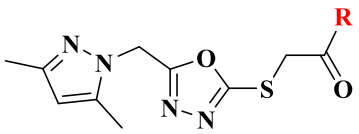
SUPPORTING DOCUMENT

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



PO1-PO22

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-trifluromethyl 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-fluro phenylamino	7	1	361.394	1.984
16	PO16	3-trifluromethyl 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-fluro 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

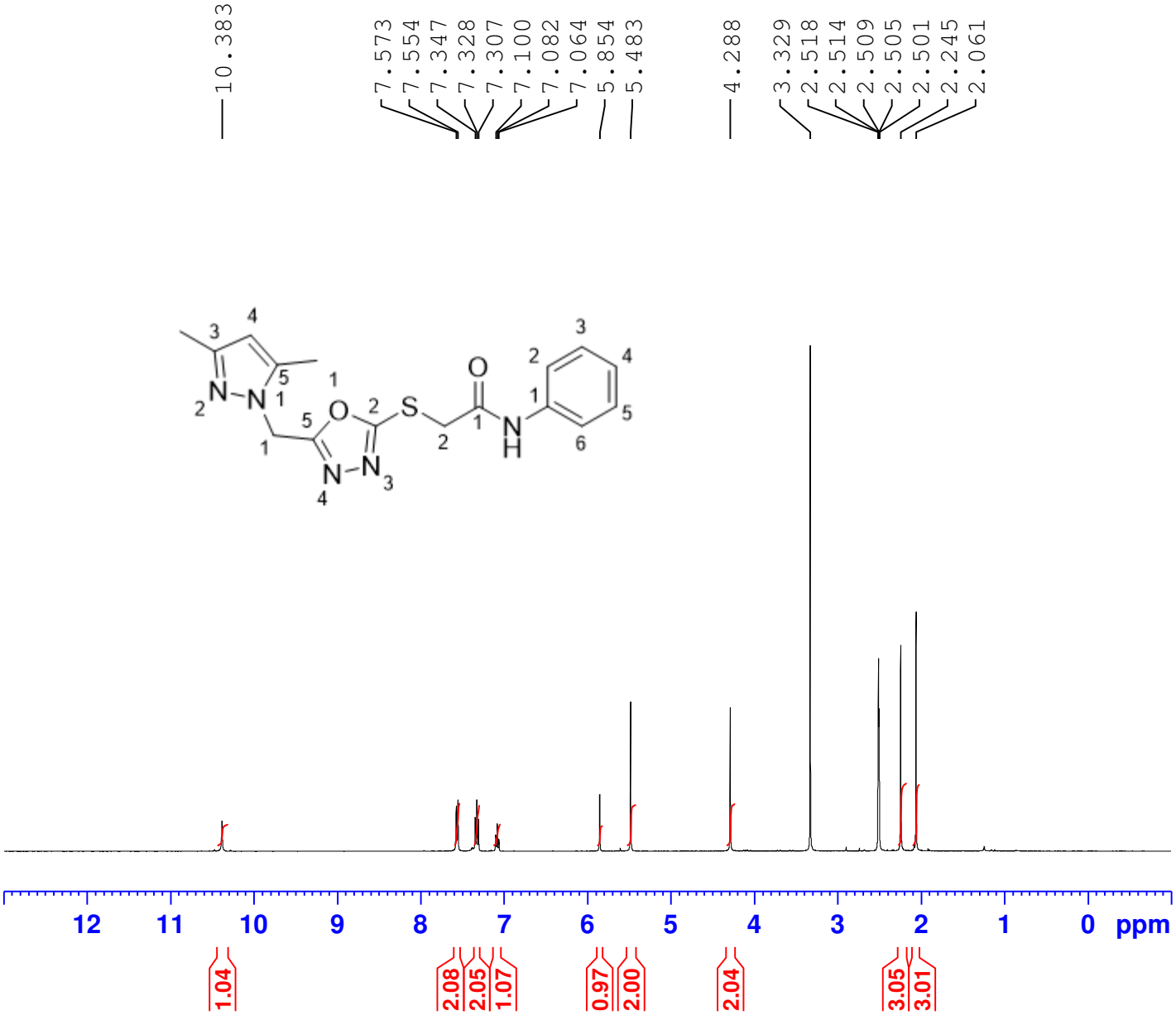
Sl	Cpd code	Solubility	Solubility Level	BBB	BBB Level	CYP2D6	CYP2D6 Prediction	HIA level
1	PO1	-3.015	3	-0.899	3	-9.95161	FALSE	0
2	PO2	-3.488	3	-0.748	3	-9.61108	FALSE	0
3	PO3	-4.172	2	-0.607	3	-5.94374	FALSE	0
4	PO4	-3.783	3	-0.667	3	-10.7456	FALSE	0
5	PO5	-3.011	3	-1.045	3	-11.189	FALSE	0
6	PO6	-3.728	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}H NMR
- ^{13}C NMR
- Mass spectra

^{1}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



BRUKER

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PROCNO 1

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SOLVENT DMSO
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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
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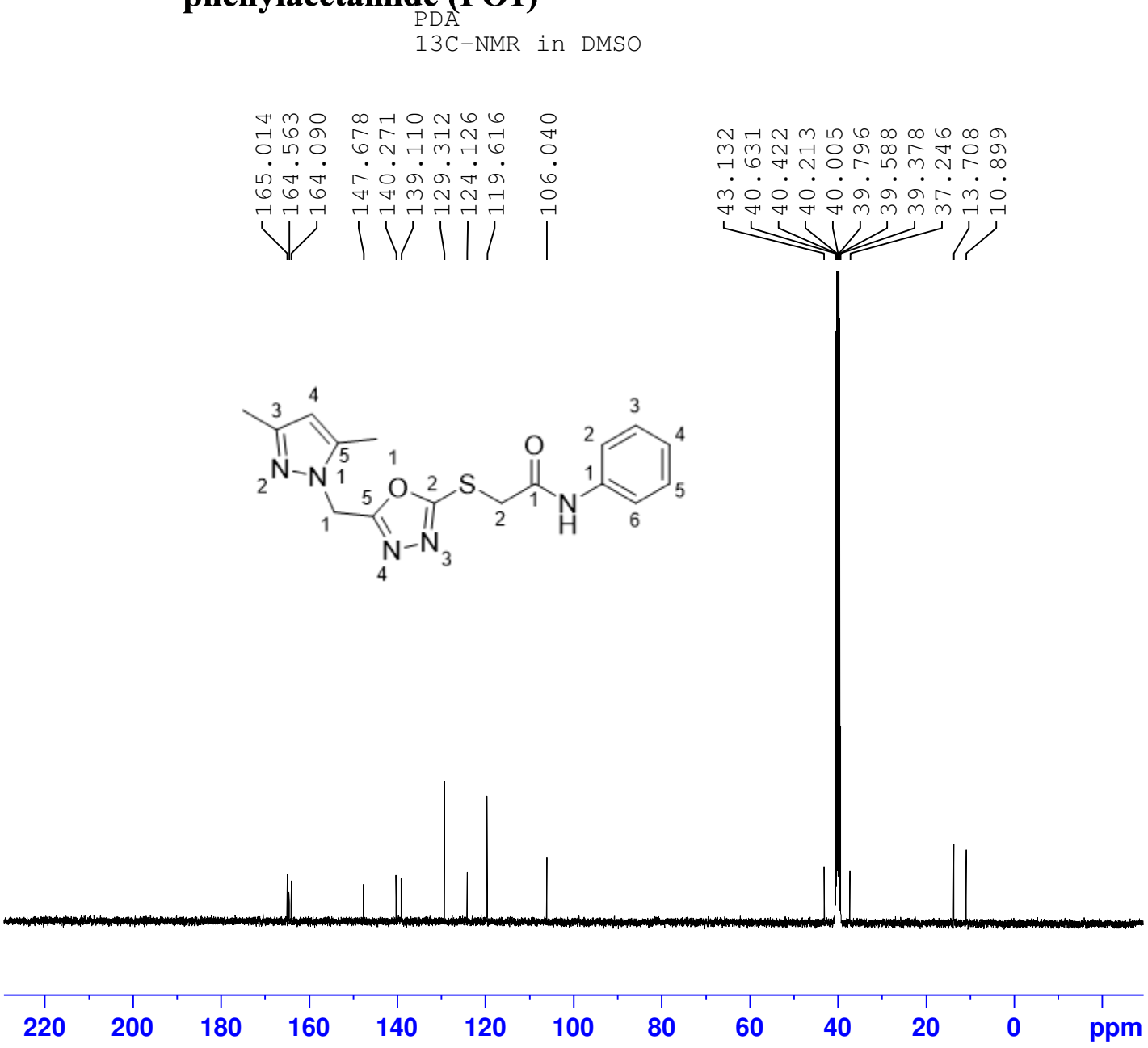
SF 400.3100000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-phenylacetamide (PO1)



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PROCNO	1

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DS	4
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DE	6.50 usec
TE	298.4 K
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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

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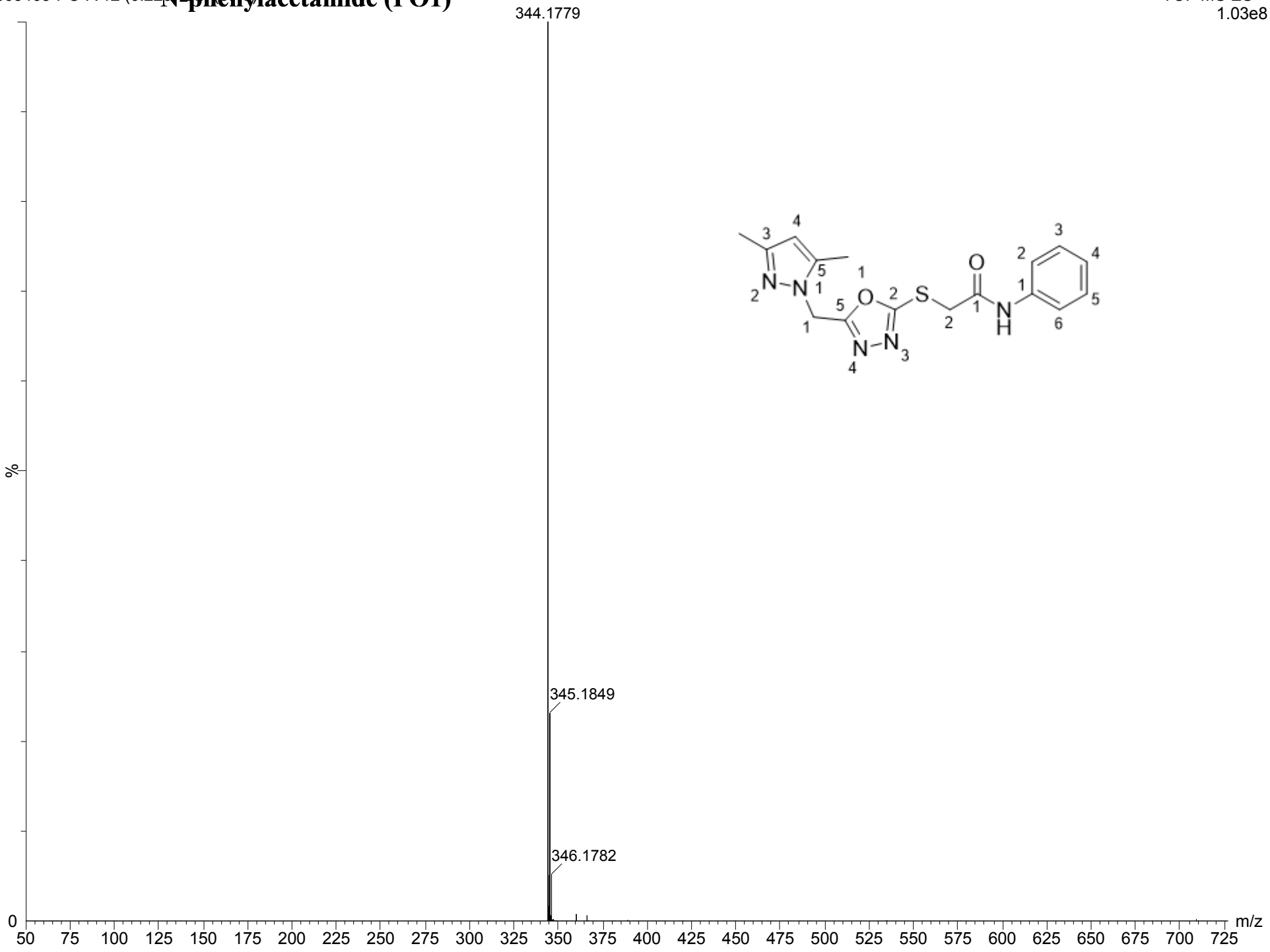
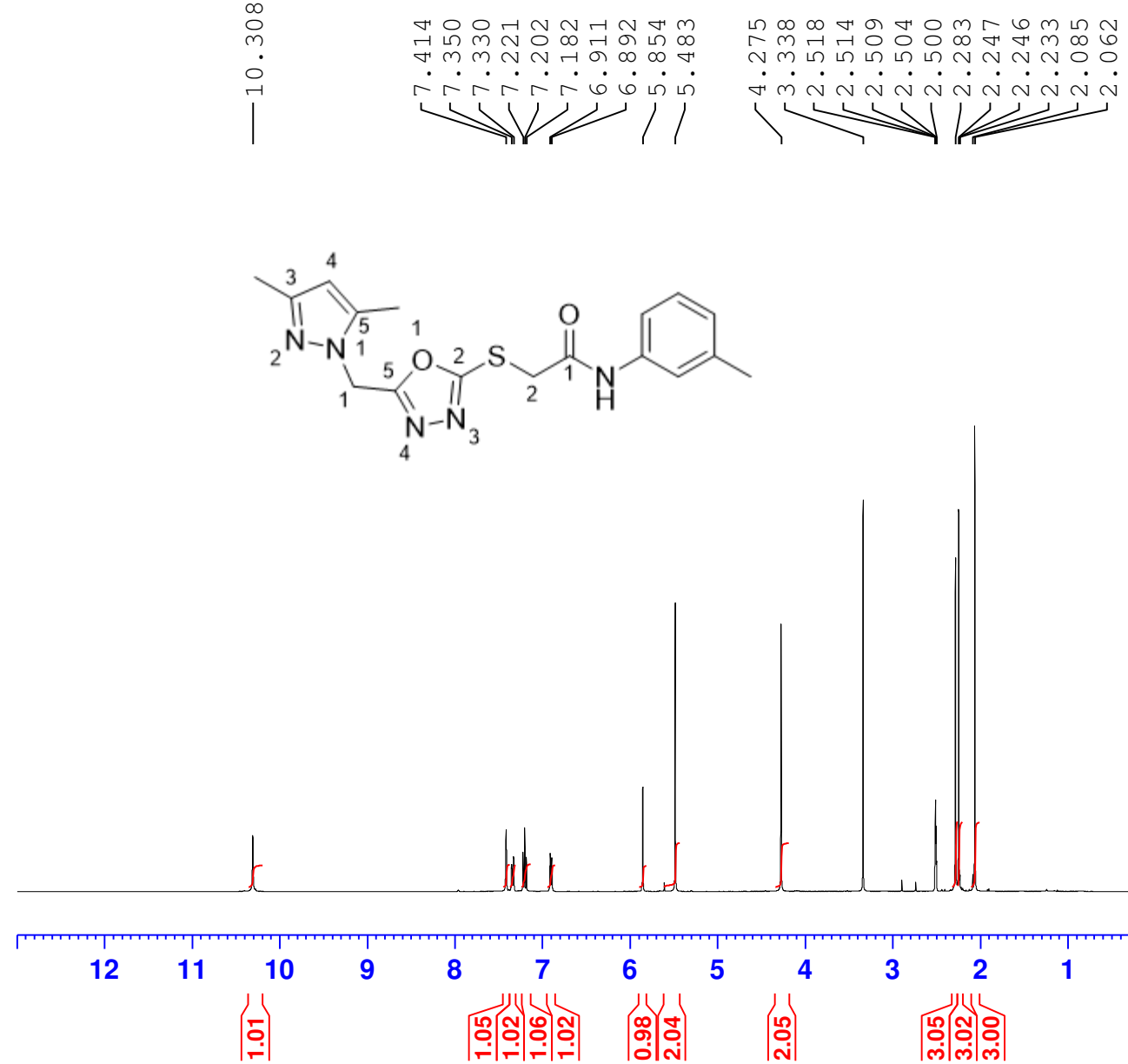
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-phenylacetamide (PO1)



^{1}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
1H-NMR in DMSO



Current Data Parameters
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EXPNO 1
PROCNO 1

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TD 65536
SOLVENT DMSO
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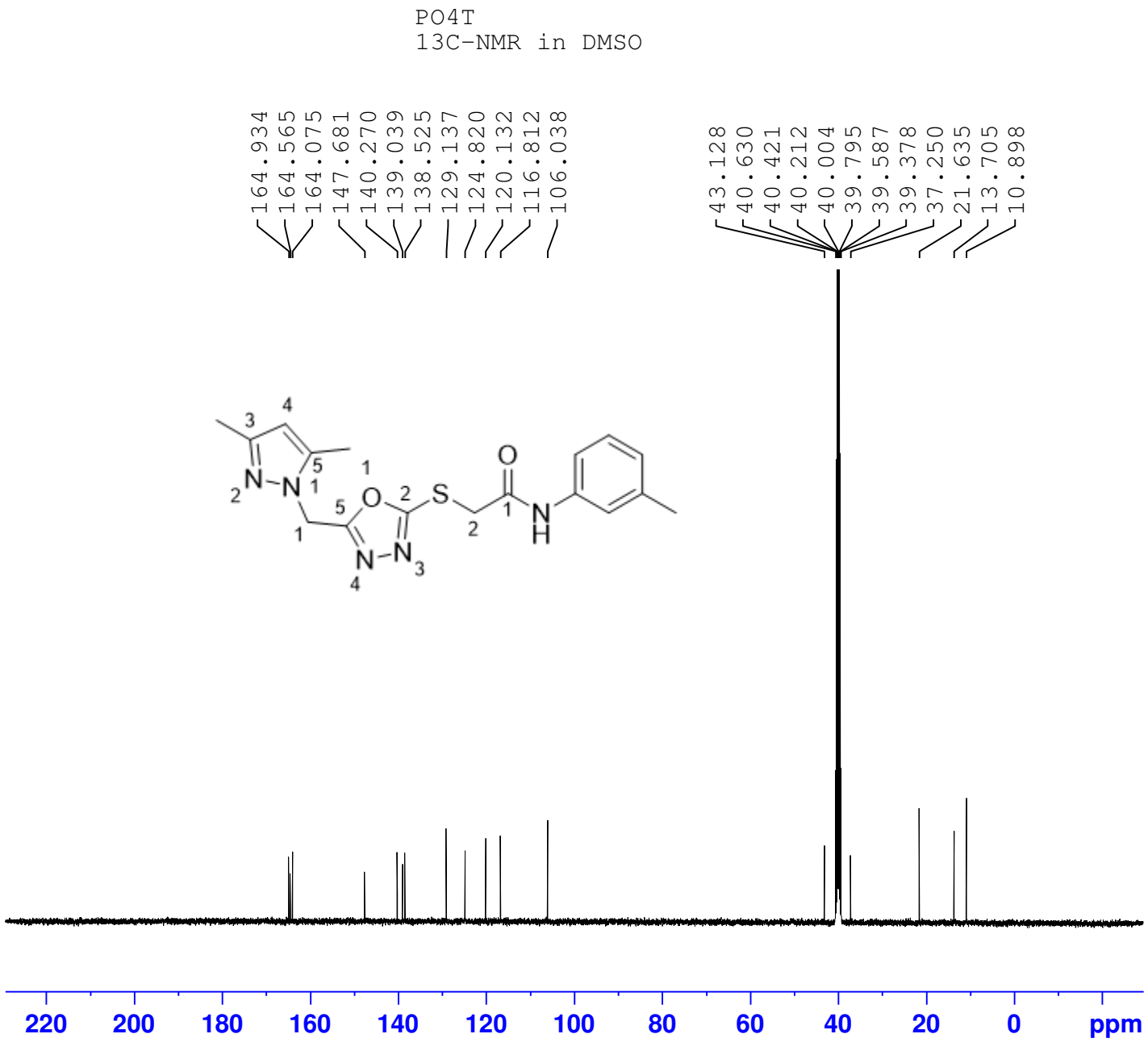
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 32.13
DW 62.400 usec
DE 17.09 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.3124719 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 11.28999996 W

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

^{13}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)



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EXPNO 2
PROCNO 1

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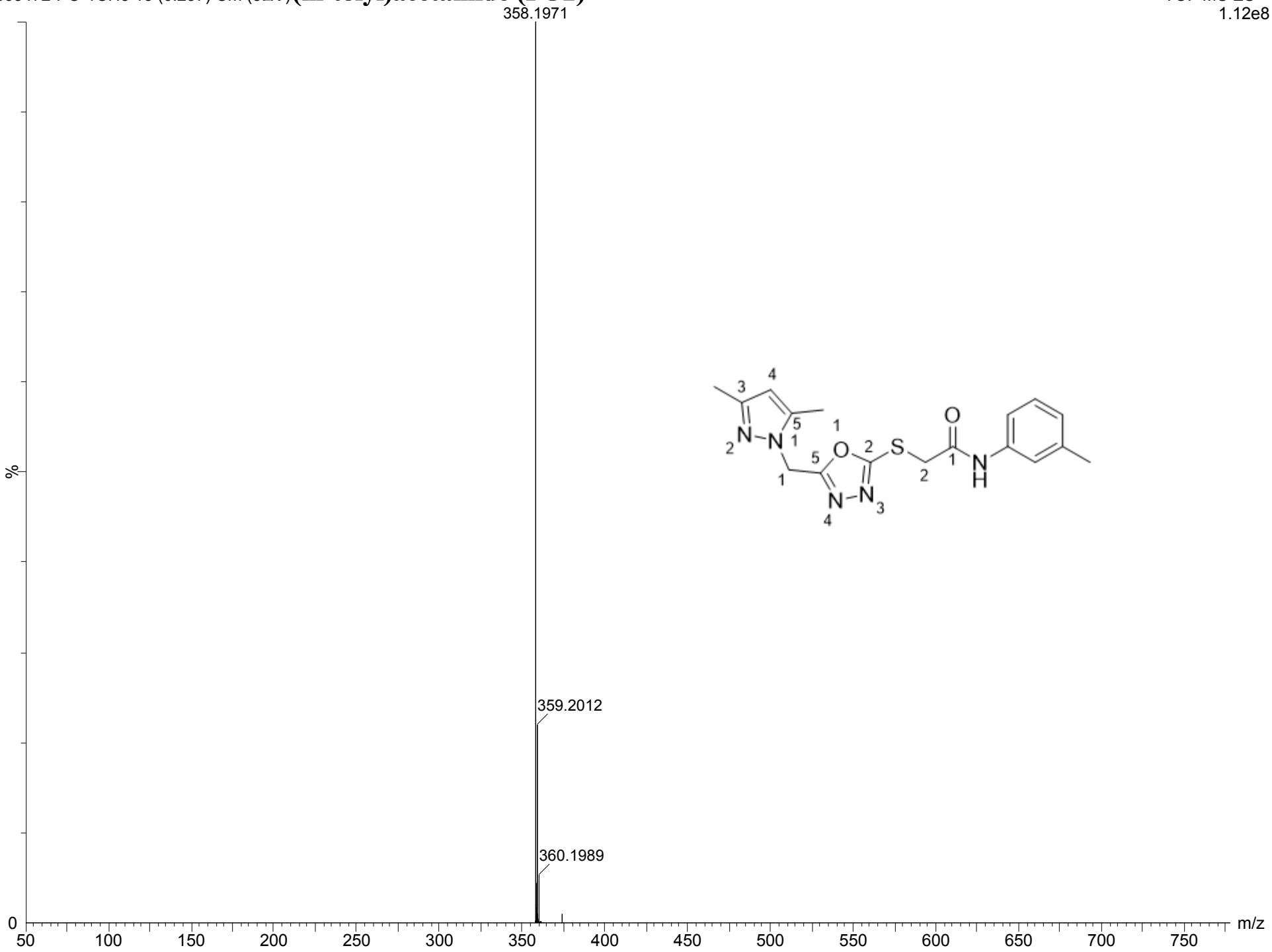
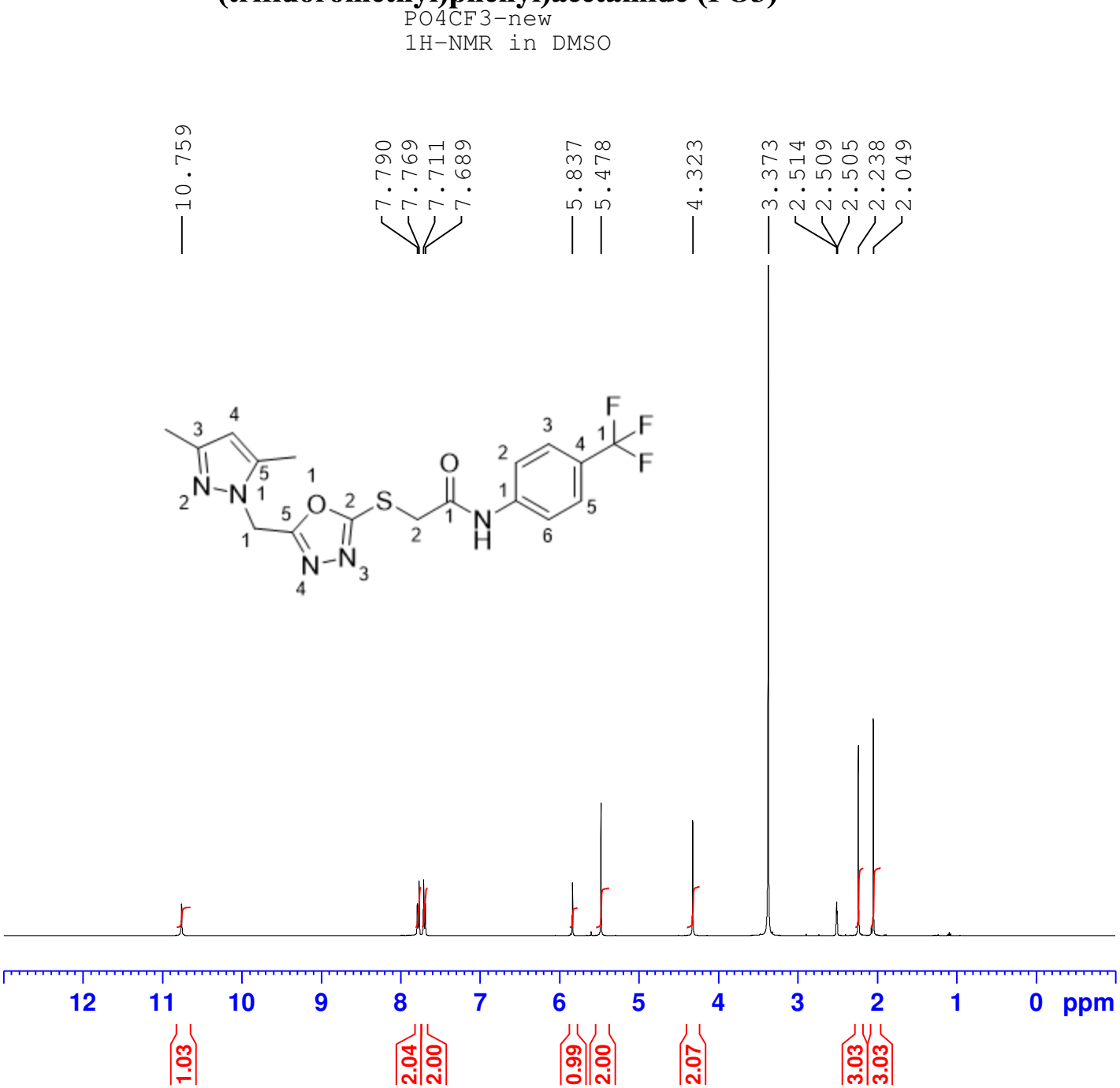
SWH 26041.666 Hz
FIDRES 0.794729 Hz
AQ 1.2582912 sec
RG 202.84
DW 19.200 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6680954 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 51.02600098 W
SFO2 400.3116012 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 11.28999996 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-(m-tolyl)acetamide (PO2)



^{1}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)

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PROCNO                      1

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TD                   65536
SOLVENT               DMSO
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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
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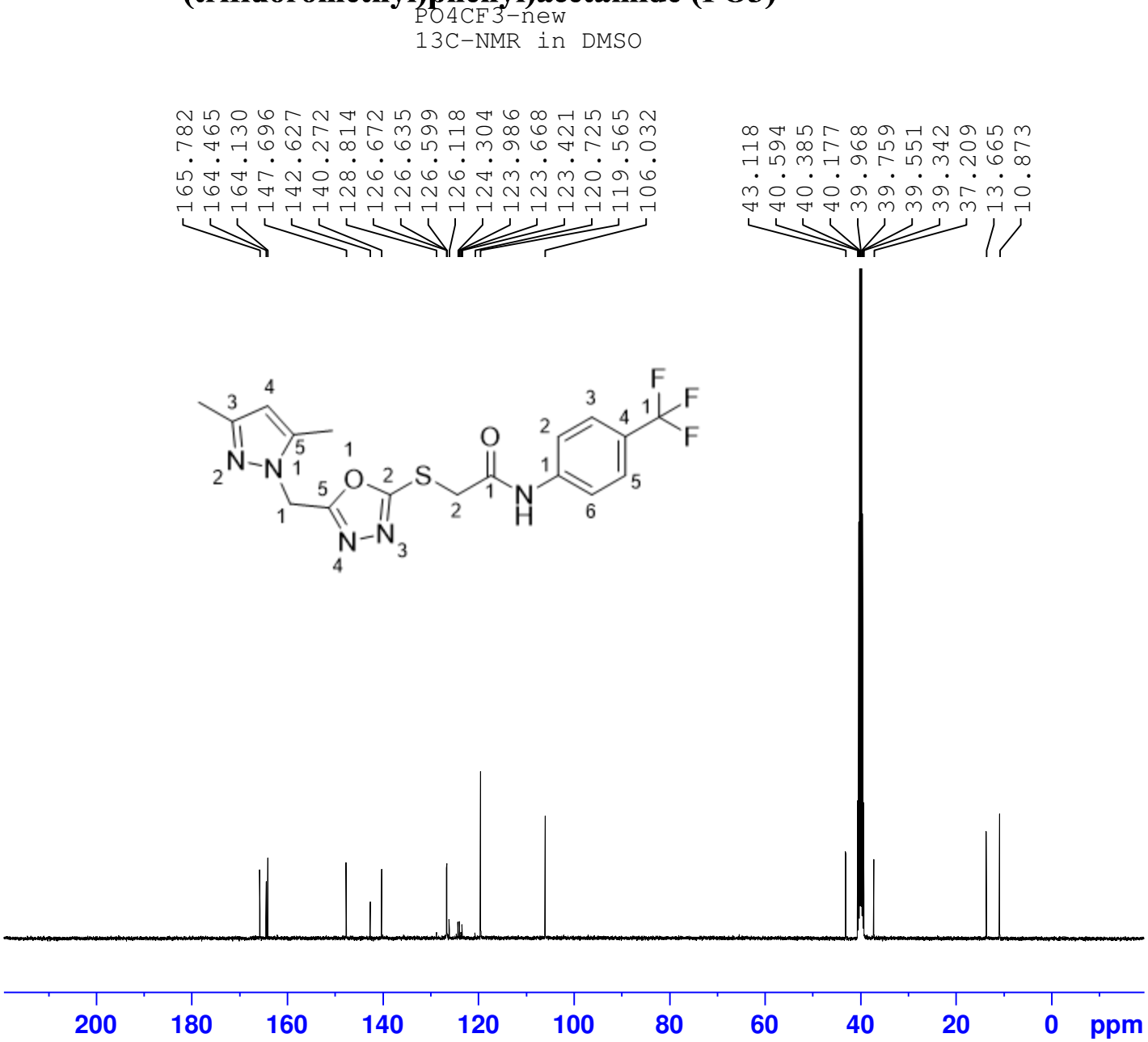
^{13}C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-(trifluoromethyl)phenyl)acetamide (PO3)



Current Data Parameters

NAME	23000506-PO4CF3-new
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

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SOLVENT	DMSO
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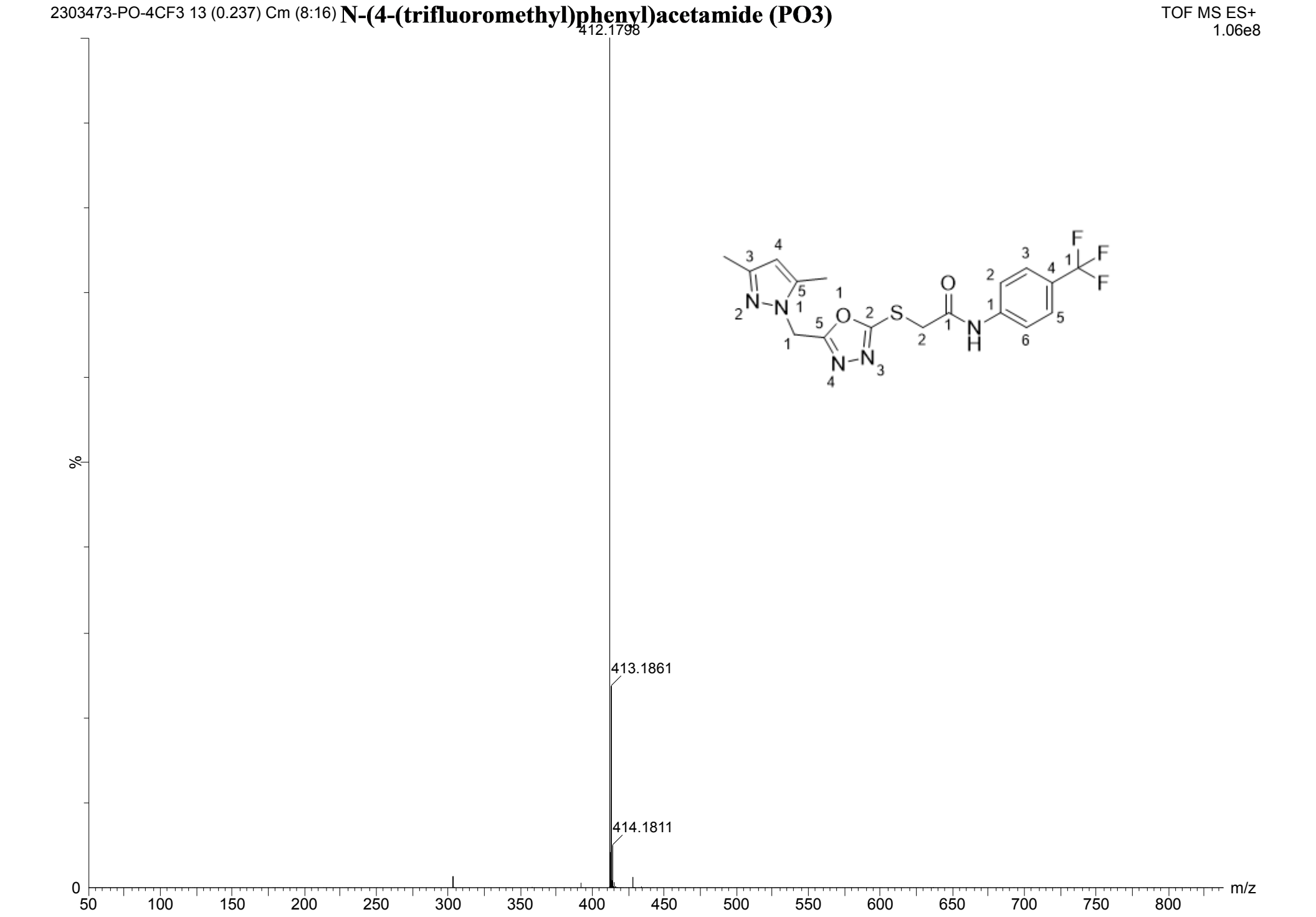
FIDRES	0.733596 Hz
AQ	1.3631488 sec
RG	202.84
DW	20.800 usec
DE	6.50 usec
TE	298.5 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6680954 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
PLW1	51.02600098 W
SFO2	400.3116012 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	90.00 usec
PLW2	11.28999996 W
PLW12	0.27318001 W
PLW13	0.13741000 W

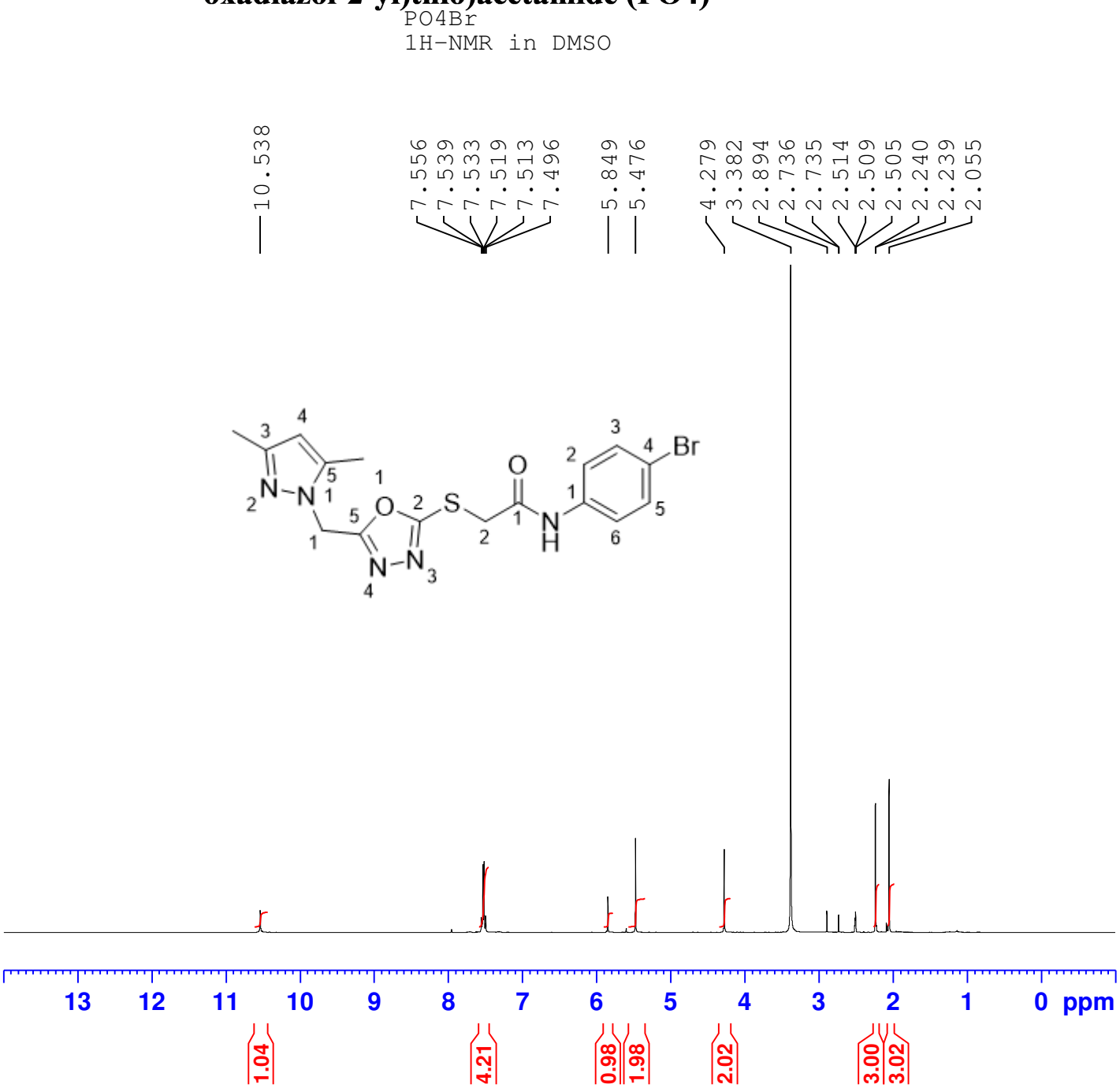
F2 - Processing parameters

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

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)



^{1}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)

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PROCNO                 1

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TD                 65536
SOLVENT             DMSO
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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
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WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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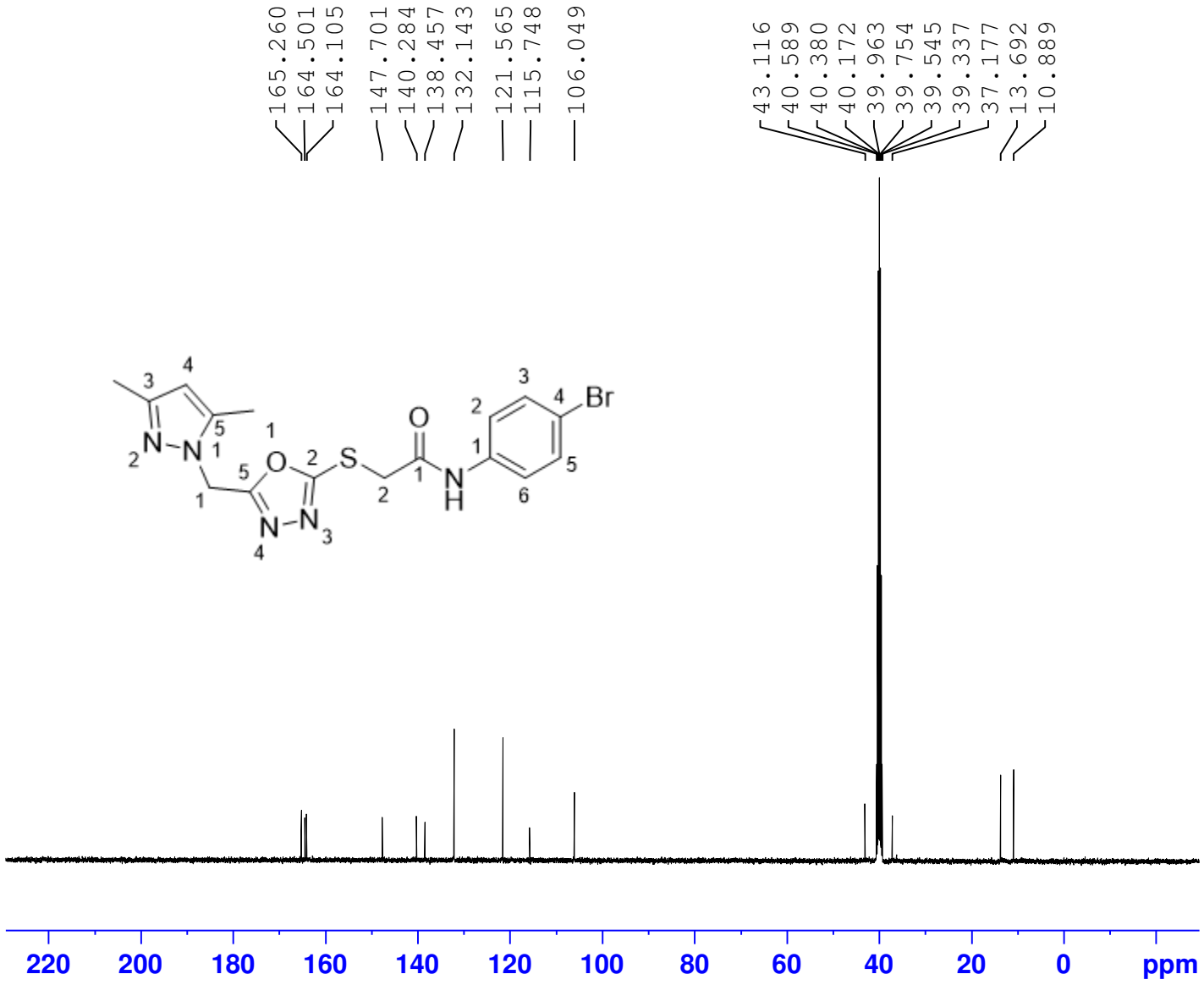
^{13}C NMR of N-(4-bromophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO4)

PO4Br
13C-NMR in DMSO



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PROCNO 1

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RG 202.84
DW 19.200 usec
DE 6.50 usec
TE 298.5 K
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D11 0.03000000 sec
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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
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PLW13 0.13741000 W

F2 - Processing parameters
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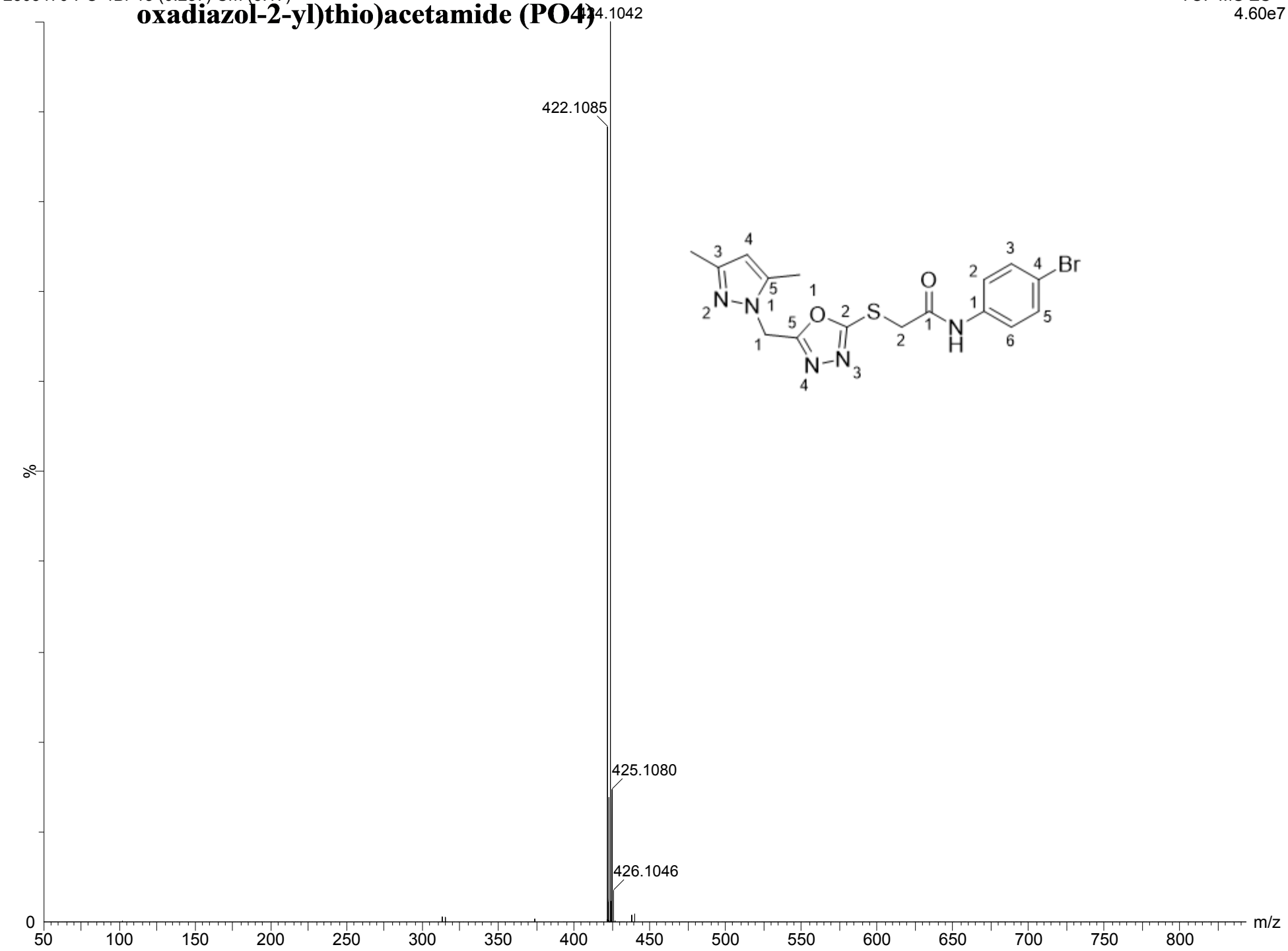
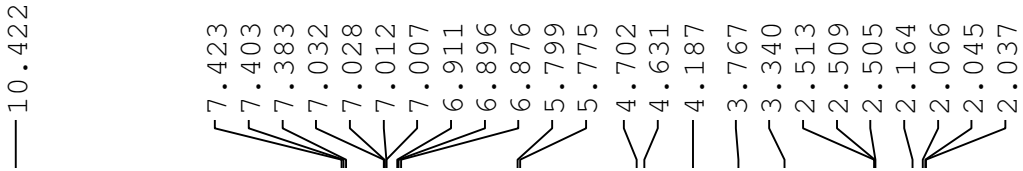
PC 1.40

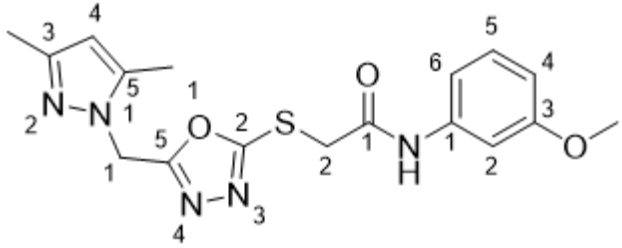
Mass spectrum of N-(4-bromophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO4)

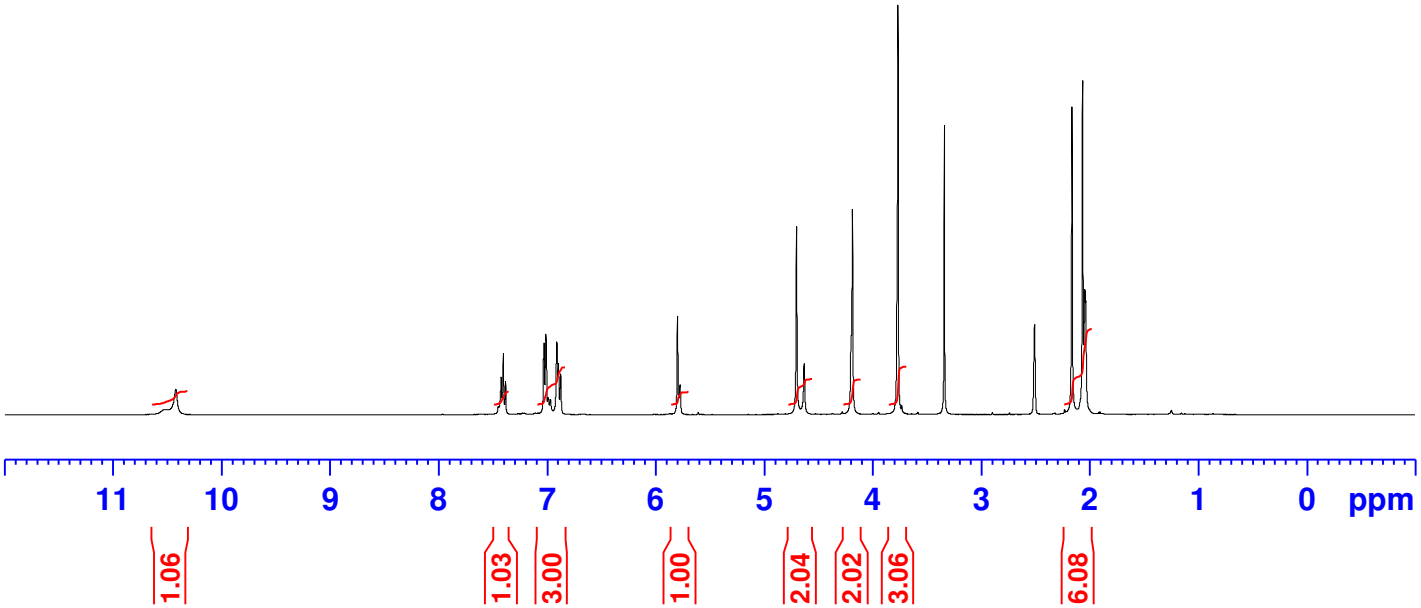


^{1}H NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3-methoxyphenyl)acetamide (PO5)

PO3MO
1H-NMR in DMSO







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PROCNO 1

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SOLVENT DMSO
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SWH 8012.820 Hz
FIDRES 0.244532 Hz
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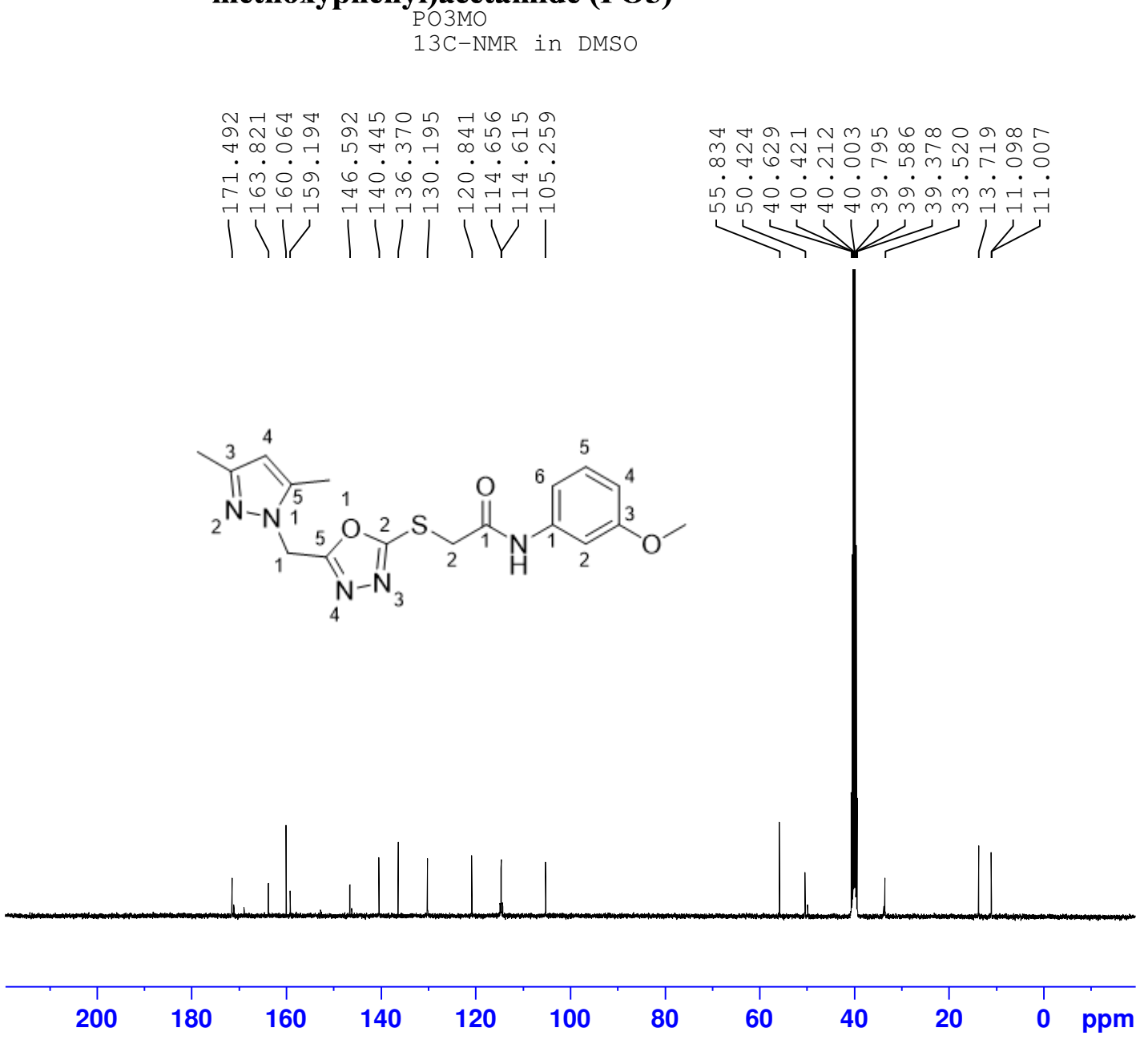
RG 32.13
DW 62.400 usec
DE 17.09 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.3124719 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 11.28999996 W

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

^{13}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)



BRUKER

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PROCNO                 1

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SWH           24038.461 Hz
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RG                202.84
DW                20.800 usec
DE                 6.50 usec
TE                298.1 K
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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
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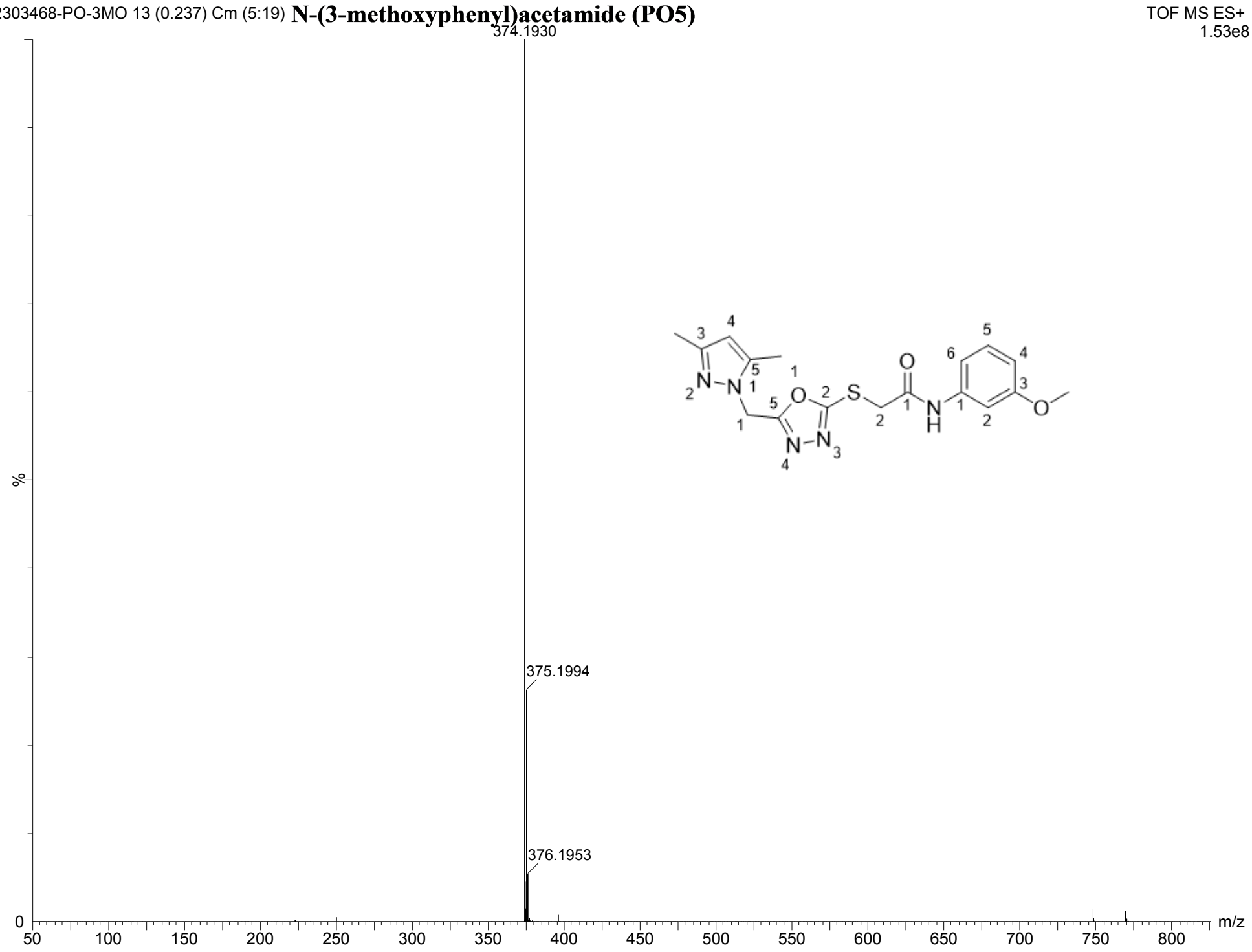
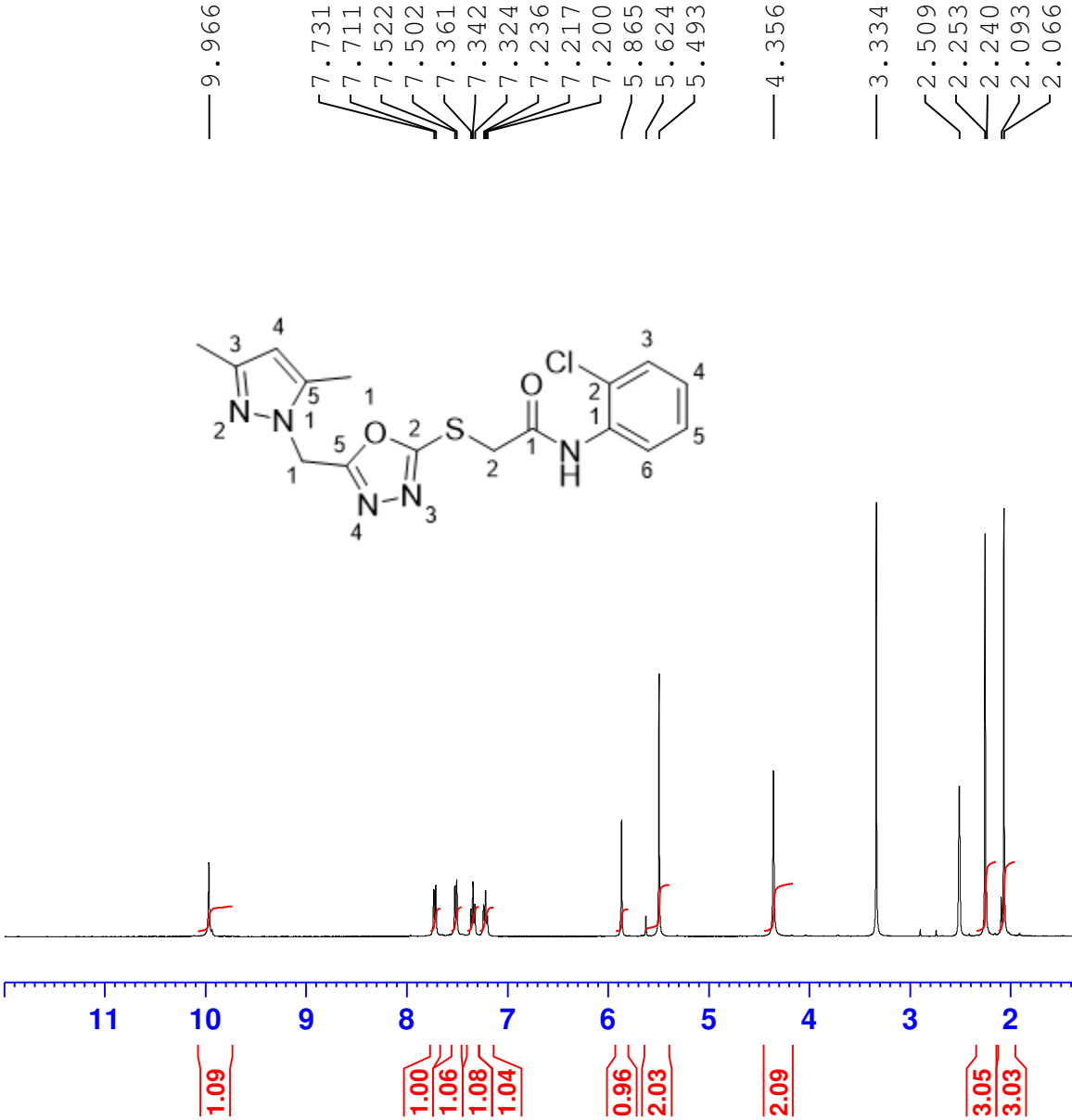
Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3-methoxyphenyl)acetamide (PO5)



^{1}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)

PO2Cl
1H-NMR in DMSO

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Current Data Parameters
NAME      23000460-PO2Cl
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          400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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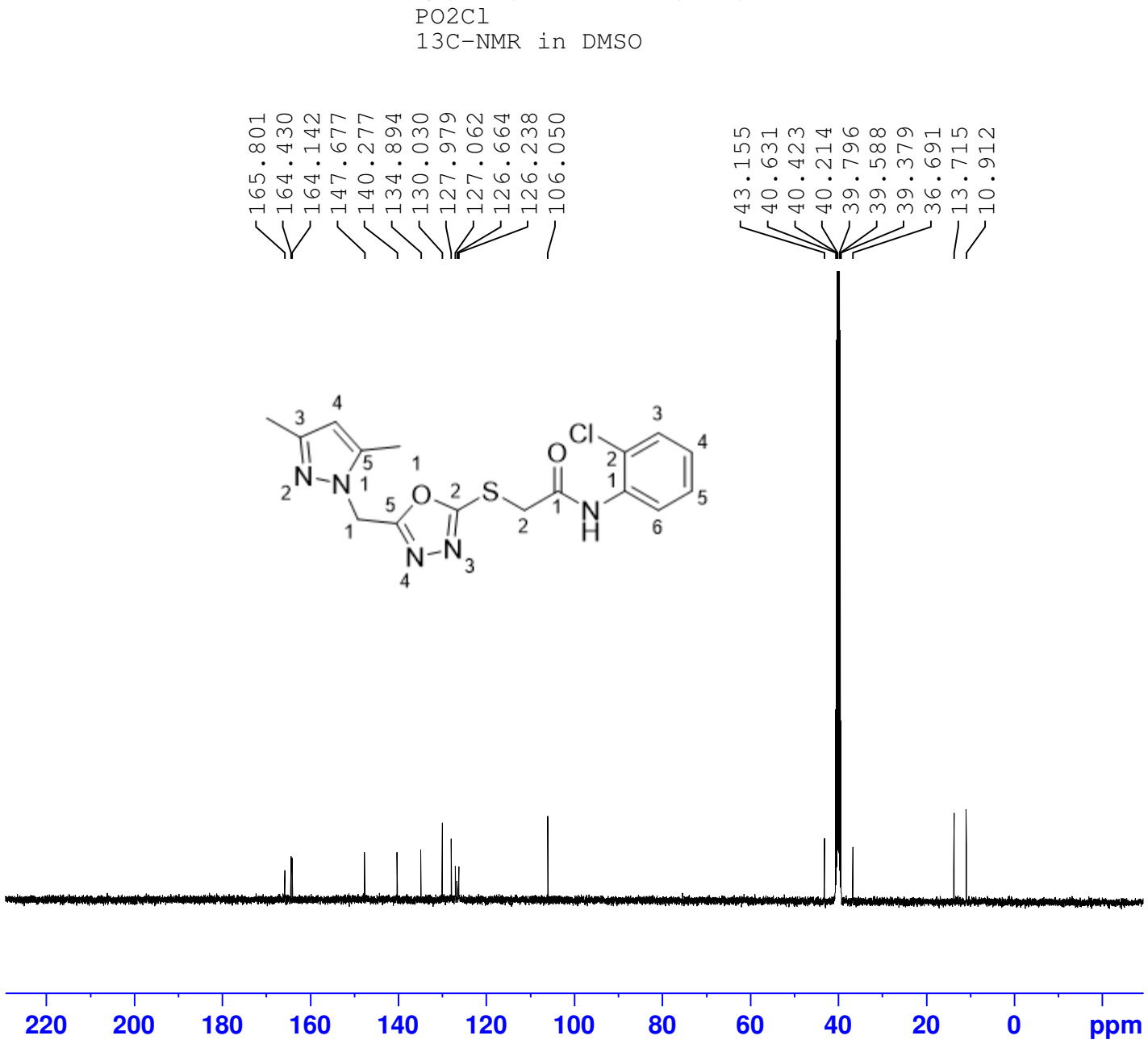
^{13}C NMR of N-(2-chlorophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO6)

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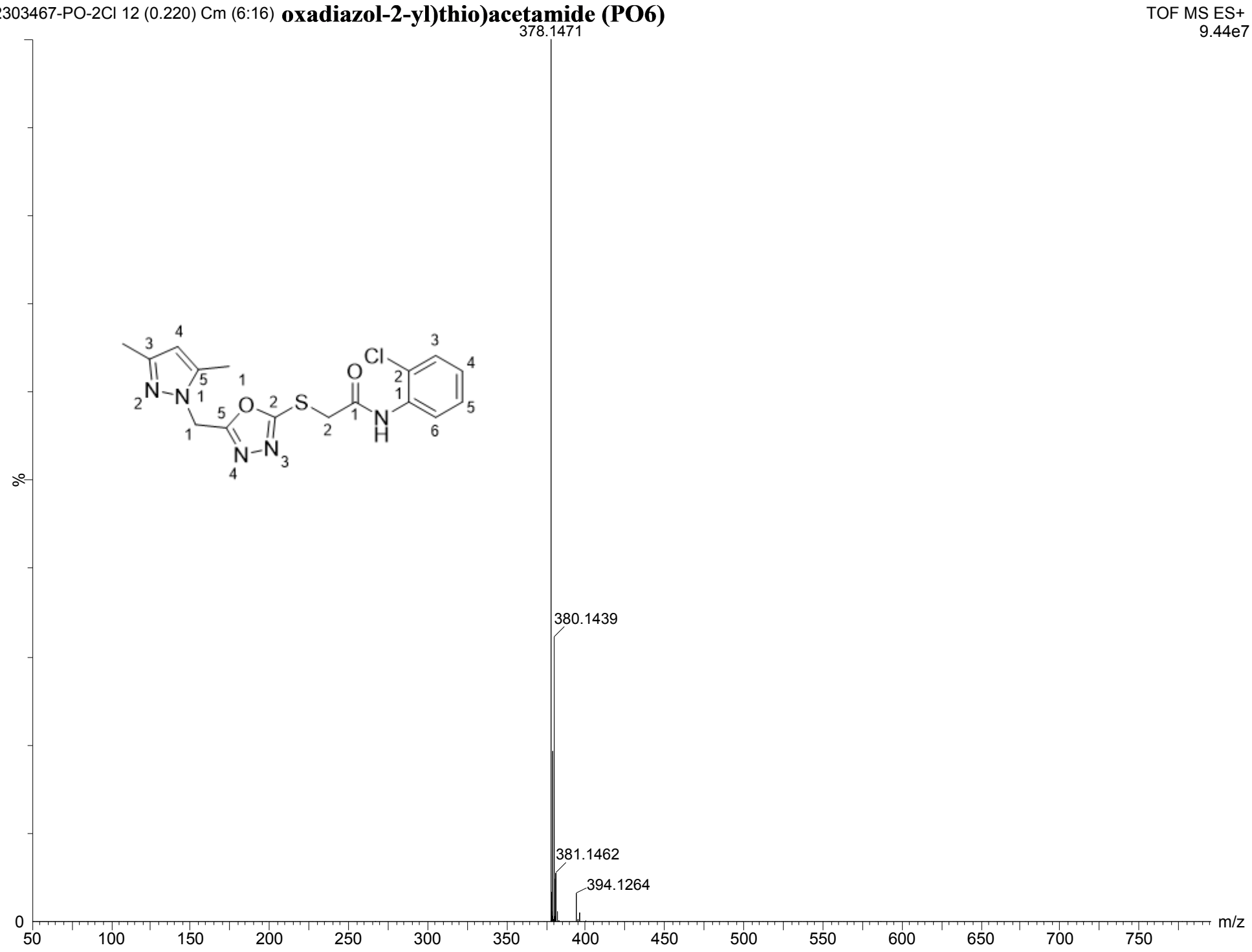
Current Data Parameters
NAME      23000460-PO2Cl
EXPNO                  2
PROCNO                 1

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                 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

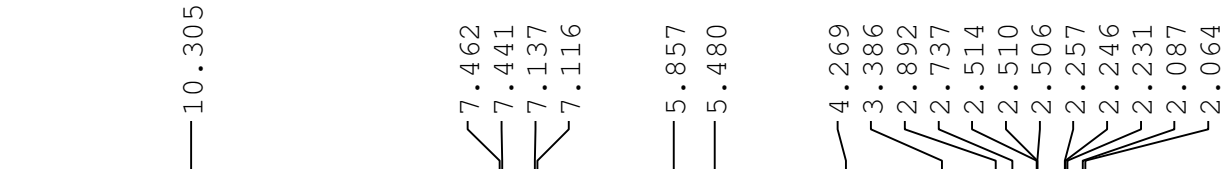
F2 - Processing parameters
SI                 32768
SF           100.6580296 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

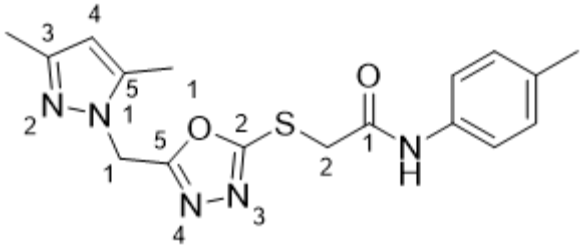
Mass spectrum of N-(2-chlorophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO6)



^{1}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





Current Data Parameters
NAME 23000494-PO4CH3
EXPNO 1
PROCNO 1

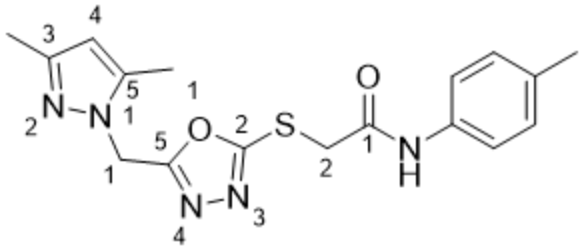
F2 - Acquisition Parameters
Date_ 20230513
Time 15.36 h
INSTRUM spect
PROBHD Z108618_0984 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 32.13
DW 62.400 usec
DE 17.09 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.3124719 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 11.28999996 W

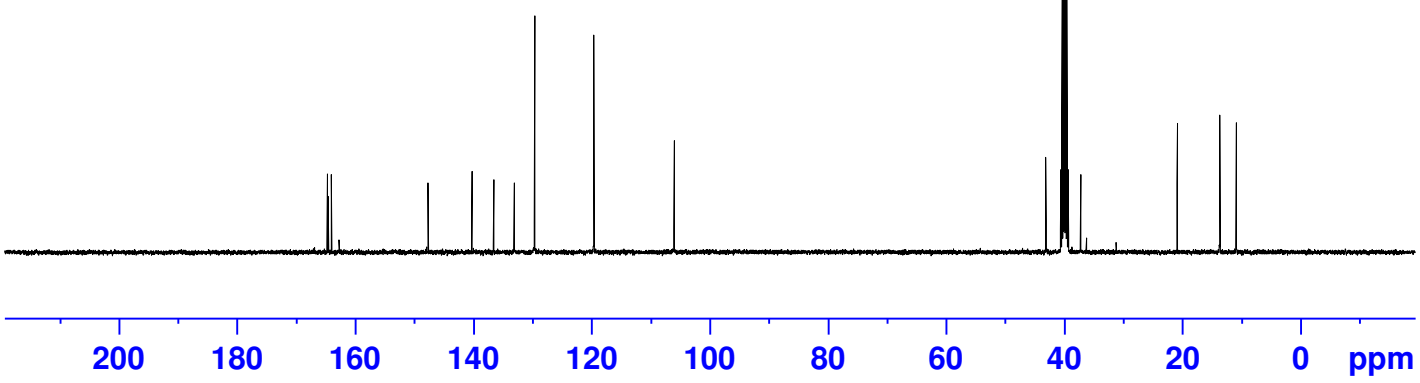
F2 - Processing parameters
SI 65536
SF 400.3100000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}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
13C-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



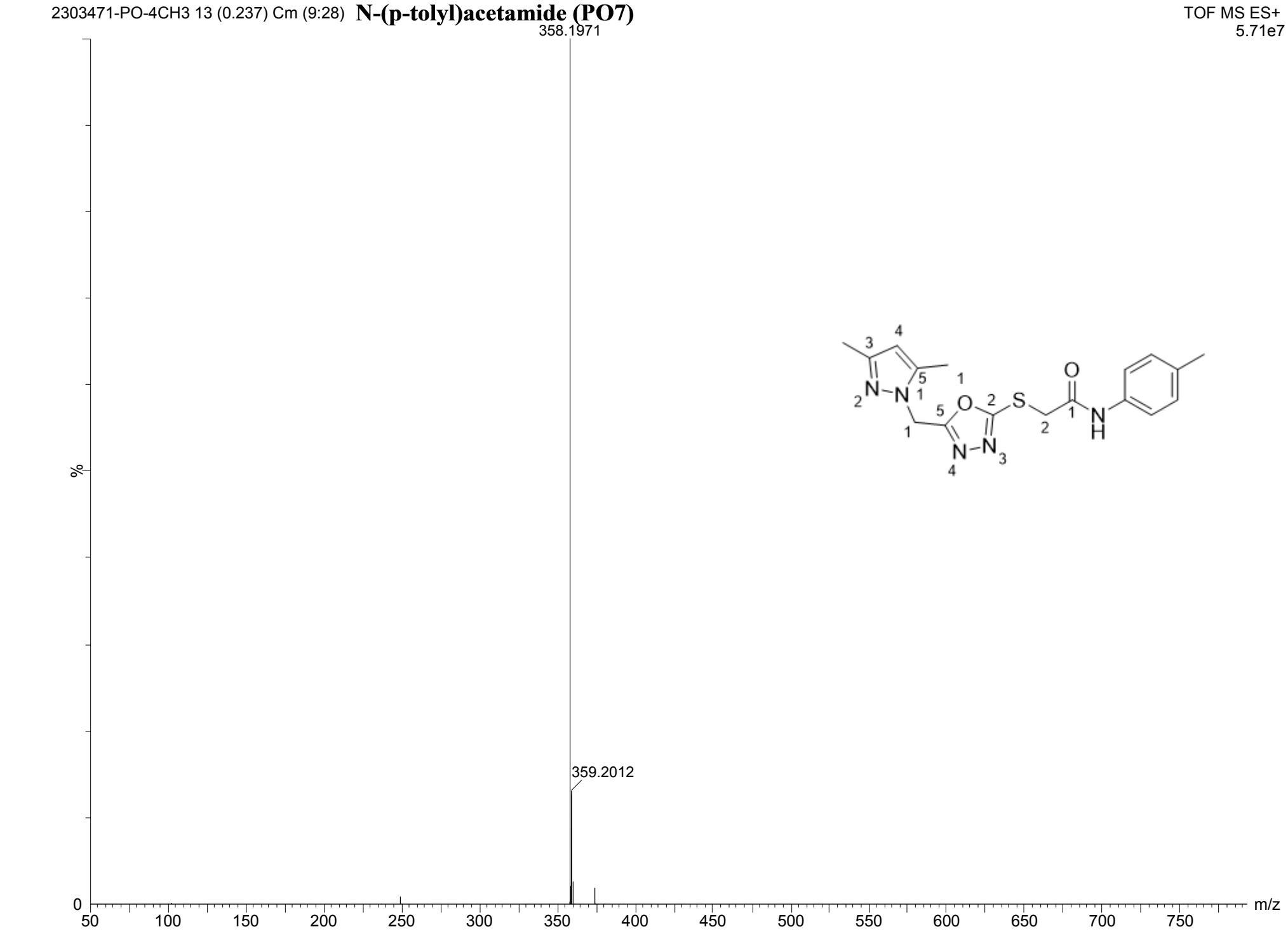


Current Data Parameters
NAME 23000494-PO4CH3
EXPNO 2
PROCNO 1

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

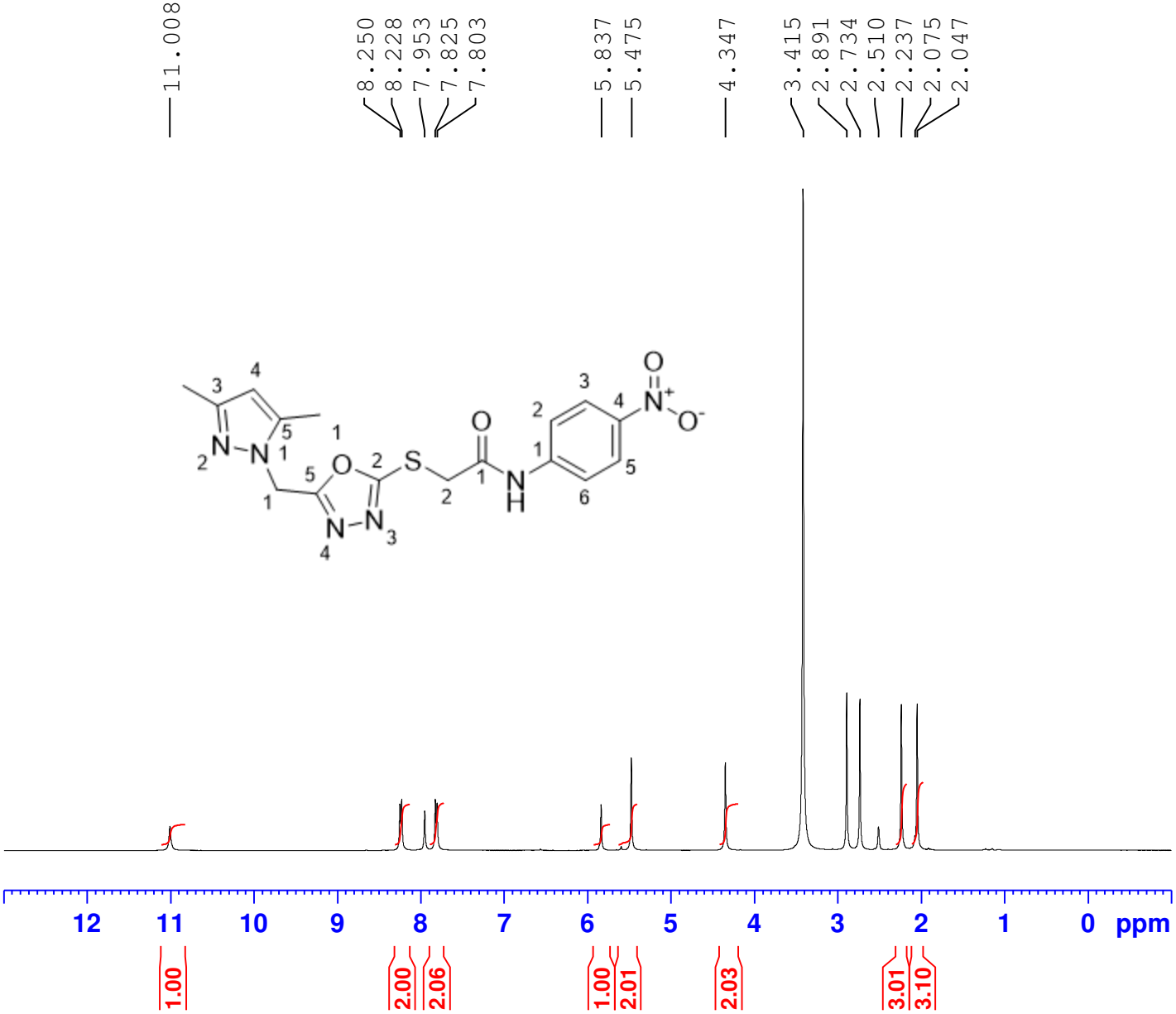
F2 - Processing parameters
SI 32768
SF 100.6580296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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)



^{1}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
1H-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

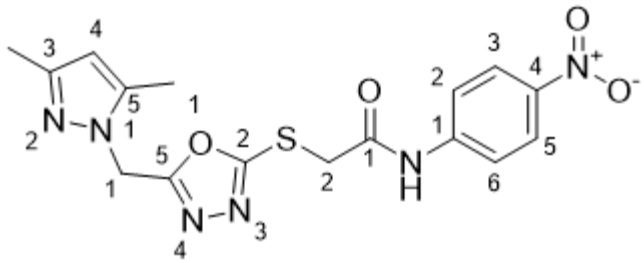
F2 - Processing parameters
SI 65536
SF 400.3100000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}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

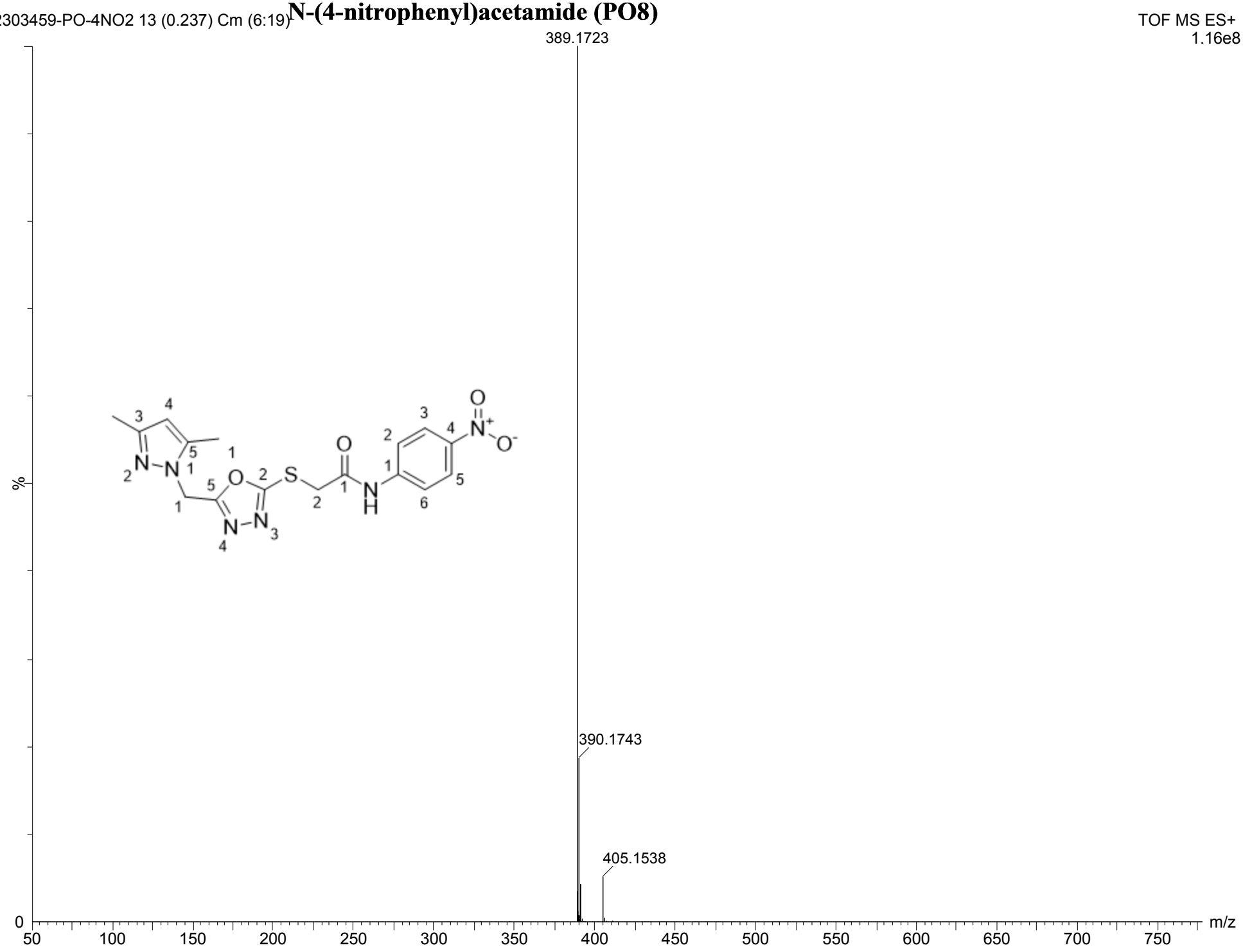


Current Data Parameters
NAME 23000462-PO4NO2
EXPNO 2
PROCNO 1

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

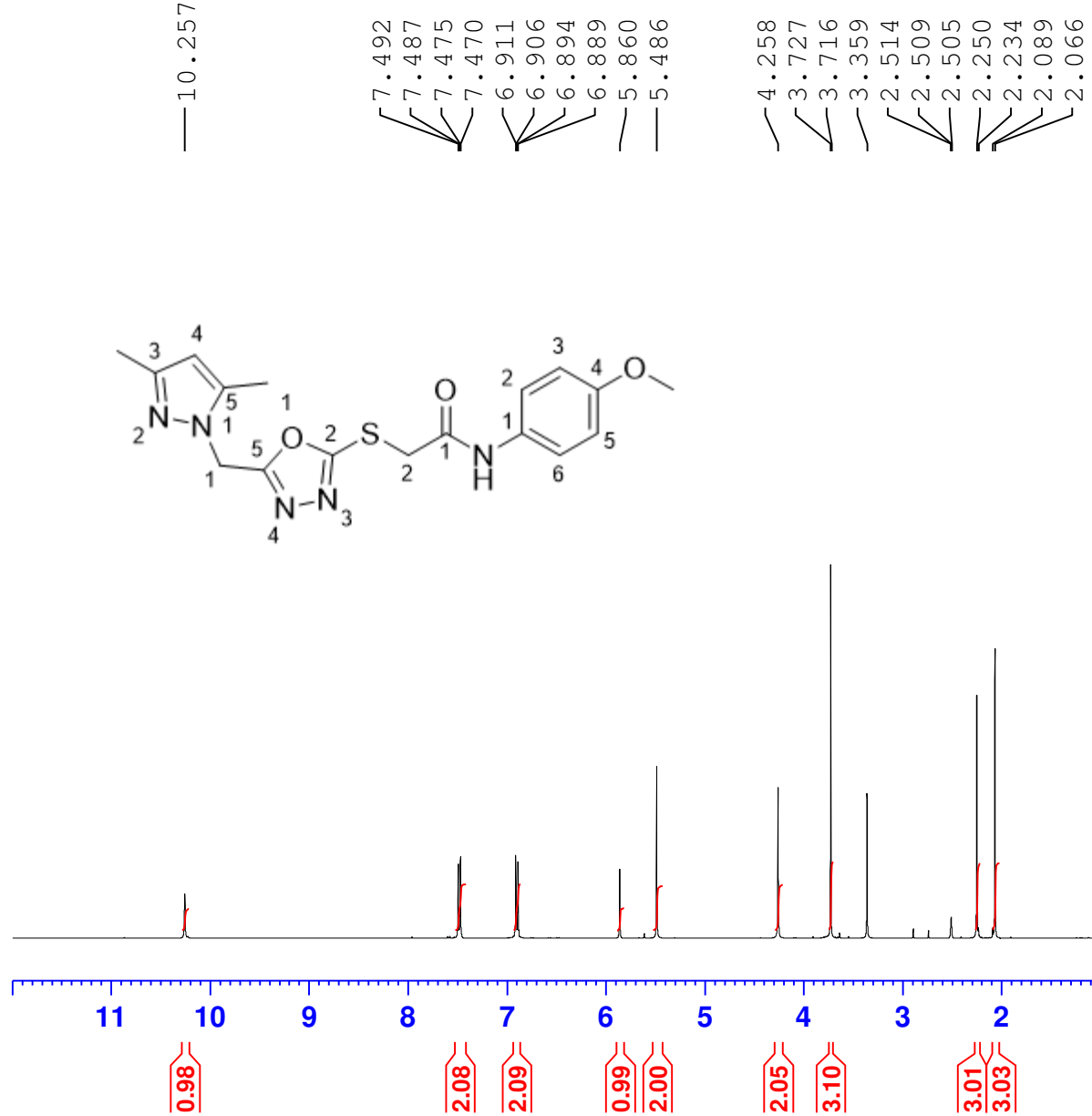
F2 - Processing parameters
SI 32768
SF 100.6580296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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)



^{1}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

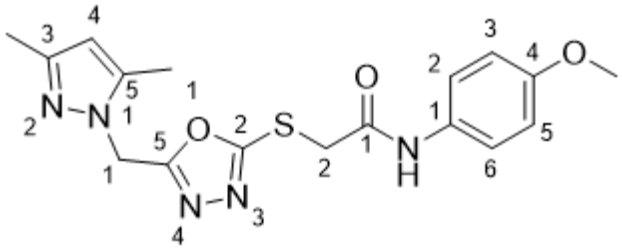
F2 - Processing parameters
SI 65536
SF 400.3100000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

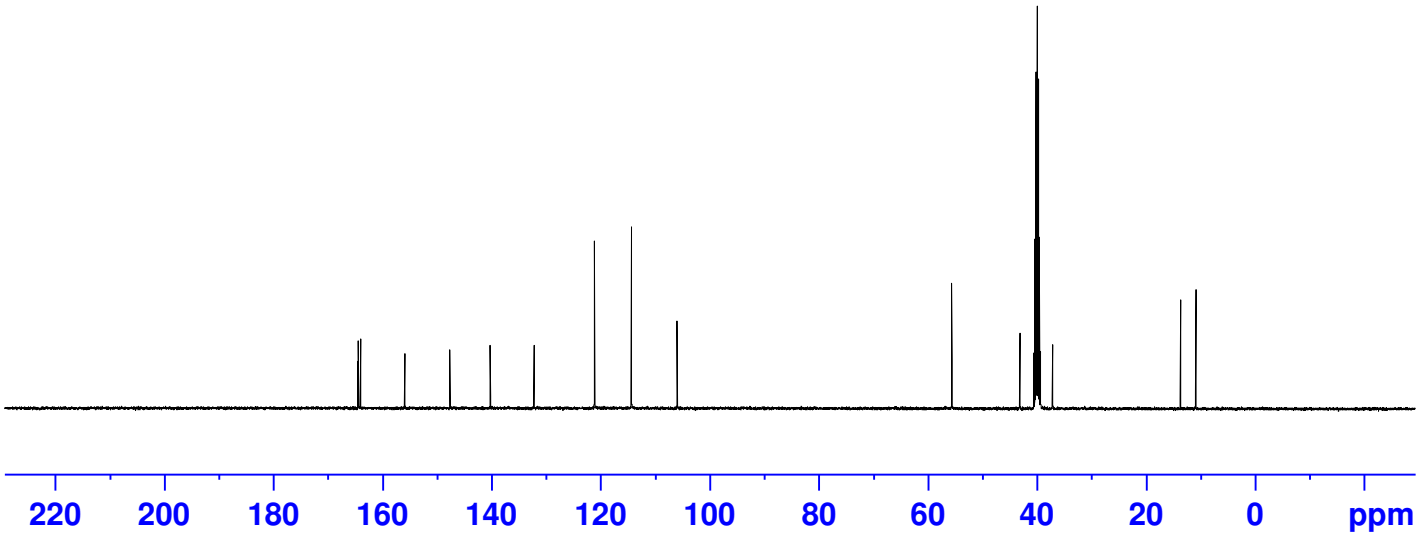
^{13}C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-methoxyphenyl)acetamide (PO9)

PO4MO
13C-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



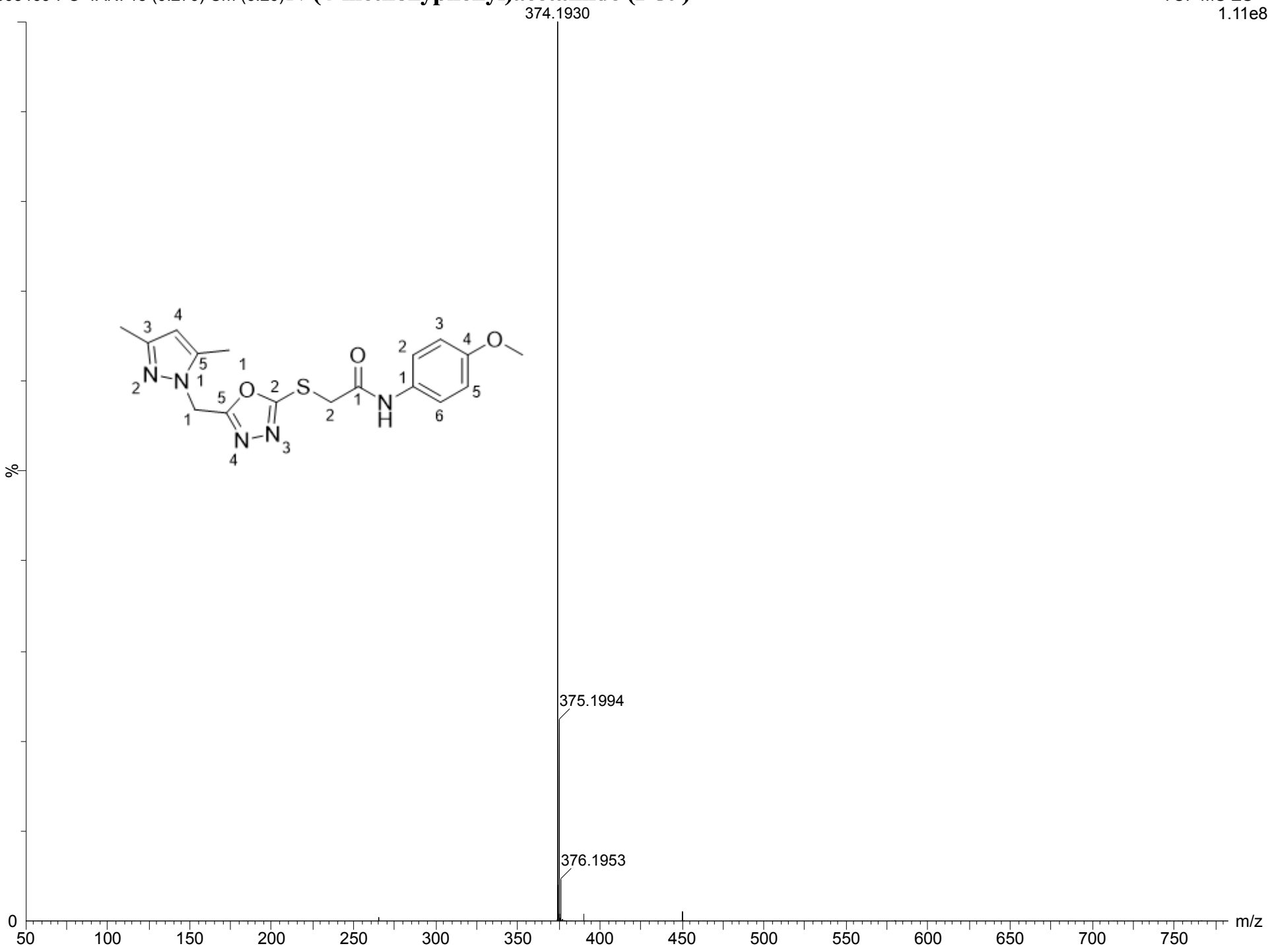


Current Data Parameters
NAME 23000459-PO4MO
EXPNO 2
PROCNO 1

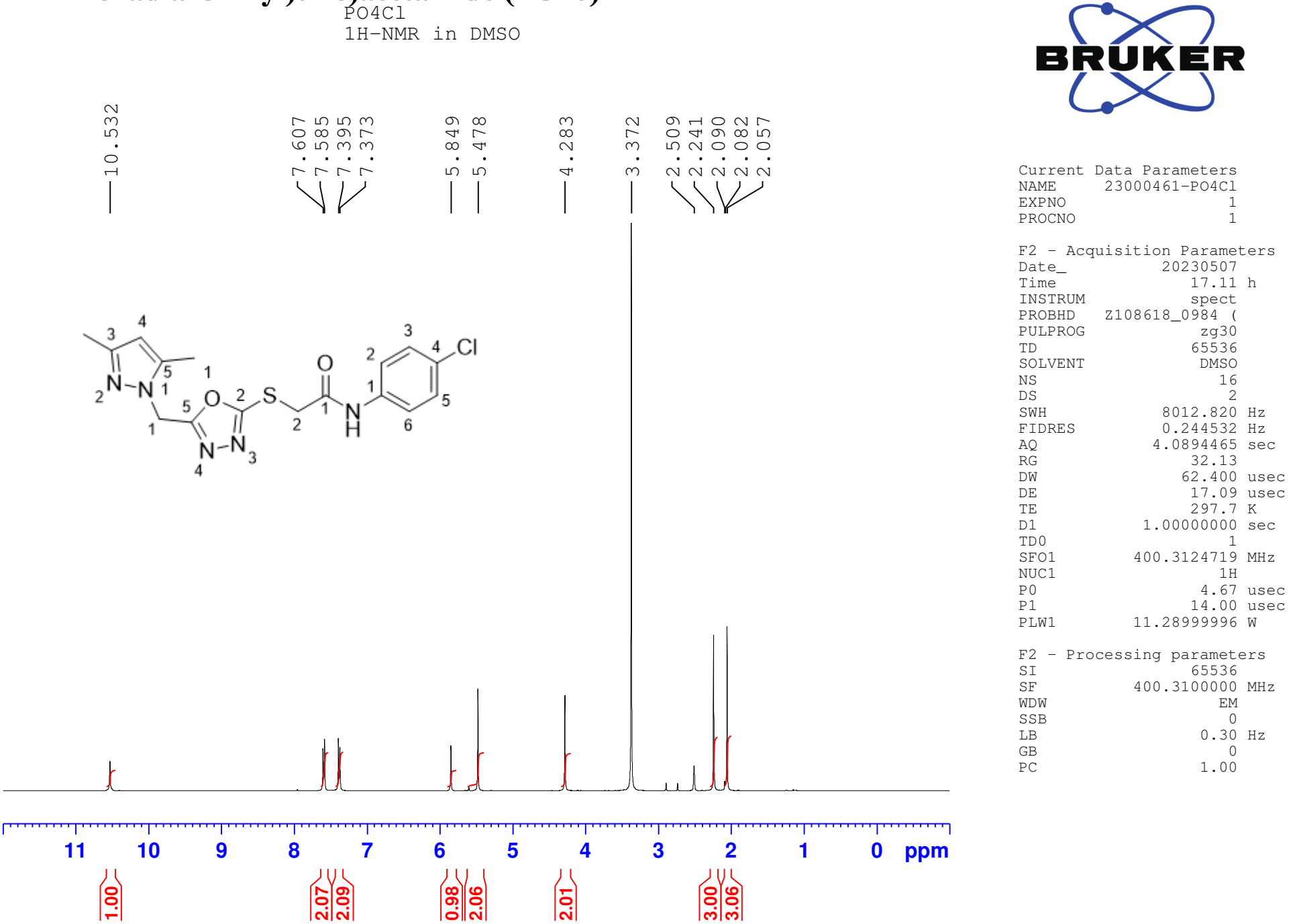
F2 - Acquisition Parameters
Date_ 20230508
Time 11.16 h
INSTRUM spect
PROBHD Z108618_0984 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 600
DS 4
SWH 26041.666 Hz
FIDRES 0.794729 Hz
AQ 1.2582912 sec
RG 202.84
DW 19.200 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6680954 MHz
NUC1 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-methoxyphenyl)acetamide (PO9)



^{1}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)

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Current Data Parameters
NAME      23000461-PO4Cl
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
```
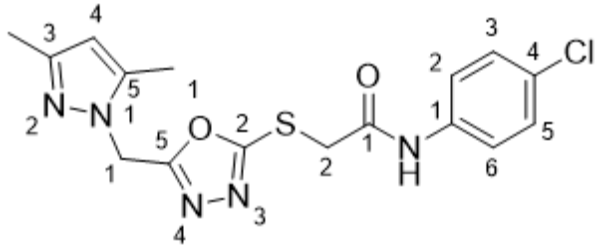
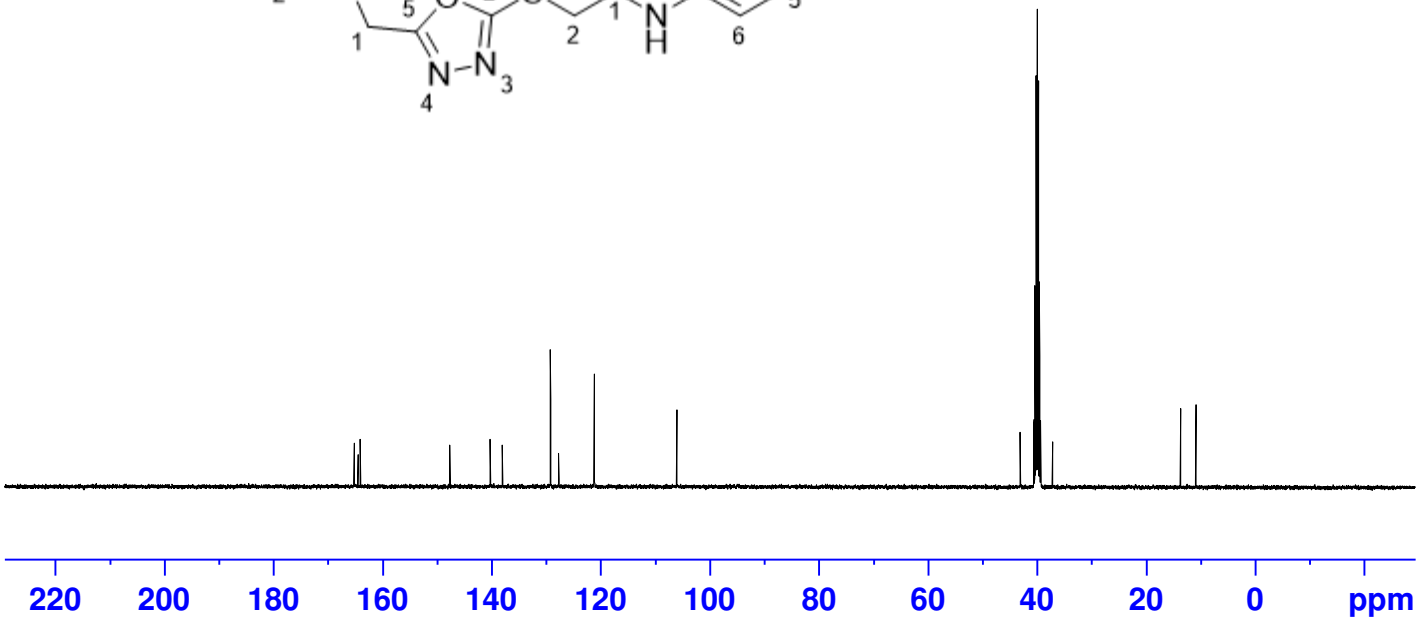

^{13}C NMR of N-(4-chlorophenyl)-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO10)

PO4Cl
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-PO4Cl
EXPNO 2
PROCNO 1

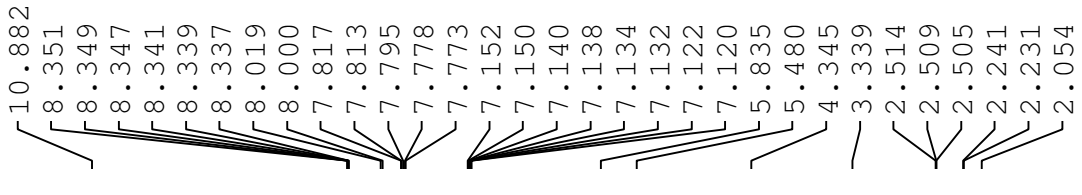
F2 - Acquisition Parameters
Date_ 20230508
Time 12.22 h
INSTRUM spect
PROBHD Z108618_0984 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 600
DS 4
SWH 26041.666 Hz
FIDRES 0.794729 Hz
AQ 1.2582912 sec
RG 202.84
DW 19.200 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6680954 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

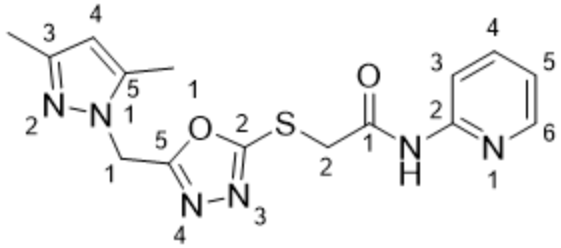
F2 - Processing parameters
SI 32768
SF 100.6580296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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)

^{1}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
1H-NMR in DMSO





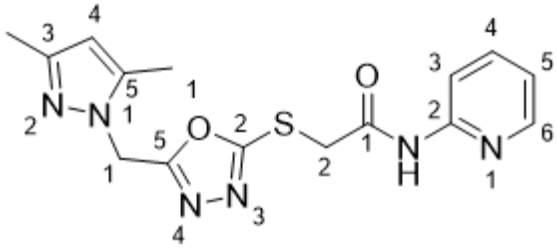
Current Data Parameters
NAME 23000441-PO2AP
EXPNO 1
PROCNO 1

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

^{13}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
13C-NMR in DMSO

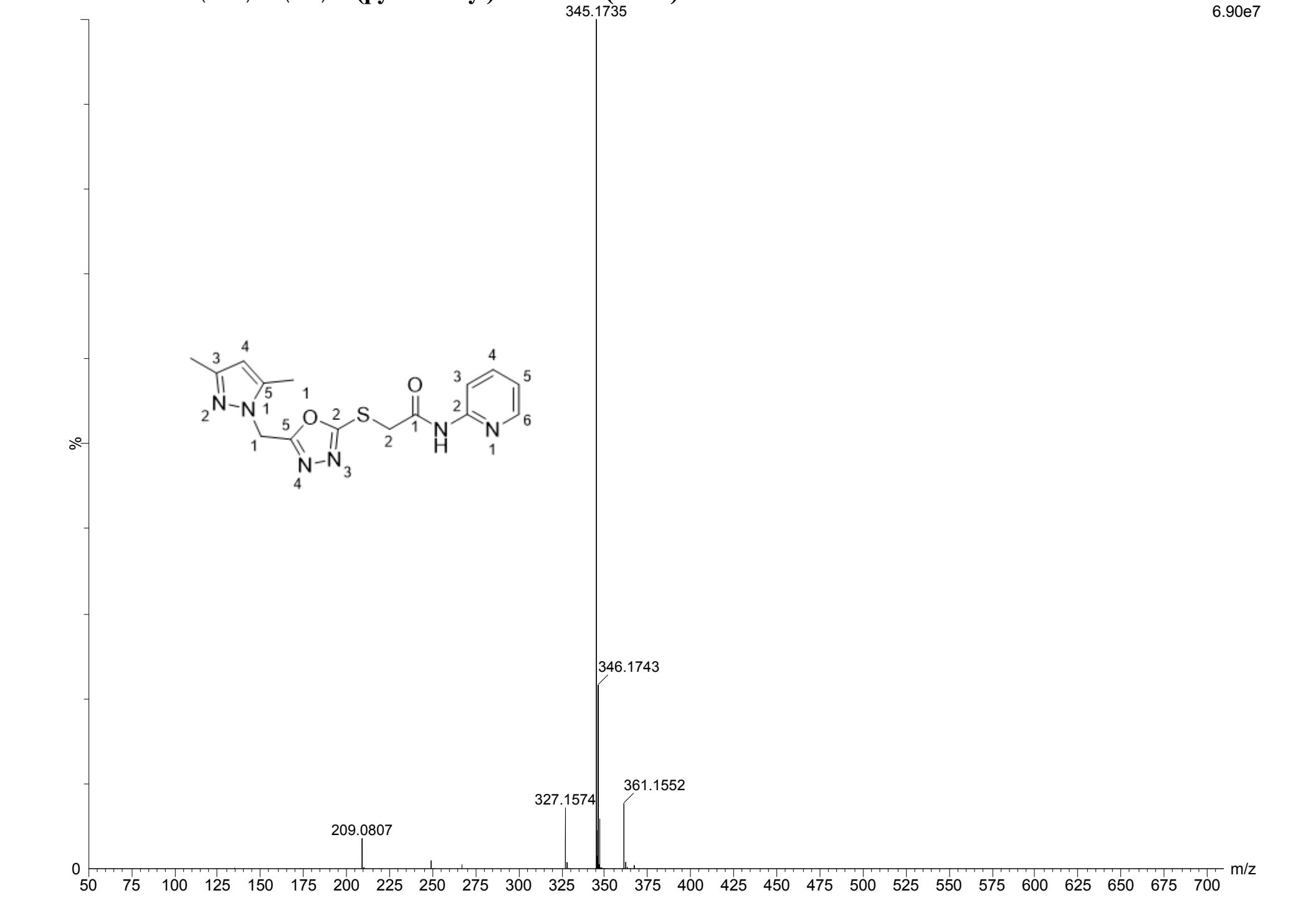


Current Data Parameters
NAME 23000441-PO2AP
EXPNO 2
PROCNO 1

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

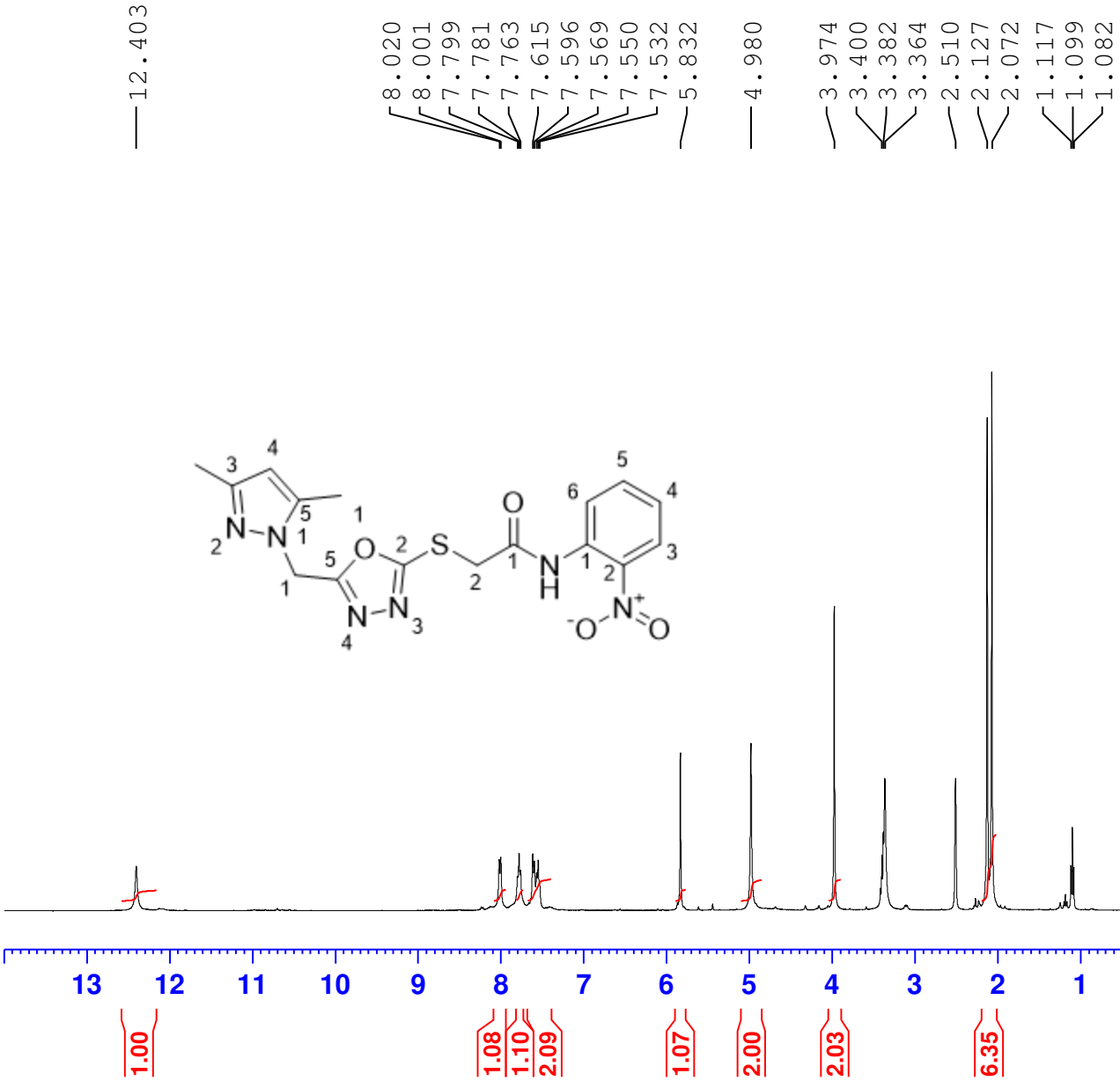
F2 - Processing parameters
SI 32768
SF 100.6580296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(pyridin-2-yl)acetamide (PO11)



^{1}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
1H-NMR in DMSO

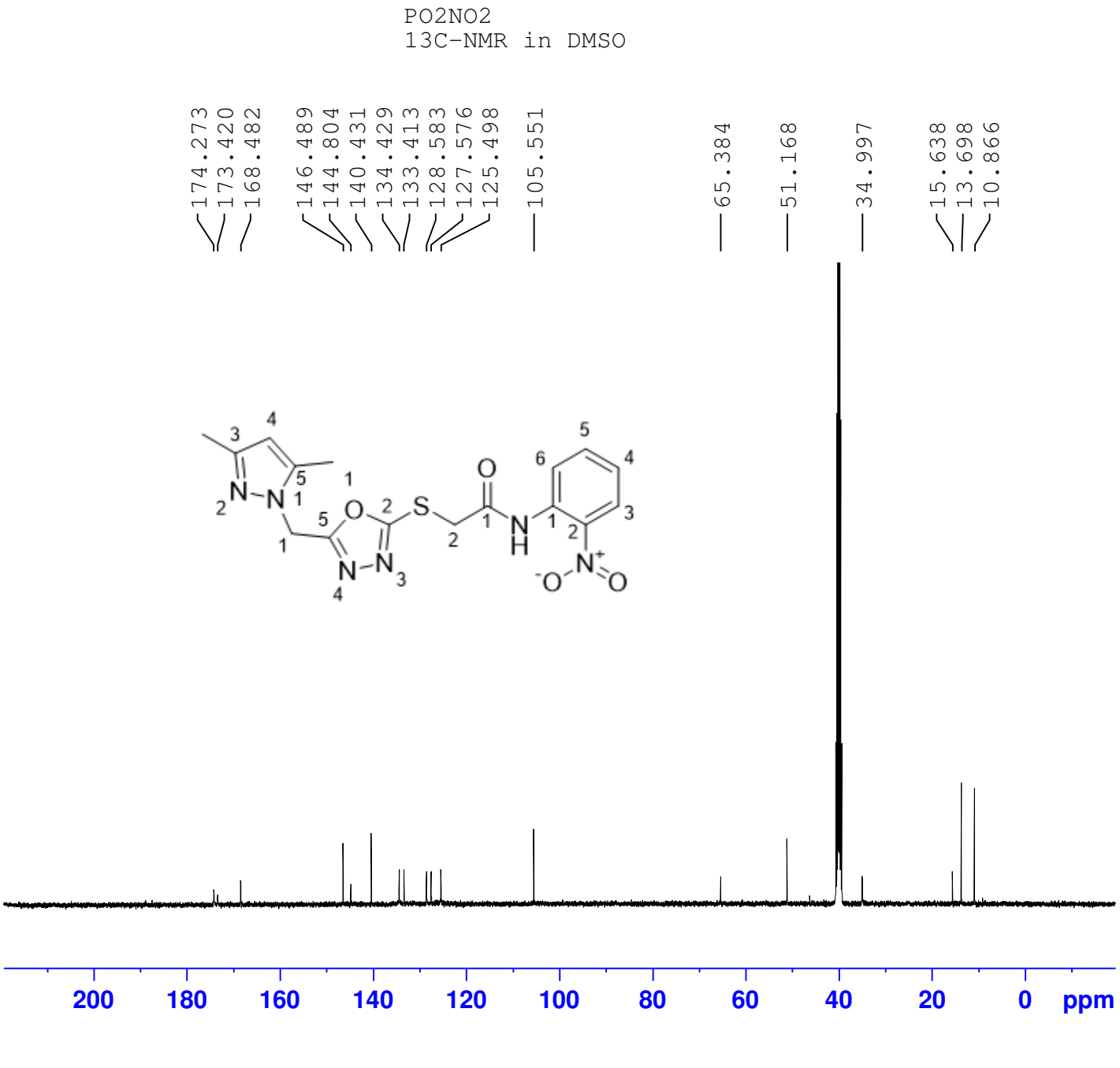


Current Data Parameters
NAME 23000438-PO2NO2
EXPNO 1
PROCNO 1

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

^{13}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)



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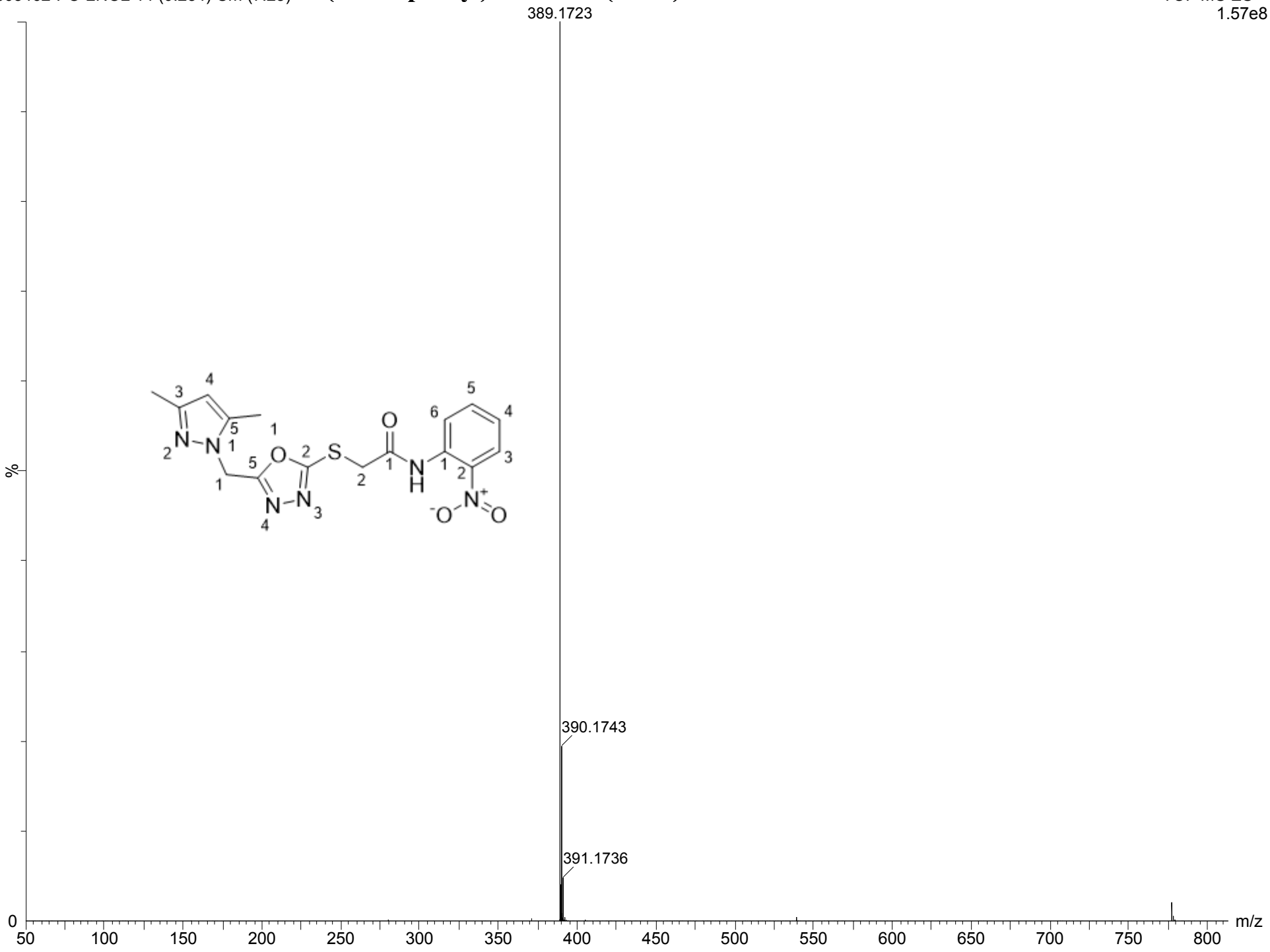
Current Data Parameters
NAME      23000438-PO2NO2
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230430
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

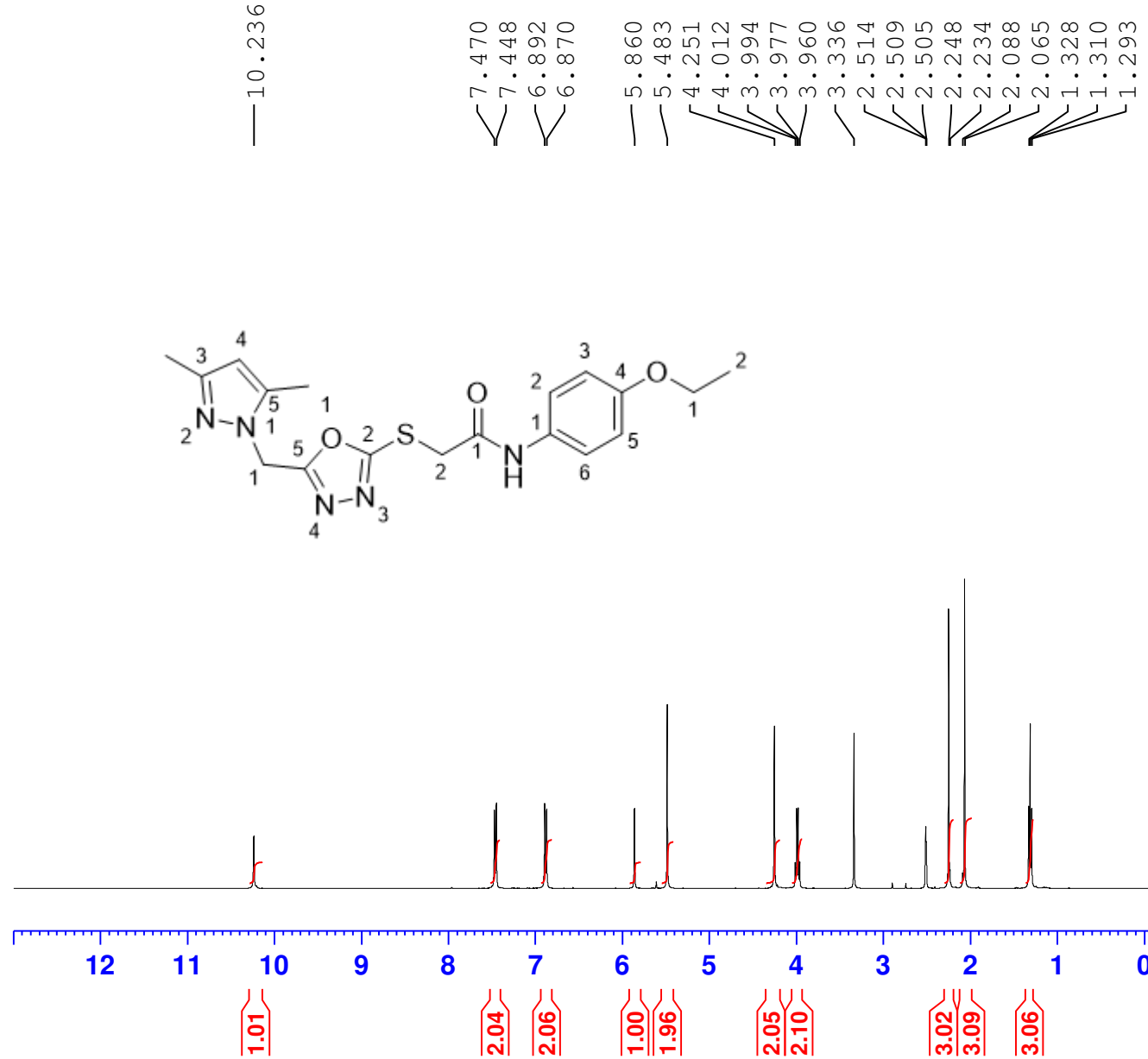
F2 - Processing parameters
SI                32768
SF          100.6580296 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

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)



^{1}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

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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
```
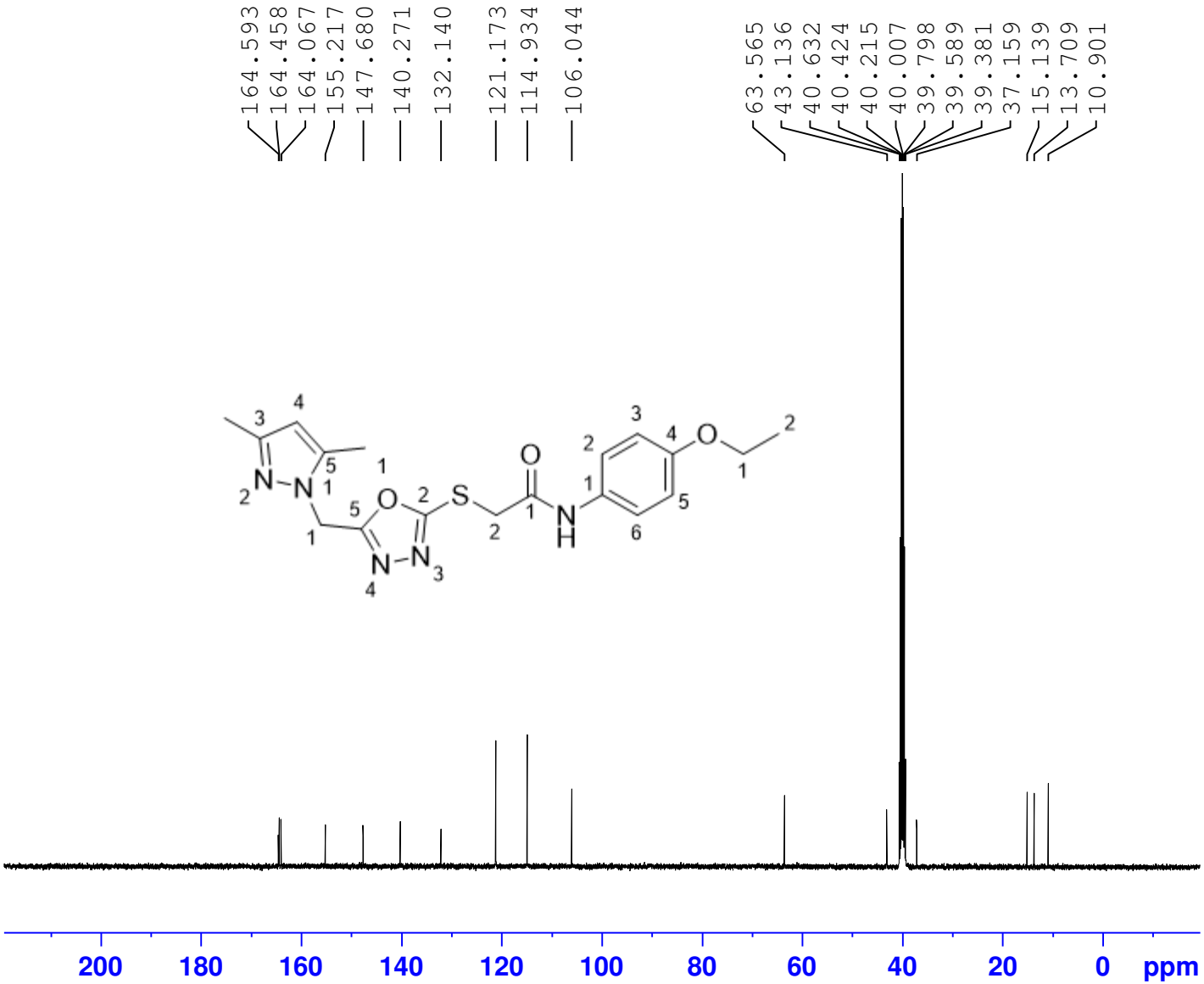

^{13}C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-ethoxyphenyl)acetamide (PO13)

POPP
13C-NMR in DMSO



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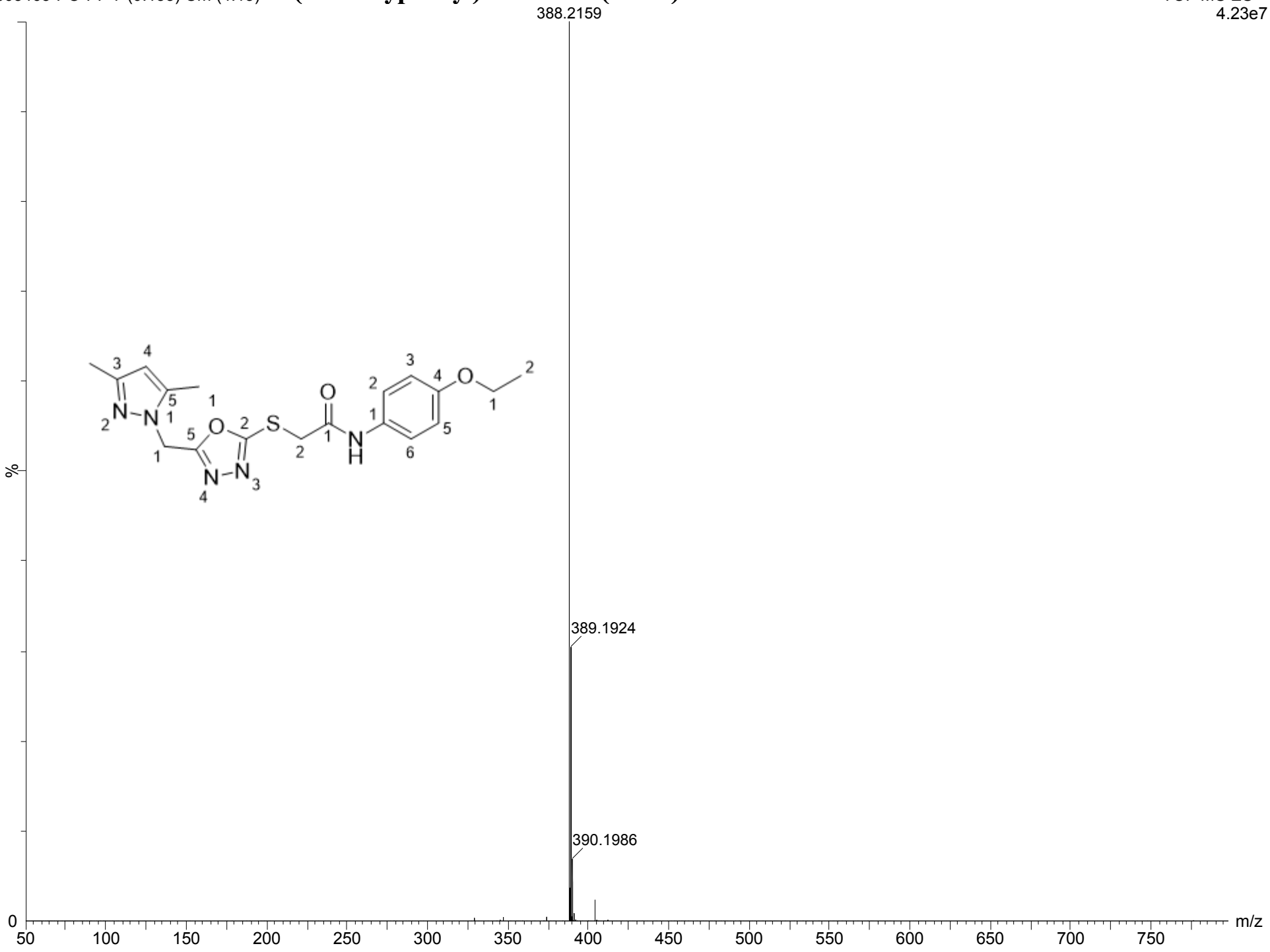
Current Data Parameters
NAME      23000435-POPP
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20230429
Time              17.26 h
INSTRUM            spect
PROBHD   Z108618_0984 (
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

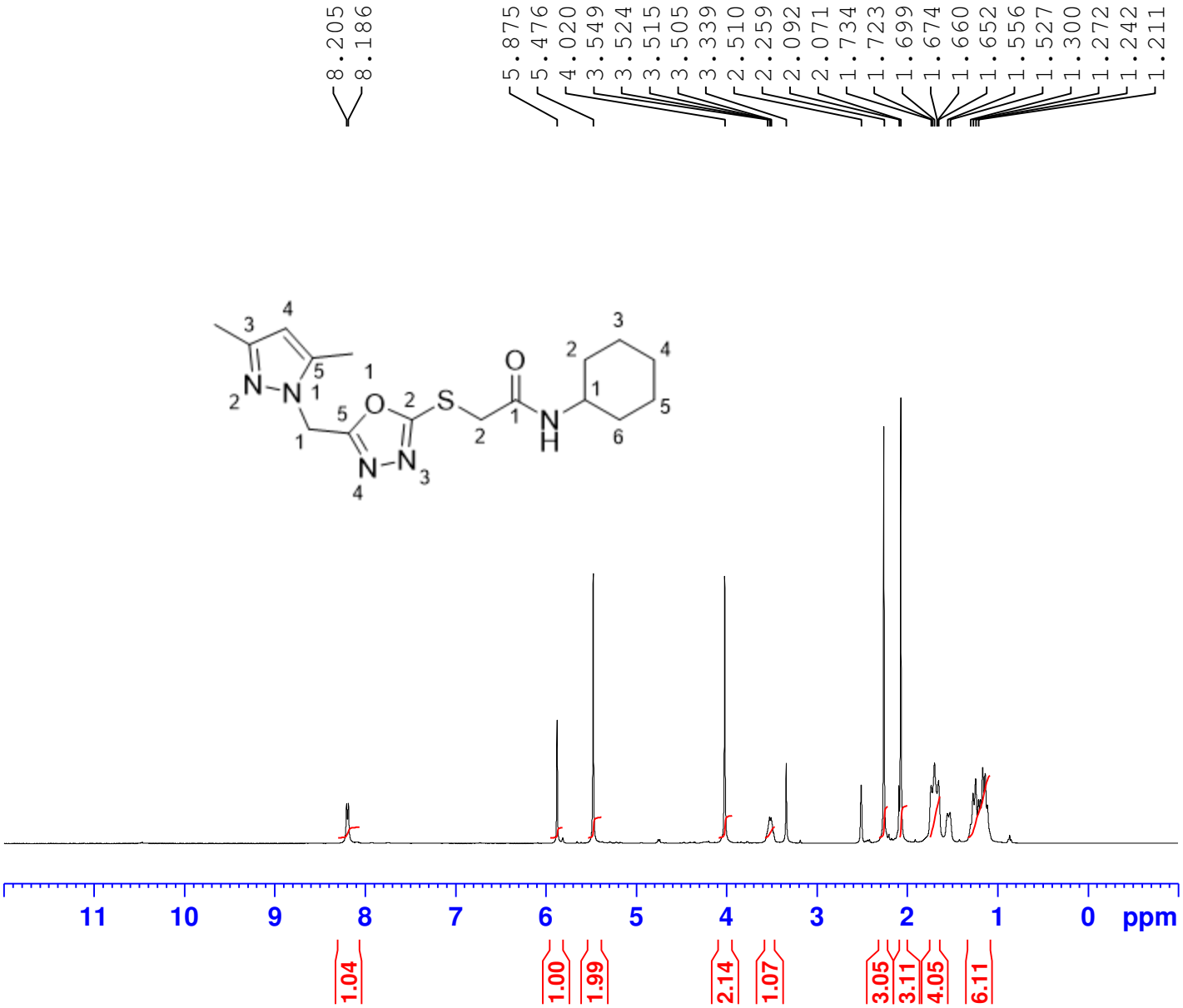
F2 - Processing parameters
SI                 32768
SF           100.6580296 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-ethoxyphenyl)acetamide (PO13)



^{1}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

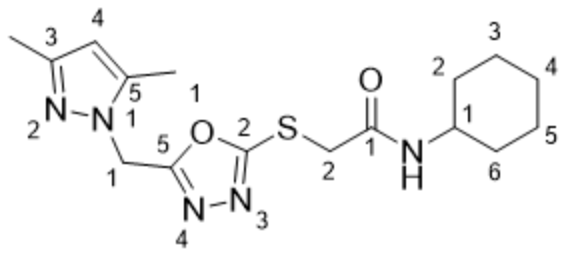
F2 - Acquisition Parameters
Date_ 20230428
Time 18.52 h
INSTRUM spect
PROBHD Z108618_0984 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 32.13
DW 62.400 usec
DE 17.09 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.3124719 MHz
NUC1 1H
P0 4.67 usec
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

^{13}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

165.042
164.641
163.956
147.646
140.264
106.032
48.615
43.149
40.635
40.426
40.218
40.009
39.800
39.592
39.383
36.459
32.645
25.605
24.845
13.707
10.912

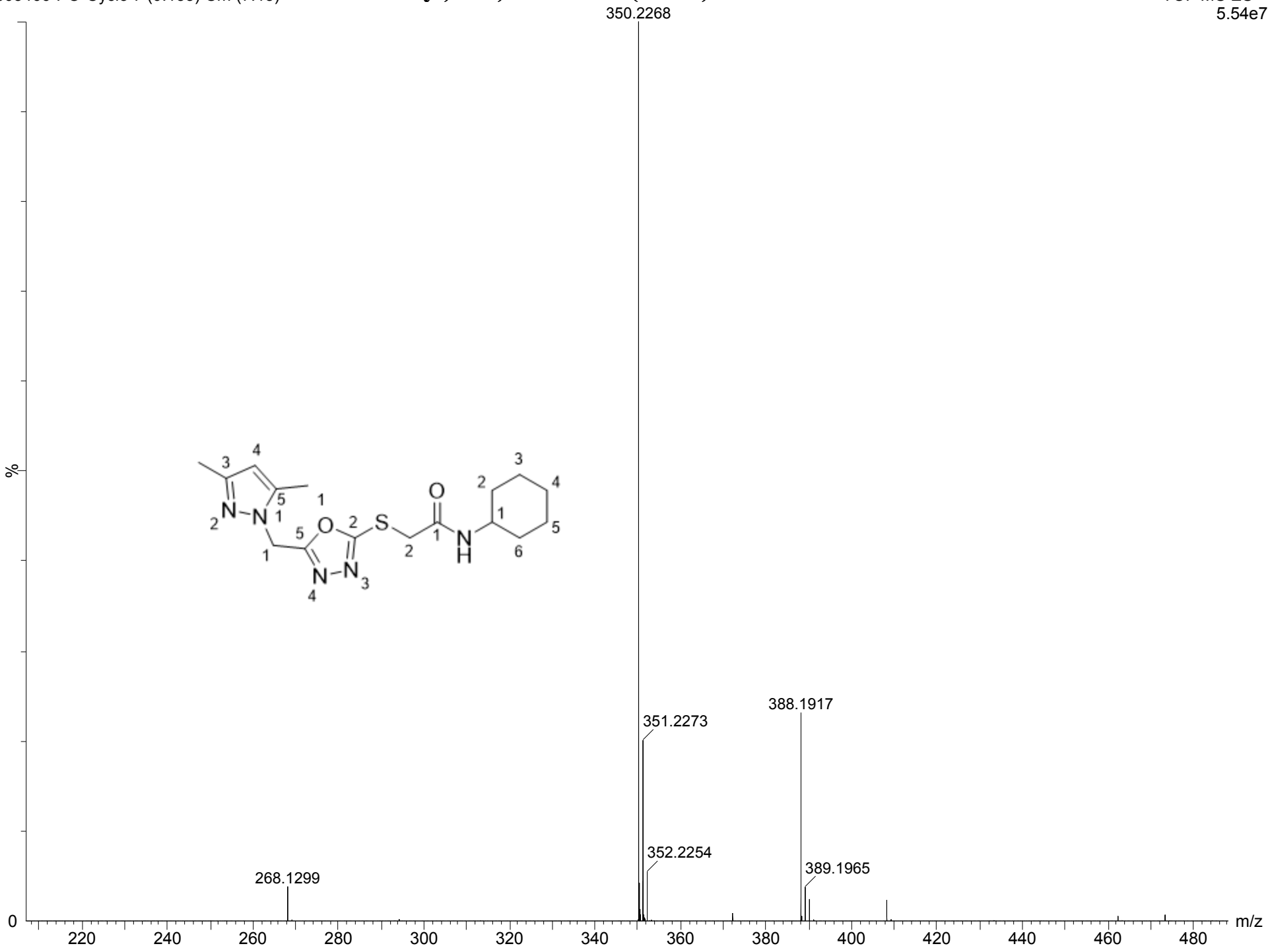


Current Data Parameters
NAME 23000433-POCyclo
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230429
Time 12.35 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 299.1 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

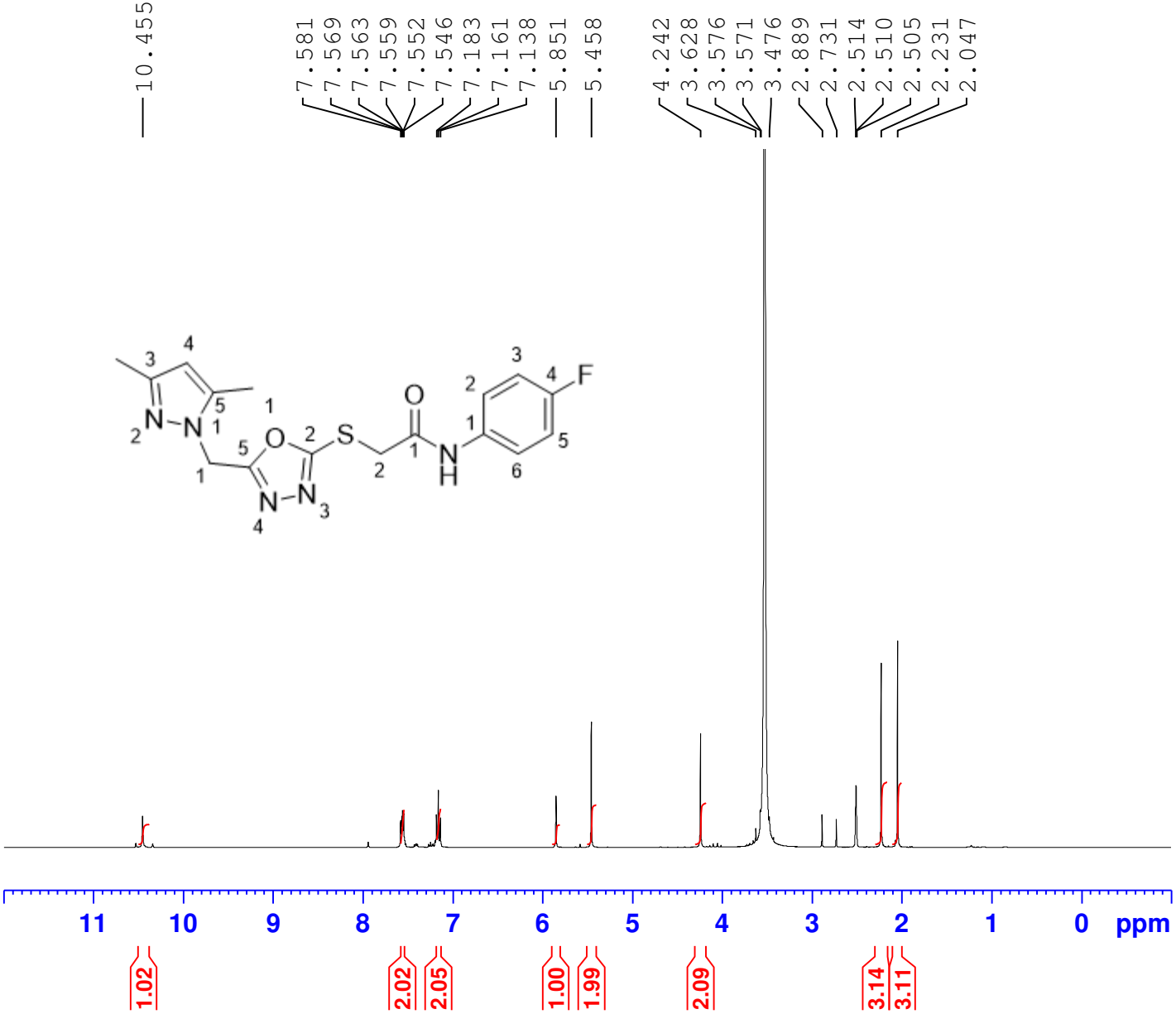
F2 - Processing parameters
SI 32768
SF 100.6580296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mass spectrum of N-cyclohexyl-2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)acetamide (PO14)



^{1}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



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Current Data Parameters
NAME        23000429-POF
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230427
Time              14.11 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                297.5 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
```
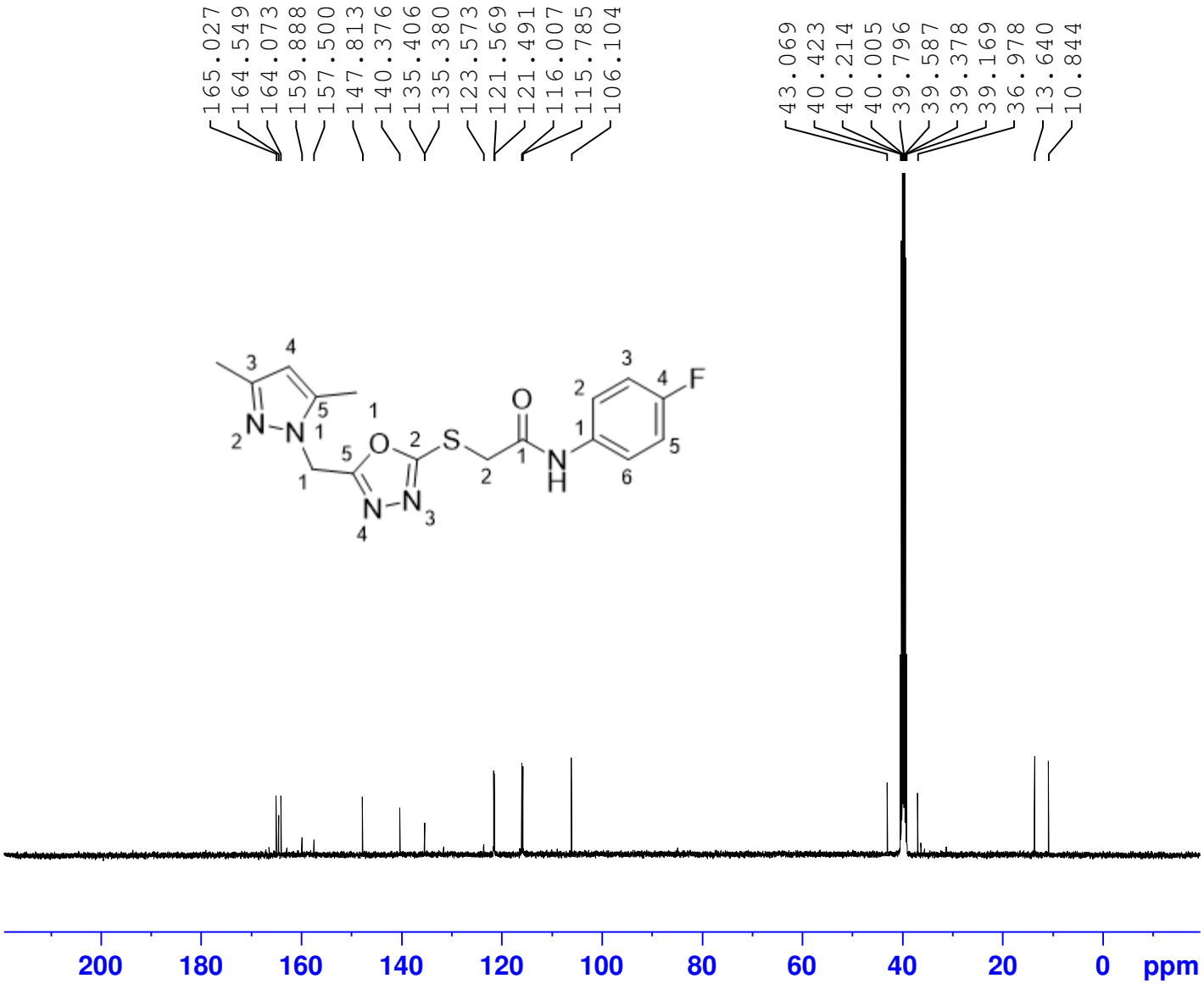

^{13}C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-fluorophenyl)acetamide (PO15)

POF
13C-NMR in DMSO

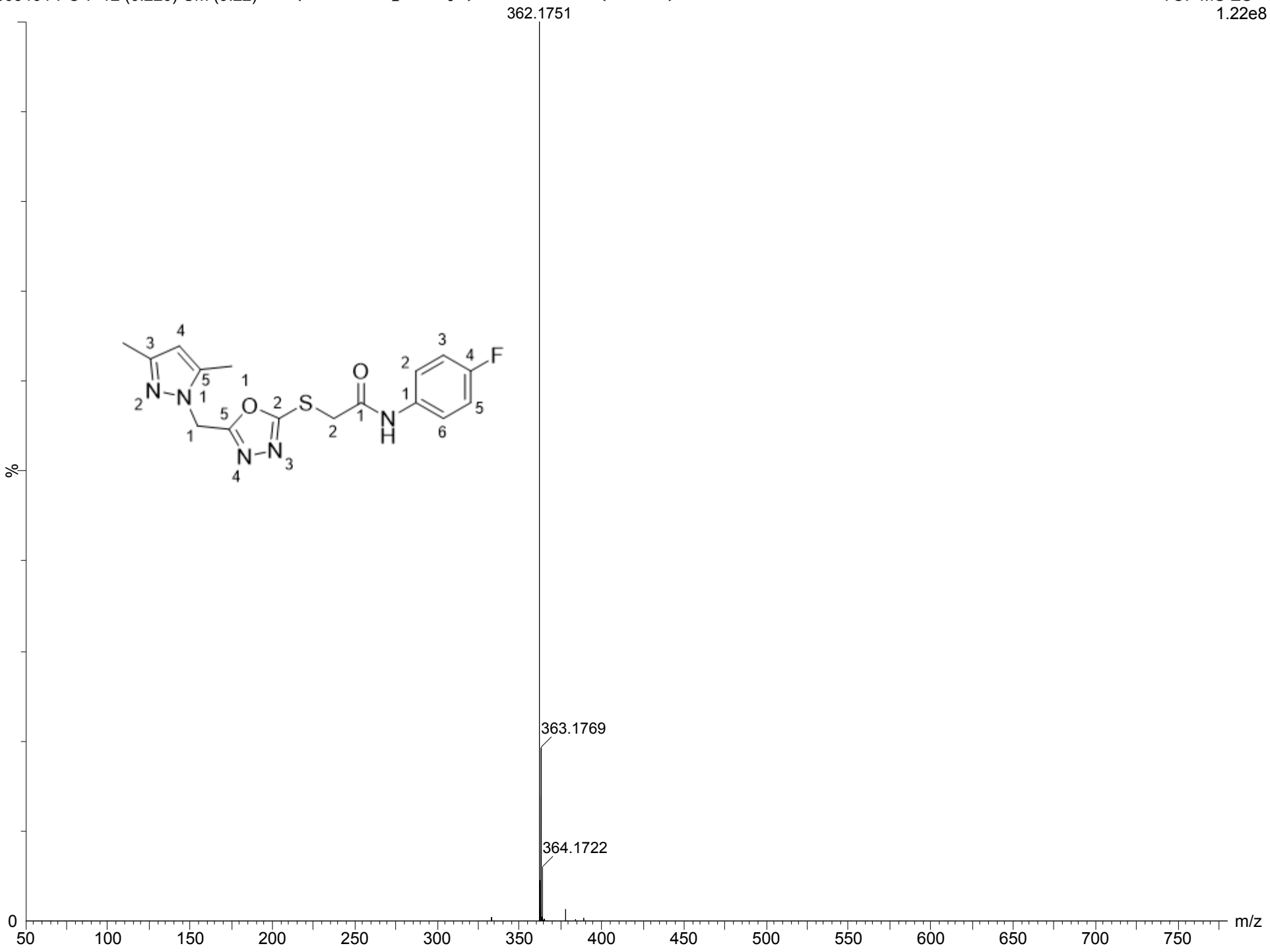


Current Data Parameters
NAME 23000429-POF
EXPNO 2
PROCNO 1

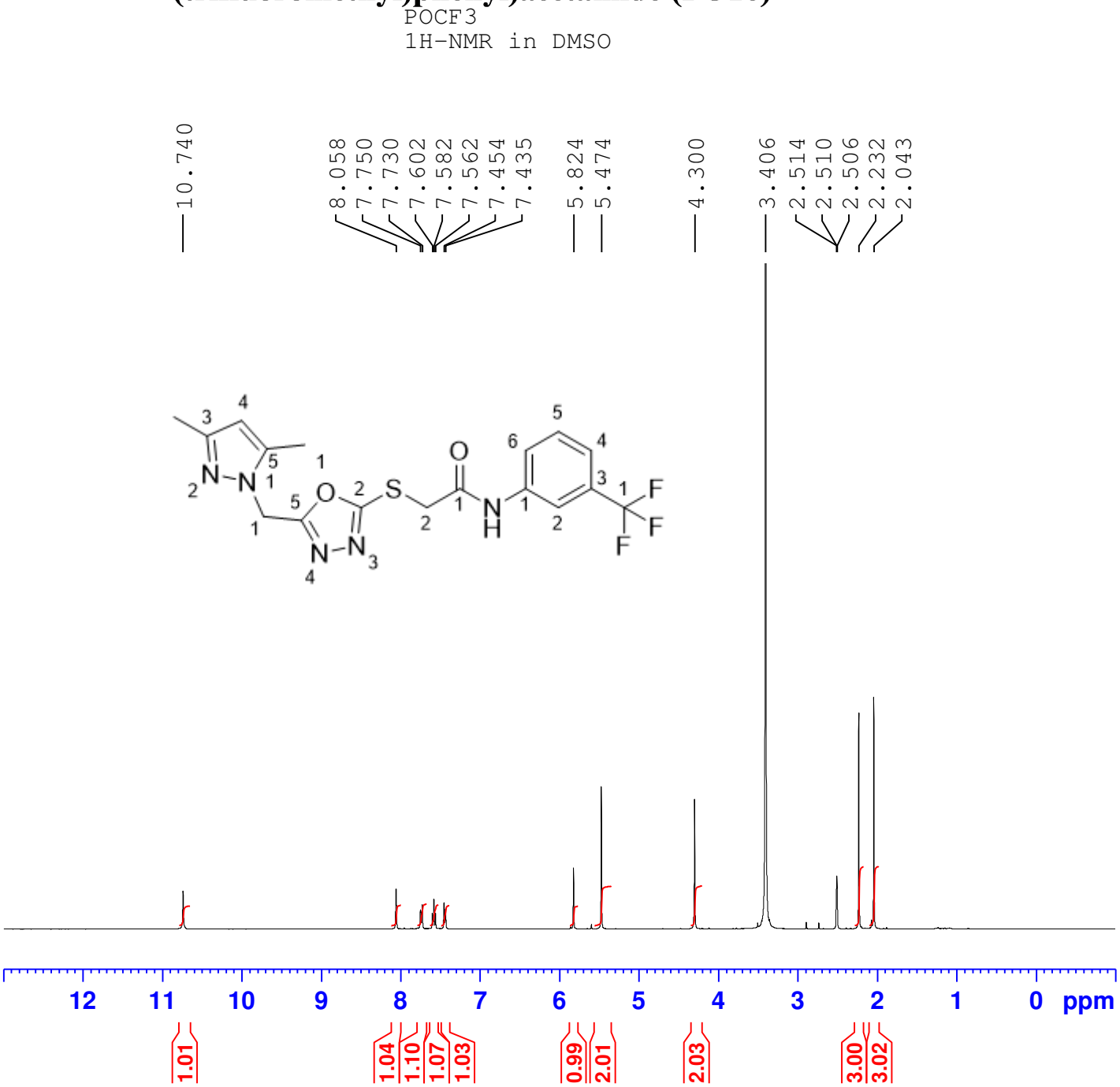
F2 - Acquisition Parameters
Date_ 20230427
Time 17.18 h
INSTRUM spect
PROBHD Z108618_0984 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1684
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 202.84
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6680954 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

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)



^{1}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)

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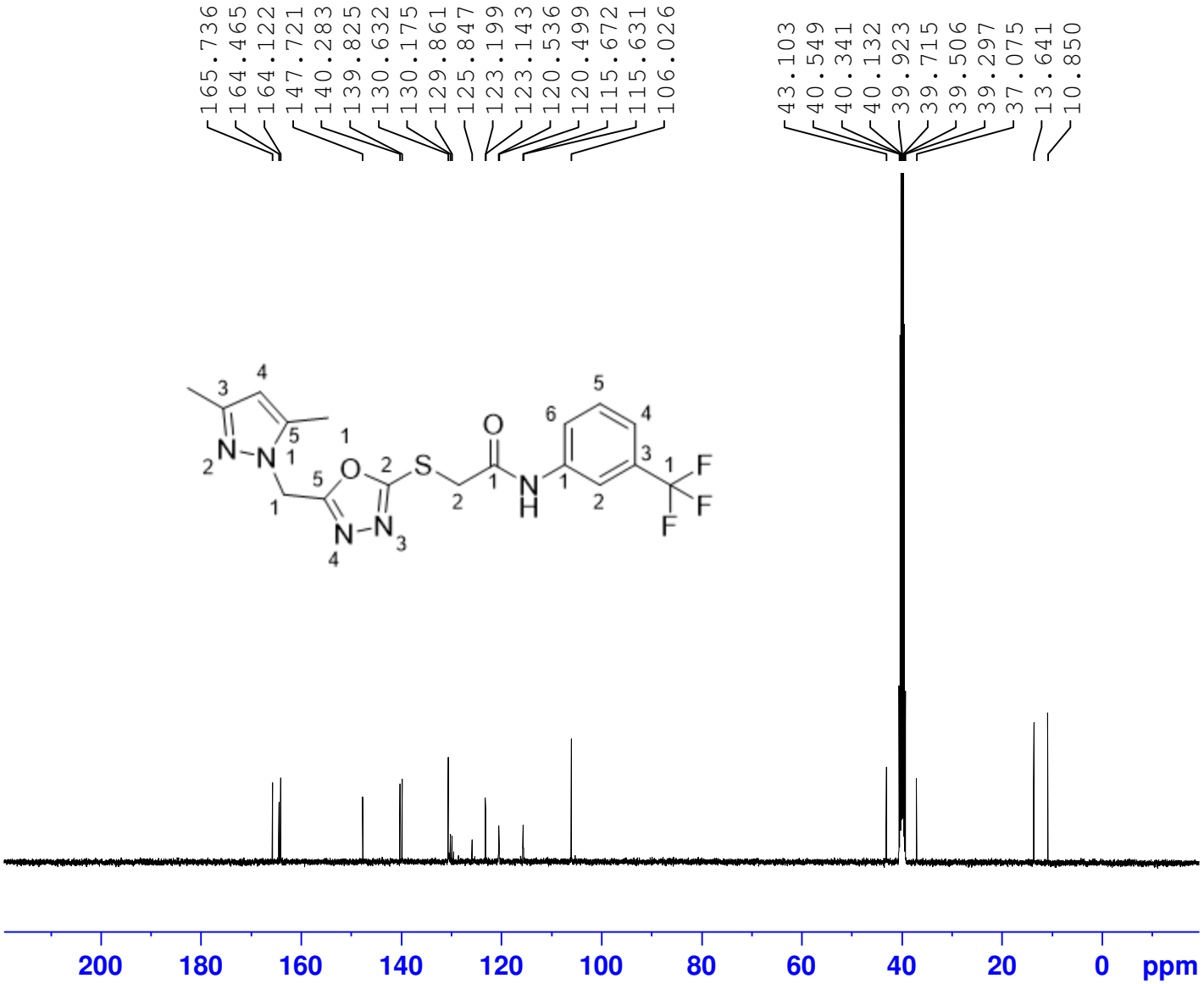
Current Data Parameters
NAME      23000428-POCF3
EXPNO                  1
PROCNO                 1

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
```

^{13}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
13C-NMR in DMSO



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```
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
```

Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3-(trifluoromethyl)phenyl)acetamide (PO16)

^{1}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)

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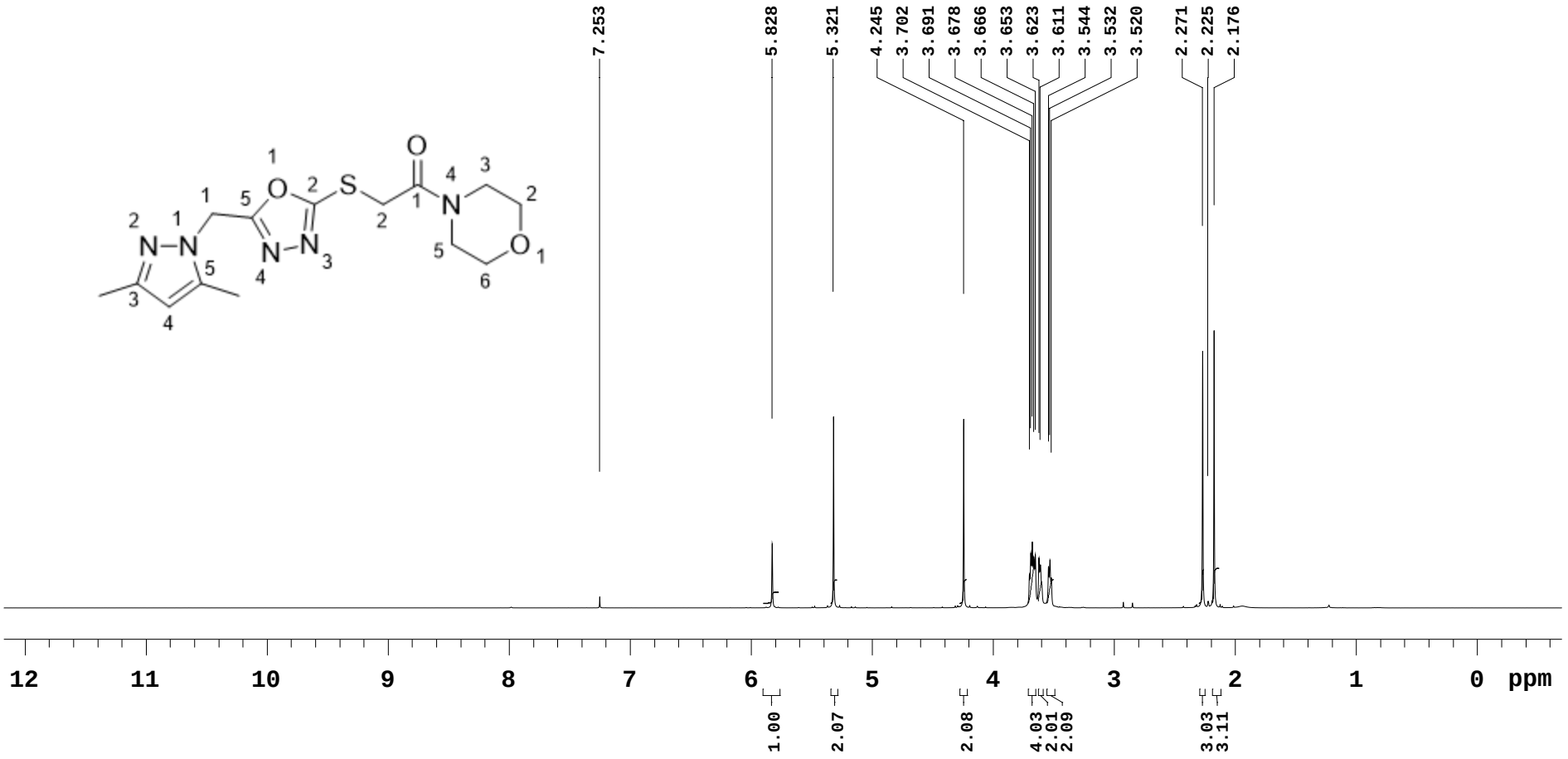
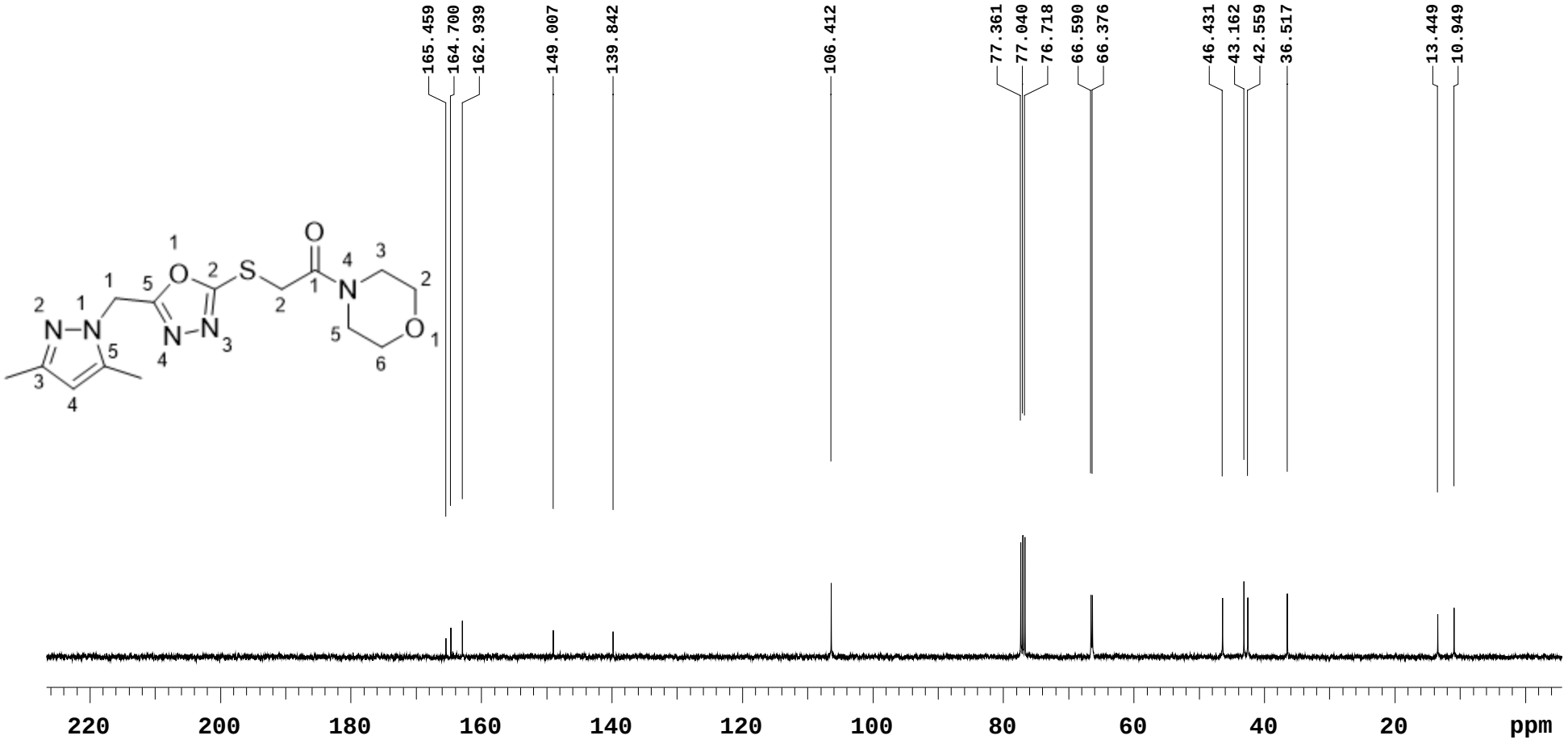


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 3.146 sec Width 10416.7 Hz 8 repetitions	OBSERVE H1, 399.8212911	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 1 minute		2001317-MD1-1H Solvent: cdcl3 Ambient temperature Operator: IOE File: 2001317-MD1-1H VNMRS-400 "Agilent-NMR"

^{13}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)

UNIVERSITY OF MYSORE

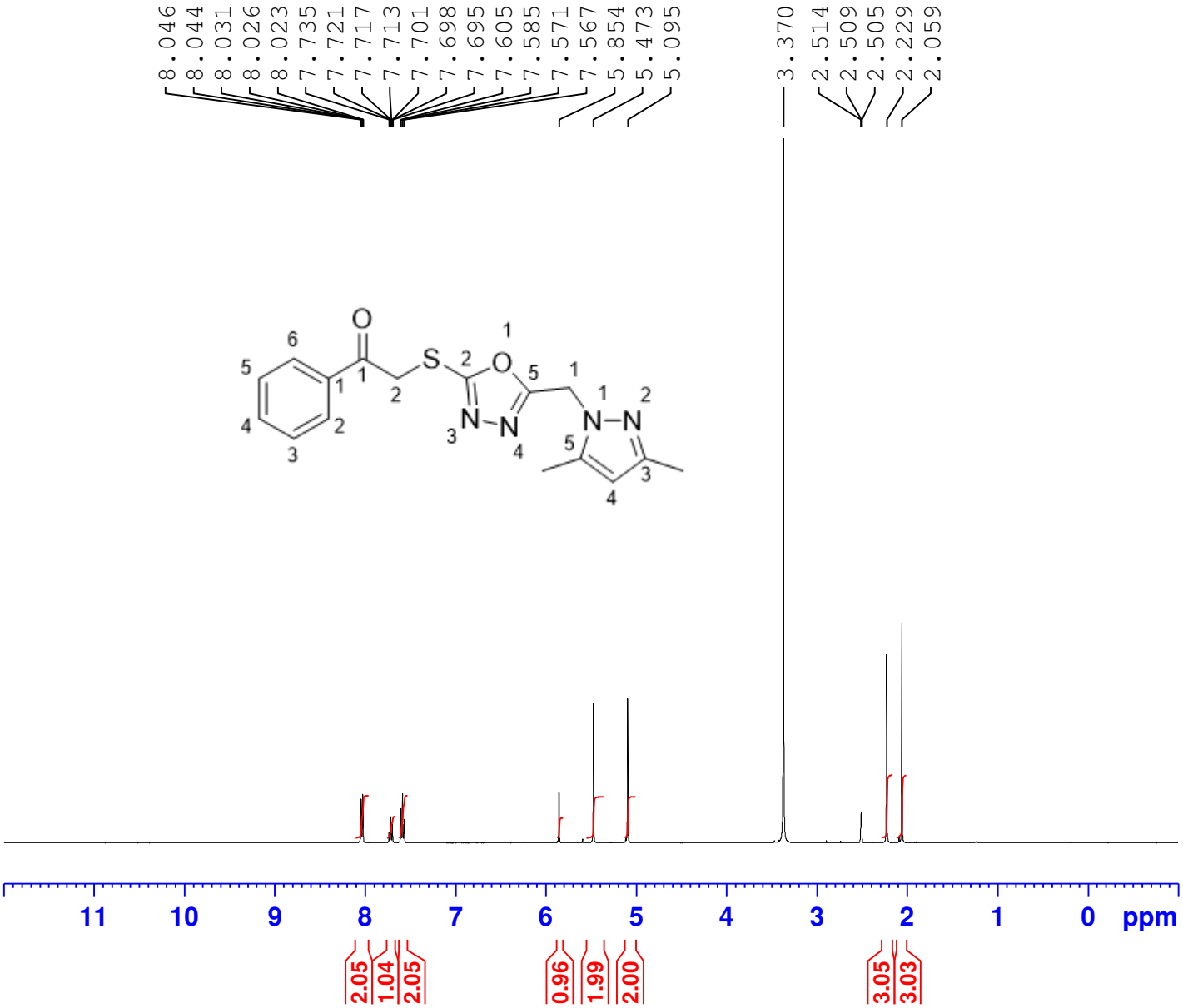


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.022 sec Width 32051.3 Hz 332 repetitions	OBSERVE C13, 100.5351436 DECOUPLE H1, 399.8232903 Power 39 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 2.5 Hz FT size 65536 Total time 11 minutes		2001318-MD1-13C Solvent: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

^{1}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



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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
```
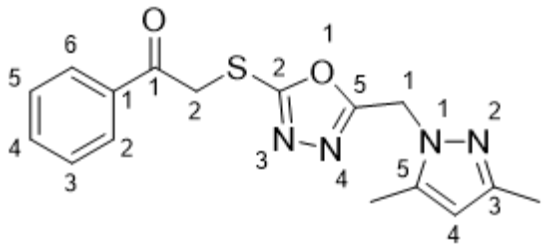

^{13}C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-phenylethan-1-one (PO18)

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

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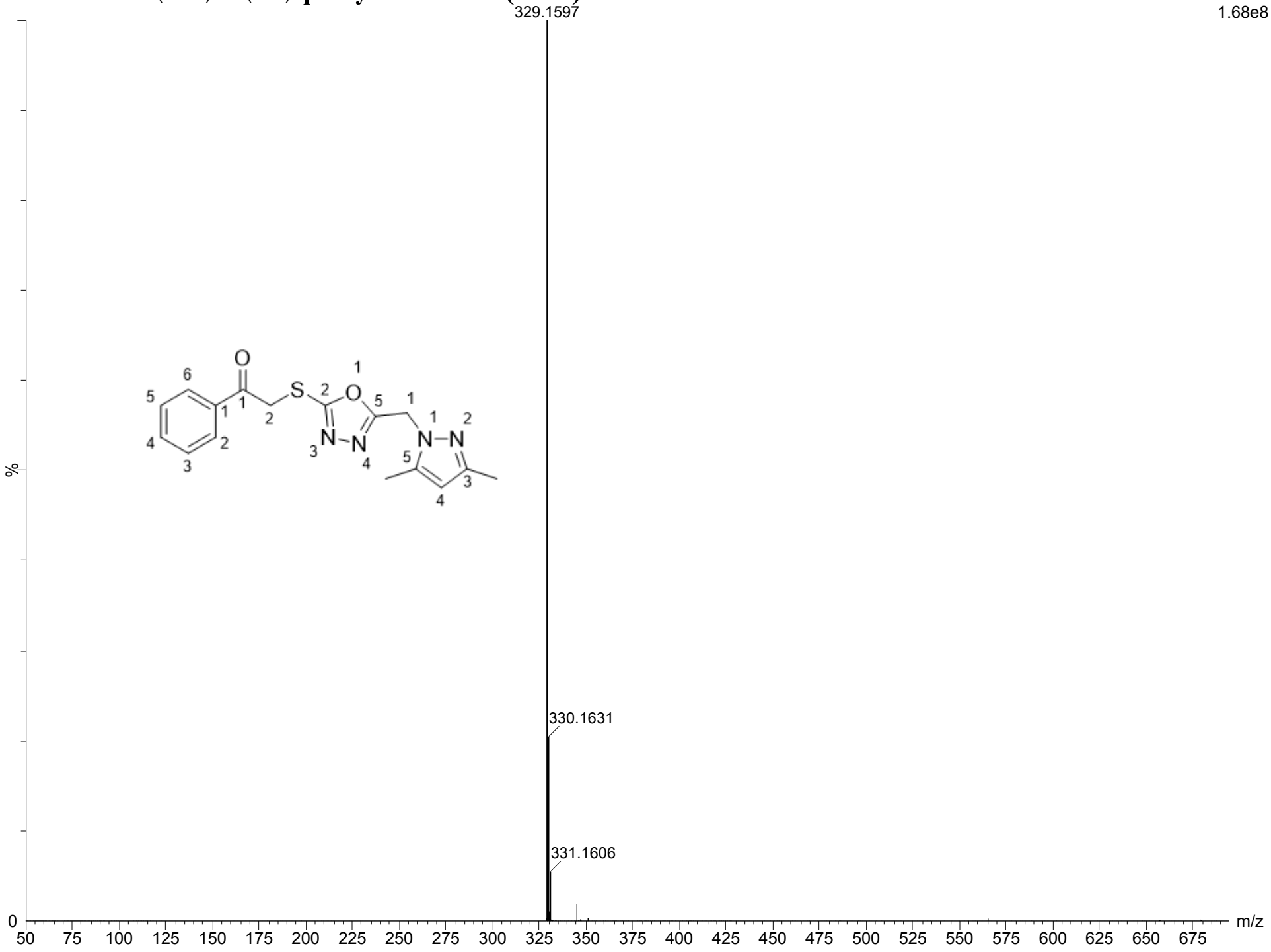
Current Data Parameters
NAME      23000477-POACP
EXPNO                  2
PROCNO                 1

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

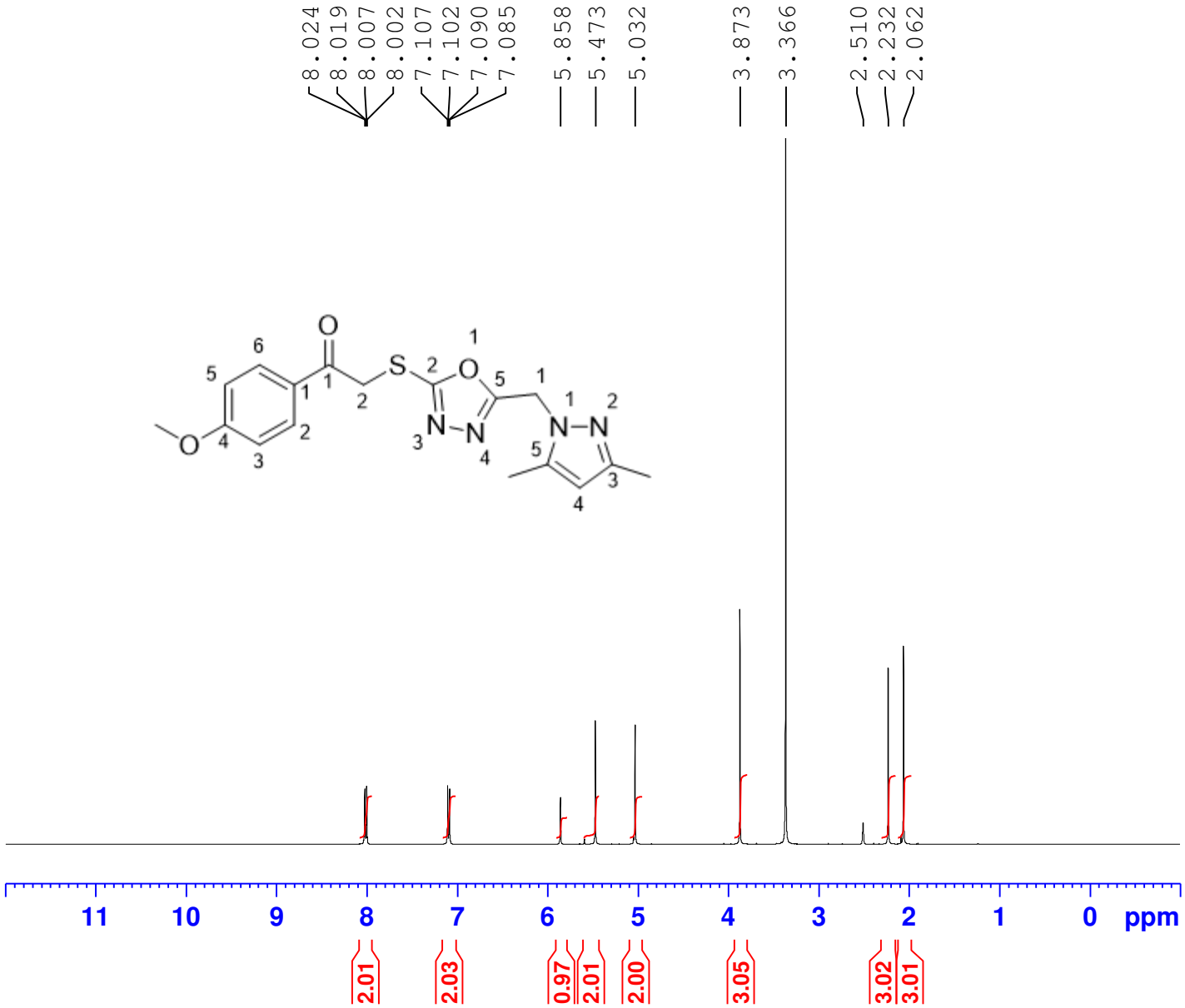
F2 - Processing parameters
SI                 32768
SF           100.6580296 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

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)



^{1}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)

PO4OCH3-ACP
1H-NMR in DMSO



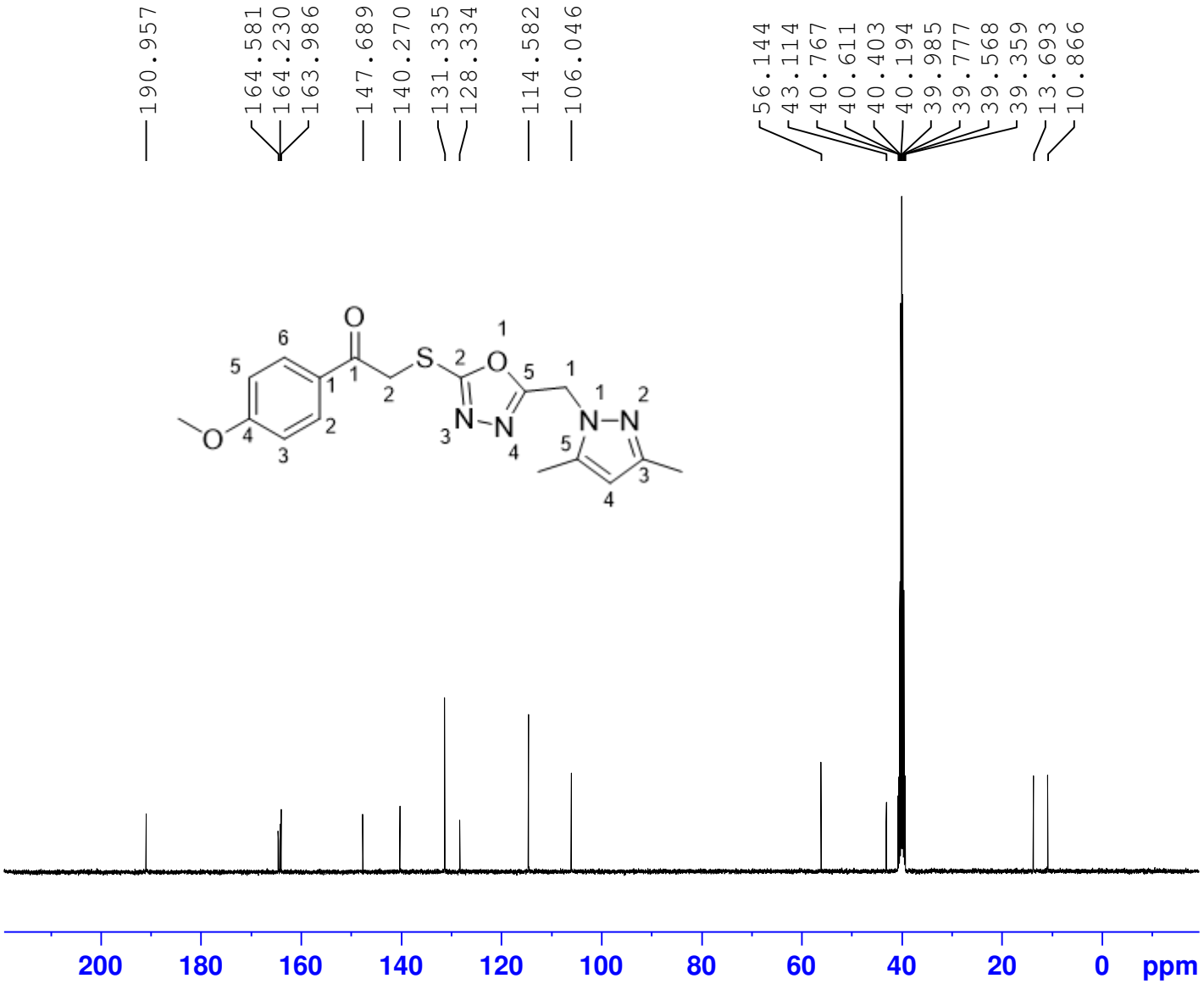
Current Data Parameters
NAME 23000495-PO4OCH3-ACP
EXPNO 1
PROCNO 1

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

^{13}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)

PO4OCH3-ACP
13C-NMR in DMSO



Current Data Parameters

NAME	23000495-PO4OCH3-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

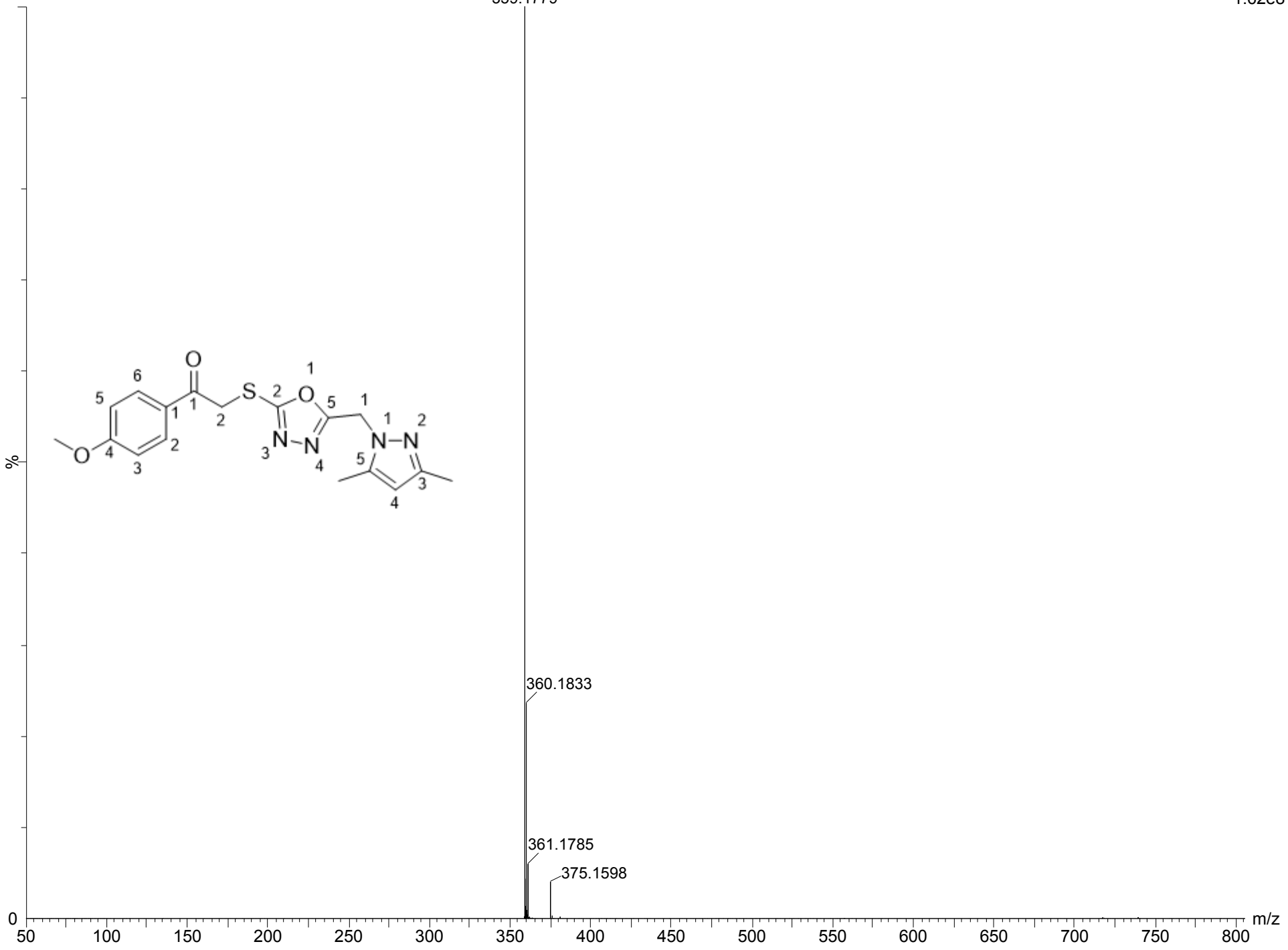
F2 - Processing parameters

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-

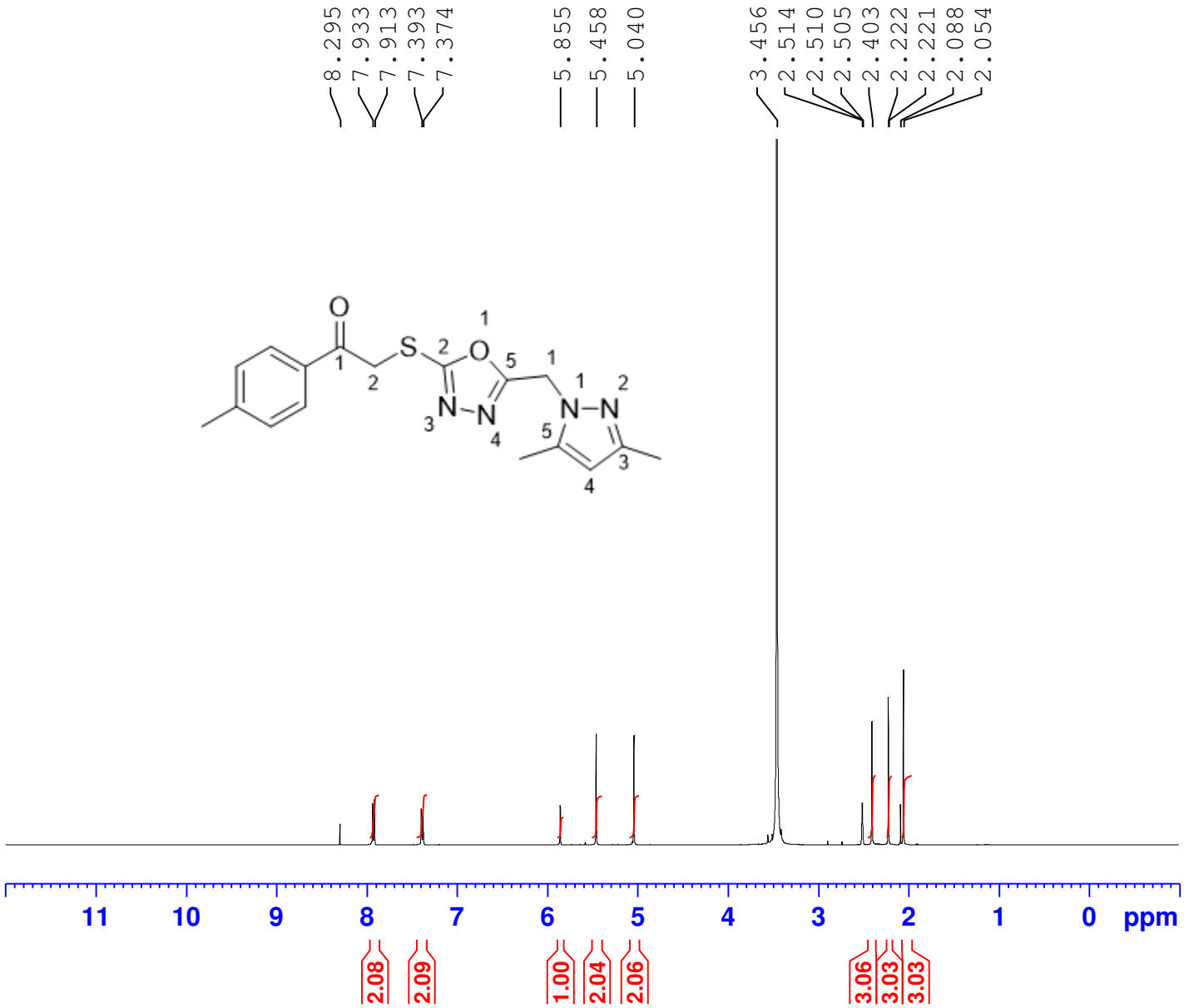
2303456-PO-4OCH3-ACP 12 (0.220) Cm (8:24) **(4-methoxyphenyl)ethan-1-one (PO19)**

TOF MS ES+
1.62e8



^{1}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
1H-NMR in DMSO

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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
```
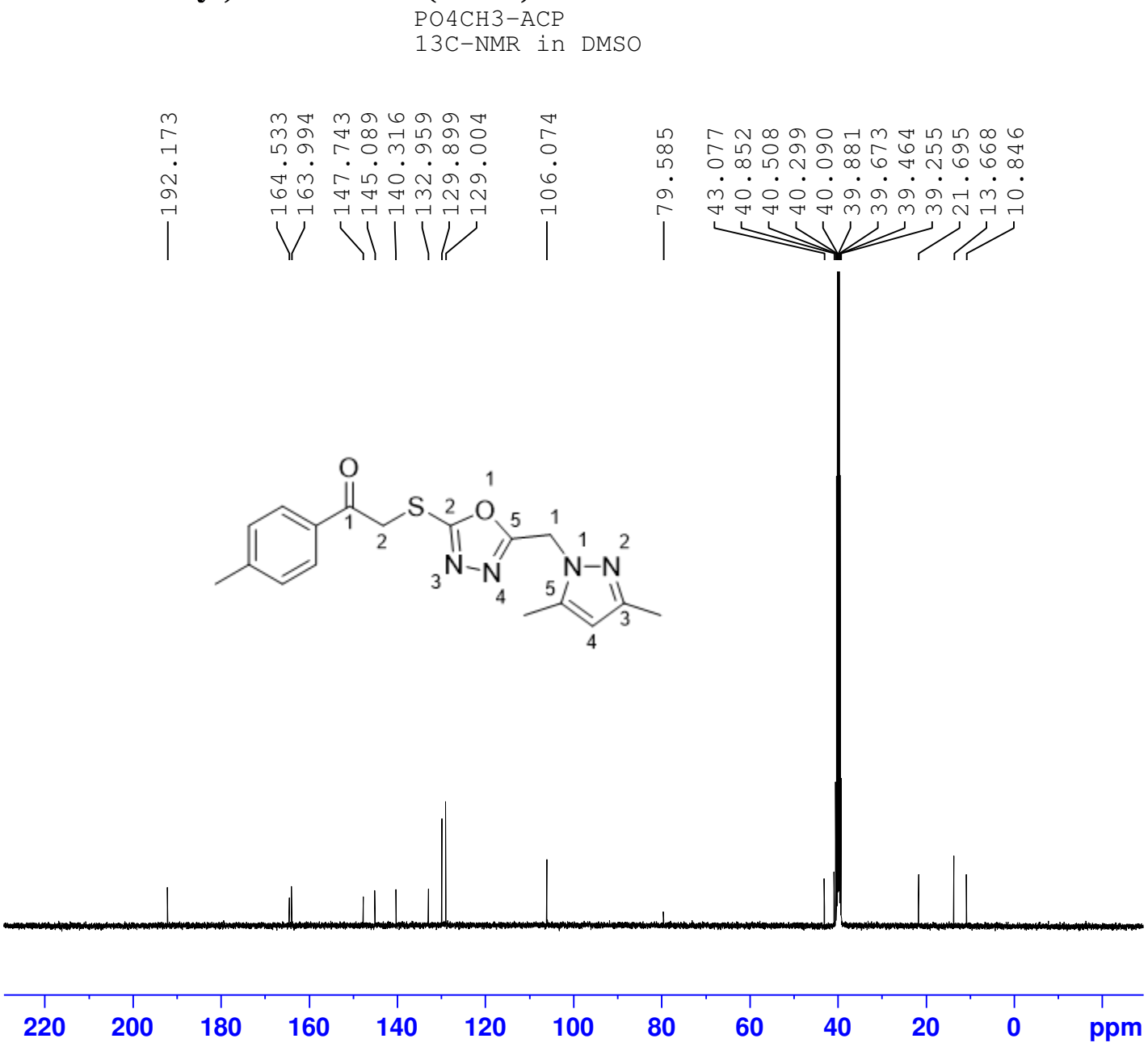

^{13}C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(p-tolyl)ethan-1-one (PO20)

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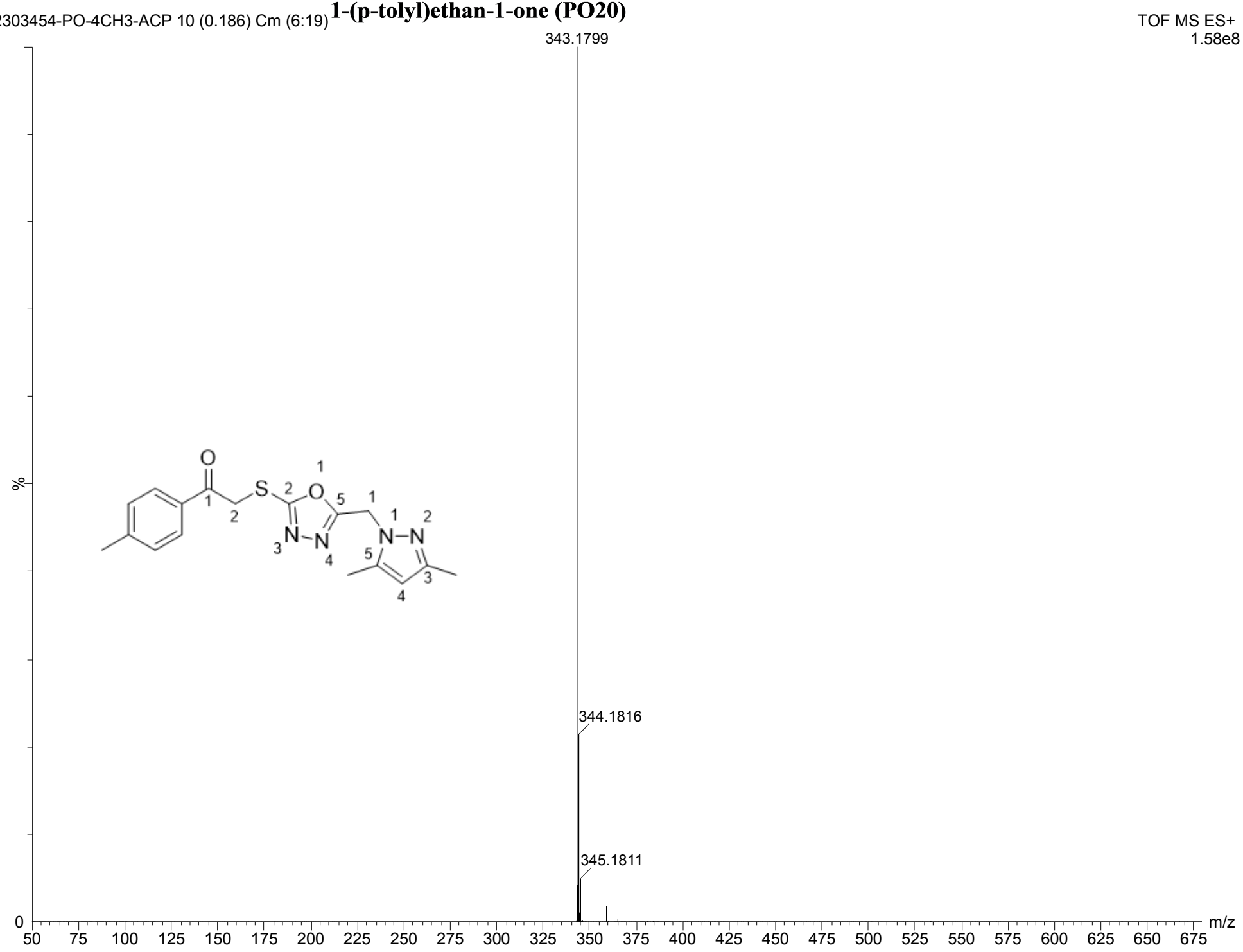
Current Data Parameters
NAME      23000491-PO4CH3-ACP
EXPNO                      2
PROCNO                     1

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

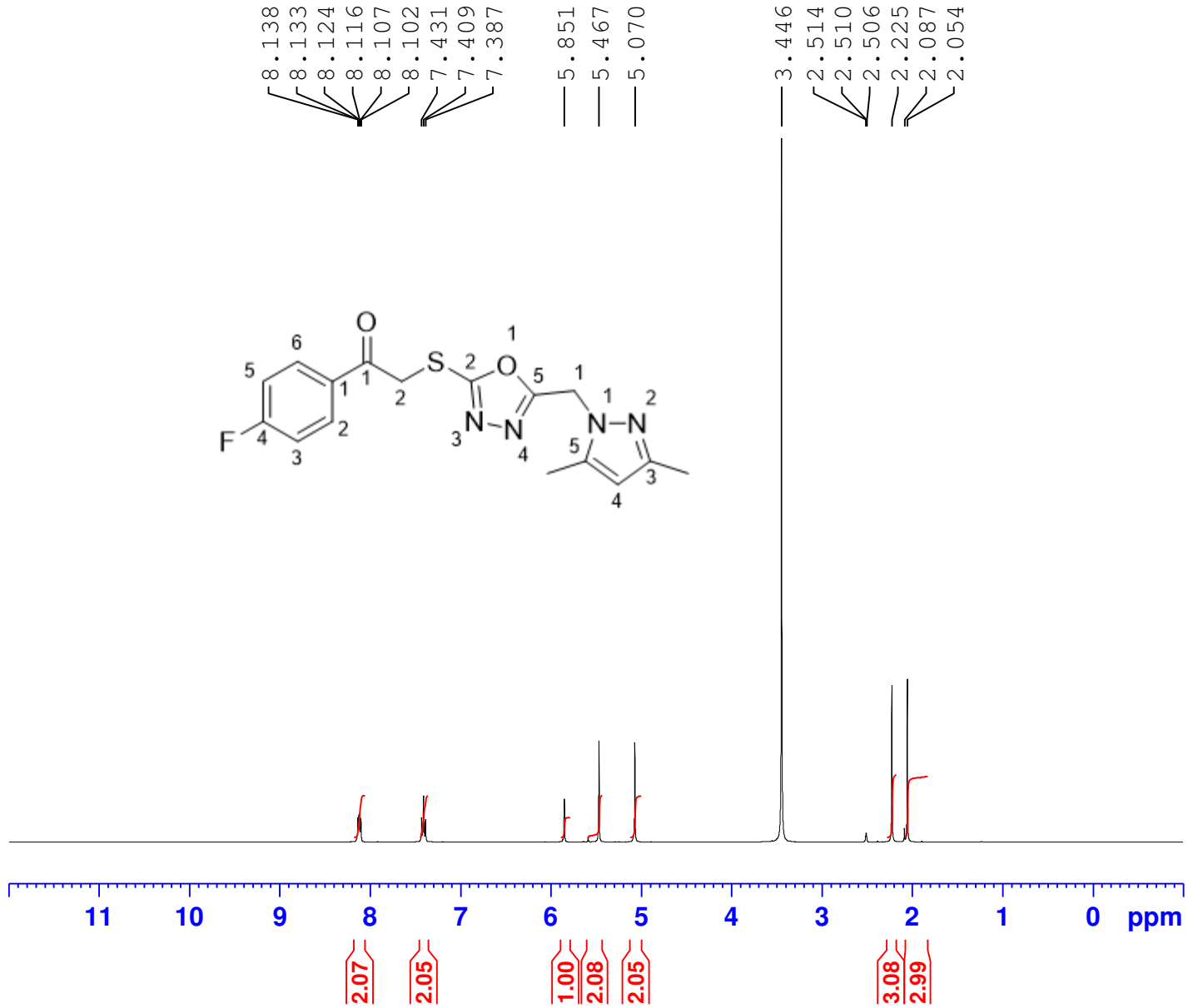
F2 - Processing parameters
SI                 32768
SF           100.6580296 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

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)



^{1}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

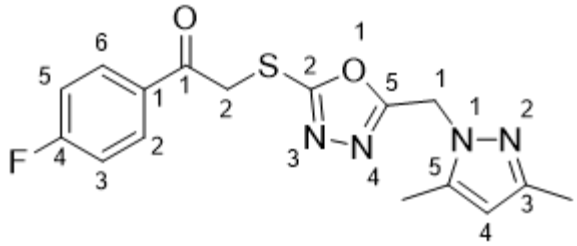
F2 - Acquisition Parameters
Date_ 20230512
Time 18.04 h
INSTRUM spect
PROBHD Z108618_0984 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 32.13
DW 62.400 usec
DE 17.09 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.3124719 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 11.28999996 W

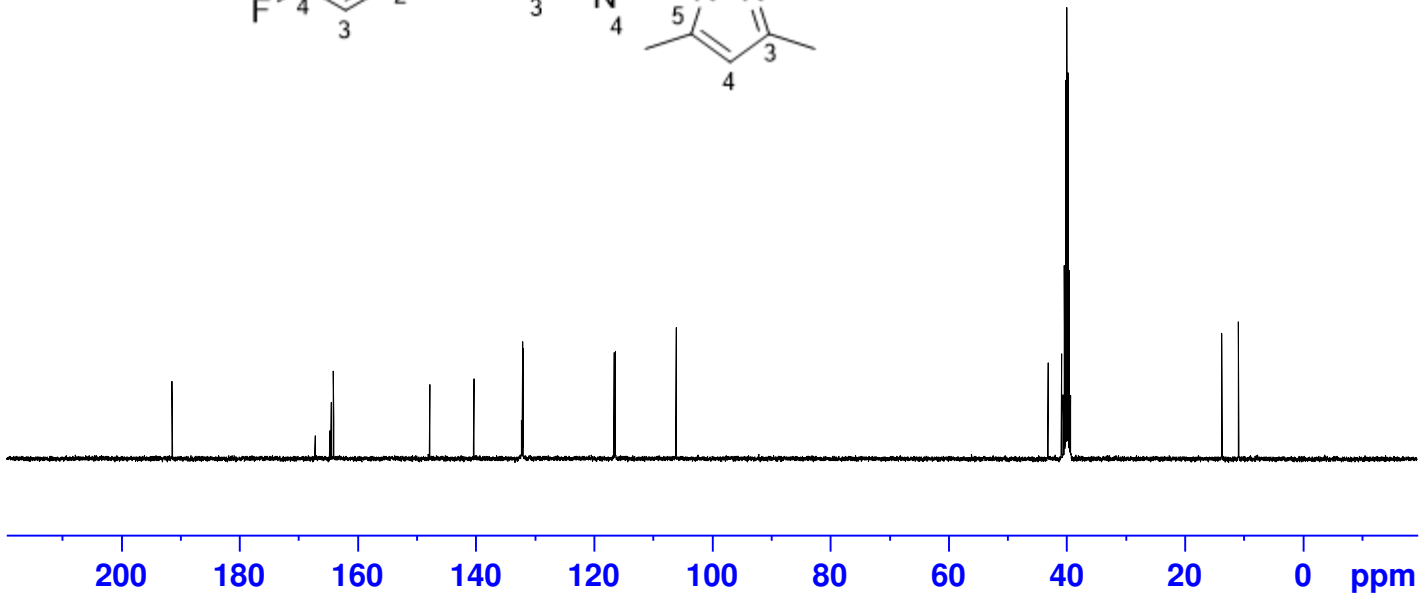
F2 - Processing parameters
SI 65536
SF 400.3100000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}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
13C-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



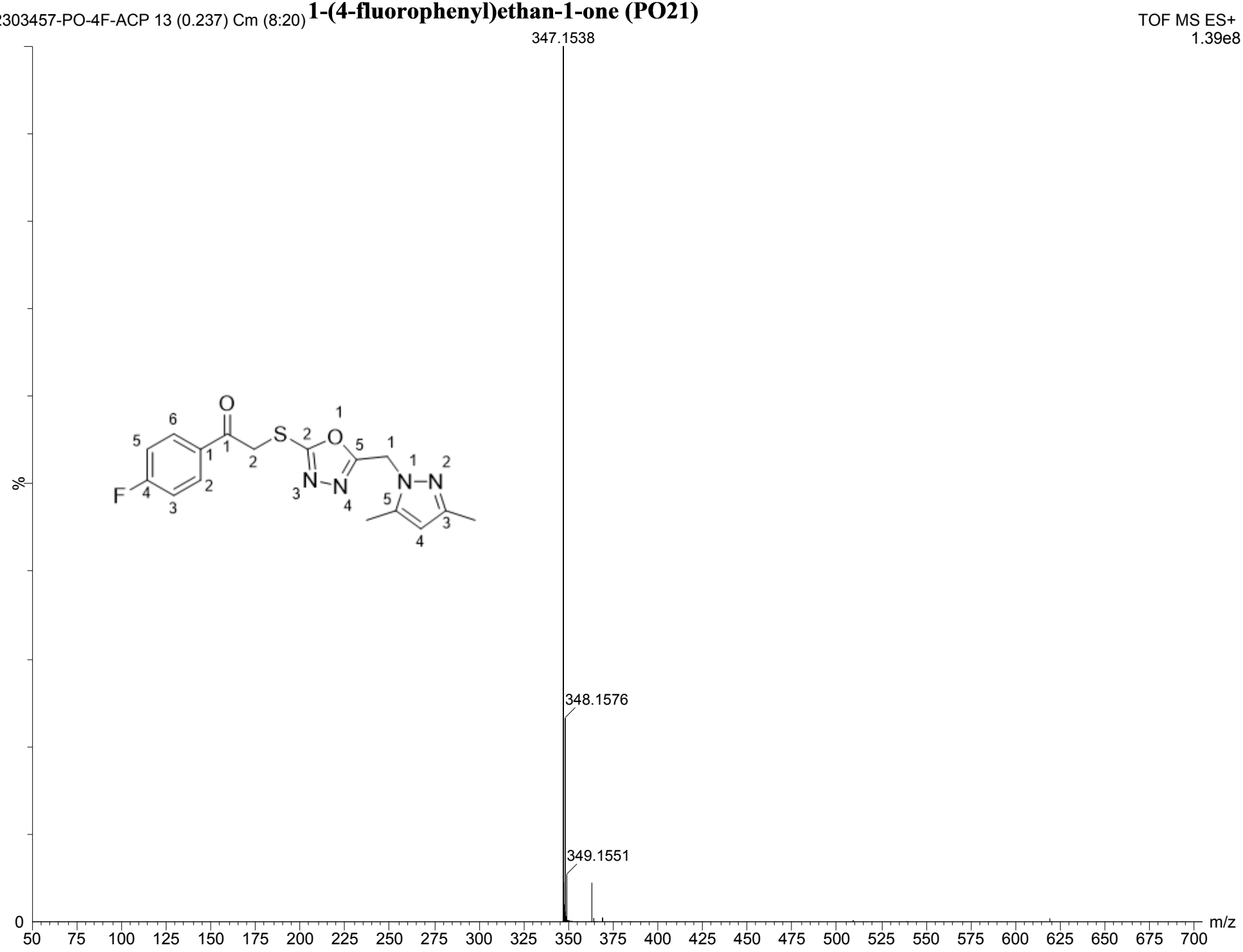


Current Data Parameters
NAME 23000490-PO4F-ACP
EXPNO 2
PROCNO 1

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

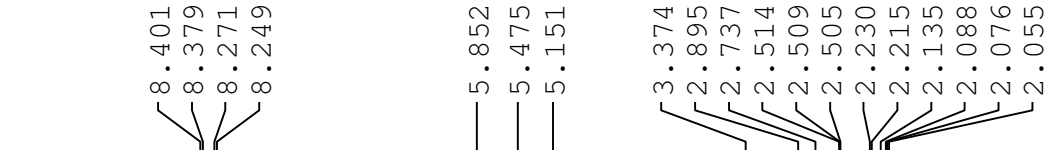
F2 - Processing parameters
SI 32768
SF 100.6580296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

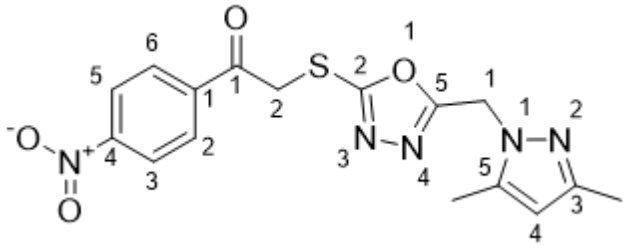
Mass spectrum of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-fluorophenyl)ethan-1-one (PO21)



^{1}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
1H-NMR in DMSO



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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
```
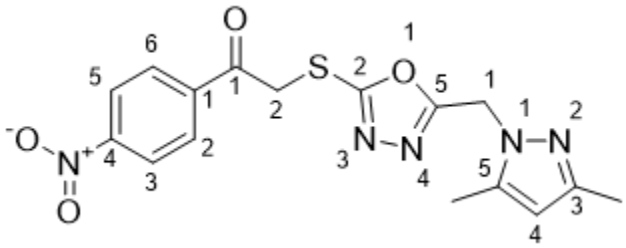
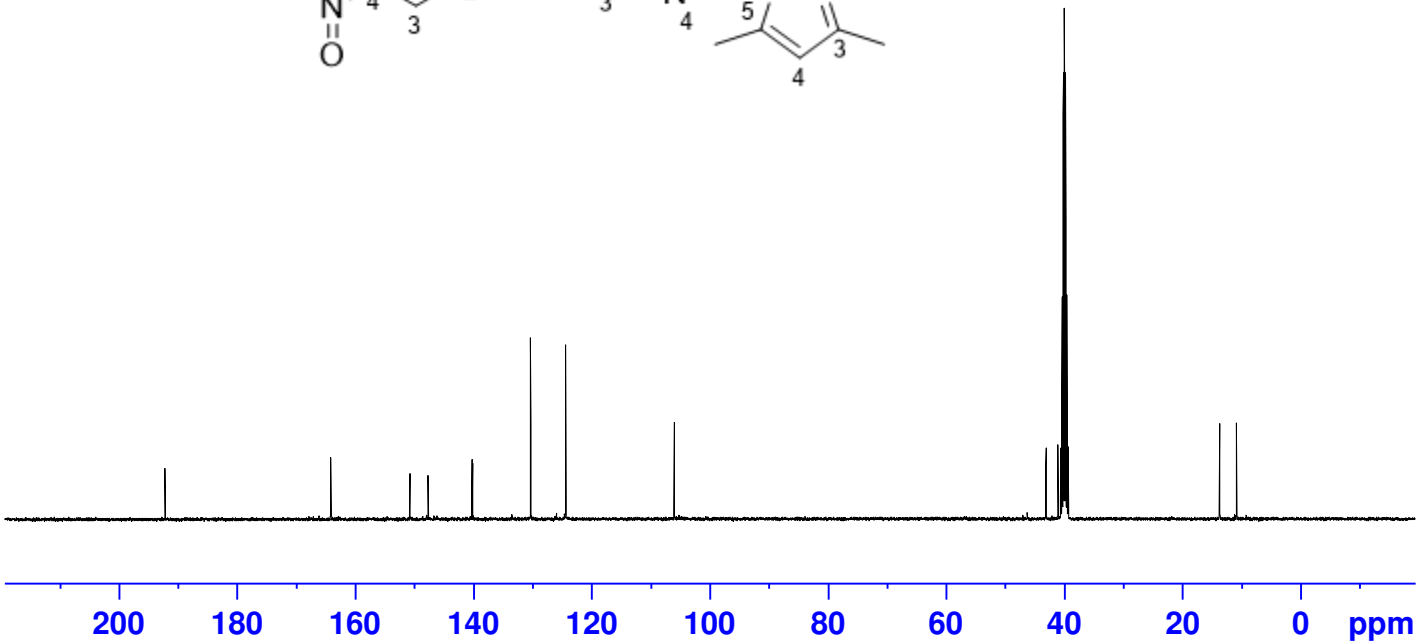

^{13}C NMR of 2-((5-((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-1-(4-nitrophenyl)ethan-1-one (PO22)

PO4NO2-ACP
13C-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)