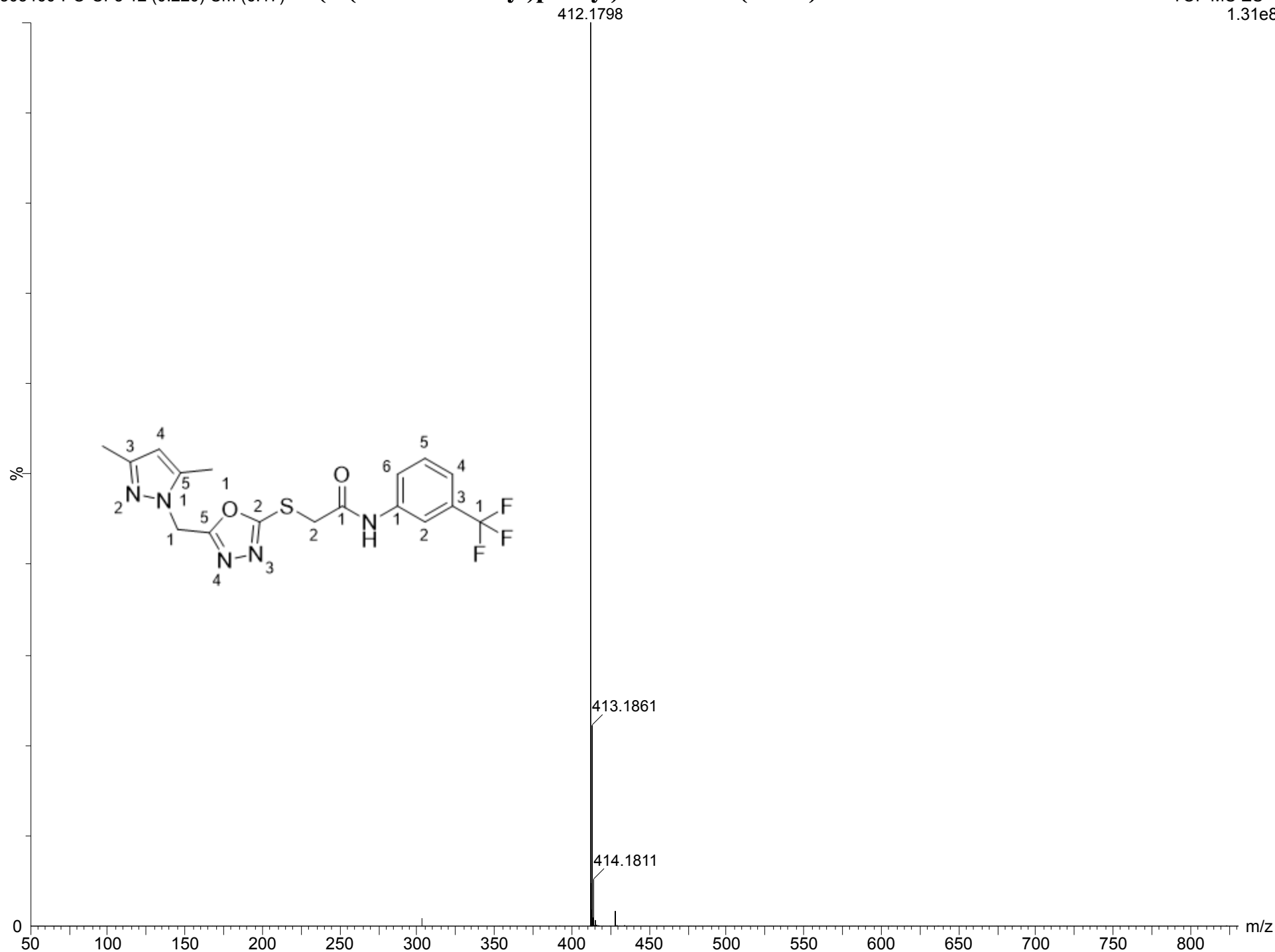
NAME 23000428-POCF3  
EXPNO 2  
PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20230427  
Time 18.12 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1302  
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 298.9 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

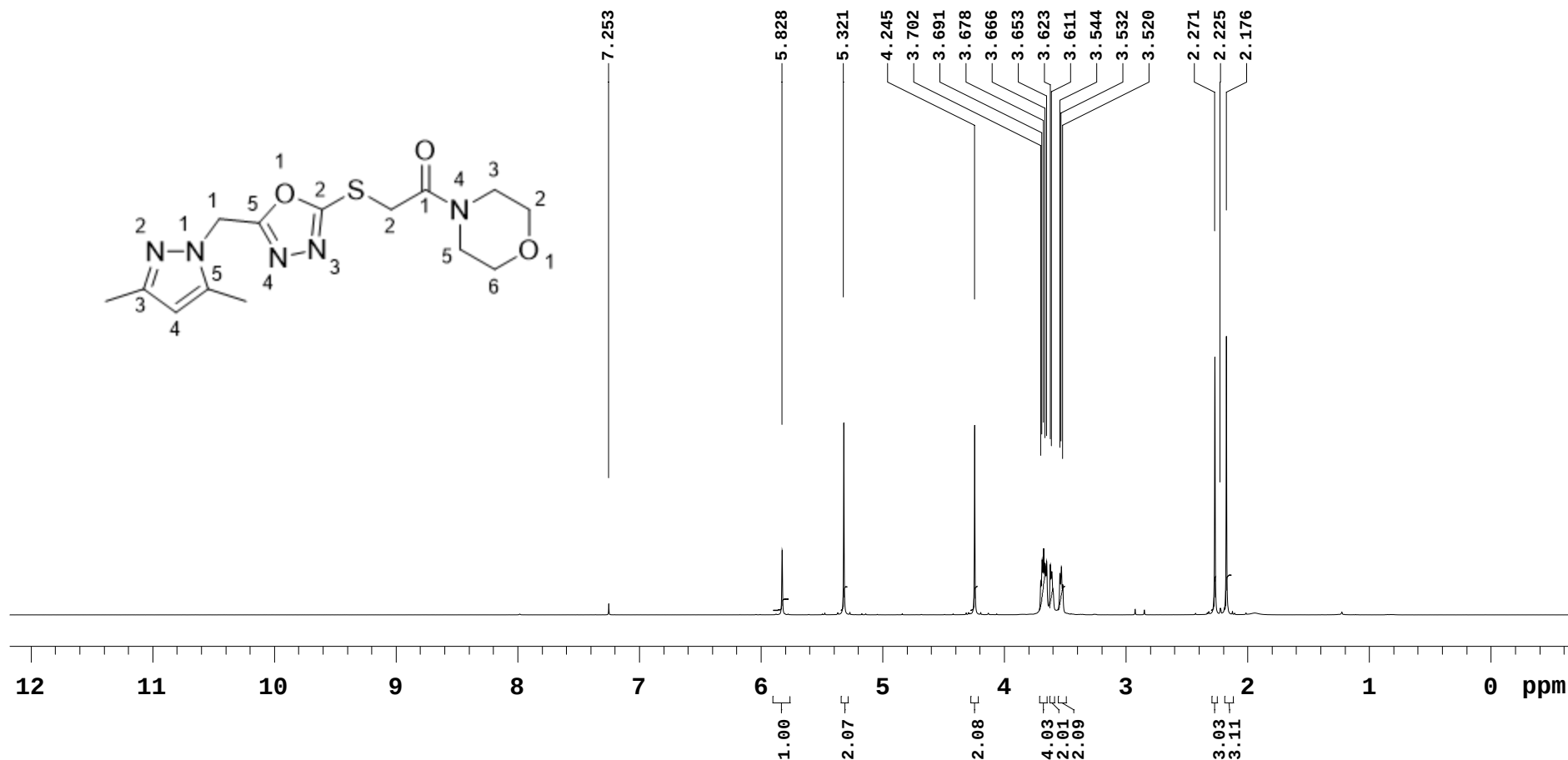
## F2 - Processing parameters

SI 32768  
SF 100.6580296 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-morpholinoethan-1-one (PO17)



**PULSE SEQUENCE**  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.146 sec  
Width 10416.7 Hz  
8 repetitions

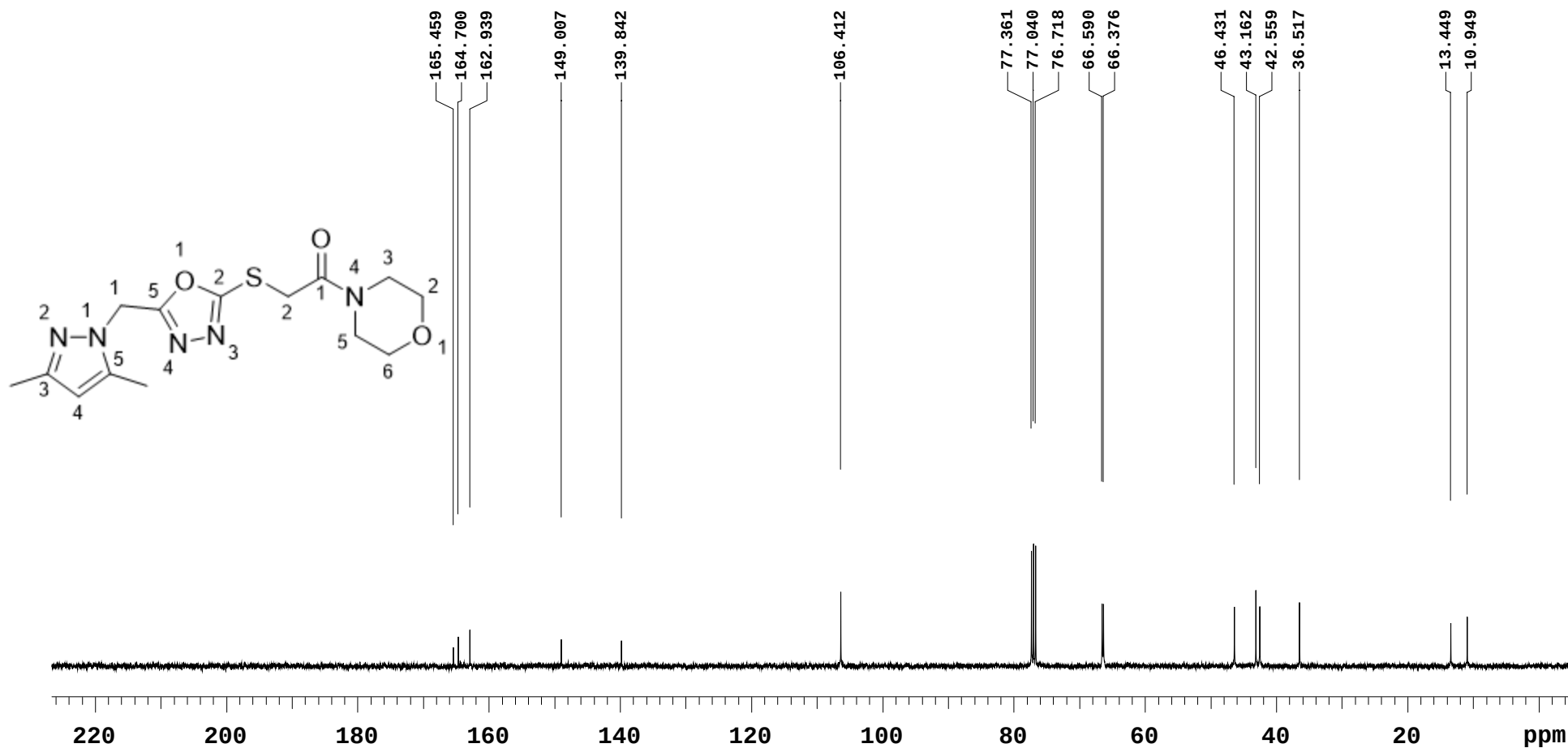
**OBSERVE** H1, 399.8212911

**DATA PROCESSING**  
Line broadening 1.0 Hz  
FT size 65536  
Total time 1 minute

2001317-MD1-1H

Solvent: cdcl3  
Ambient temperature  
Operator: IOE  
File: 2001317-MD1-1H  
VNMR-400 "Agilent-NMR"

# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-morpholinoethan-1-one (PO17)



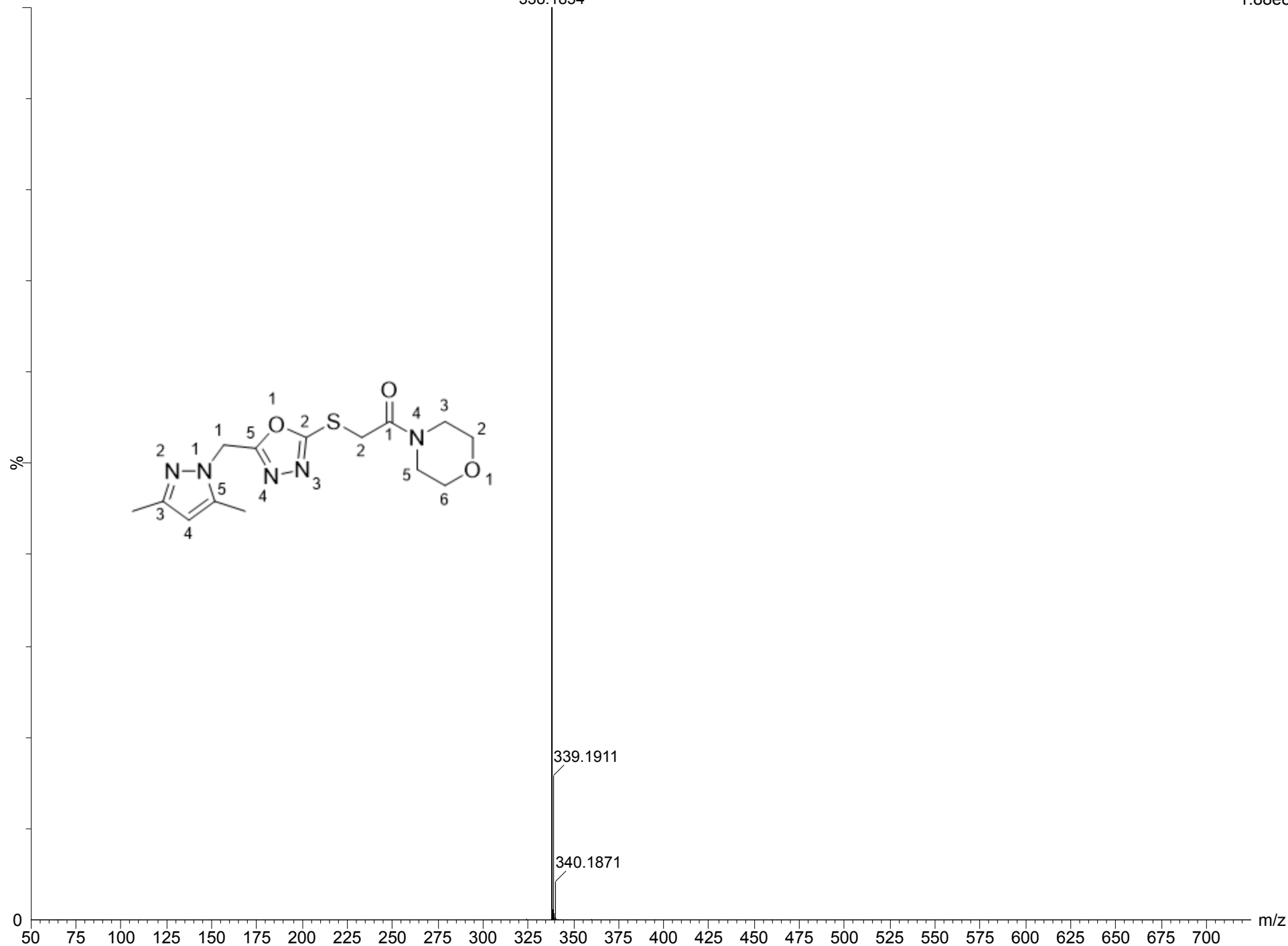
|                                                                                                                                     |                                                                                                                            |                                                                                            |                                                                                                                |
|-------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|
| <b>PULSE SEQUENCE</b><br>Relax. delay 1.000 sec<br>Pulse 45.0 degrees<br>Acq. time 1.022 sec<br>Width 32051.3 Hz<br>332 repetitions | <b>OBSERVE</b> C13, 100.5351436<br><b>DECOUPLE</b> H1, 399.8232903<br>Power 39 dB<br>continuously on<br>WALTZ-16 modulated | <b>DATA PROCESSING</b><br>Line broadening 2.5 Hz<br>FT size 65536<br>Total time 11 minutes | <b>2001318-MD1-13C</b><br><br>Solvent: cdcl3<br>Ambient temperature<br>Operator: IOE<br>VNMR-400 "Agilent-NMR" |
|-------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|

Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-morpholinoethan-1-one (PO17)

2303475-PO-M 13 (0.237) Cm (8:34)

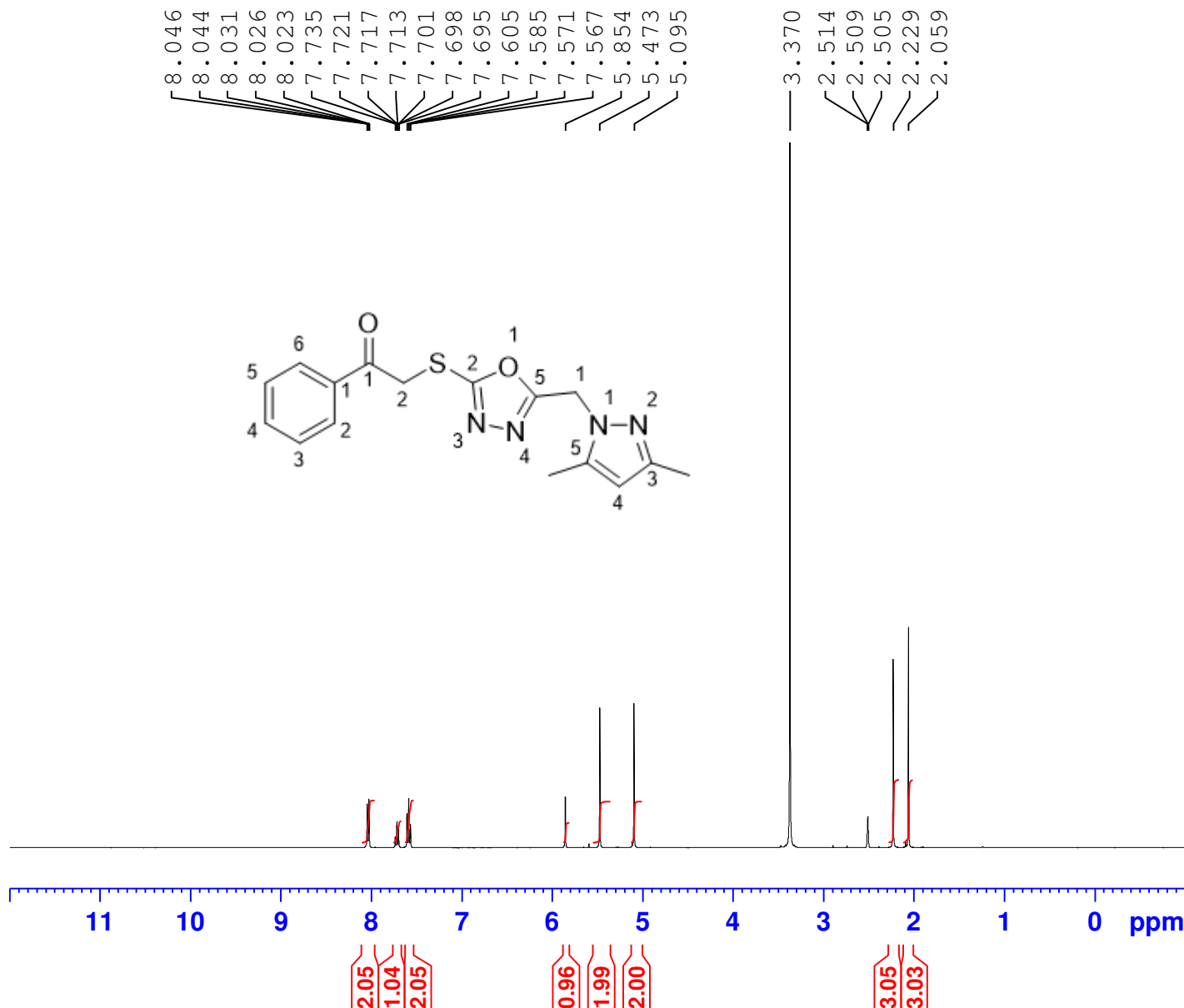
TOF MS ES+  
1.88e8

338.1854



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-phenylethan-1-one (PO18)

POACP  
1H-NMR in DMSO



Current Data Parameters  
NAME 23000477-POACP  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230509  
Time 18.01 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 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

# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-phenylethan-1-one (PO18)

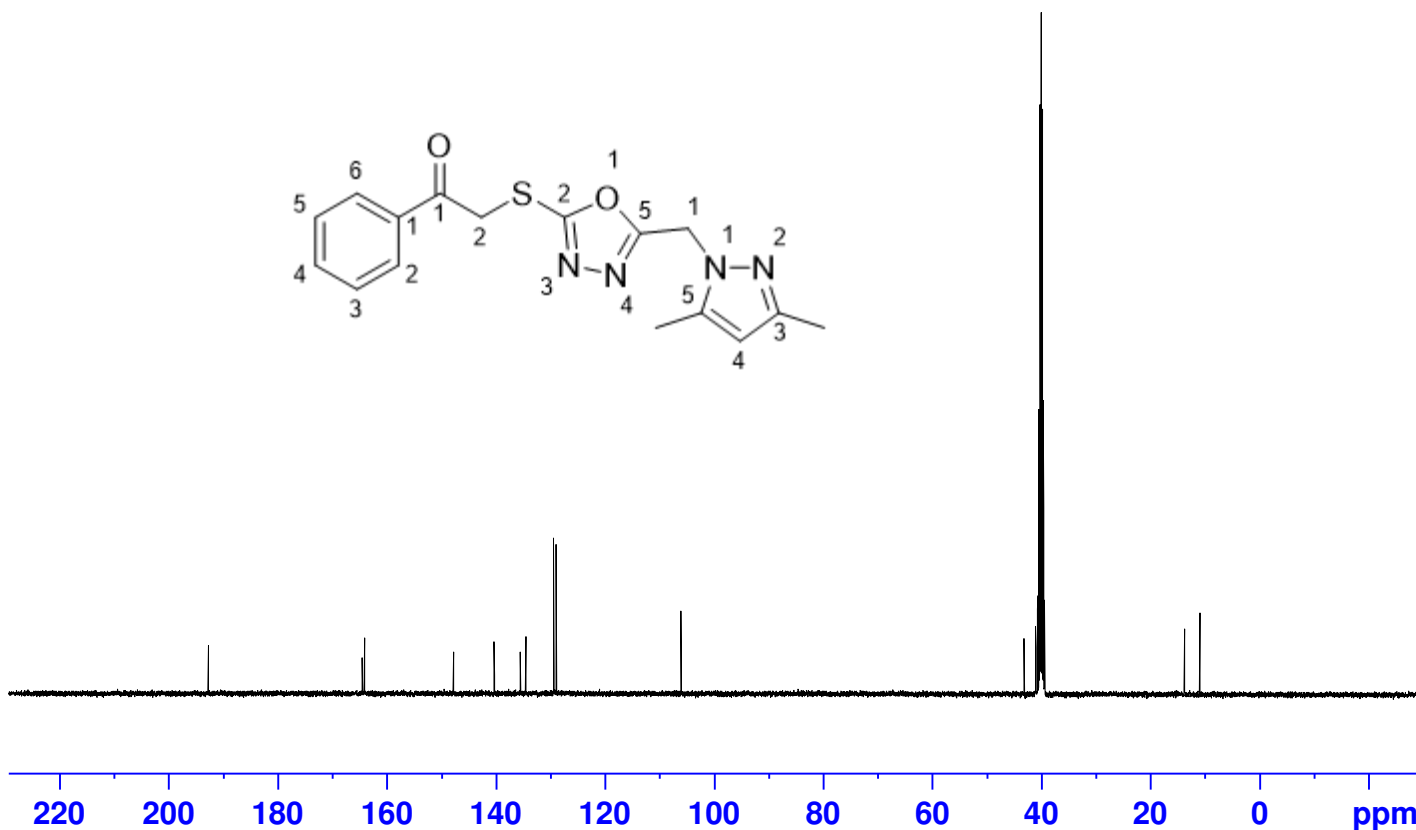
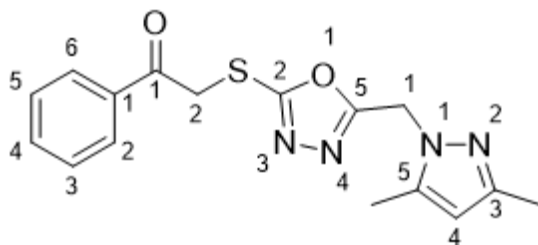
POACP  
13C-NMR in DMSO



— 192.680  
164.469  
164.035  
147.692  
140.270  
135.478  
134.462  
129.366  
128.894  
— 106.044  
43.105  
40.962  
40.599  
40.391  
40.182  
39.973  
39.764  
39.556  
39.347  
13.694  
10.866

Current Data Parameters  
NAME 23000477-POACP  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230509  
Time 18.21 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
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 298.4 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 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-phenylethan-1-one (PO18)

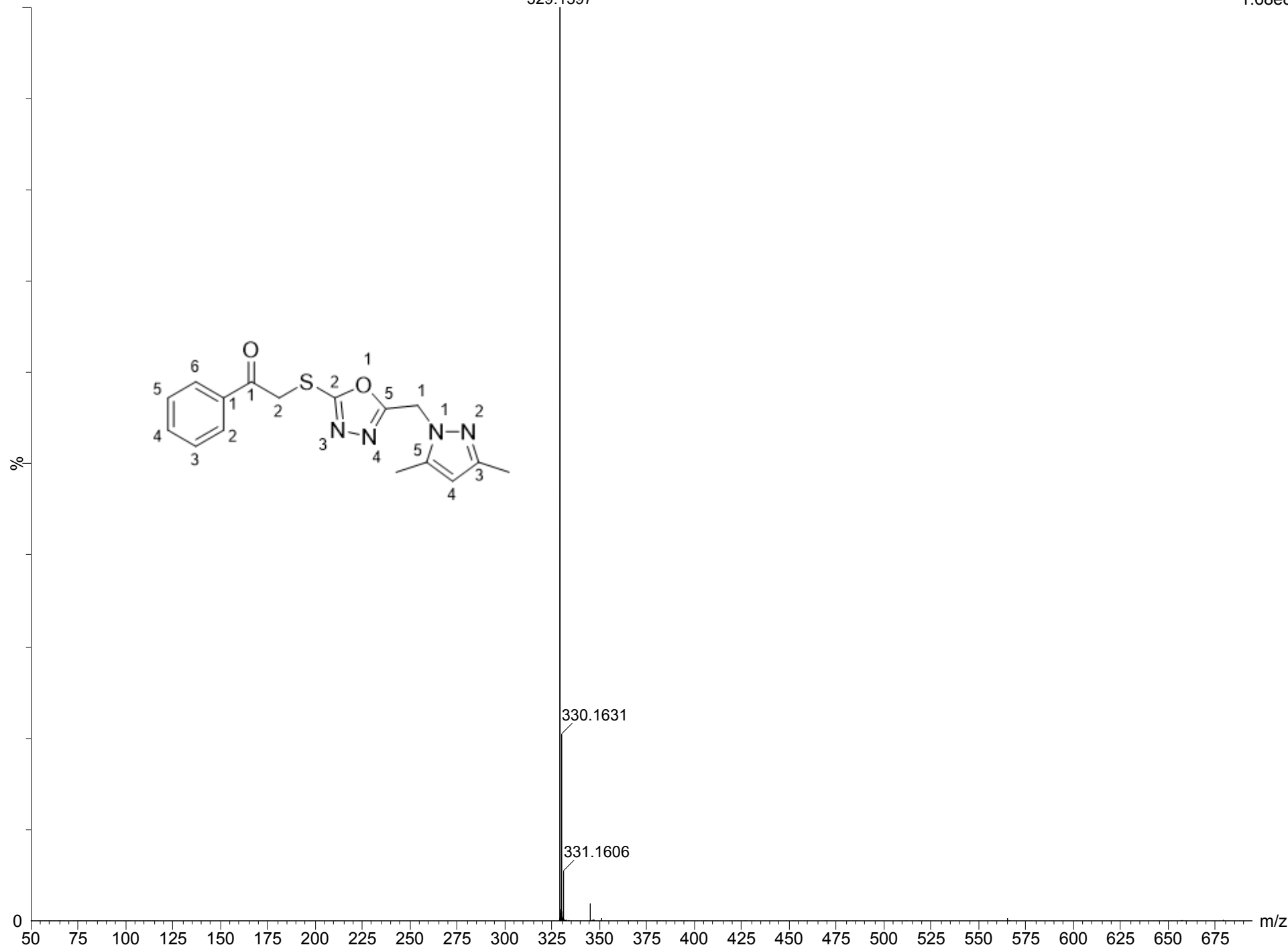
2303458-PO-ACPs 12 (0.220) Cm (7:23)

**phenylethan-1-one (PO18)**

TOF MS ES+

1.68e8

329.1597

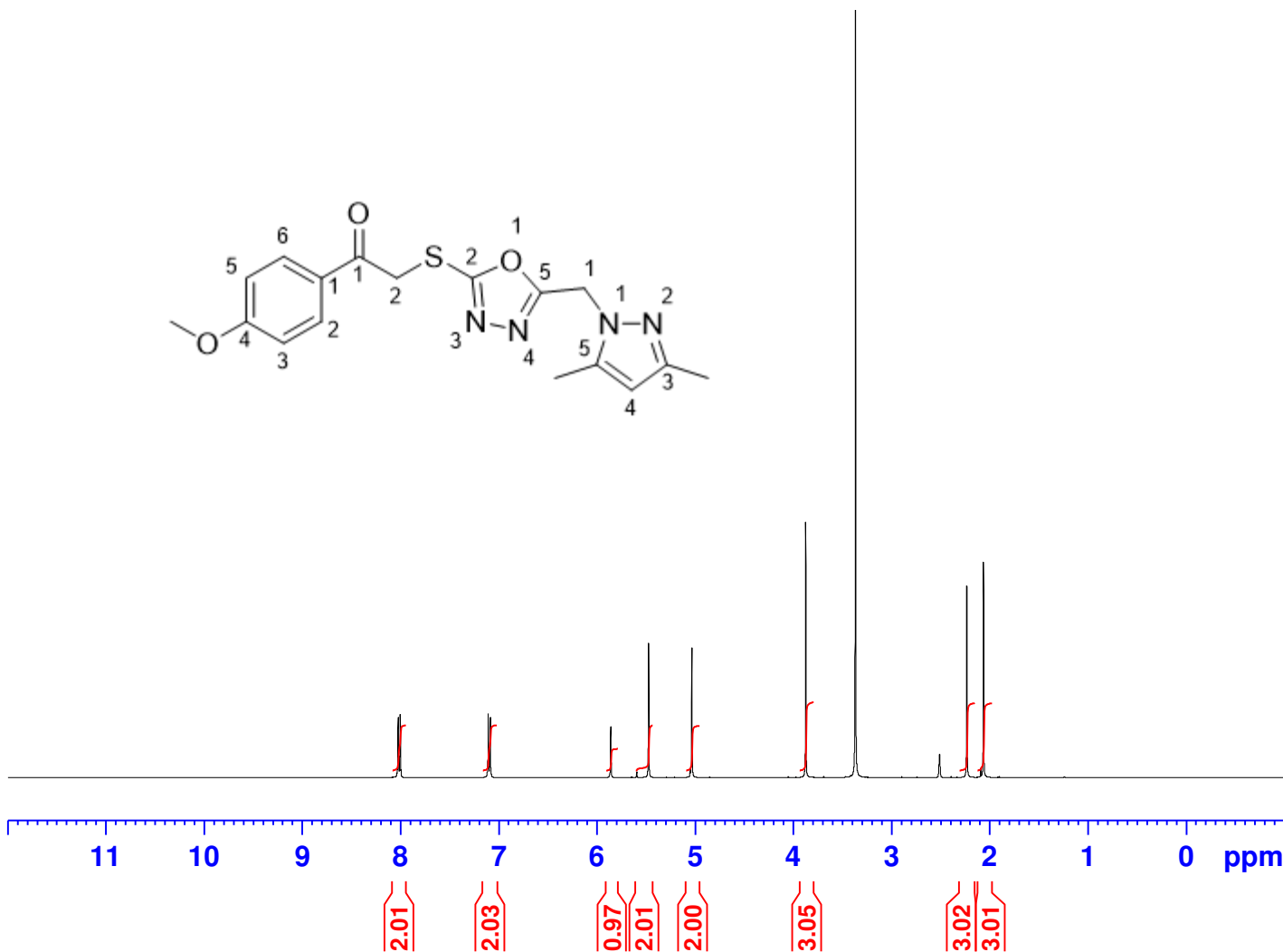
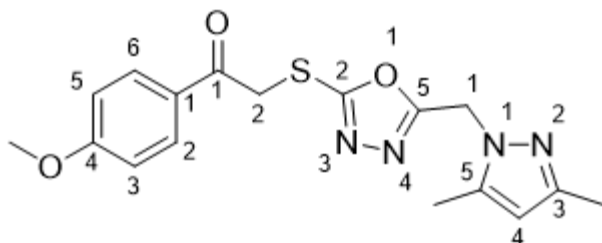


**<sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-methoxyphenyl)ethan-1-one (PO19)**

PO40CH3-ACP  
1H-NMR in DMSO



8.024  
8.019  
8.007  
8.002  
7.107  
7.102  
7.090  
7.085  
— 5.858  
— 5.473  
— 5.032  
— 3.873  
— 3.366  
2.510  
2.232  
2.062



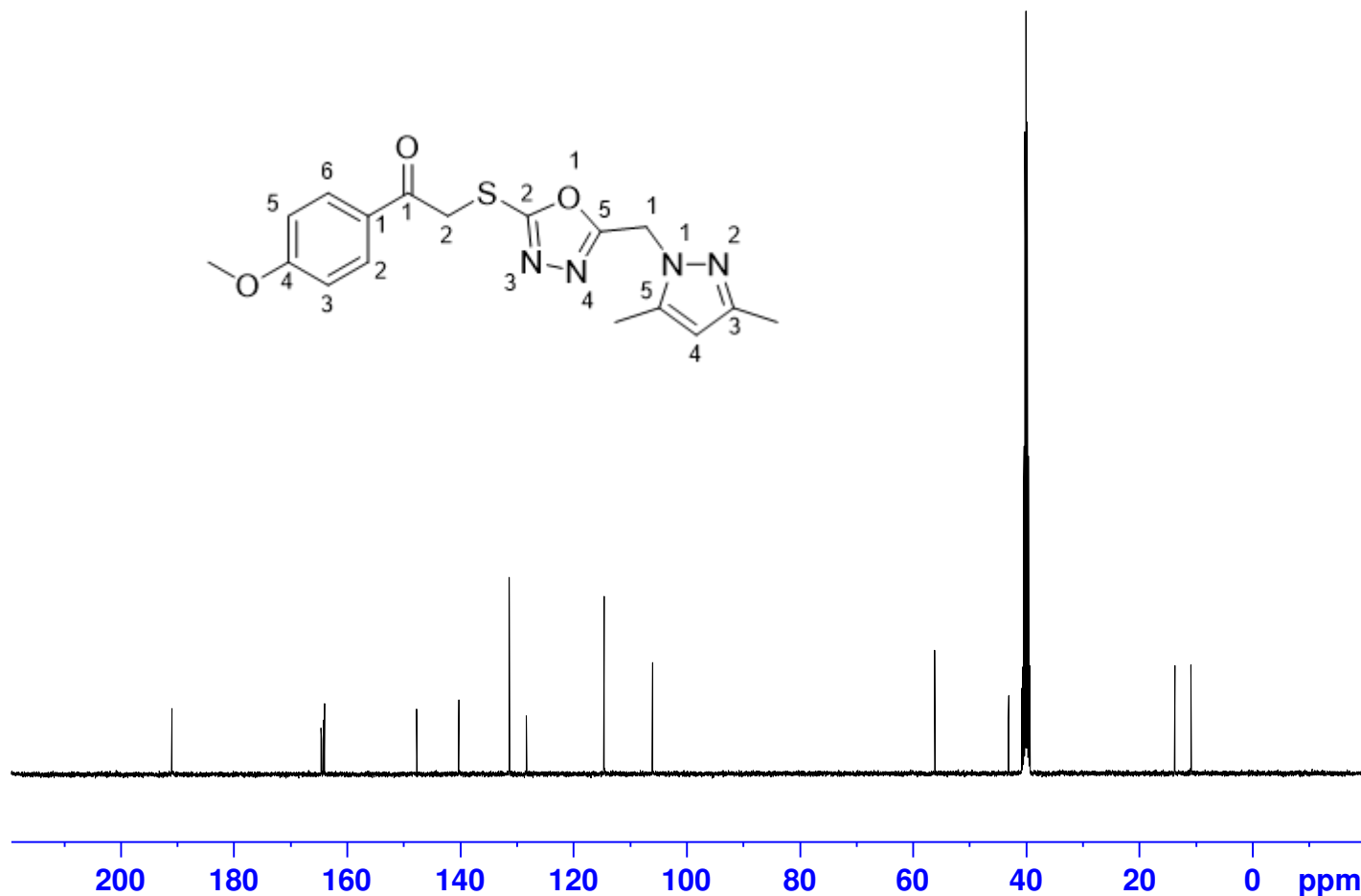
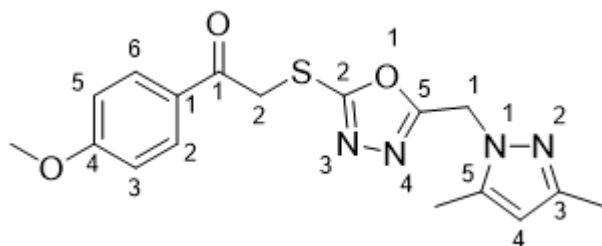
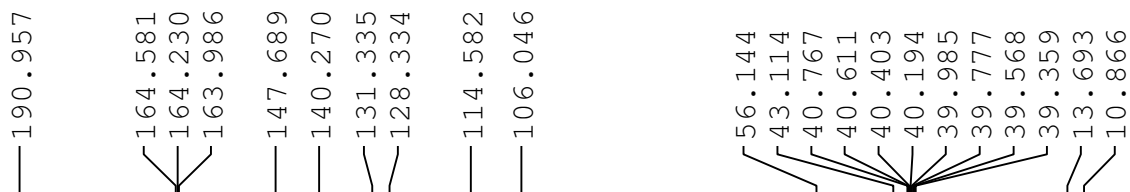
Current Data Parameters  
NAME 23000495-PO40CH3-ACP  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230513  
Time 15.49 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 298.4 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

# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-methoxyphenyl)ethan-1-one (PO19)

PO40CH3-ACP  
13C-NMR in DMSO



Current Data Parameters  
NAME 23000495-PO40CH3-ACP  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230513  
Time 16.17 h  
INSTRUM spect  
PROBHD Z108618\_0984 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 661  
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 299.7 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

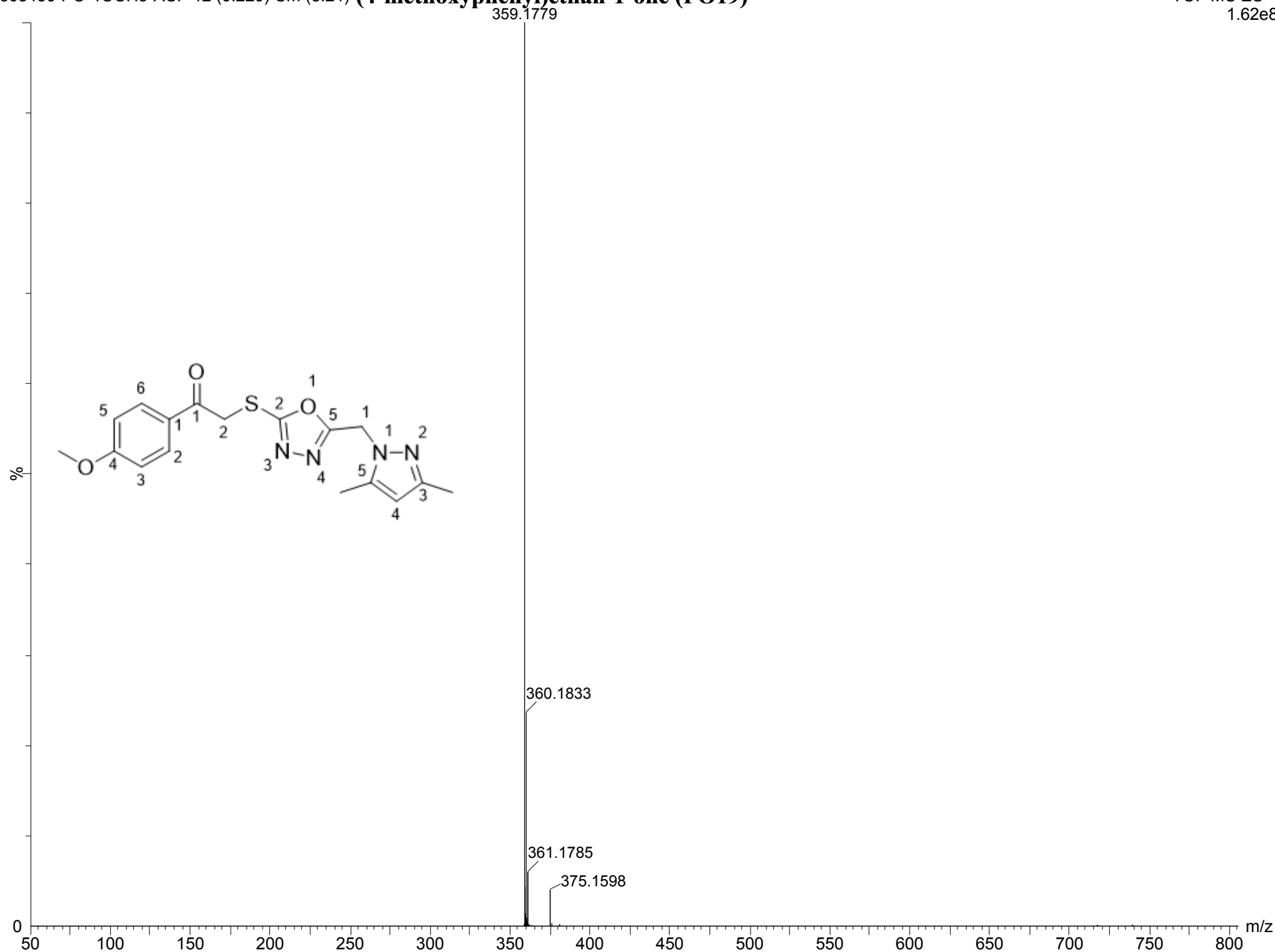
F2 - Processing parameters  
SI 32768  
SF 100.6580296 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



# Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-methoxyphenyl)ethan-1-one (PO19)

2303456-PO-4OCH3-ACP 12 (0.220) Cm (8:24)

TOF MS ES+  
1.62e8



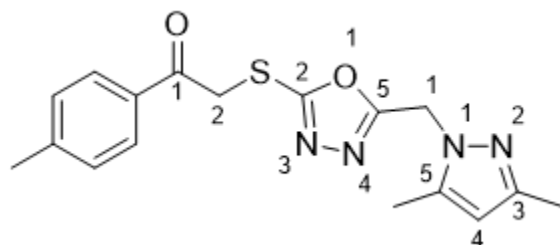
# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(p-tolyl)ethan-1-one (PO20)

PO4CH3-ACP

<sup>1</sup>H-NMR in DMSO



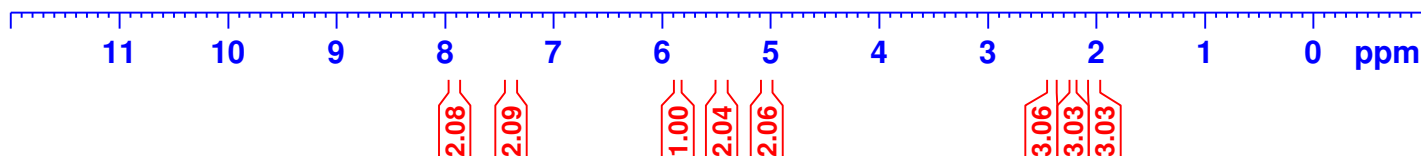
8.295  
7.933  
7.913  
7.393  
7.374  
5.855  
5.458  
5.040  
3.456  
2.514  
2.510  
2.505  
2.403  
2.222  
2.221  
2.088  
2.054



Current Data Parameters  
NAME 23000491-PO4CH3-ACP  
EXPNO 1  
PROCNO 1

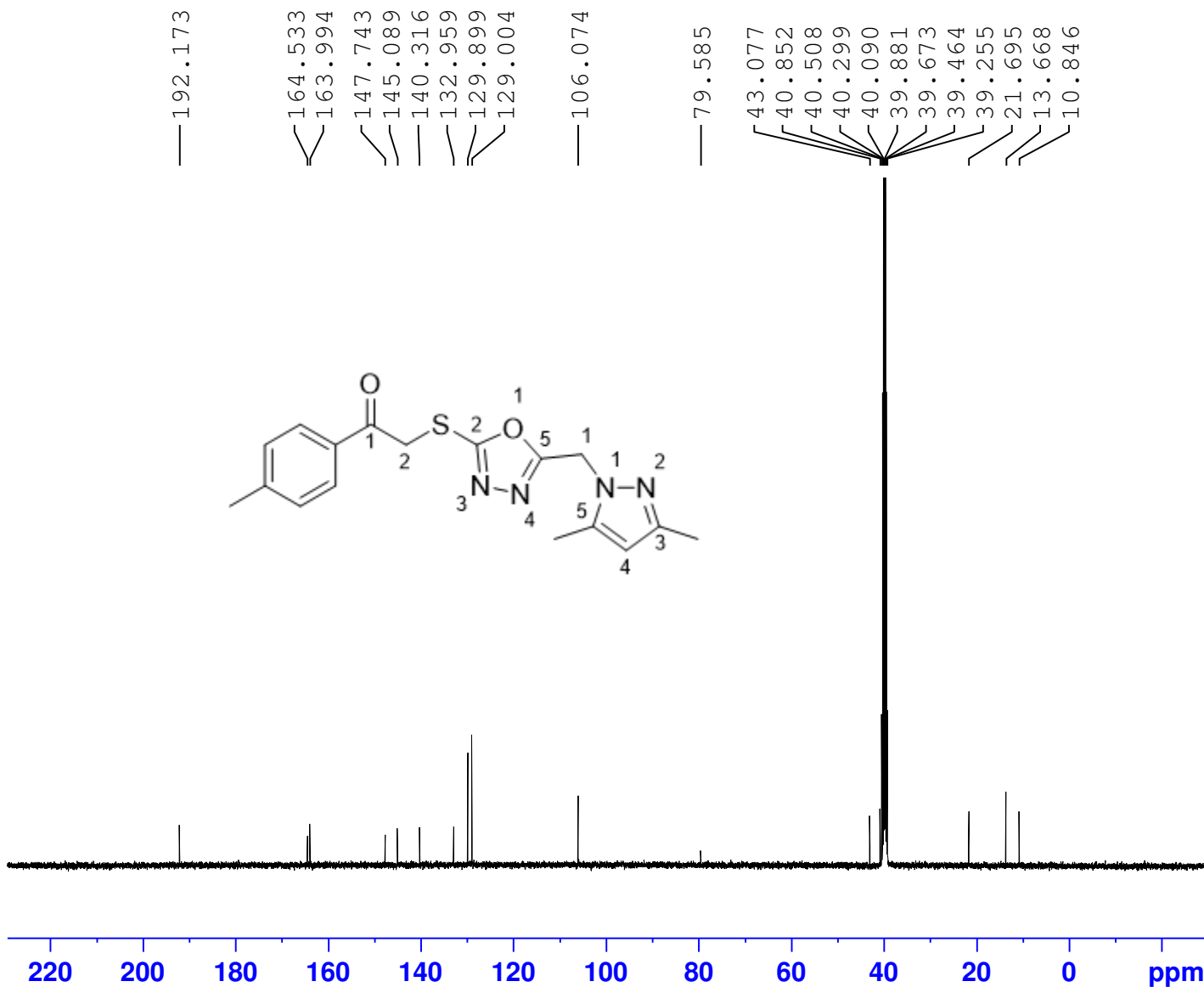
F2 - Acquisition Parameters  
Date\_ 20230512  
Time 18.21 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 32  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 32.13  
DW 62.400 usec  
DE 17.09 usec  
TE 297.8 K  
D1 1.00000000 sec  
TD0 1  
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



# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(p-tolyl)ethan-1-one (PO20)

PO4CH3-ACP  
<sup>13</sup>C-NMR in DMSO



Current Data Parameters  
NAME 23000491-PO4CH3-ACP  
EXPNO 2  
PROCNO 1

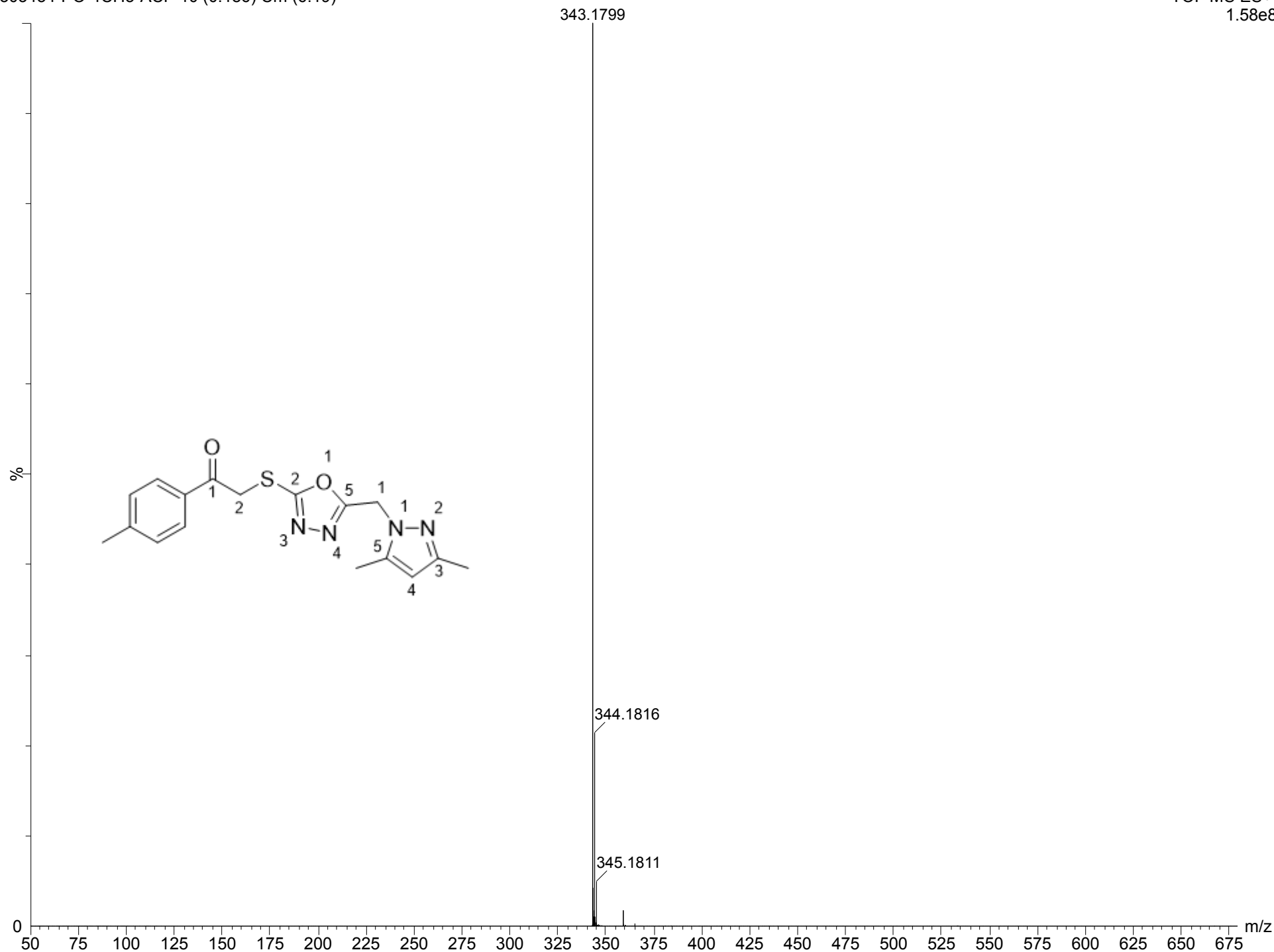
F2 - Acquisition Parameters  
Date\_ 20230512  
Time 18.57 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 932  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.794729 Hz  
AQ 1.2582912 sec  
RG 202.84  
DW 19.200 usec  
DE 6.50 usec  
TE 298.9 K  
D1 1.00000000 sec  
D11 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

Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(p-tolyl)ethan-1-one (PO20)

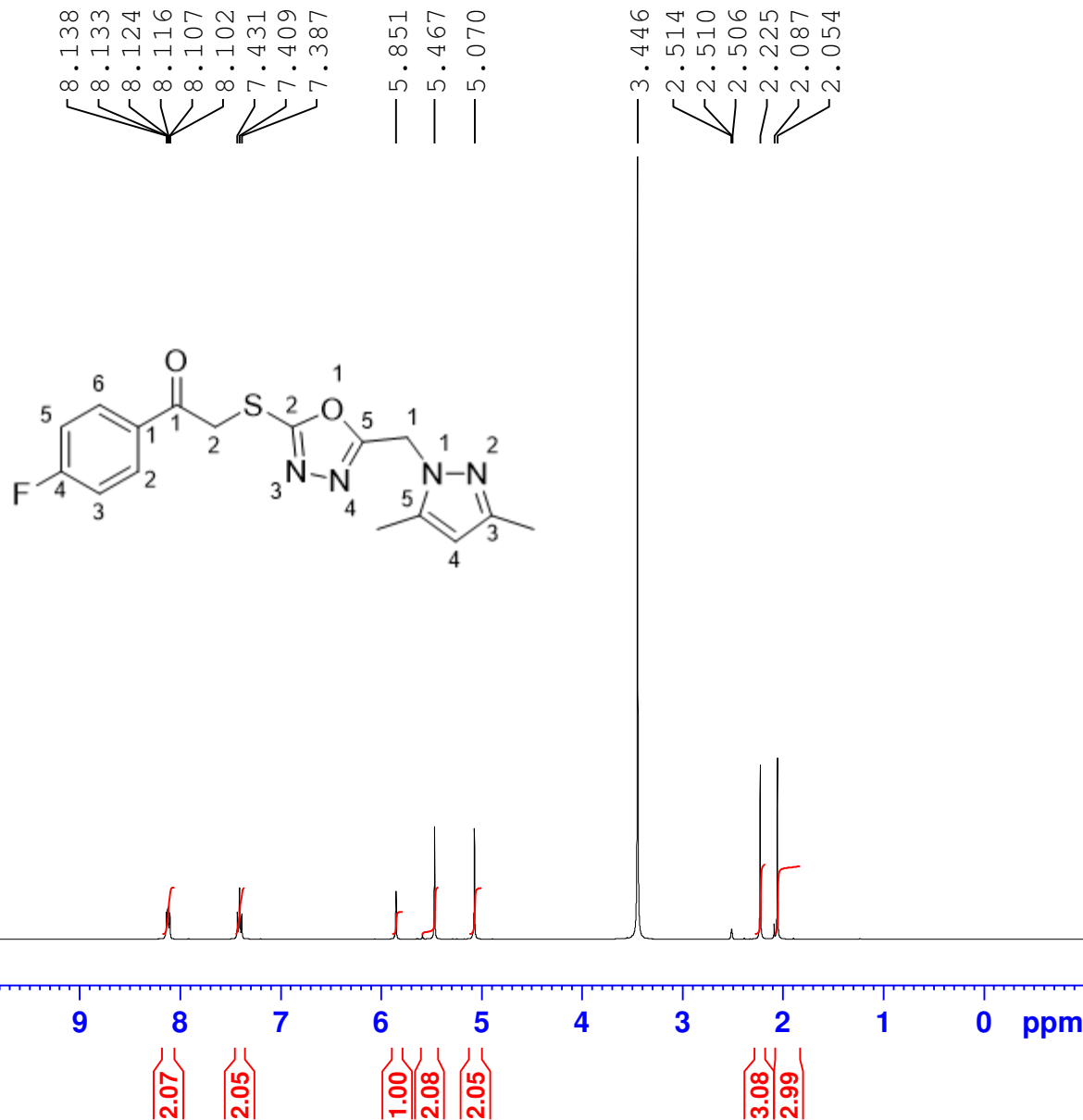
2303454-PO-4CH3-ACP 10 (0.186) Cm (6:19)

TOF MS ES+  
1.58e8



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-fluorophenyl)ethan-1-one (PO21)

PO4F-ACP  
1H-NMR in DMSO



Current Data Parameters  
NAME 23000490-PO4F-ACP  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230512  
Time 18.04 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 297.7 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

# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-fluorophenyl)ethan-1-one (PO21)

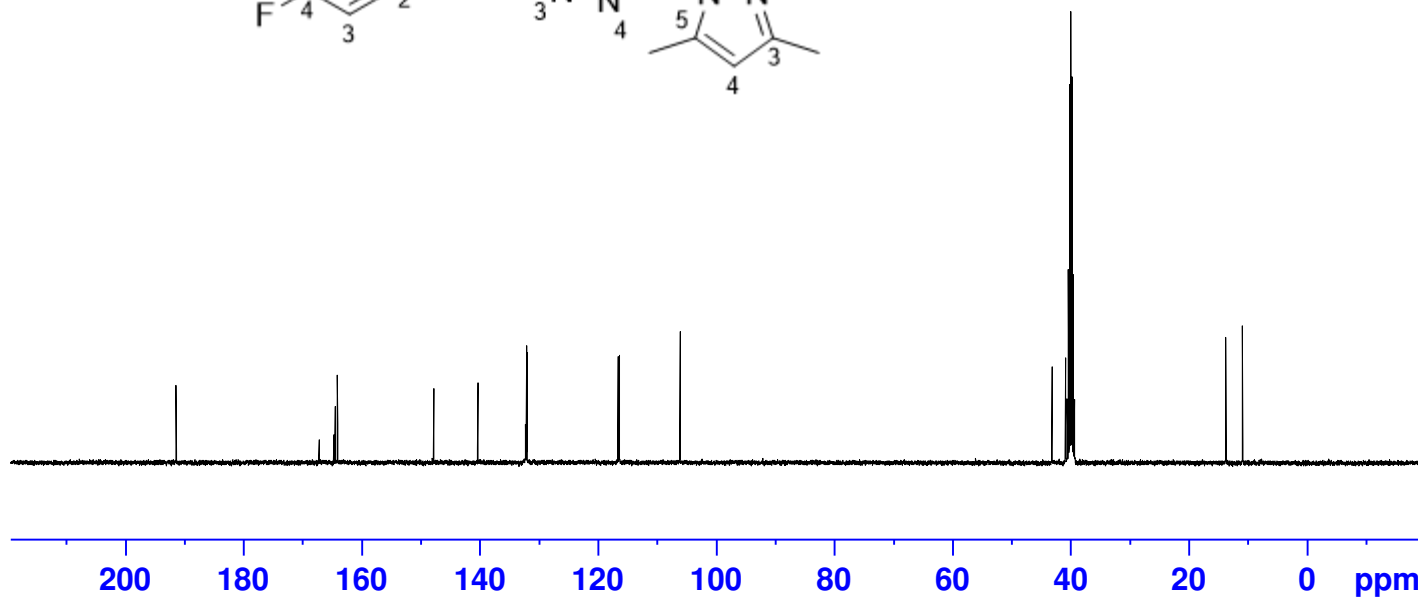
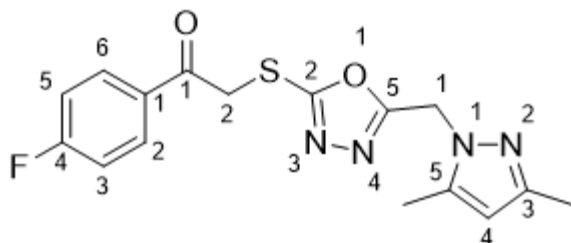
PO4F-ACP

<sup>13</sup>C-NMR in DMSO



— 191.358  
167.168  
164.655  
164.438  
164.043  
147.741  
140.298  
132.253  
132.225  
132.055  
131.959  
116.544  
116.324  
— 106.060

43.091  
40.789  
40.532  
40.323  
40.114  
39.905  
39.696  
39.488  
39.279  
13.657  
10.841



Current Data Parameters  
NAME 23000490-PO4F-ACP  
EXPNO 2  
PROCNO 1

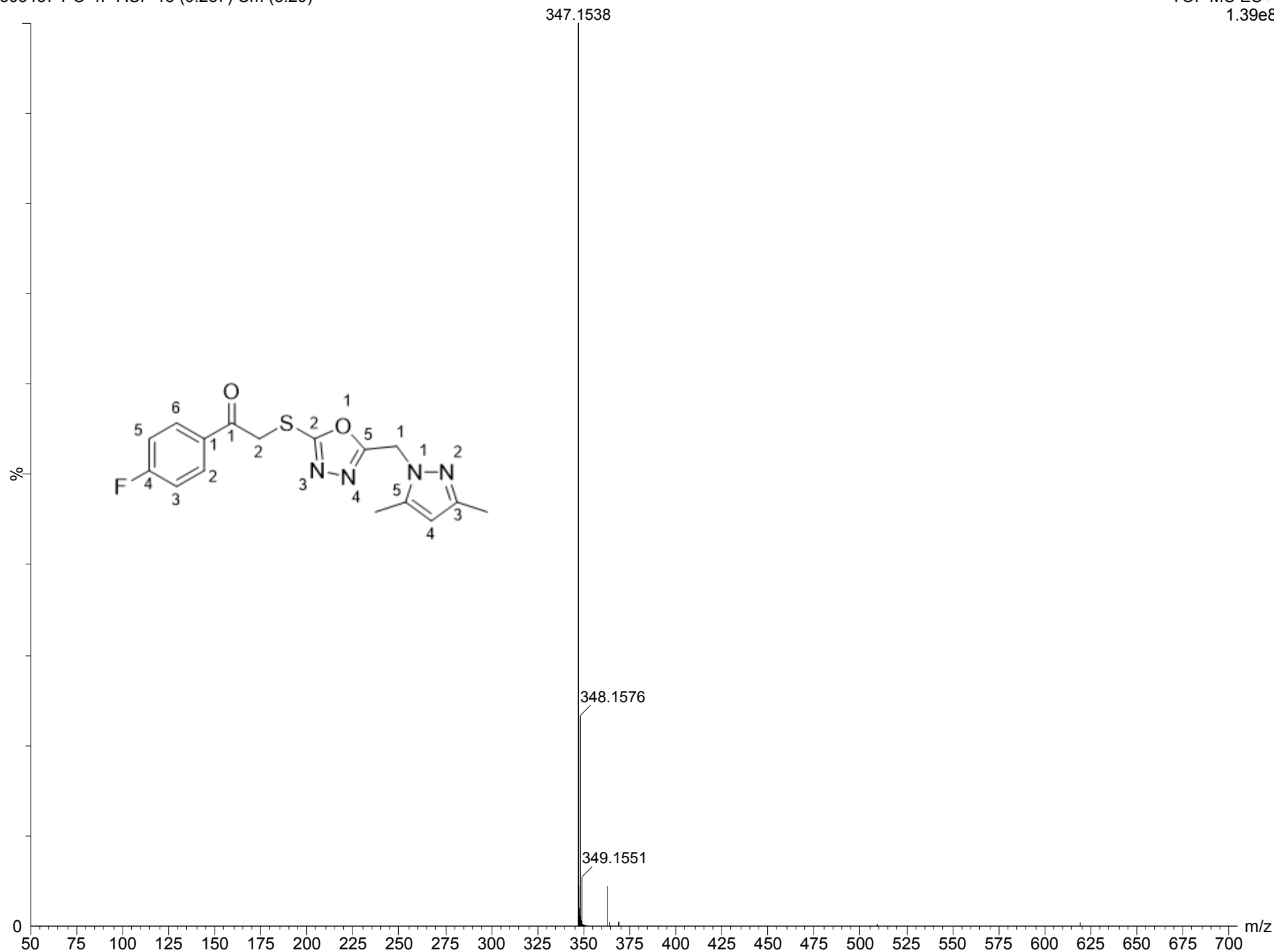
F2 - Acquisition Parameters  
Date\_ 20230512  
Time 18.15 h  
INSTRUM spect  
PROBHD Z108618\_0984 (   
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 256  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 202.84  
DW 20.800 usec  
DE 6.50 usec  
TE 298.8 K  
D1 1.00000000 sec  
D11 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

2303457-PO-4F-ACP 13 (0.237) Cm (8:20)

**Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-fluorophenyl)ethan-1-one (PO21)**

TOF MS ES+  
1.39e8



# <sup>1</sup>H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-nitrophenyl)ethan-1-one (PO22)

PO4NO2-ACP

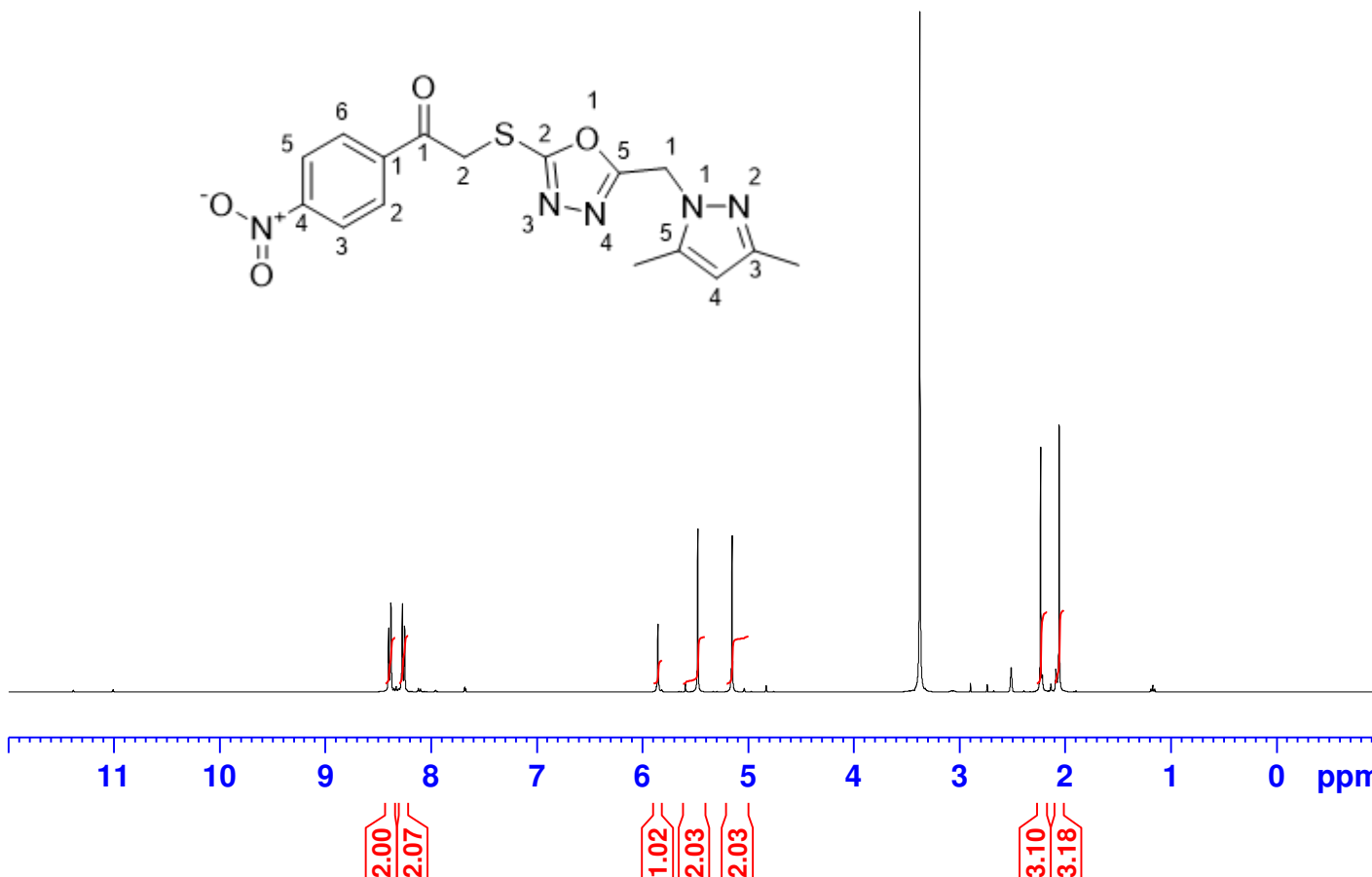
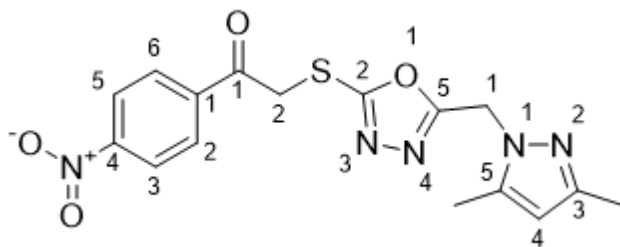
<sup>1</sup>H-NMR in DMSO



8.401  
8.379  
8.271  
8.249

5.852  
5.475  
5.151

3.374  
2.895  
2.737  
2.514  
2.509  
2.505  
2.230  
2.215  
2.135  
2.088  
2.076  
2.055



Current Data Parameters  
NAME 23000493-PO4NO2-ACP  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230513  
Time 15.30 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 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



# <sup>13</sup>C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-nitrophenyl)ethan-1-one (PO22)

PO4NO2-ACP  
<sup>13</sup>C-NMR in DMSO



— 192.232

164.211  
 164.161

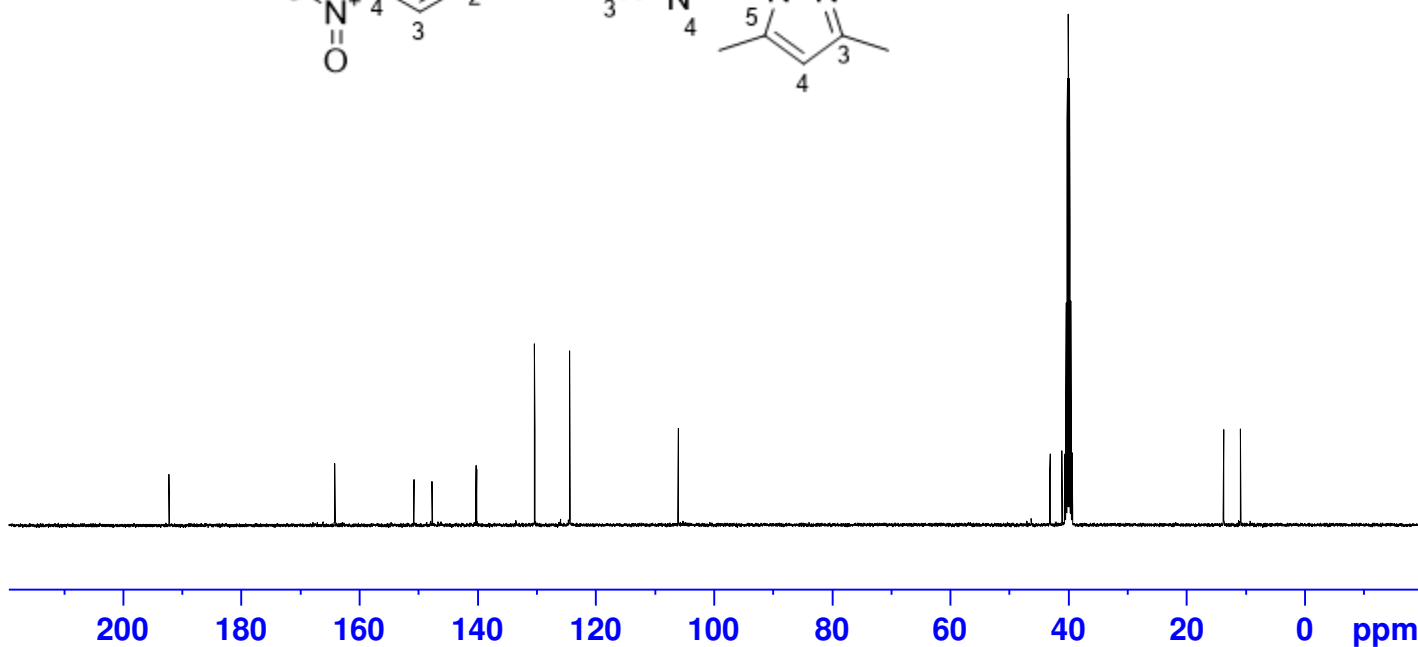
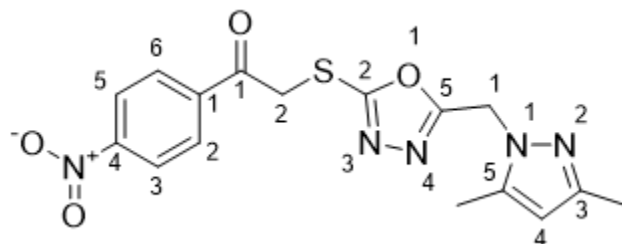
150.764  
 147.707

140.276  
 140.139

130.344  
 124.410

— 106.046

43.114  
 41.081  
 40.602  
 40.393  
 40.185  
 39.976  
 39.767  
 39.558  
 39.350  
 13.678  
 10.866



Current Data Parameters  
 NAME 23000493-PO4NO2-ACP  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230513  
 Time 17.24 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 299.2 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

Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-nitrophenyl)ethan-1-one (PO22)

2303455-PO-4NO2-ACP 15 (0.270) Cm (6:21)

TOF MS ES+  
1.29e8

