Supporting information

Exploring the Antimicrobial Properties of Synthetic Tetrahydro-2*H*-1,3,5-Thiadiazine-2-thiones (THTTs) through In-vitro and In-silico Antileishmanial and Antibacterial Studies

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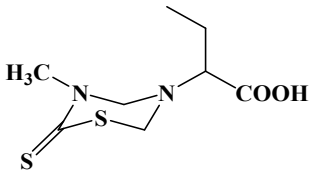
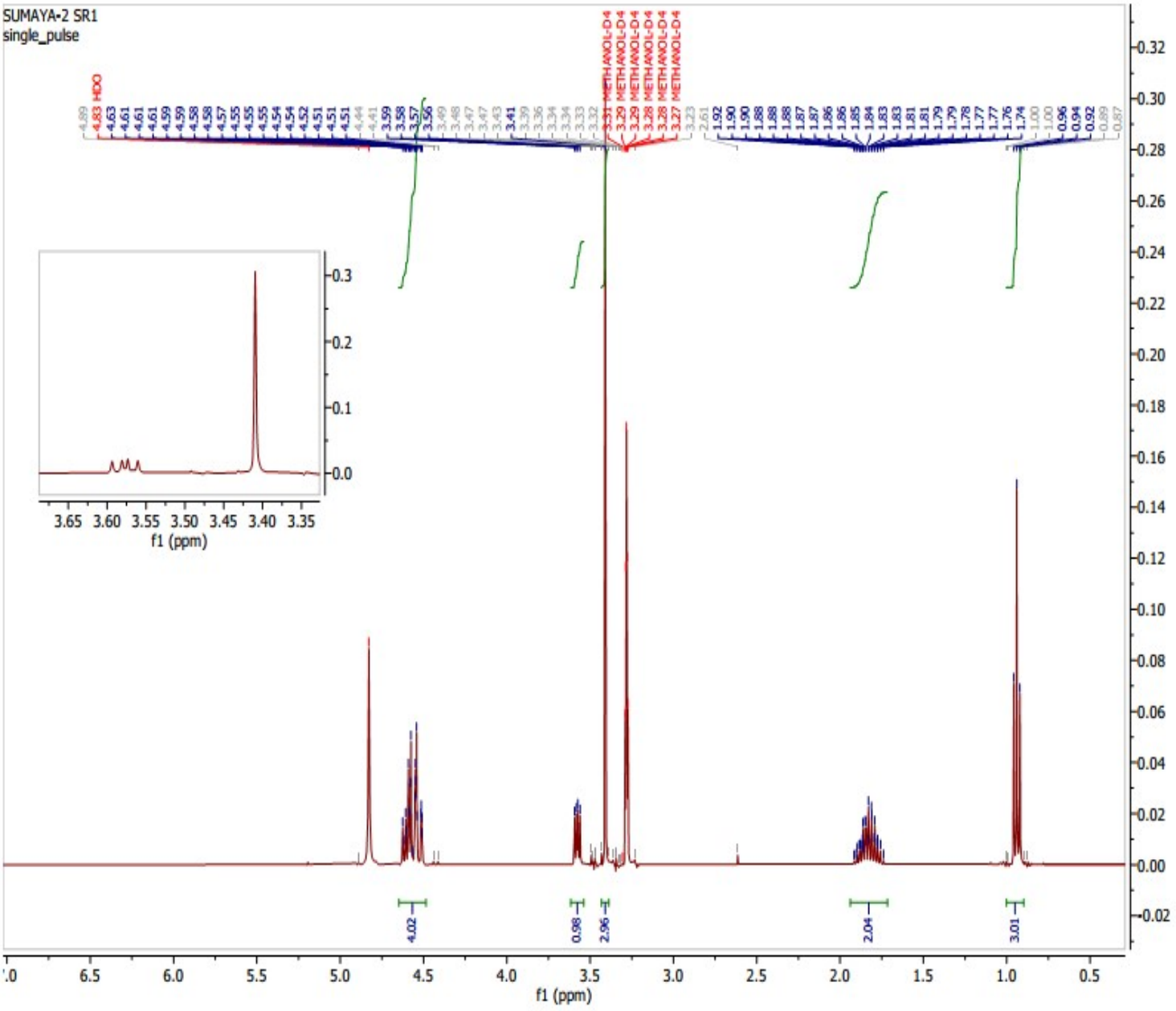
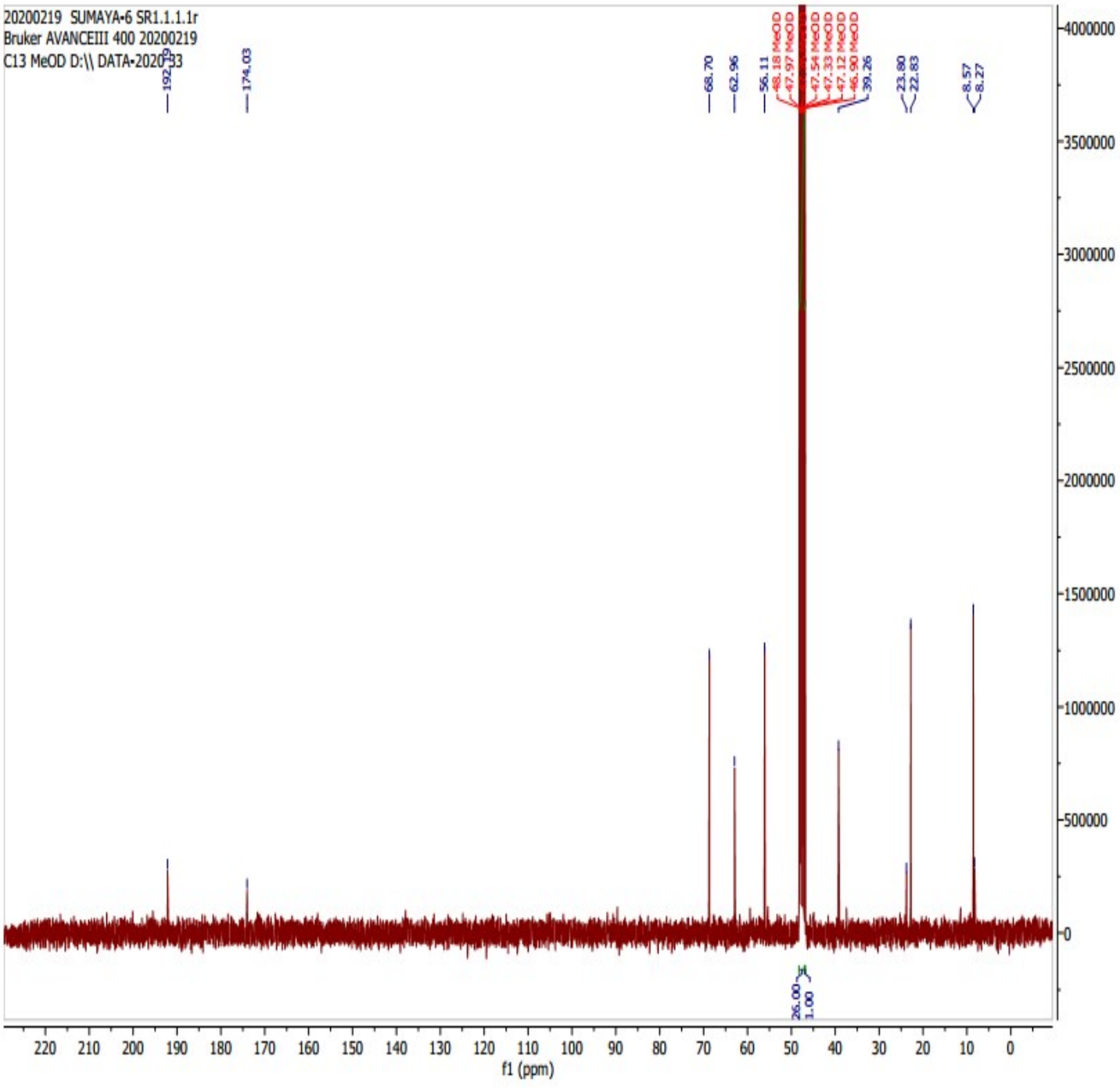
2-(5-methyl-6-thioxo-1,3,5-thiadiazinan-3-yl) butanoic acid (4a)



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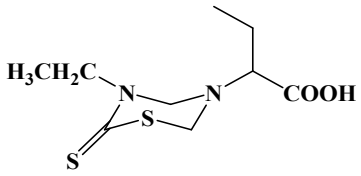
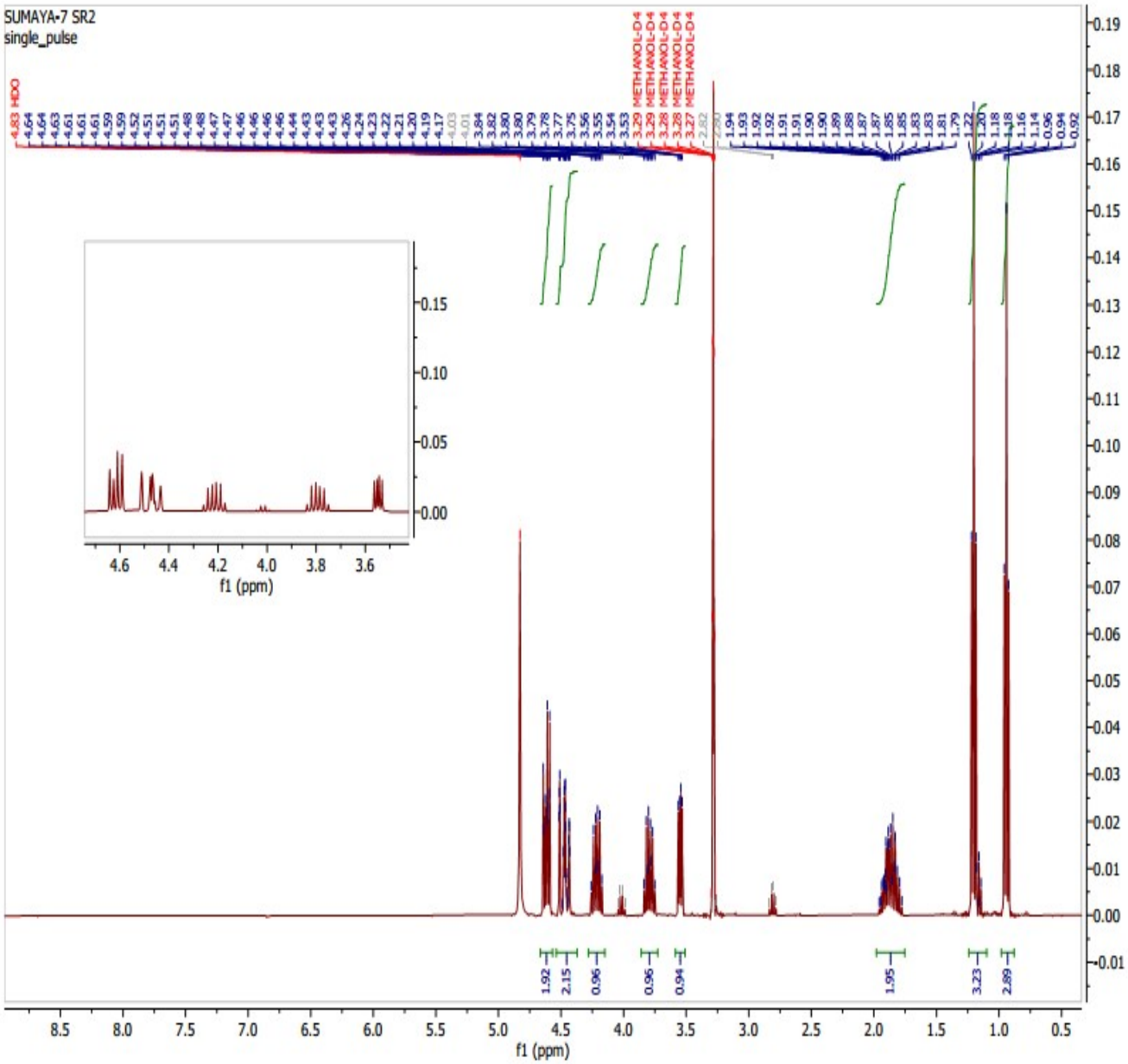
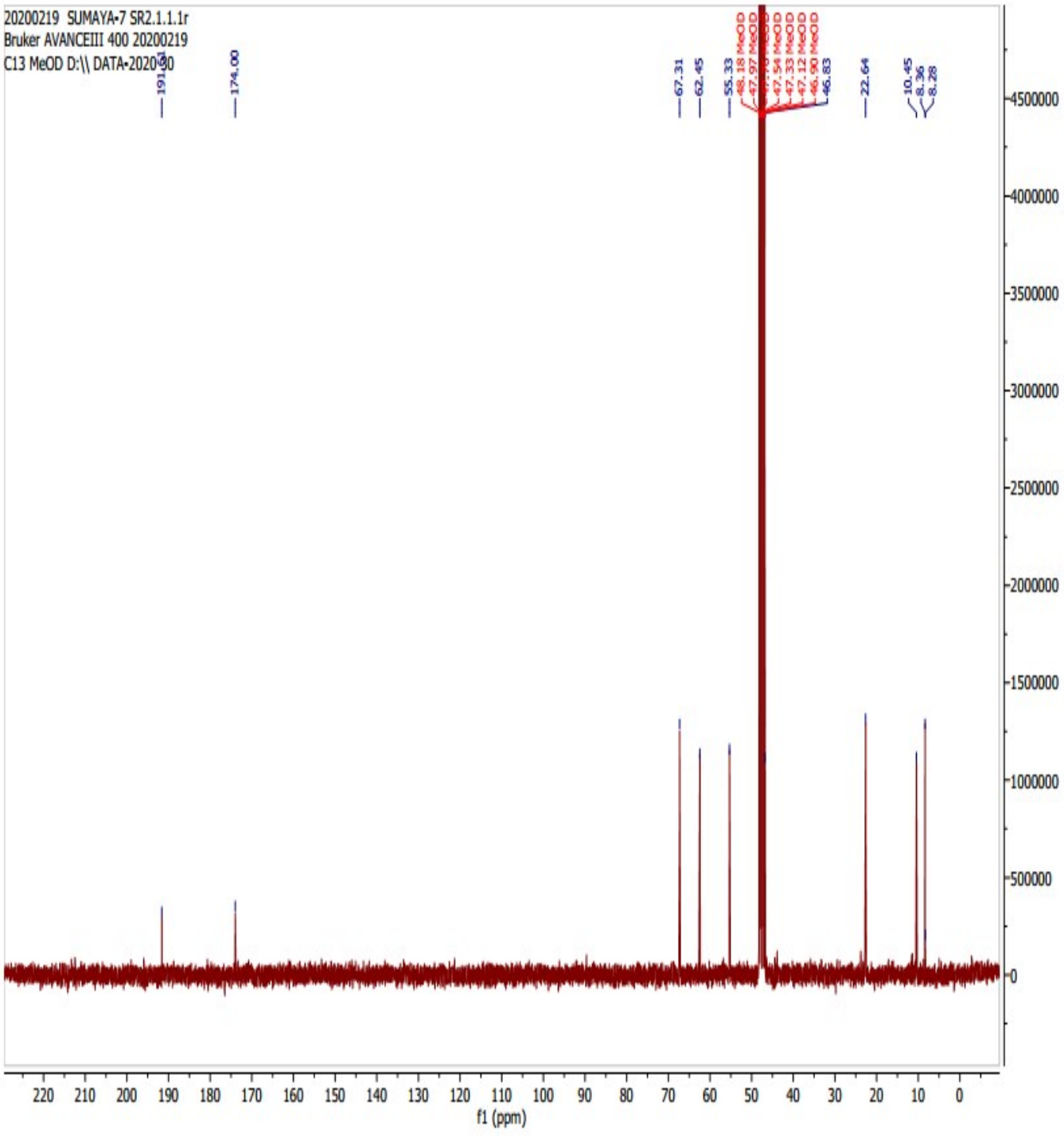
62.96
56.11
48.18 MeOD
47.97 MeOD
47.54 MeOD
47.33 MeOD
47.12 MeOD
46.90 MeOD
39.26
23.80
22.83
8.57
8.27
26.00
1.00
f1 (ppm)

2-(5-ethyl-6-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (4b)



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Bruker AVANCEIII 400 20200219
C13 MeOD D:\\ DATA-2020-0
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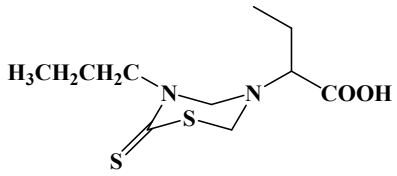
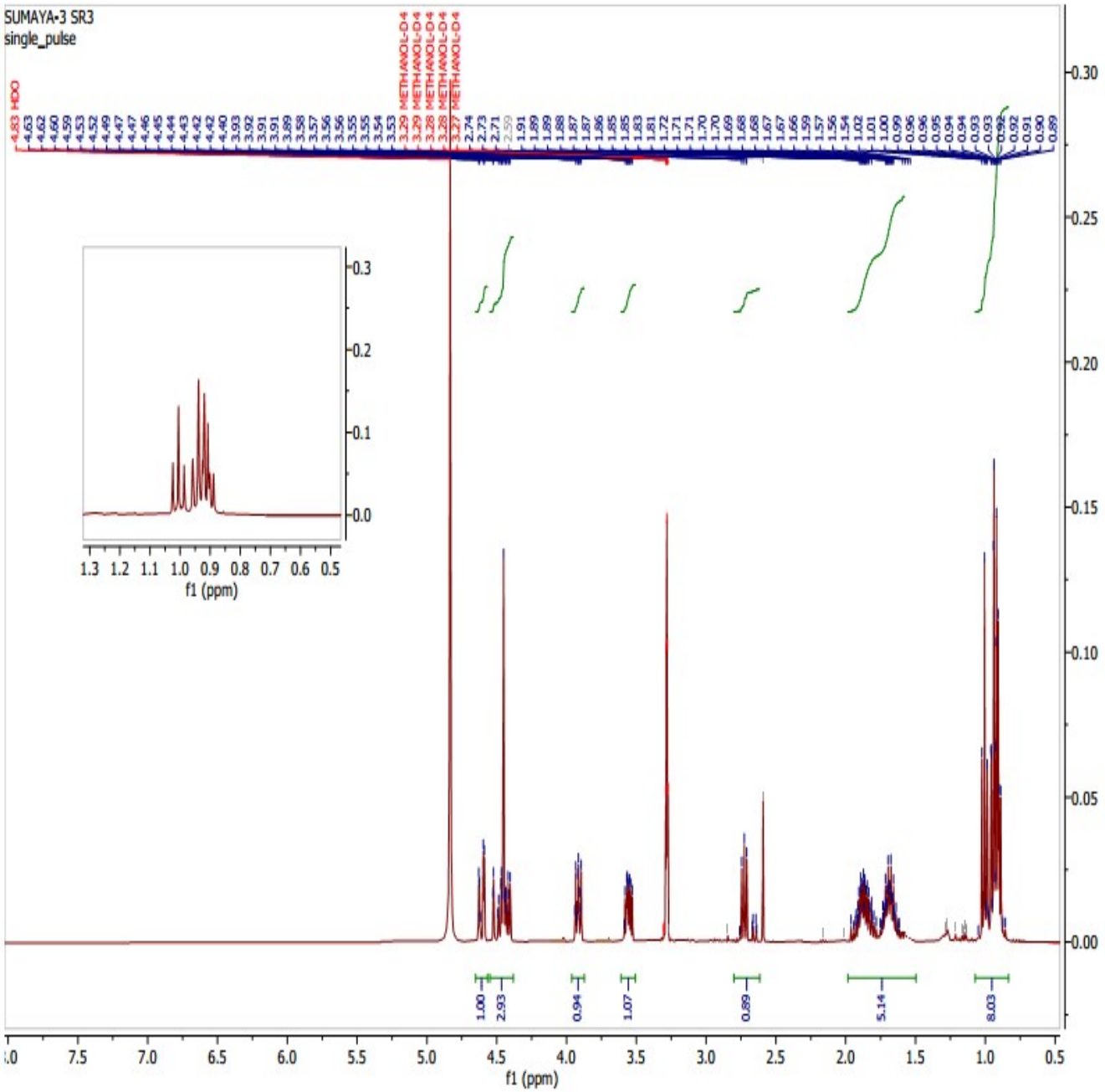
174.00
67.31
62.45
55.33
48.18 MeOD
47.97 MeOD
47.54 MeOD
47.33 MeOD
47.12 MeOD
46.90 MeOD
46.83
22.64
10.45
8.36
8.28
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2-(5-propyl-6-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (4c)





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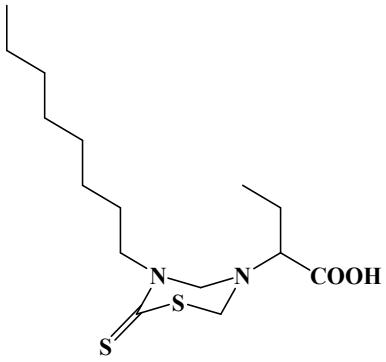
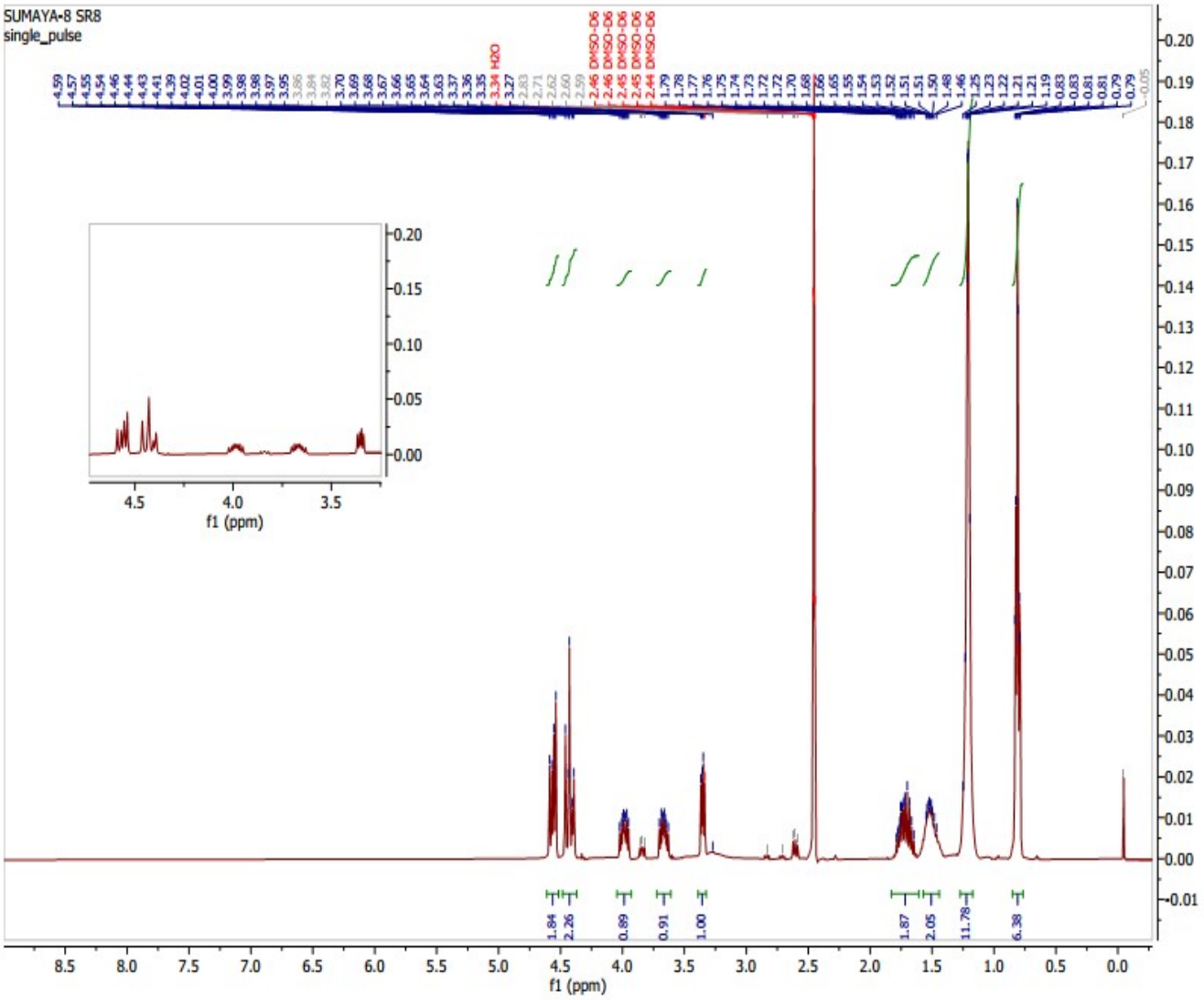
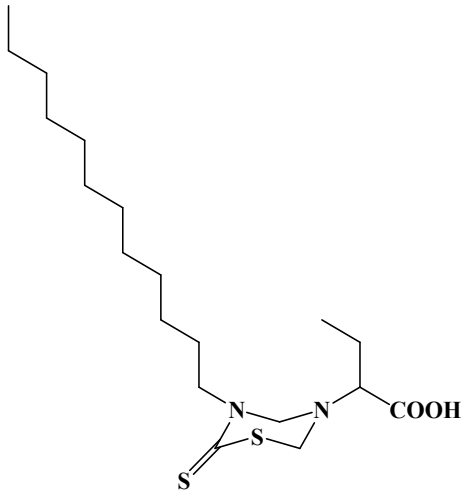
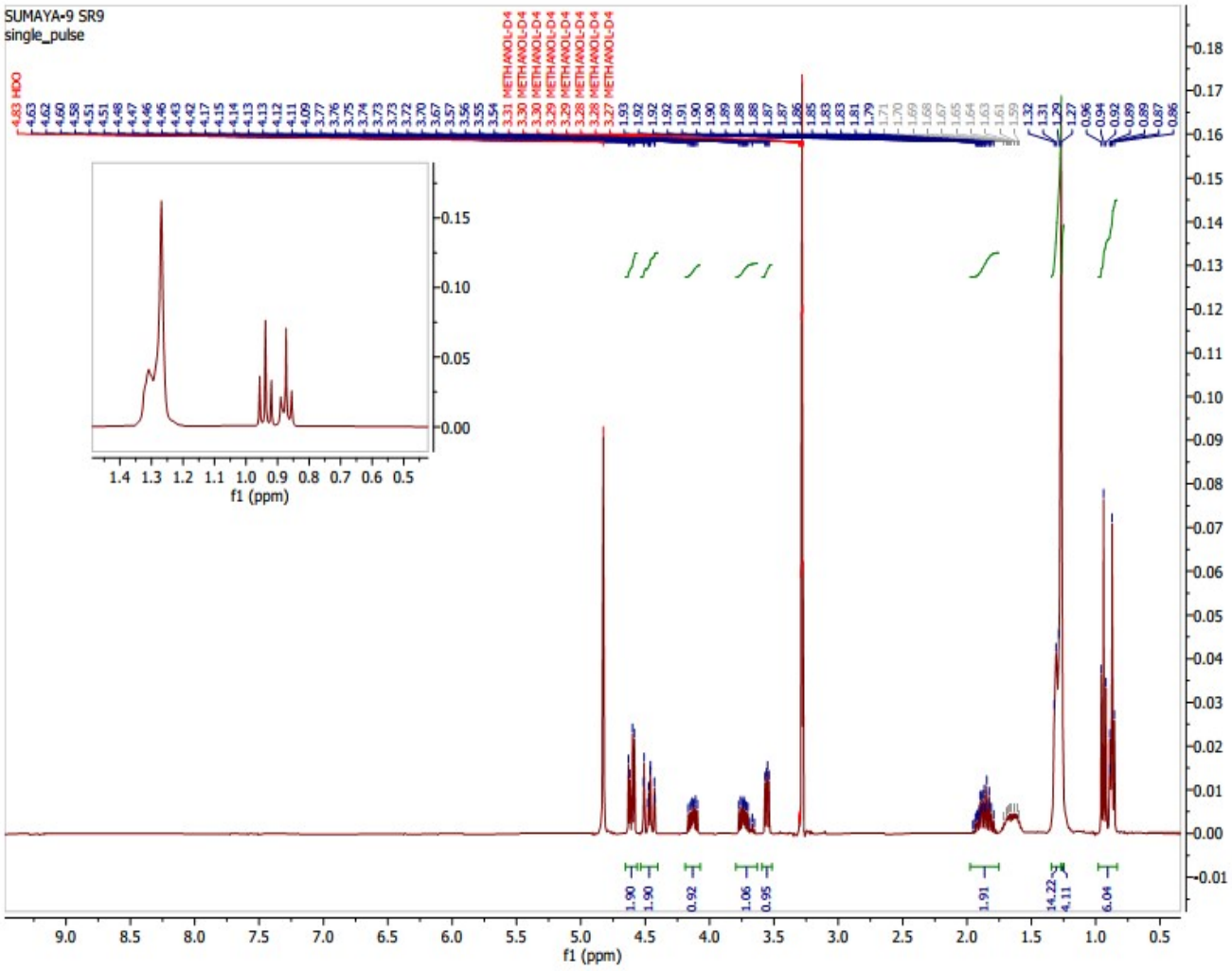
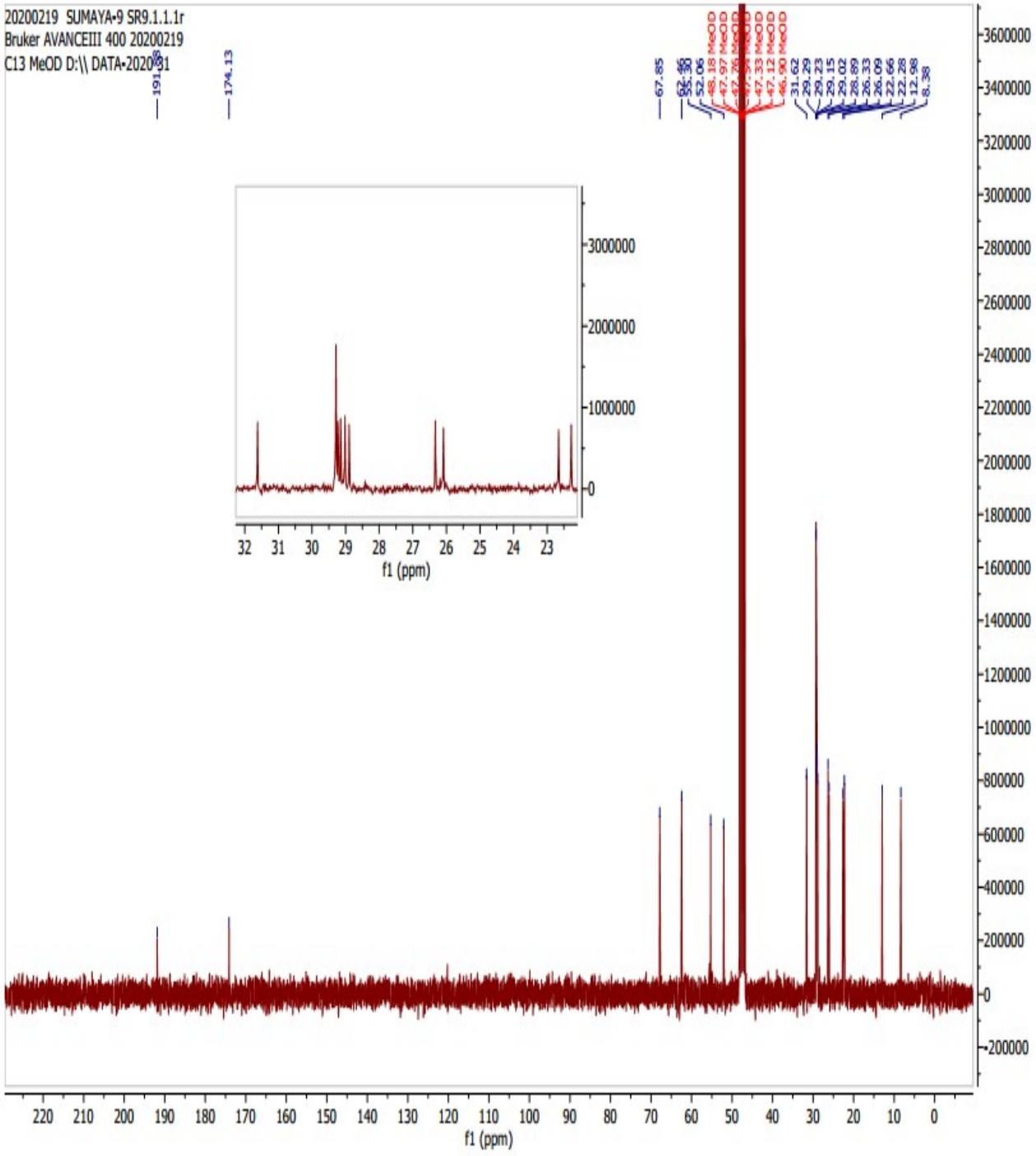




2-(5-dodecyl-6-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (4e)



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Bruker AVANCEIII 400 20200219
C13 MeOD D:\\ DATA-2020 31
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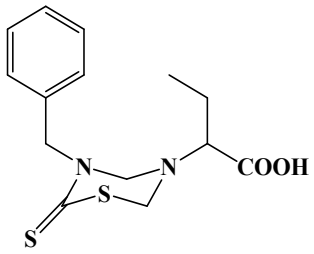
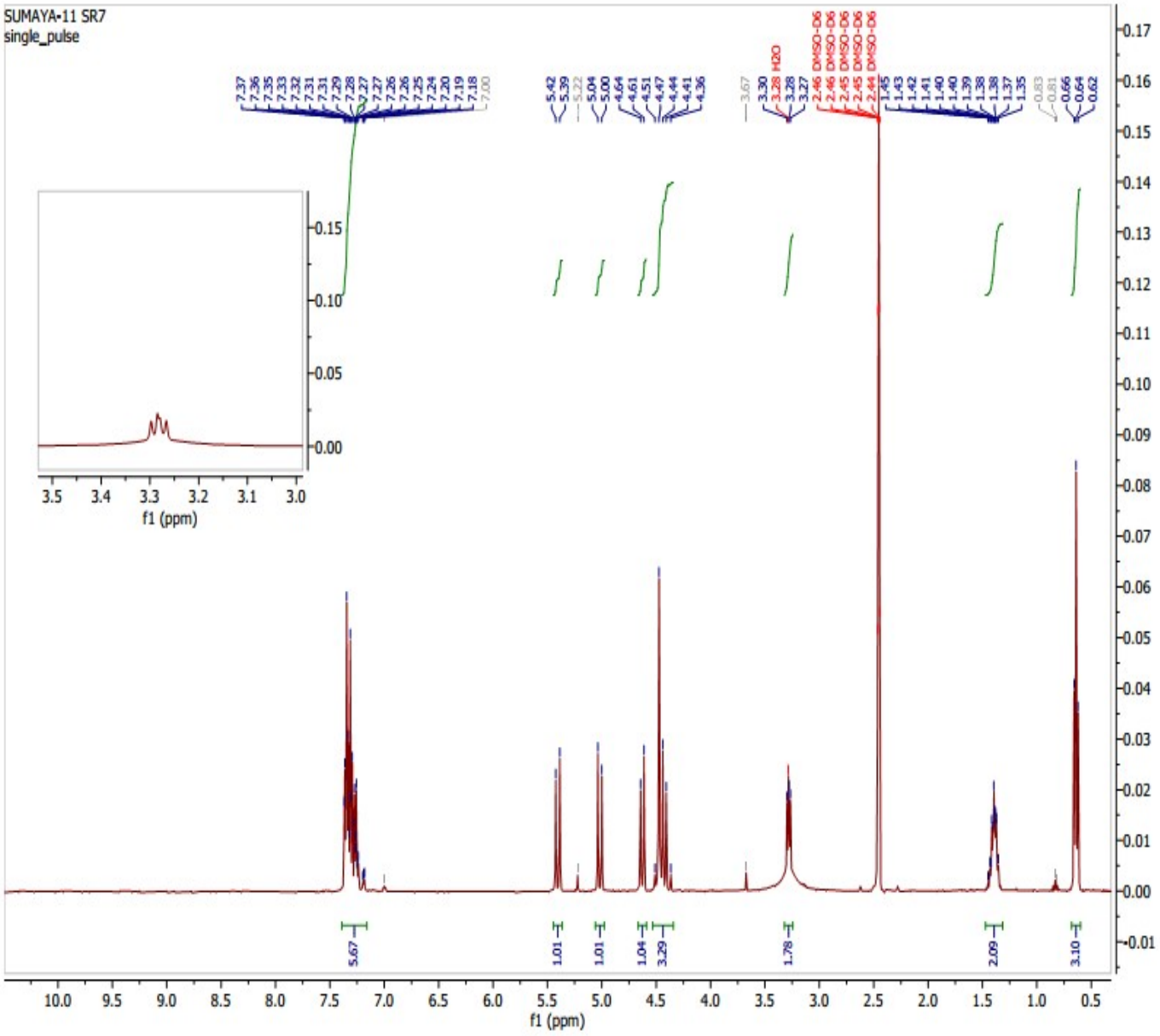
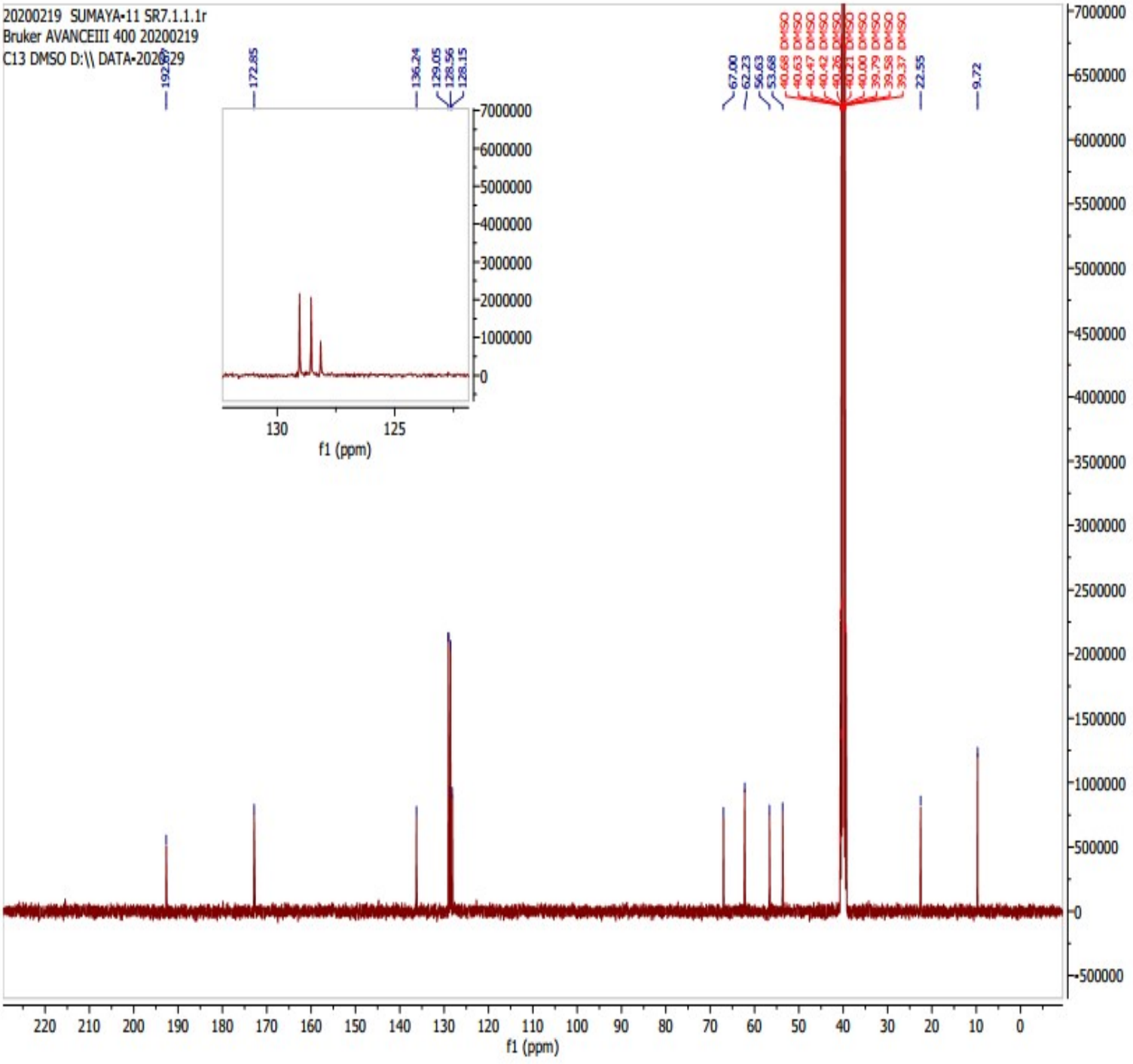
174.13
67.85
62.46
55.30
52.06
48.18 MeOD
47.97 MeOD
47.76 MeOD
47.54 MeOD
47.33 MeOD
47.12 MeOD
46.90 MeOD
31.62
29.29
29.23
29.15
29.02
28.89
26.33
26.09
22.66
22.28
12.98
8.38
f1 (ppm)
f1 (ppm)

2-(5-benzyl -6-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (4f)



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Bruker AVANCEIII 400 20200219
C13 DMSO D:\\ DATA-20200219
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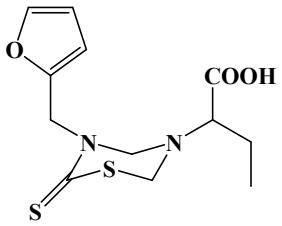
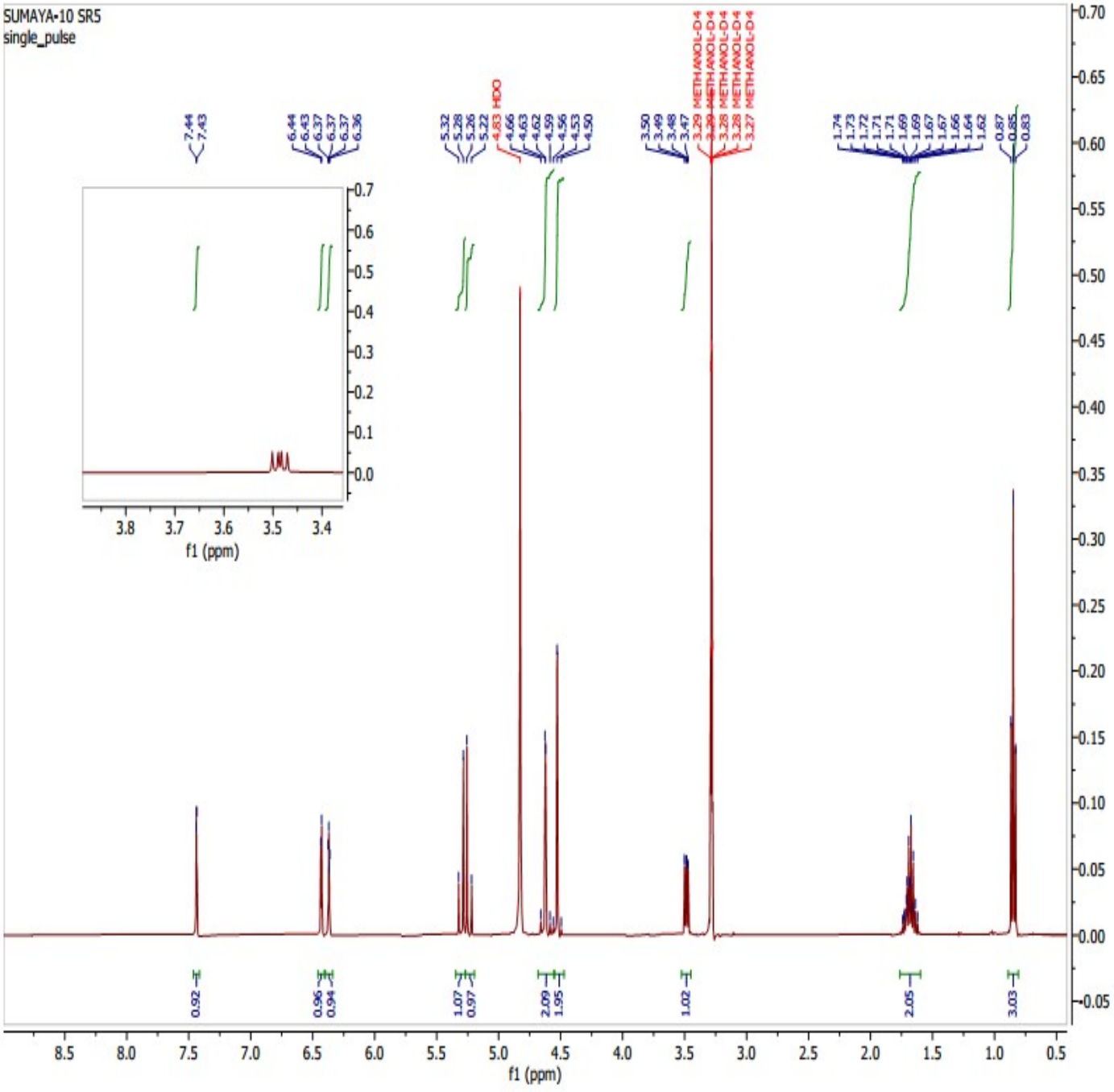
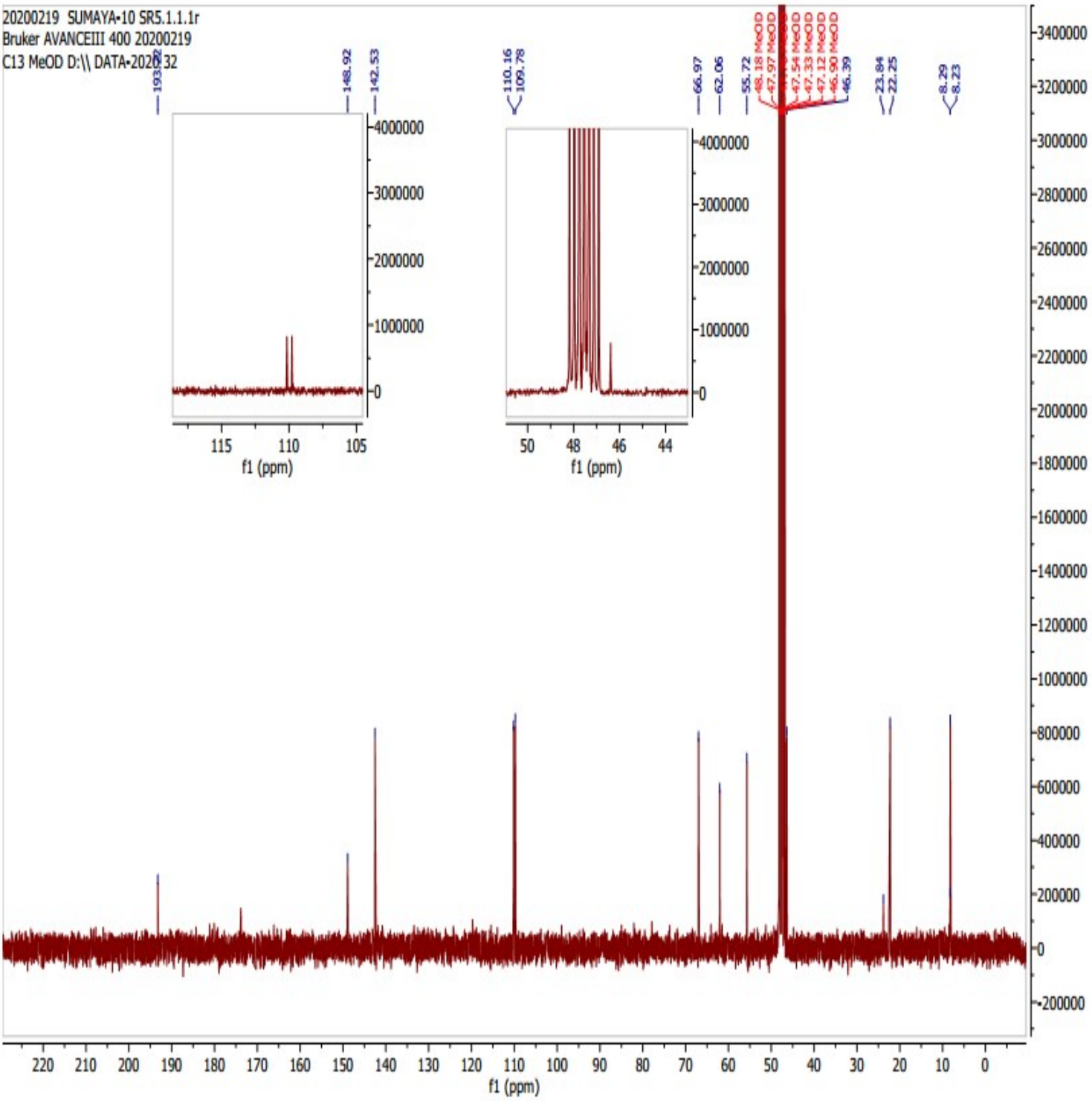
172.85
136.24
129.05
128.56
128.15
67.00
62.23
56.63
53.68
40.68 DMSO
40.63 DMSO
40.47 DMSO
40.42 DMSO
40.26 DMSO
40.21 DMSO
40.00 DMSO
39.79 DMSO
39.58 DMSO
39.37 DMSO
22.55
9.72
f1 (ppm)
f1 (ppm)

2-(5-(furan-2-ylmethyl)-6-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (4g)



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Bruker AVANCEIII 400 20200219
C13 MeOD D:\\ DATA-2020 32
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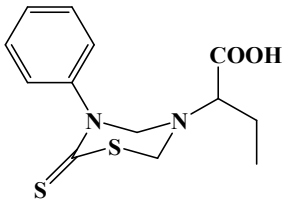
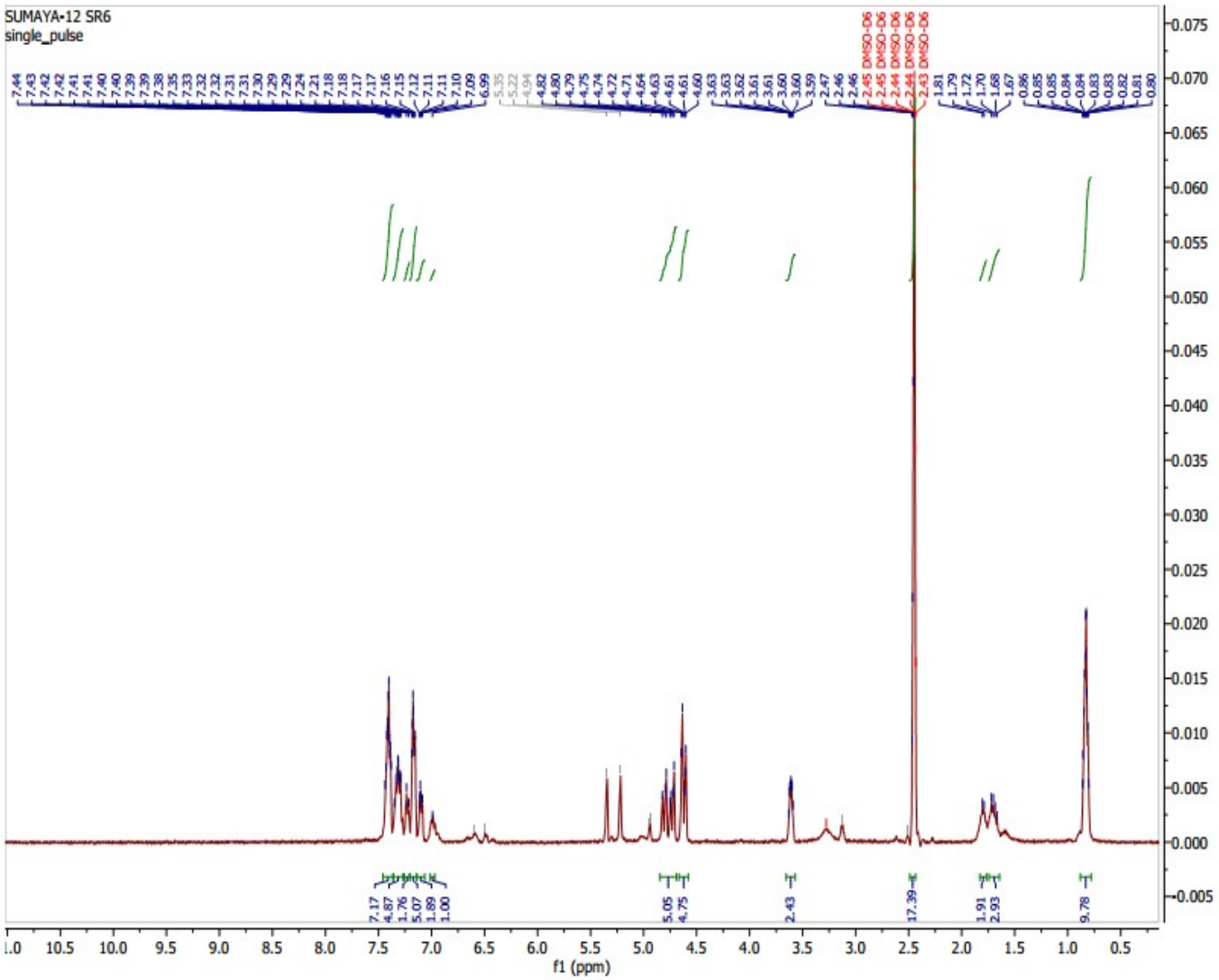
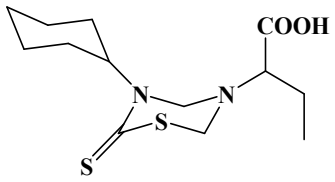
148.92
142.53
110.16
109.78
66.97
62.06
55.72
48.18 MeOD
47.97 MeOD
47.54 MeOD
47.33 MeOD
47.12 MeOD
46.90 MeOD
46.39
23.84
22.25
8.29
8.23
f1 (ppm)
f1 (ppm)
f1 (ppm)

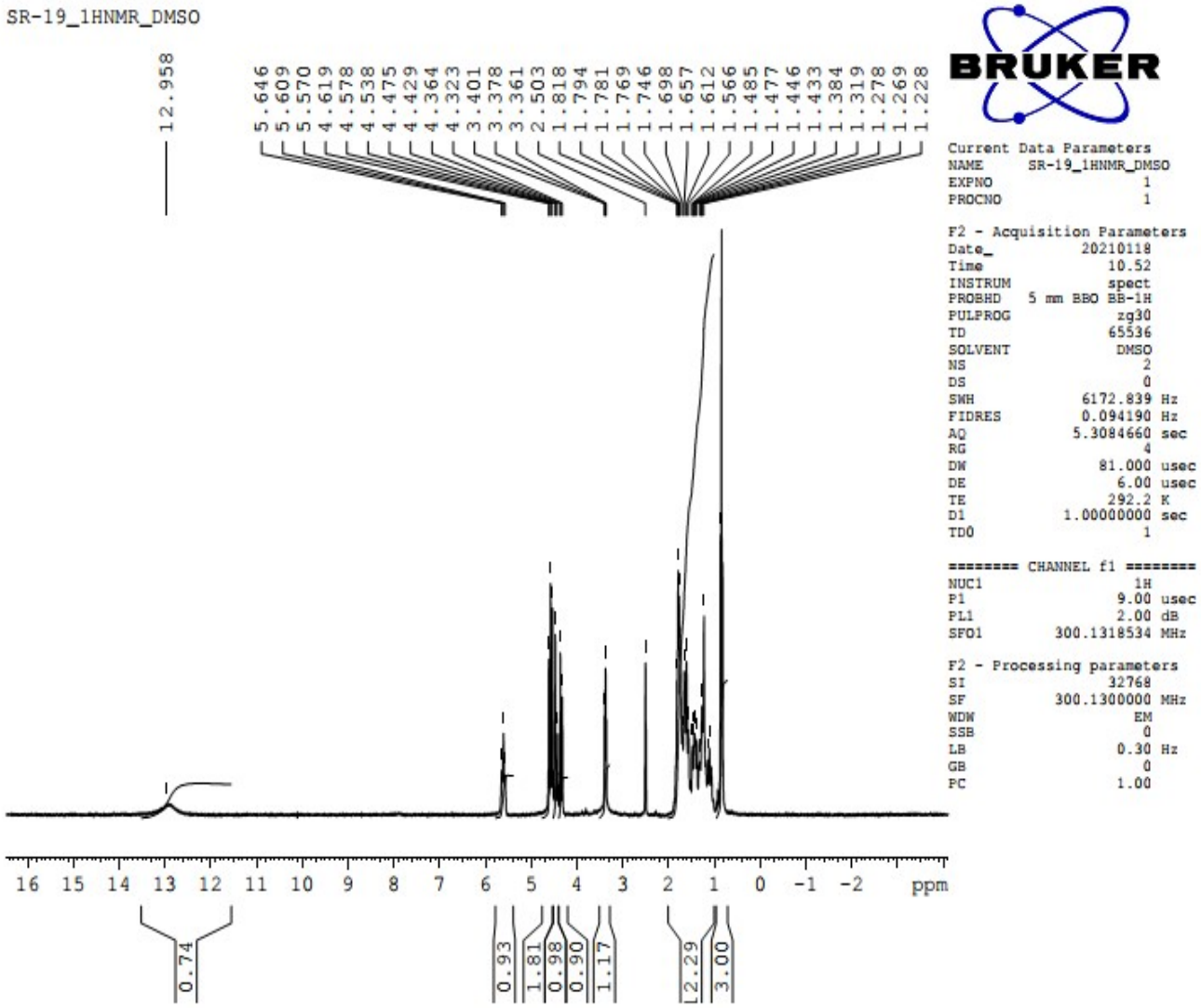
2-(5-phenyl-6-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (4h)



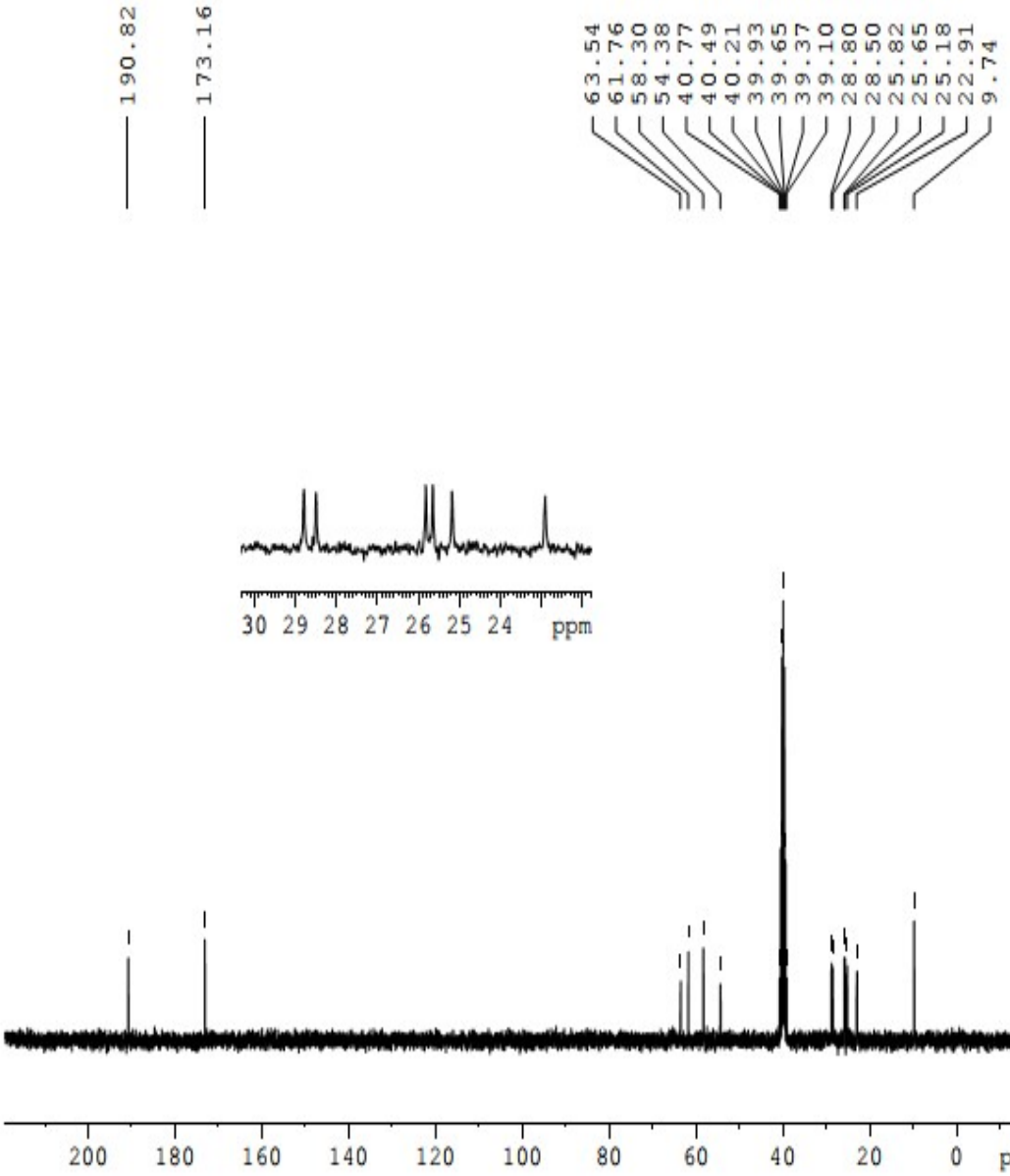


Synthesis of 2-(5-cyclohexyl-6-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (4i)





SR-19_13CNMR_DMSO



BRUKER

Current Data Parameters

NAME	SR-19_13CNMR_DMSO
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20210118
Time	10.50
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	35968
SOLVENT	DMSO
NS	46
DS	0
SWH	17985.611 Hz
FIDRES	0.500045 Hz
AQ	0.9999604 sec
RG	29193
DW	27.800 usec
DE	6.00 usec
TE	292.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	6.00 usec
PL1	-5.00 dB
SFO1	75.4752953 MHz

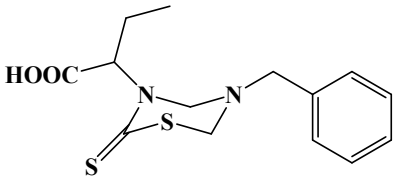
======== CHANNEL f2 ========

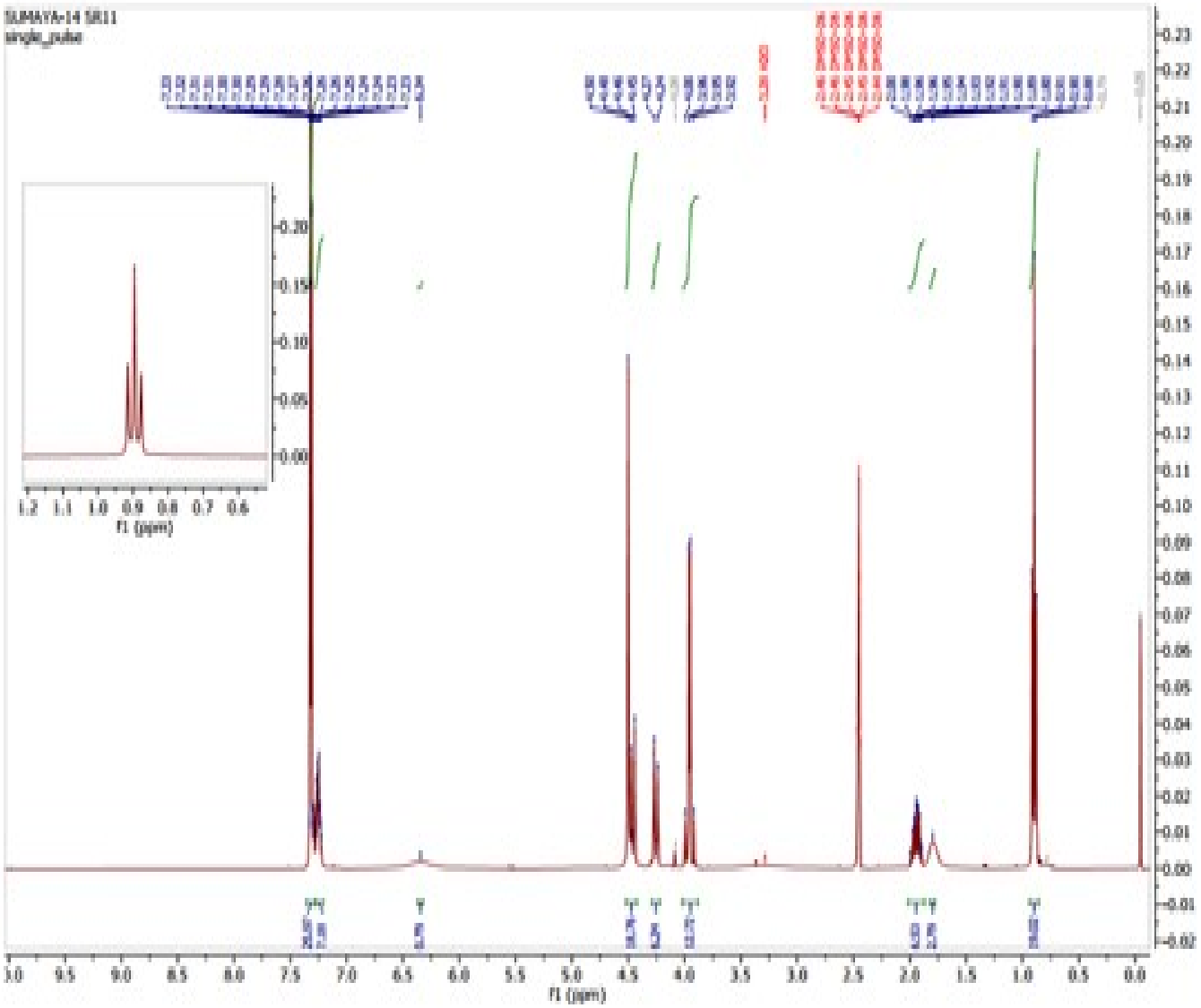
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	20.98 dB
PL13	20.00 dB
SFO2	300.1312005 MHz

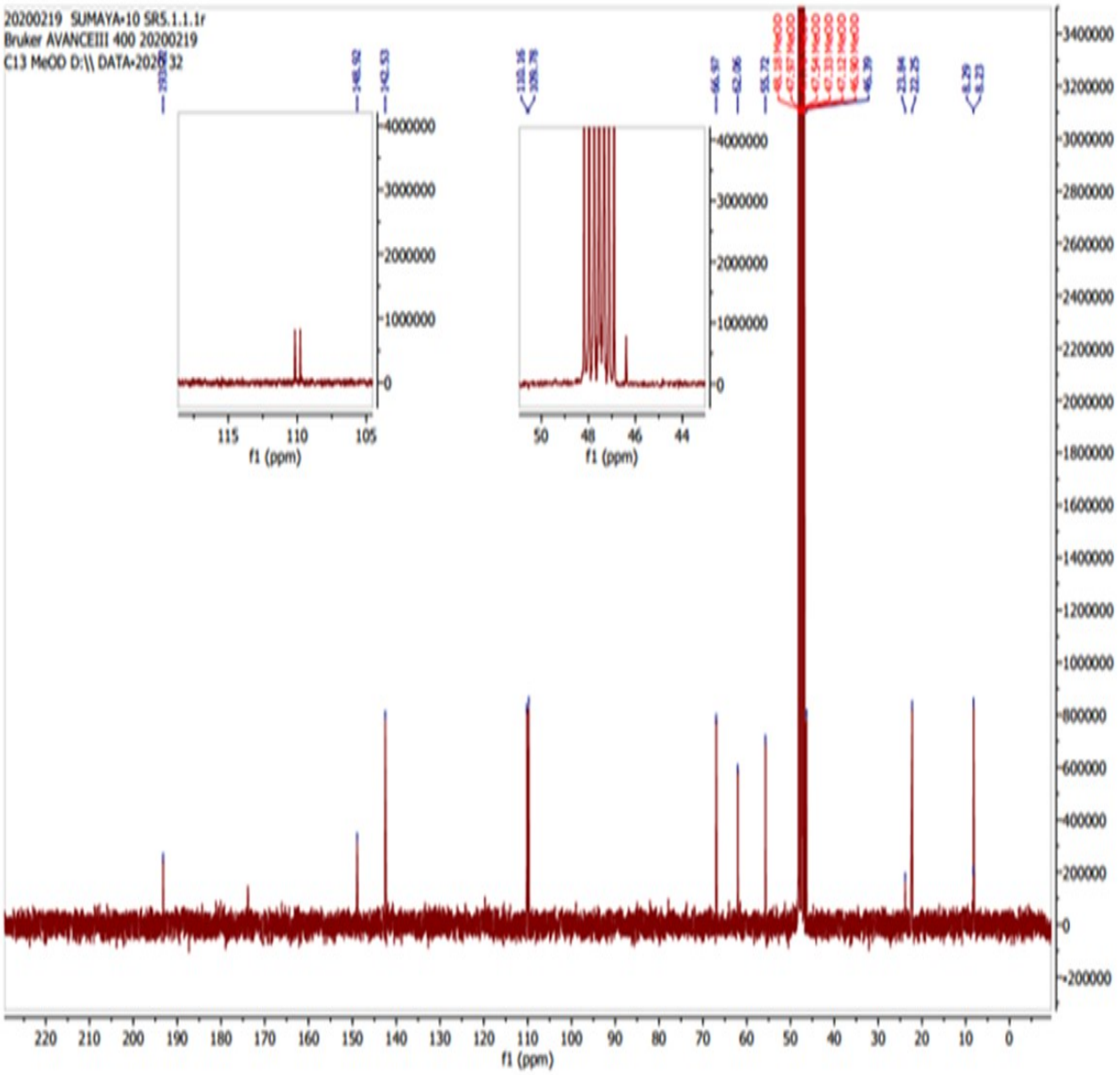
F2 - Processing parameters

SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

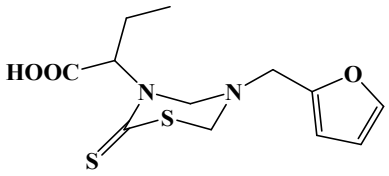
2-(5-benzyl-2-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (5a)

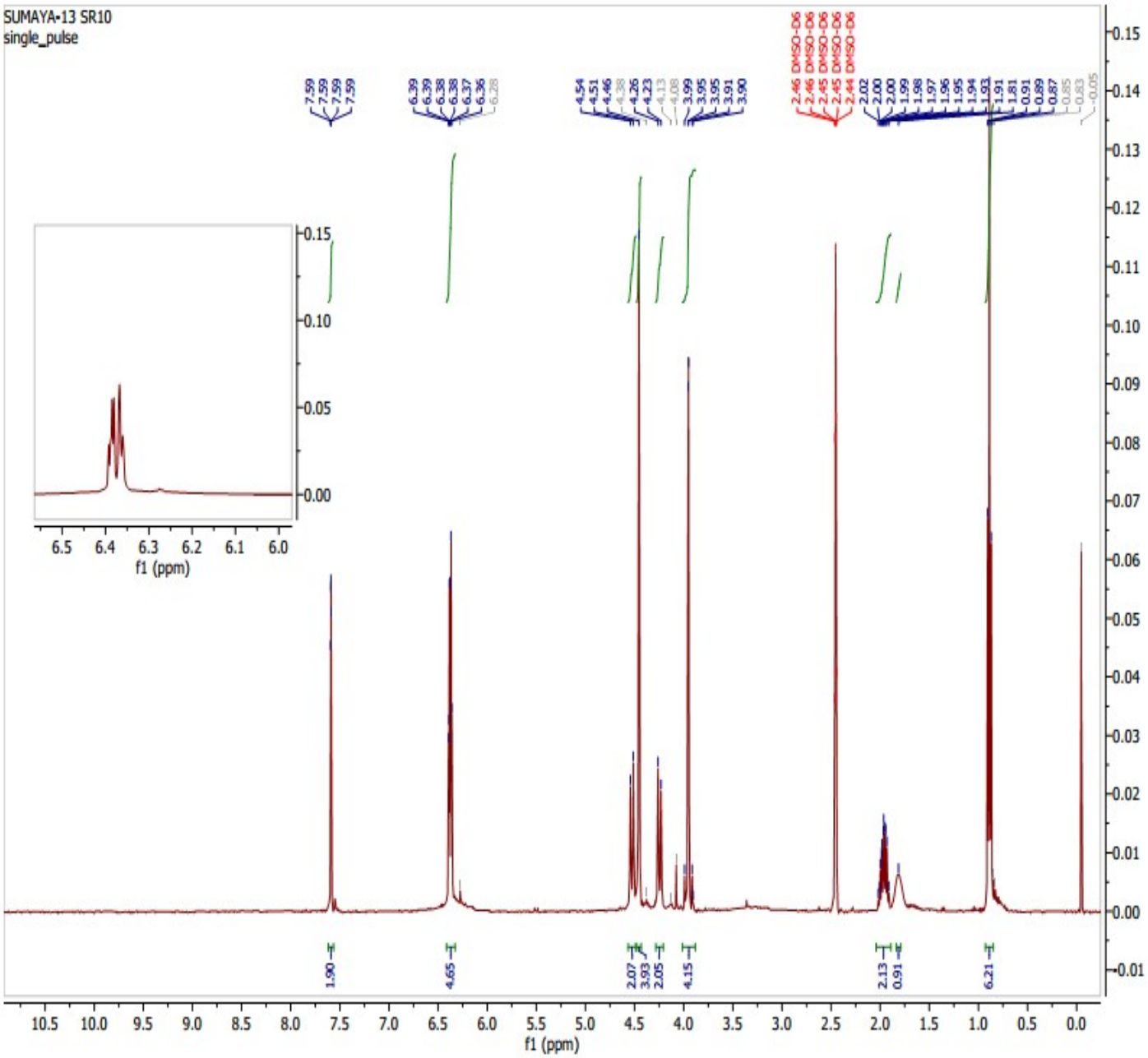




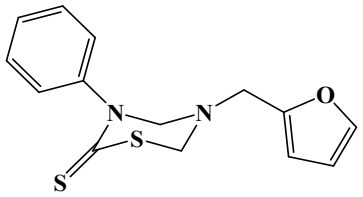

20200219 SUMAYA-10 SR5.1.1.1r
Bruker AVANCEIII 400 20200219
C13 MeOD D:\\ DATA-2020 32
148.92
142.53
110.16
106.78
56.97
52.06
55.72
46.39
21.84
22.25
6.29
6.23
f1 (ppm)
f1 (ppm)
f1 (ppm)

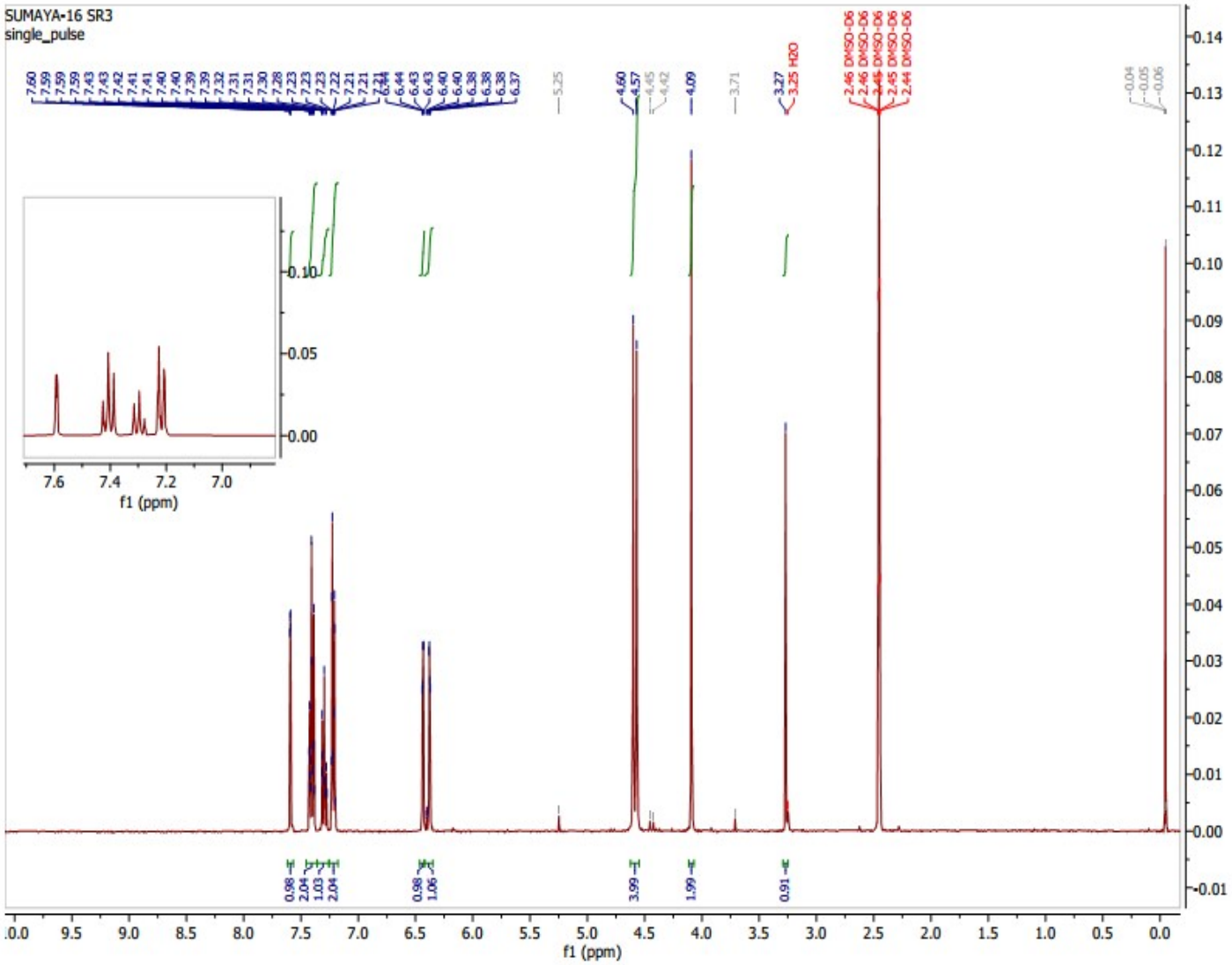
2-(5-(furan-2-ylmethyl)-2-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (5b)



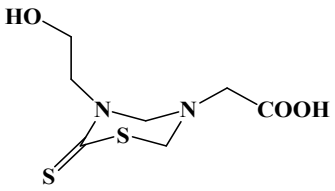


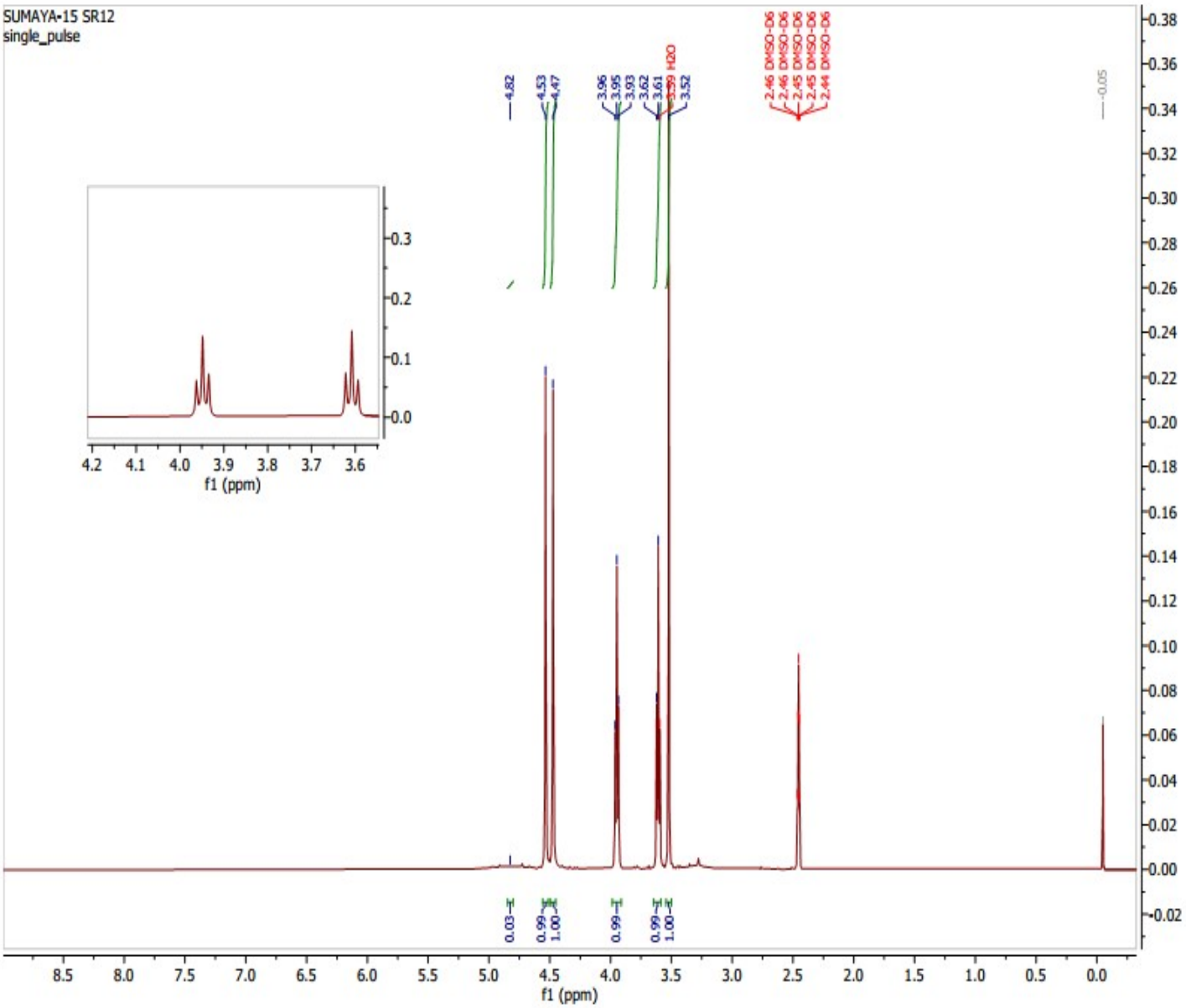
5-(furan-2-ylmethyl)-3-phenyl-1,3,5-thiadiazinane-2-thione (5c)

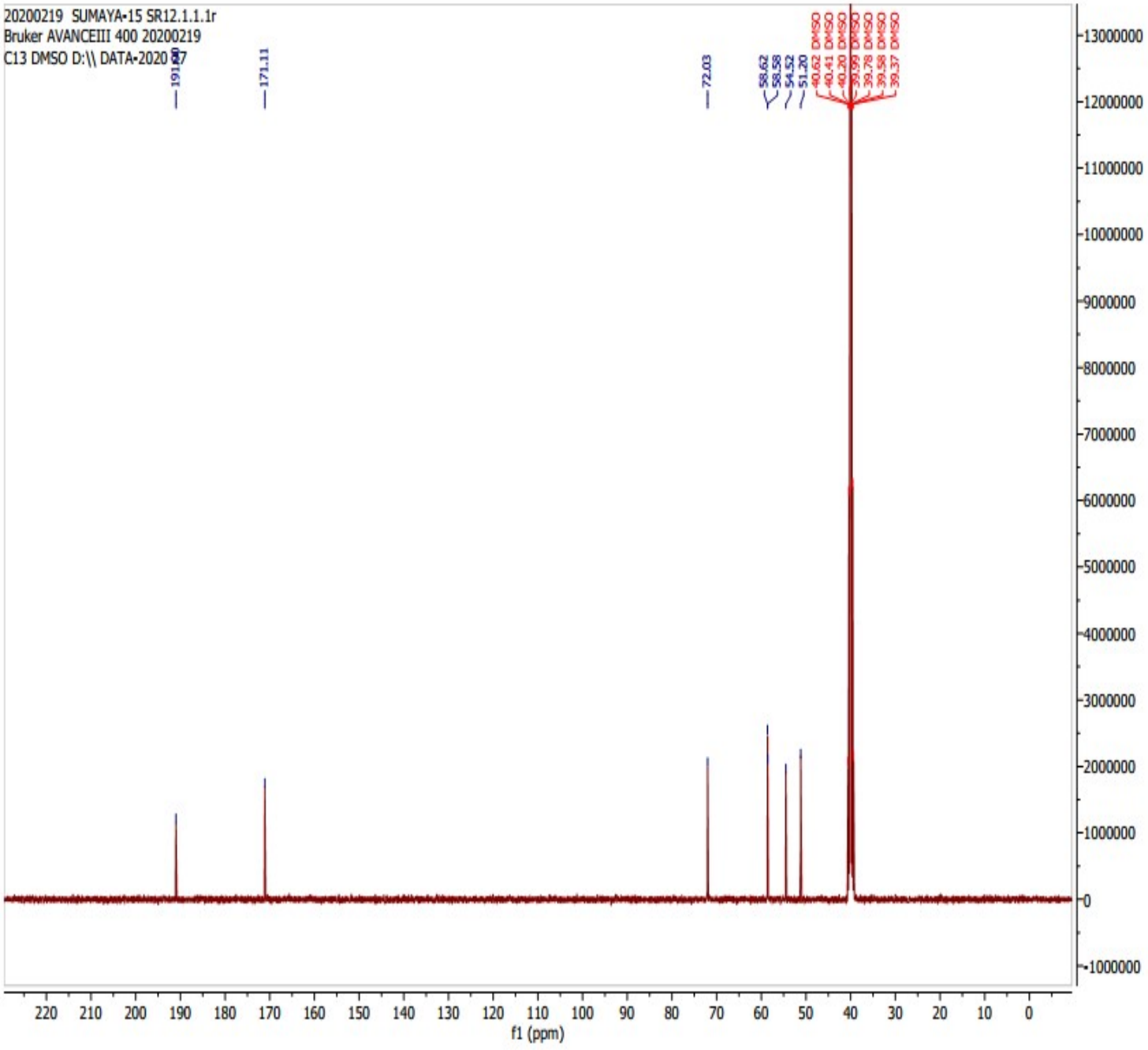




2-(5-(2-hydroxyethyl)-6-thioxo-1,3,5-thiadiazinan-3-yl)acetic acid (5d)



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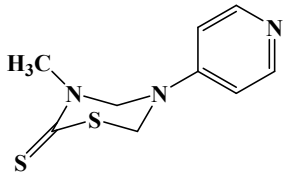
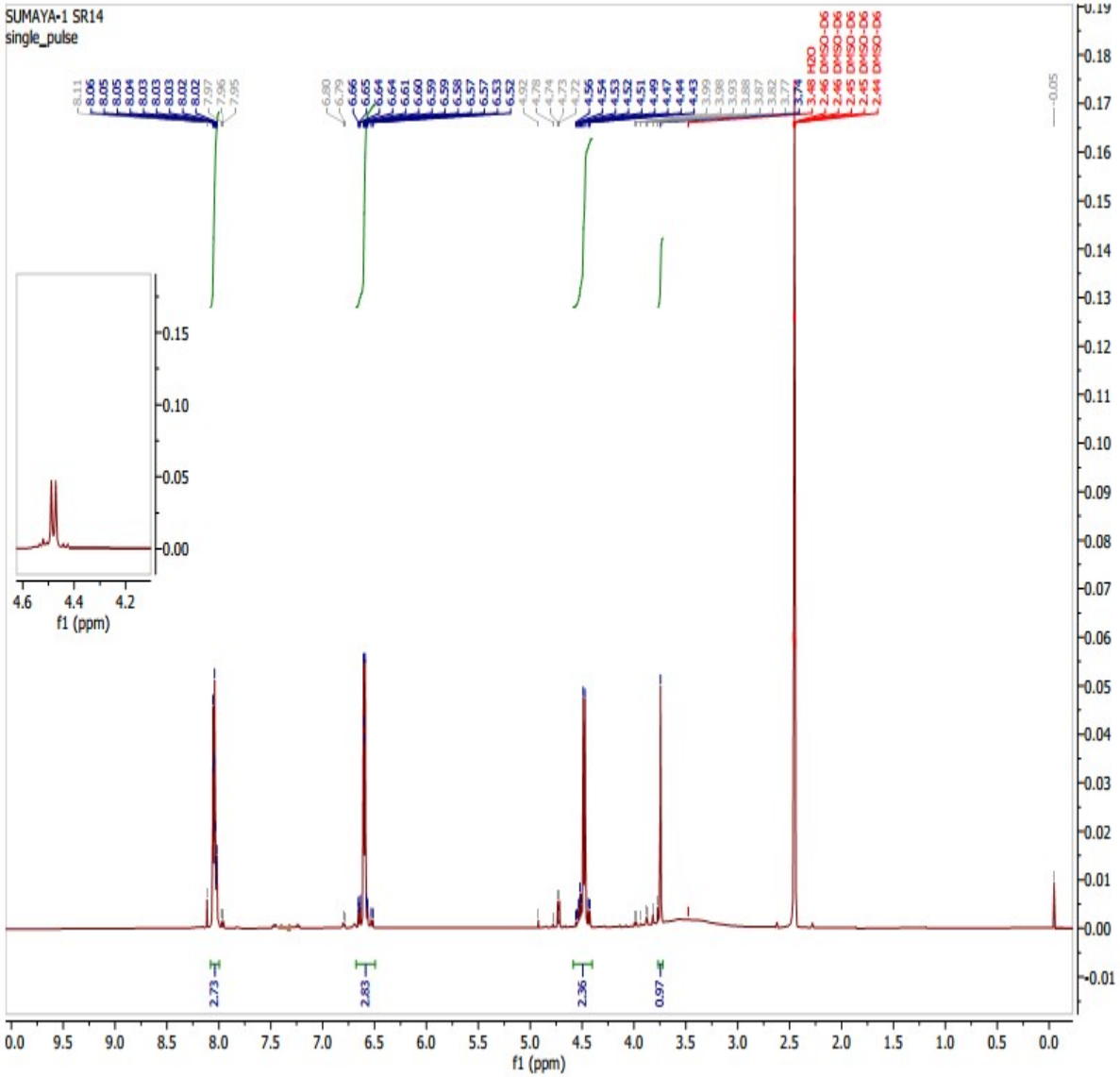
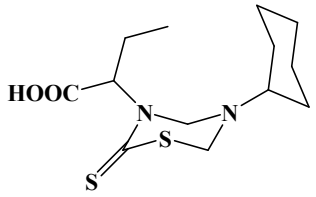
Bruker AVANCEIII 400 20200219
C13 DMSO D:\\ DATA-2020
191.60
171.11
72.03
58.62
58.58
54.52
51.20
40.62 DMSO
40.41 DMSO
40.20 DMSO
39.99 DMSO
39.78 DMSO
39.58 DMSO
39.37 DMSO
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

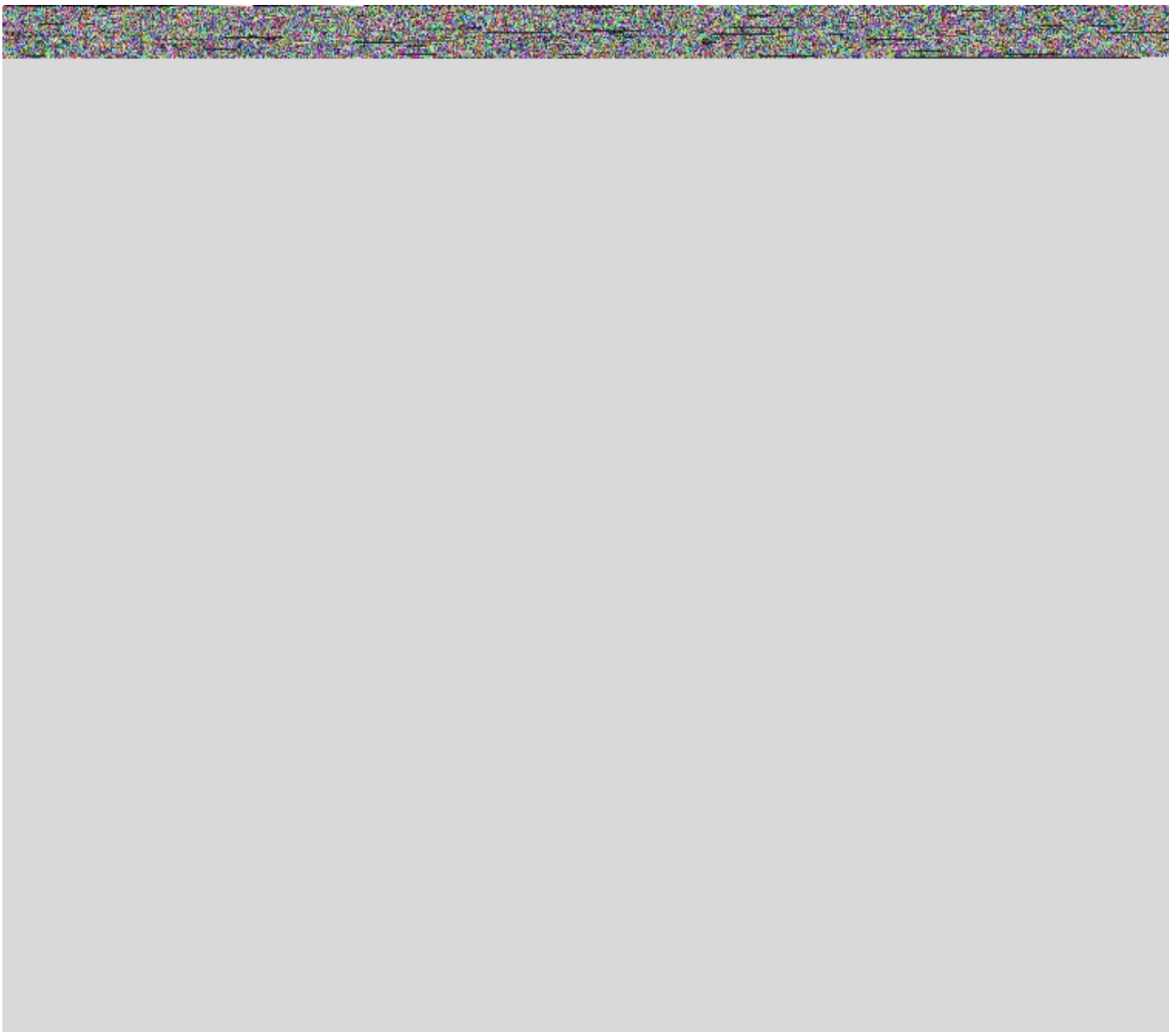
3-methyl-5-(pyridin-4-yl)-1,3,5-thiadiazinane-2-thione (5e)



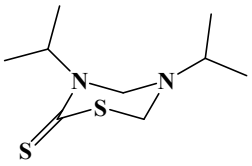


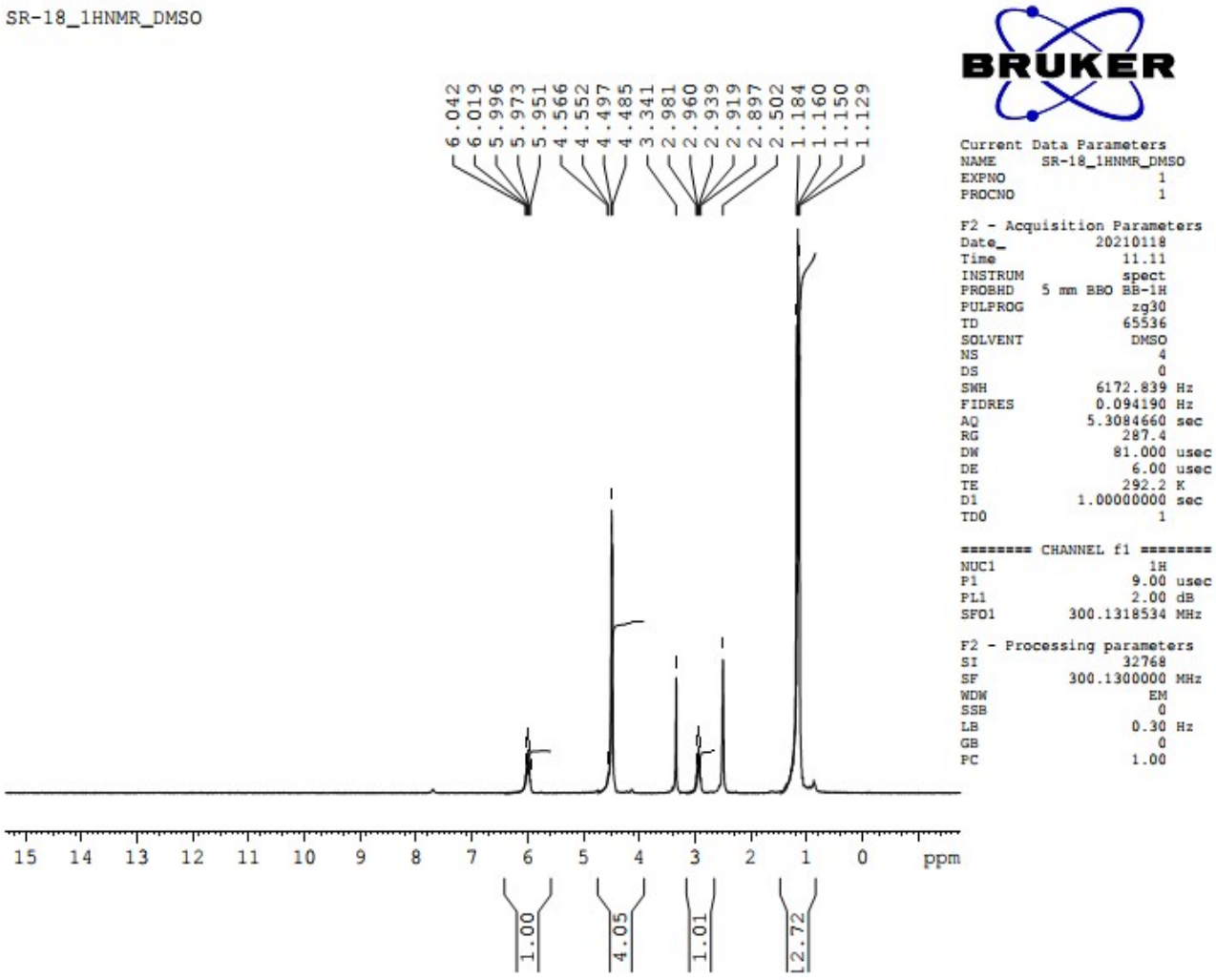
Synthesis of 2-(5-cyclohexyl-2-thioxo-1,3,5-thiadiazinan-3-yl)butanoic acid (5f)





Synthesis of 3,5-diisopropyl-1,3,5-thiadiazinane-2-thione (5g)



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Current Data Parameters
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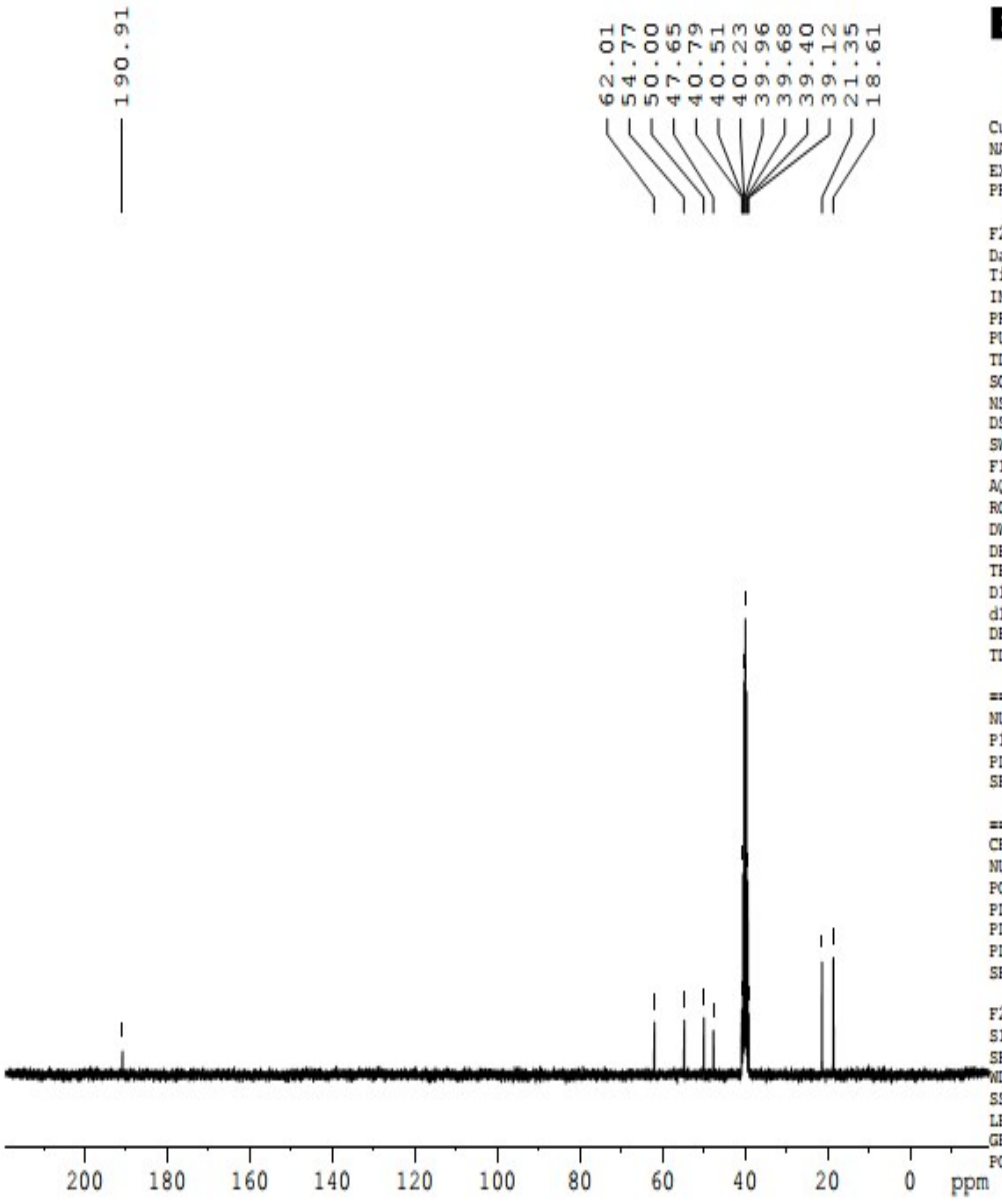
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20210118
Time              11.11
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                65536
SOLVENT            DMSO
NS                    4
DS                    0
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ             5.3084660 sec
RG                287.4
DW               81.000 usec
DE                6.00 usec
TE               292.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                9.00 usec
PL1               2.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                32768
SF          300.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

SR-18_13CNMR_DMSO



BRUKER

Current Data Parameters

NAME	SR-18_13CNMR_DMSO
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20210118
Time	11.08
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	35968
SOLVENT	DMSO
NS	262
DS	0
SWH	17985.611 Hz
FIDRES	0.500045 Hz
AQ	0.9999604 sec
RG	20642.5
DW	27.800 usec
DE	6.00 usec
TE	292.6 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	6.00 usec
PL1	-5.00 dB
SFO1	75.4752953 MHz

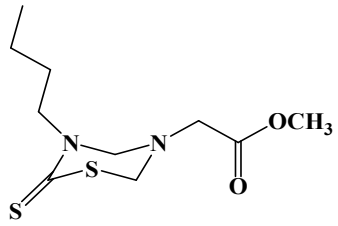
======== CHANNEL f2 ========

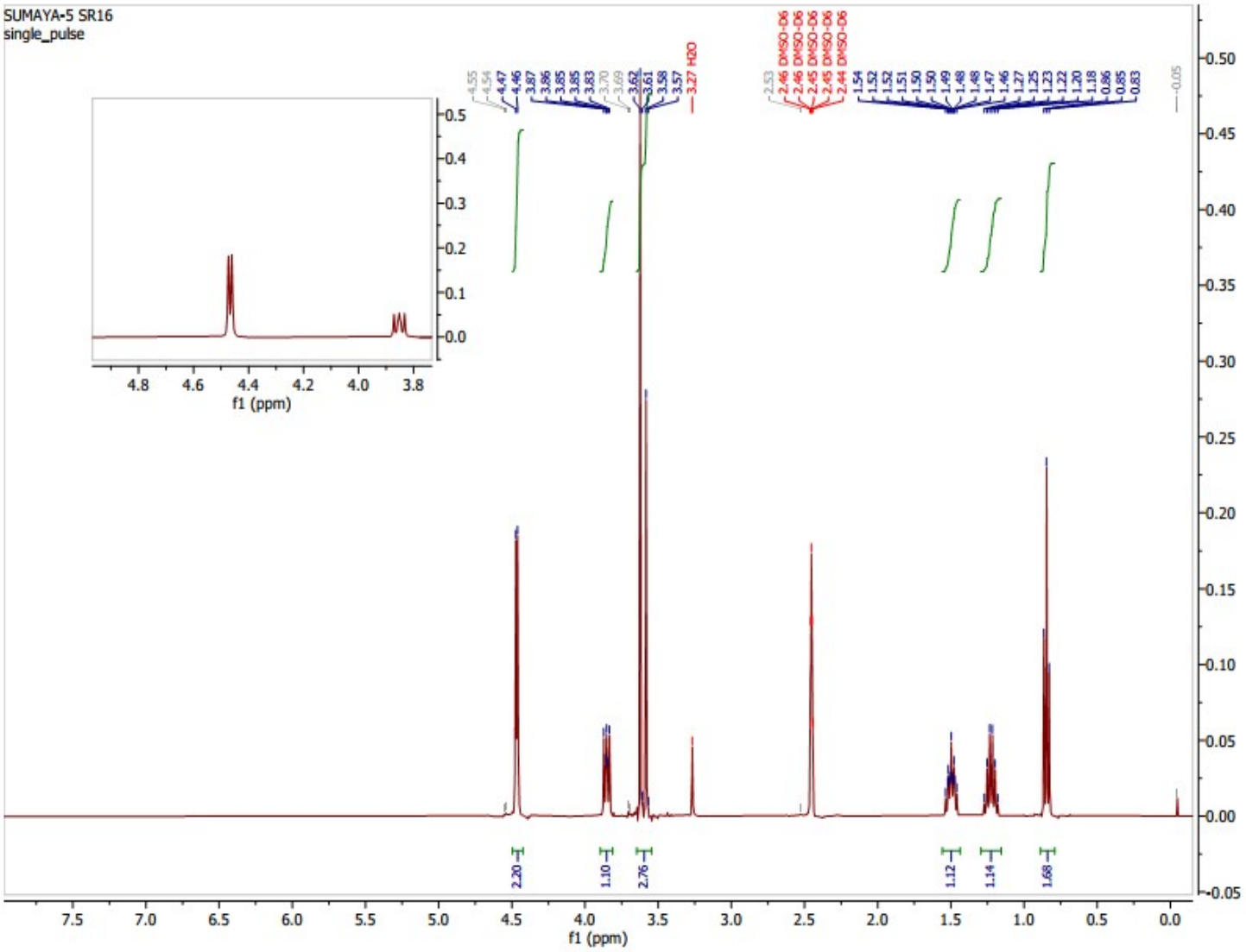
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	20.98 dB
PL13	20.00 dB
SFO2	300.1312005 MHz

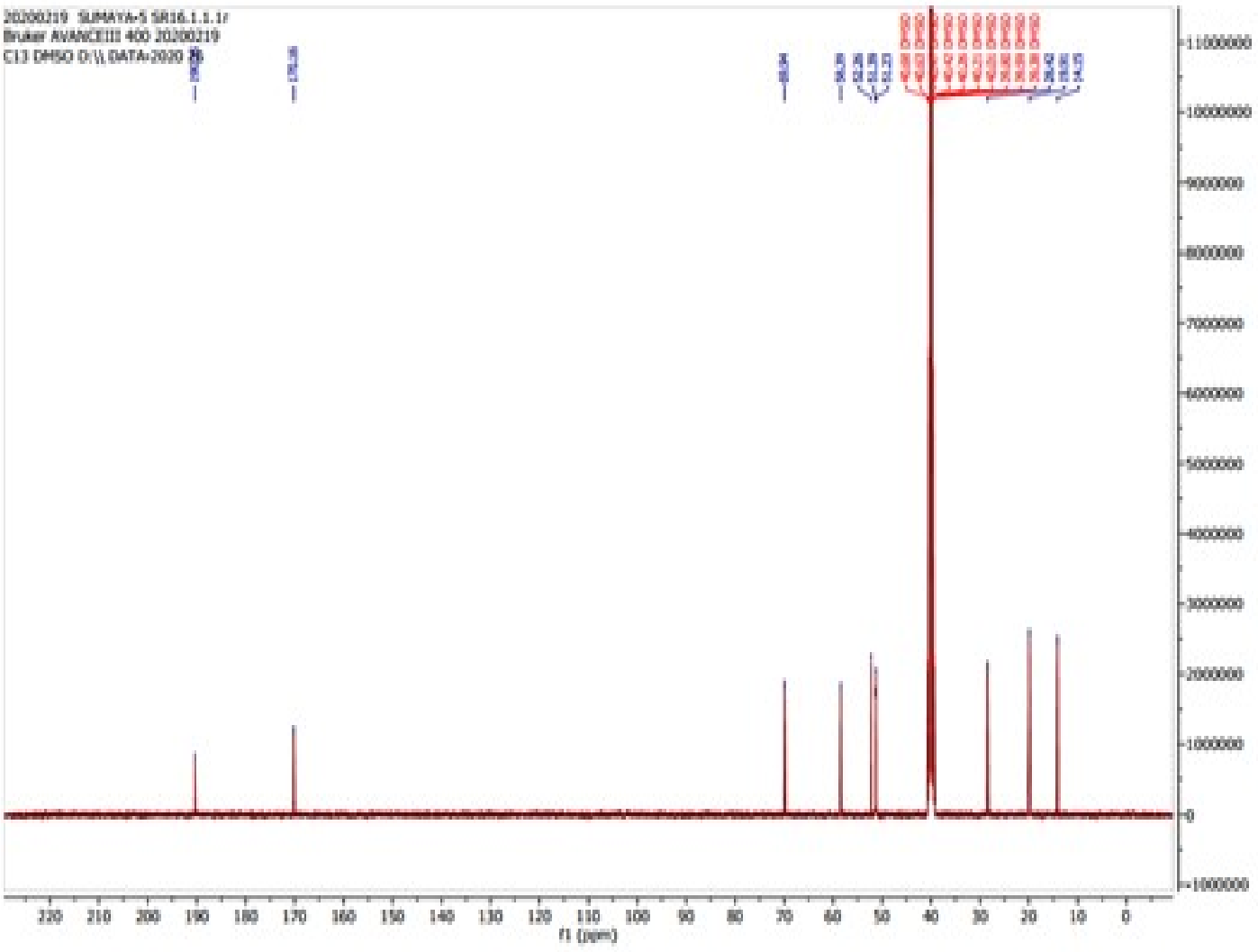
F2 - Processing parameters

SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Synthesis of methyl 2-(5-butyl-6-thioxo-1,3,5-thiadiazinan-3-yl)butanoate: An ester analogue (7)






20200219 SUMAYA-5 SR16.1.1.1r
Bruker AVANCEIII 400 20200219
C13 DMSO D:\\ DATA-2020
f1 (ppm)