

Design and Synthesis of 1,3-Diarylpyrazoles and Investigation of Their Cytotoxicity and Antiparasitic Profile

Murat Bozdag ¹, Freke Mertens ², An Matheeussen ³, Natascha Van Pelt ³, Kenn Foubert ⁴, Nina Hermans ⁴, Guido R. Y. De Meyer ², Koen Augustyns ¹, Wim Martinet ², Guy Caljon ³ and Pieter Van der Veken ^{1,*}

1 Laboratory of Medicinal Chemistry, Department of Pharmaceutical Sciences, Infla-Med Centre of Excellence, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk-Antwerp, Belgium; koen.augustyns@uantwerpen.be (K.A.)

2 Laboratory of Physiopharmacology, Department of Pharmaceutical Sciences, Infla-Med Centre of Excellence, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk-Antwerp, Belgium; freke.mertens@uantwerpen.be (F.M.); guido.demeyer@uantwerpen.be (G.R.Y.D.M.); wim.martinet@uantwerpen.be (W.M.)

3 Laboratory of Microbiology, Parasitology and Hygiene, Department of Biomedical Sciences, Infla-Med Centre of Excellence, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk-Antwerp, Belgium; an.matheeussen@uantwerpen.be (A.M.); natascha.vanpelt@uantwerpen.be (N.V.P.); guy.caljon@uantwerpen.be (G.C.)

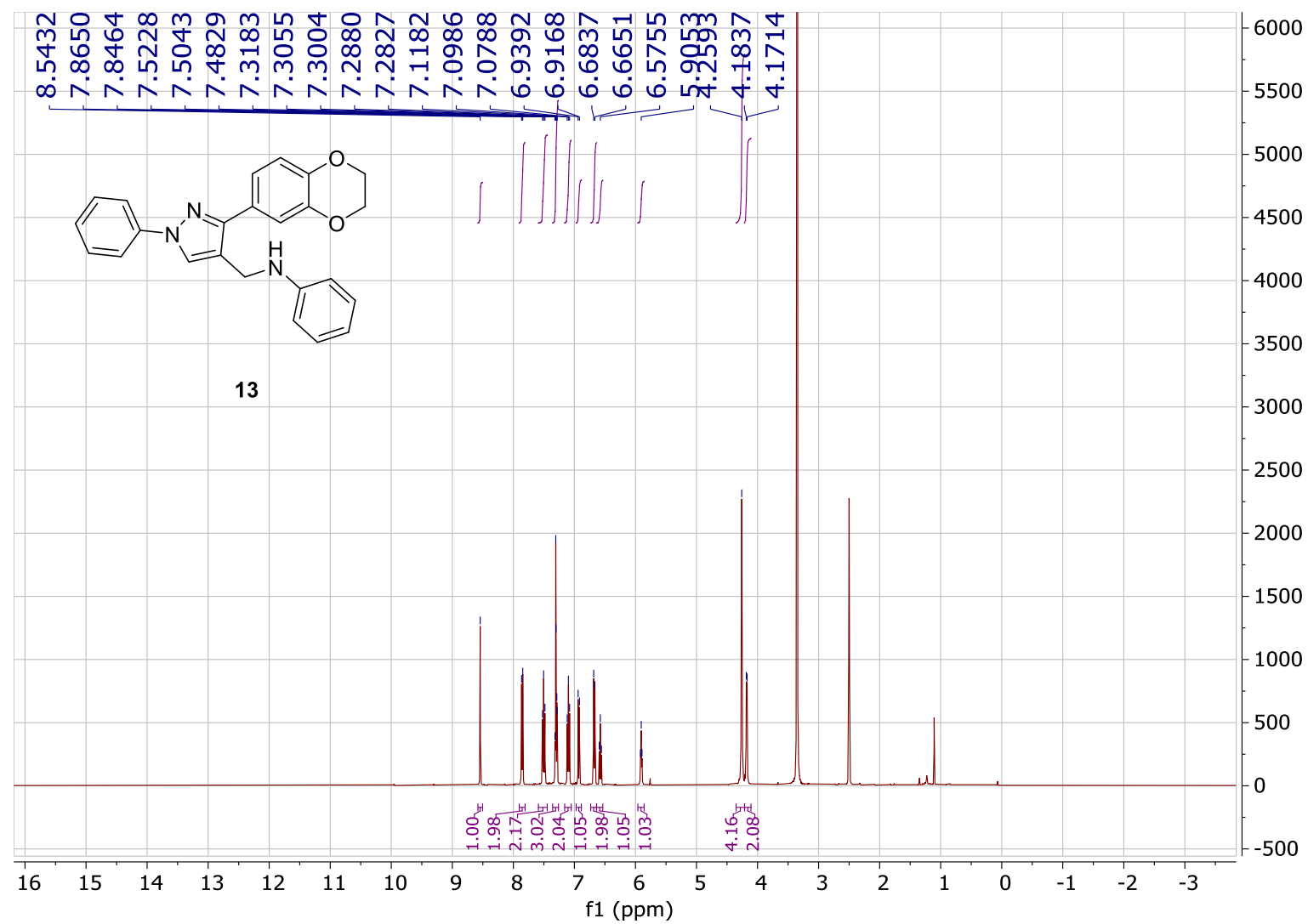
4 Natural Products and Food Research and Analysis–Pharmaceutical Technology, Department of Pharmaceutical Sciences, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk-Antwerp, Belgium; kenn.foubert@uantwerpen.be (K.F.); nina.hermans@uantwerpen.be (N.H.)

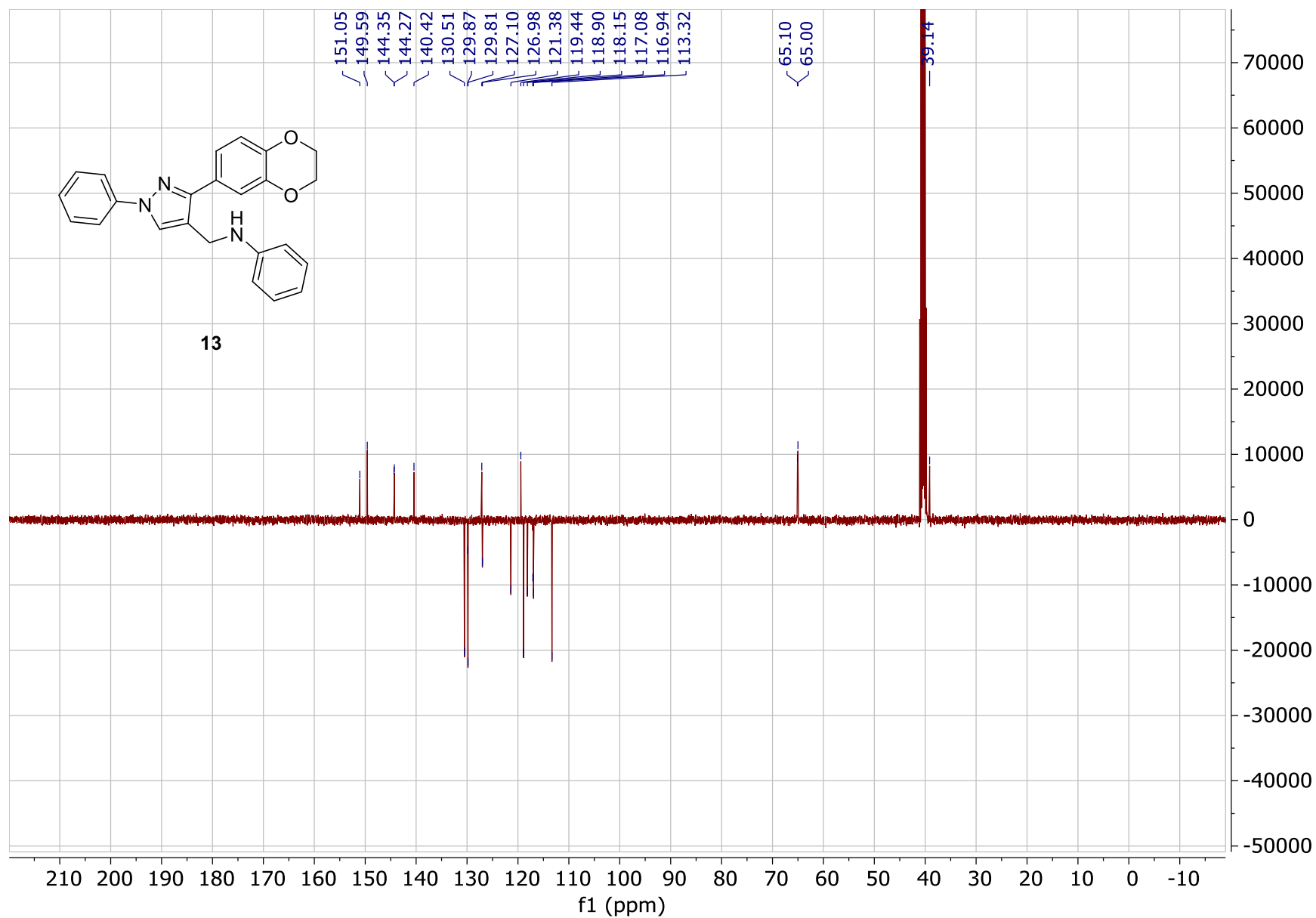
* Correspondence: pieter.vanderveken@uantwerpen.be

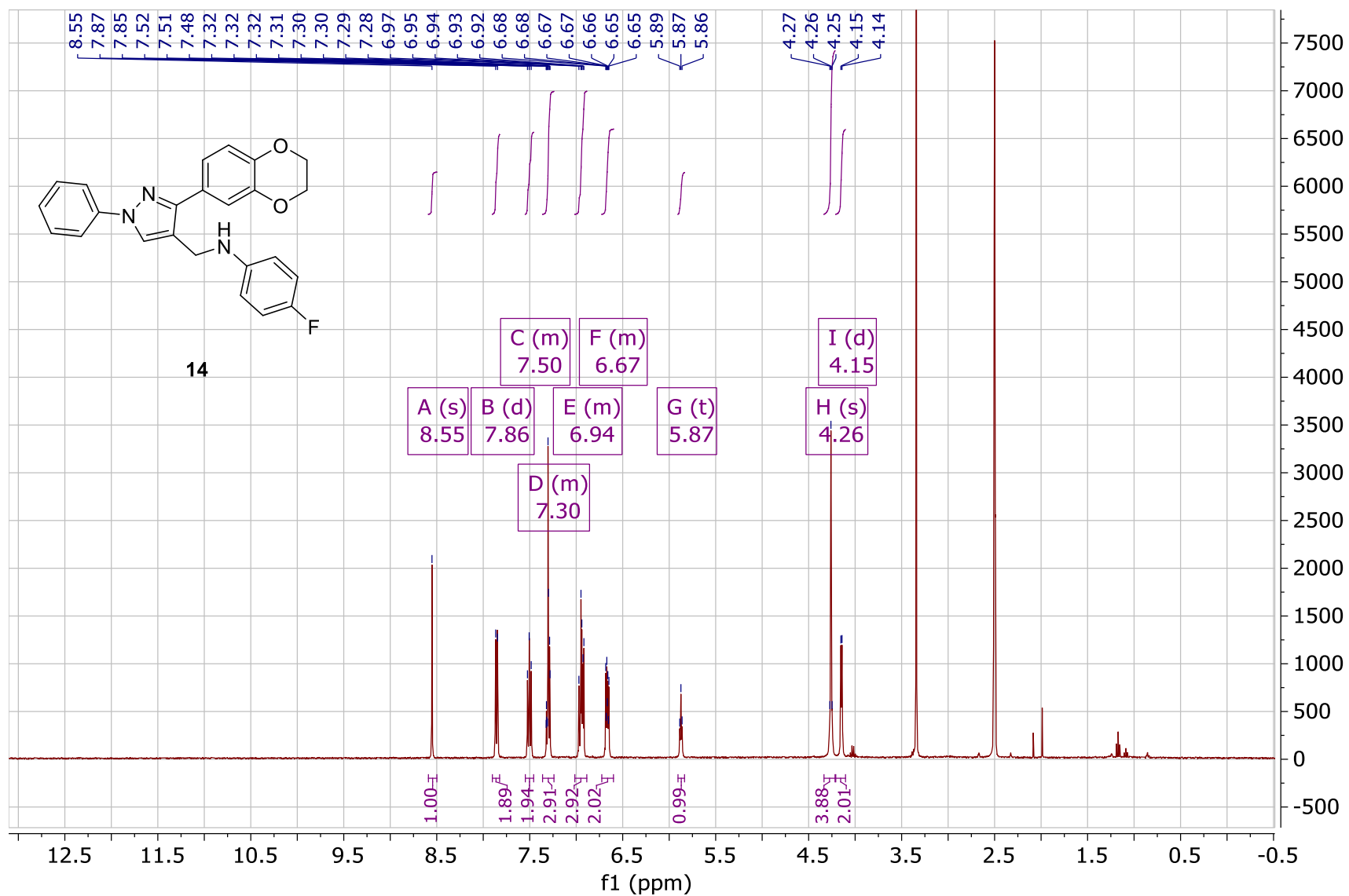
Table of Contents:

1) ¹ H and ¹³ C-NMR spectra of compounds 13–69.....	2–115
2) UPLC and HRMS spectra of the studied samples.....	116–147

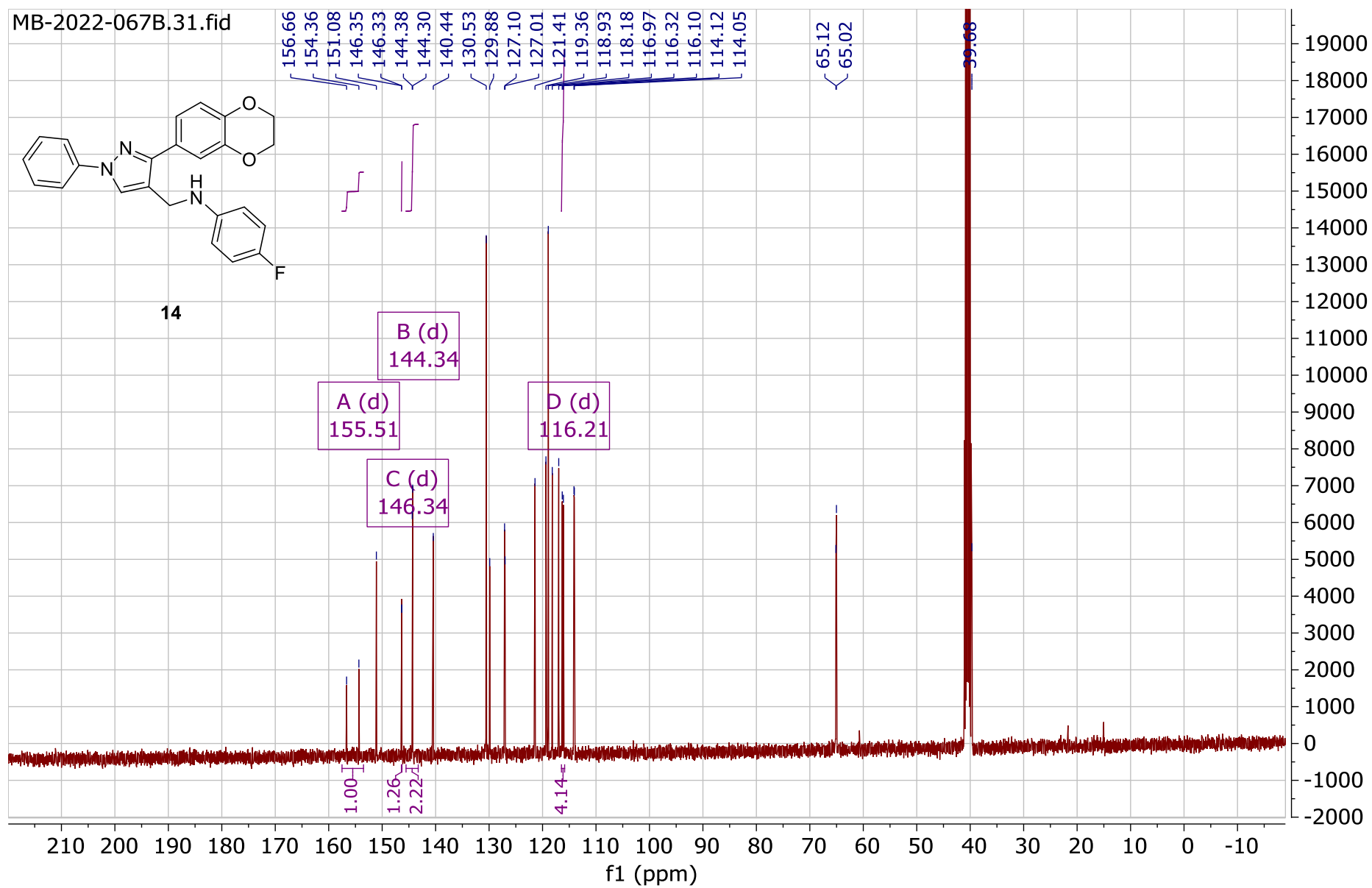
1. ^1H and ^{13}C -NMR spectra of compounds 13–69

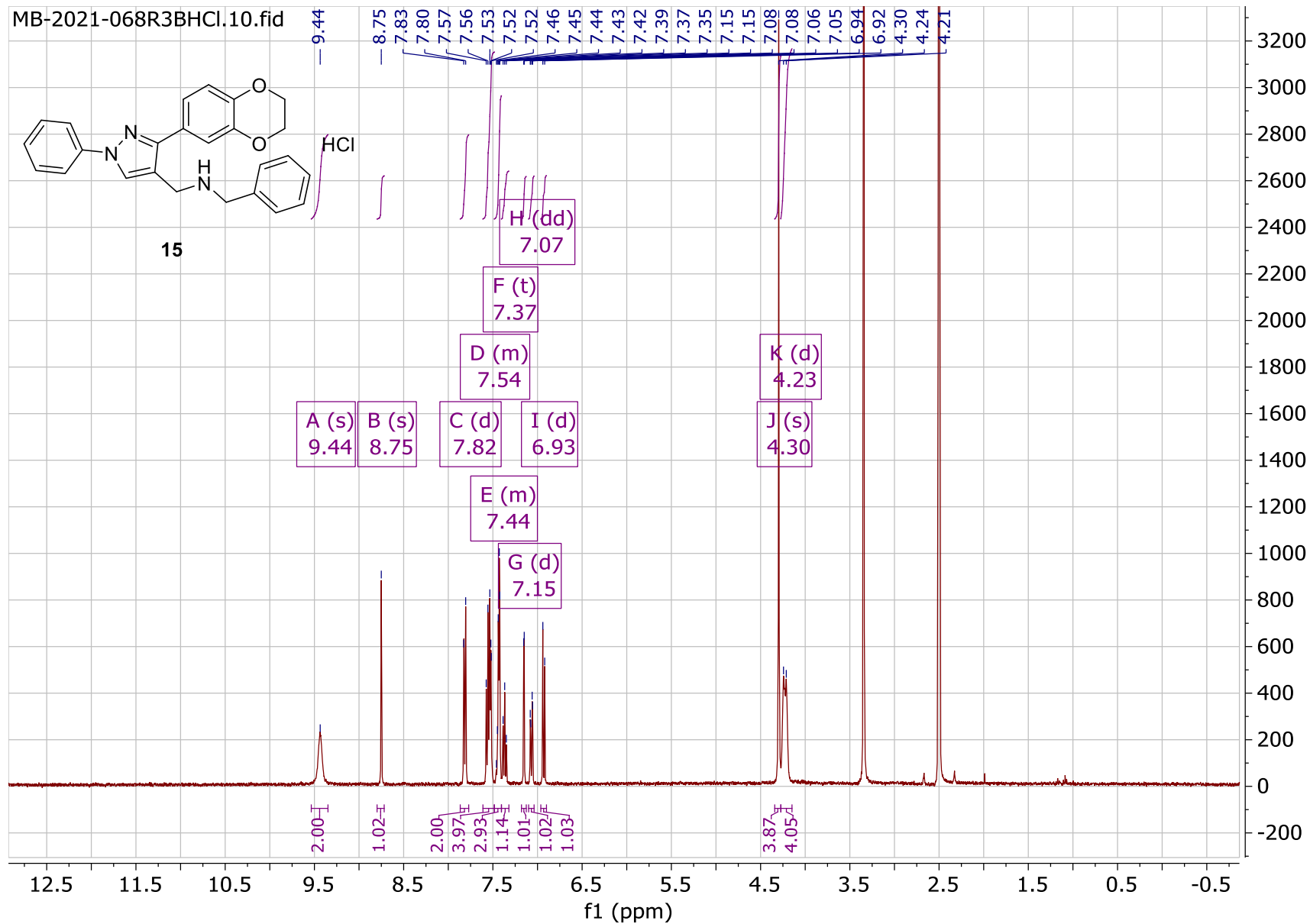


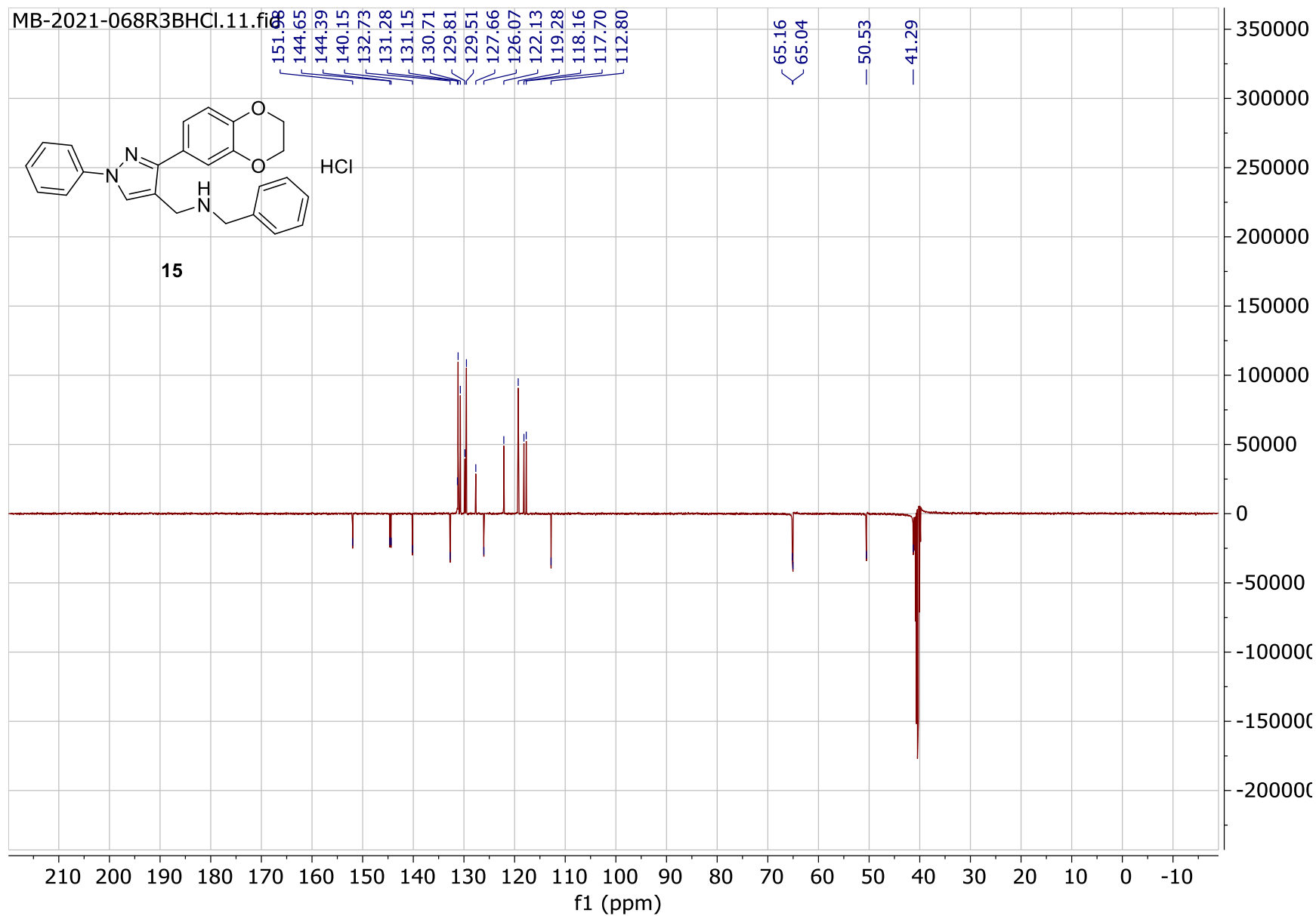


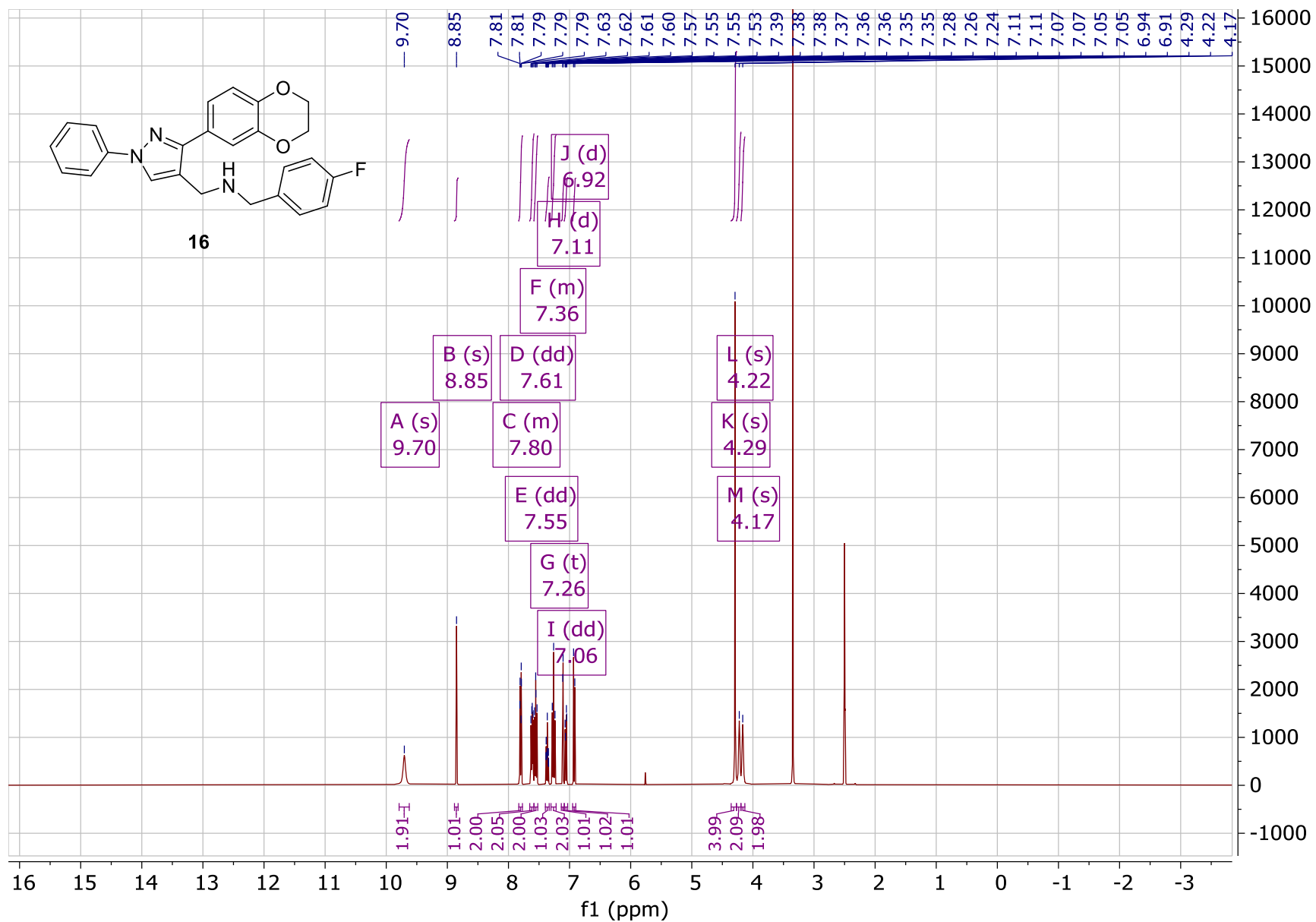


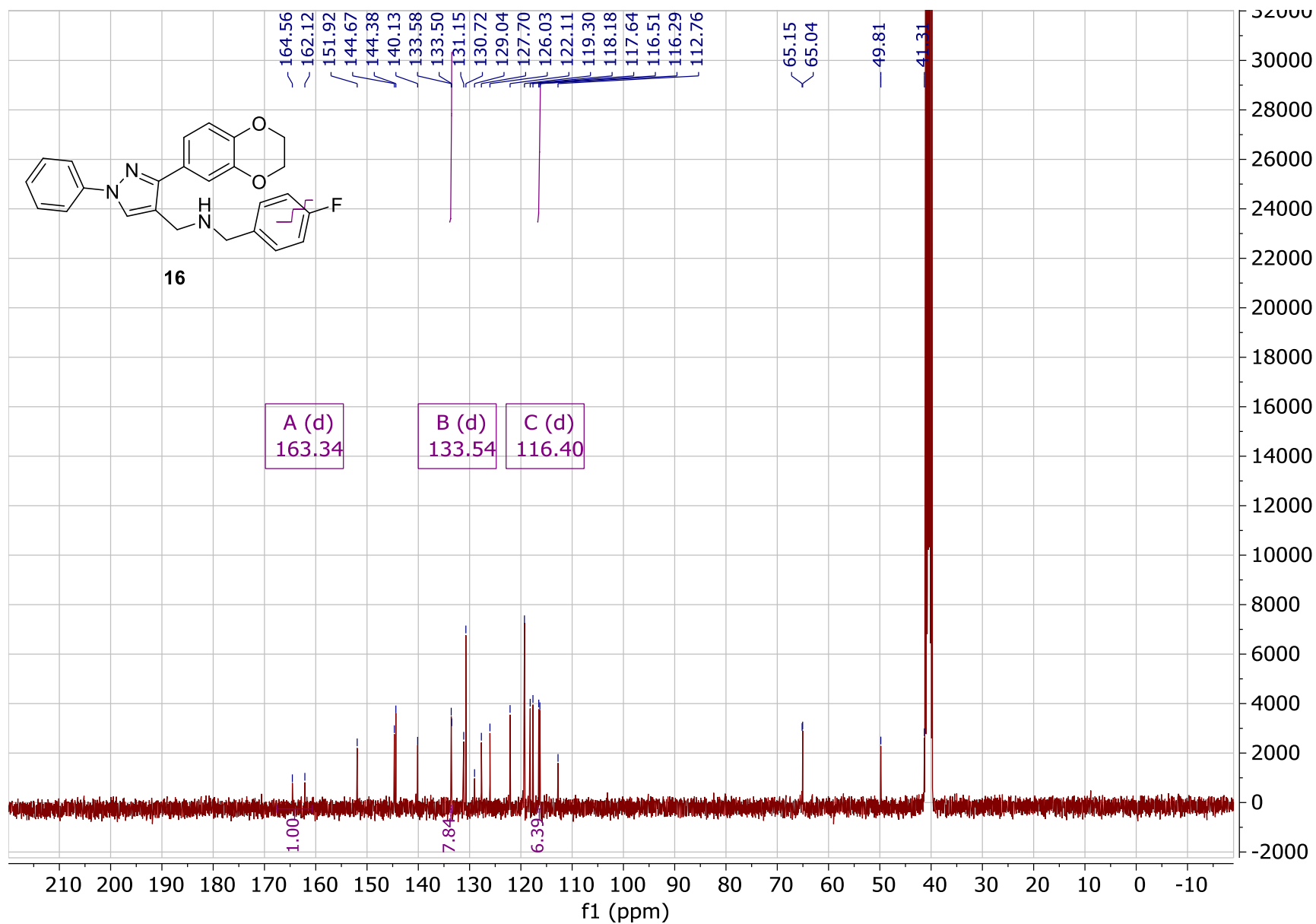
MB-2022-067B.31.fid

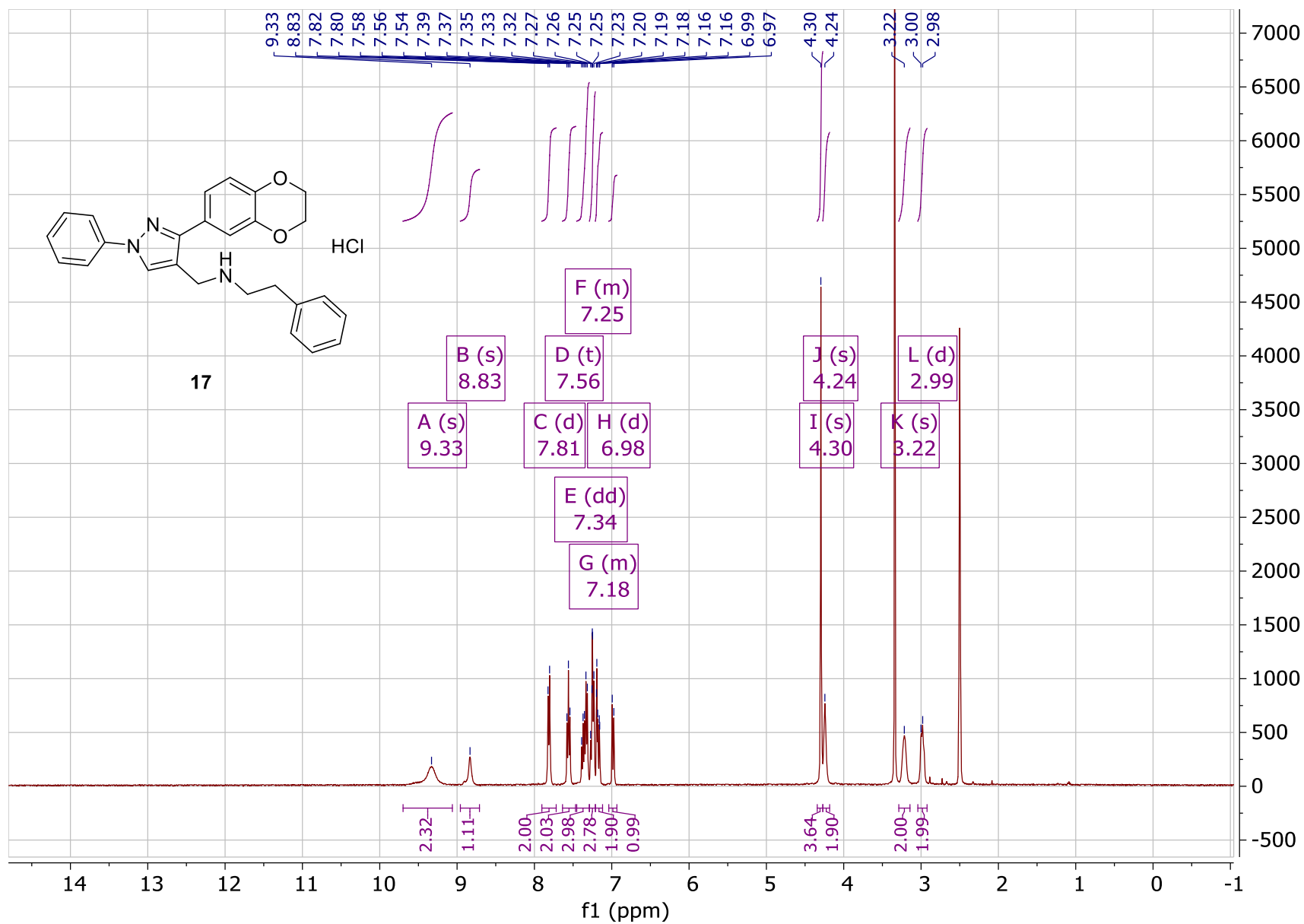


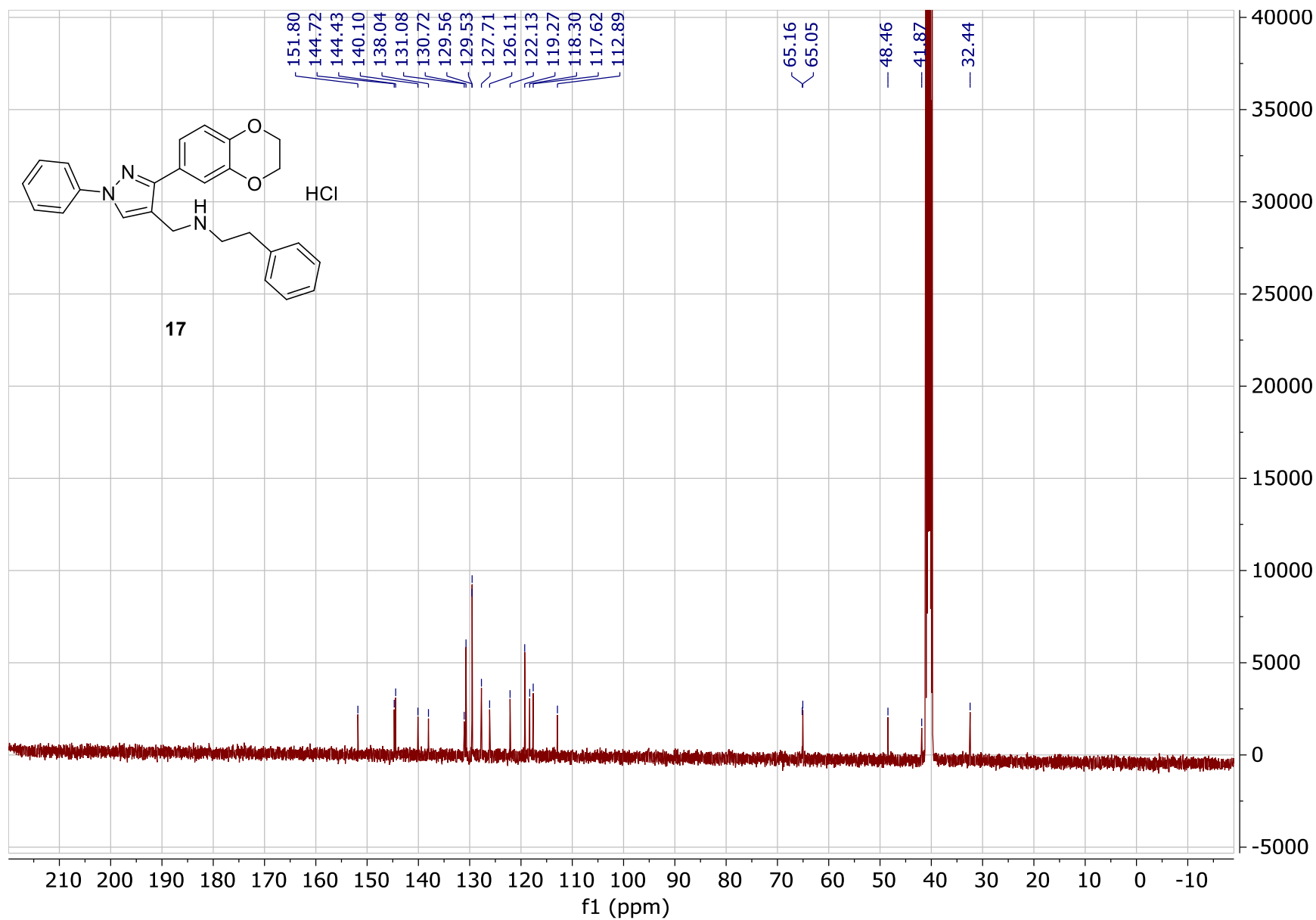


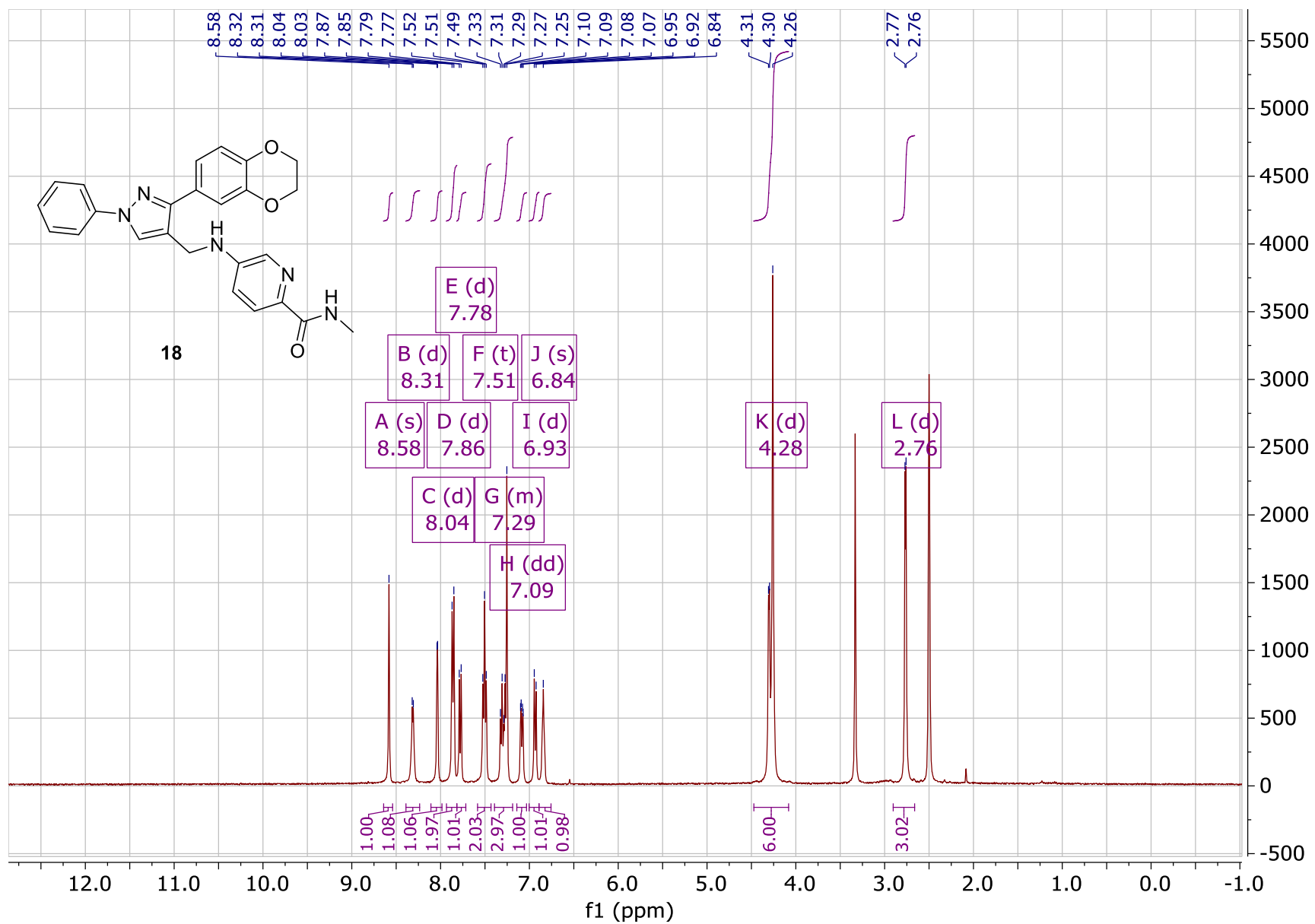




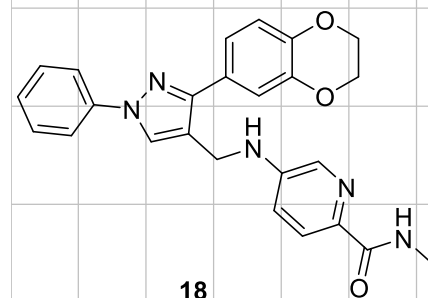








MB-2022-013B.11.fid

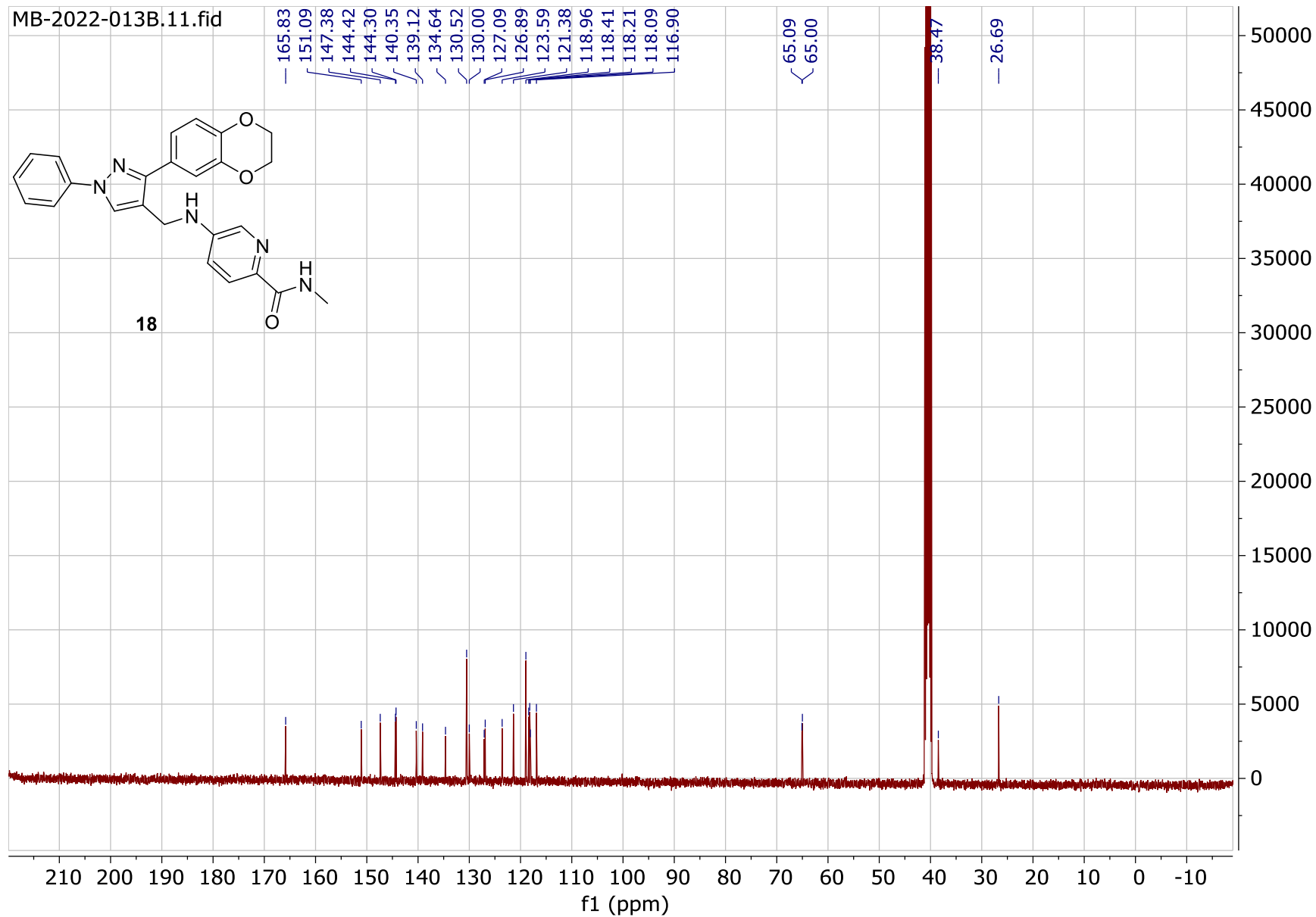


165.83
151.09
147.38
144.42
144.30
140.35
139.12
134.64
130.52
130.00
127.09
126.89
123.59
121.38
118.96
118.41
118.21
118.09
116.90

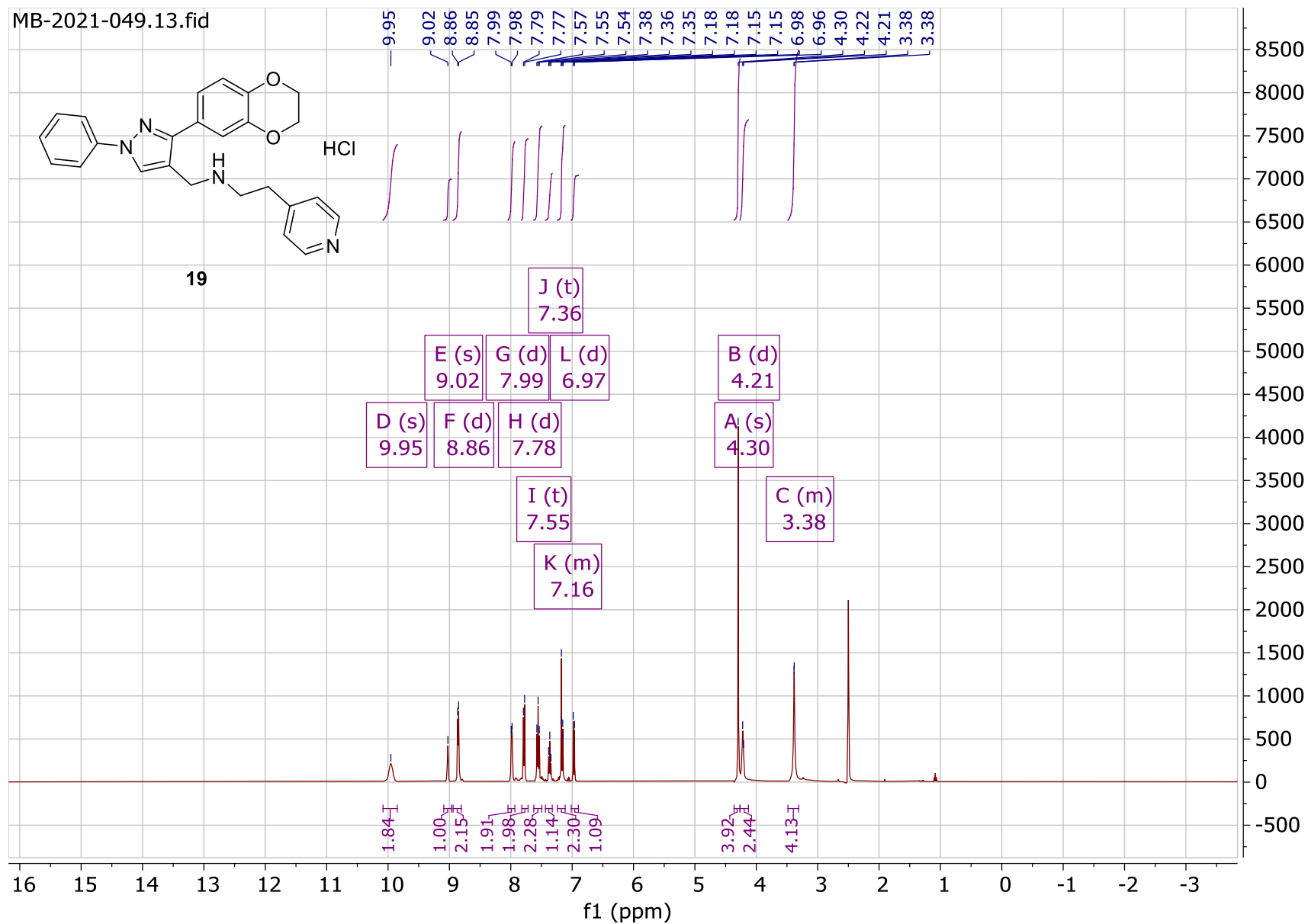
65.09
65.00

38.47

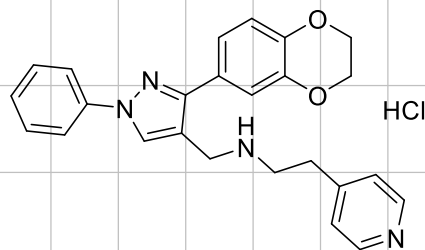
26.69



MB-2021-049.13.fid



MB-2021-049.12.fid



HCl

19

151.79
144.67
144.38
140.10
131.62
130.69
128.09
127.65
126.08
122.19
119.23
118.25
117.66
112.83

65.13
65.03

46.40
41.99

32.15

35000

30000

25000

20000

15000

10000

5000

0

-5000

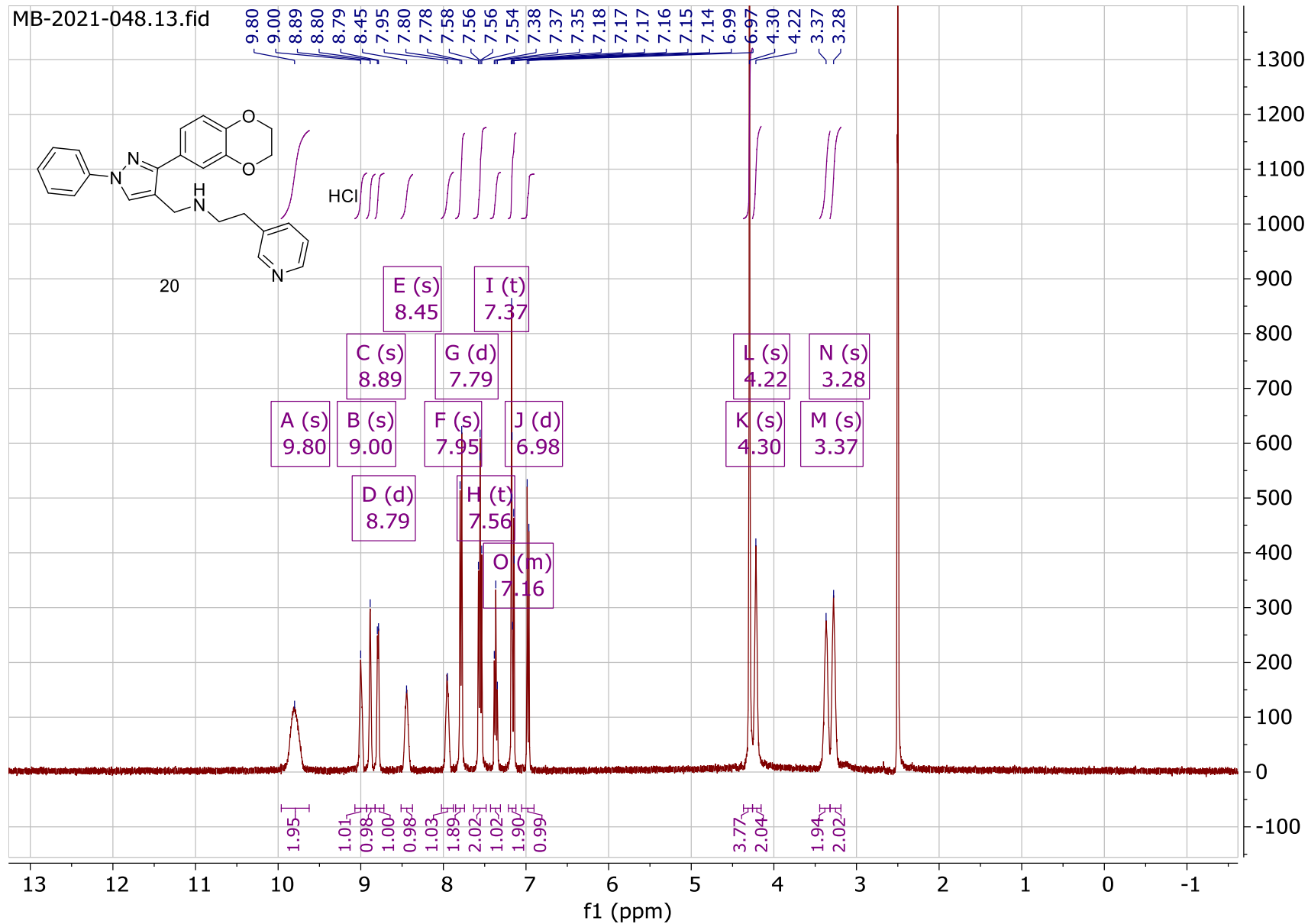
-10000

-15000

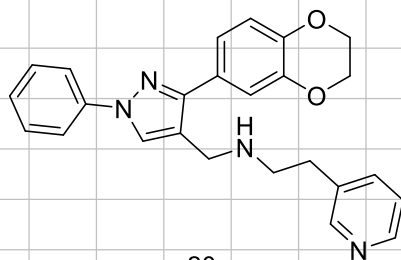
-20000

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)



MB-2021-048.12.fid



HCl

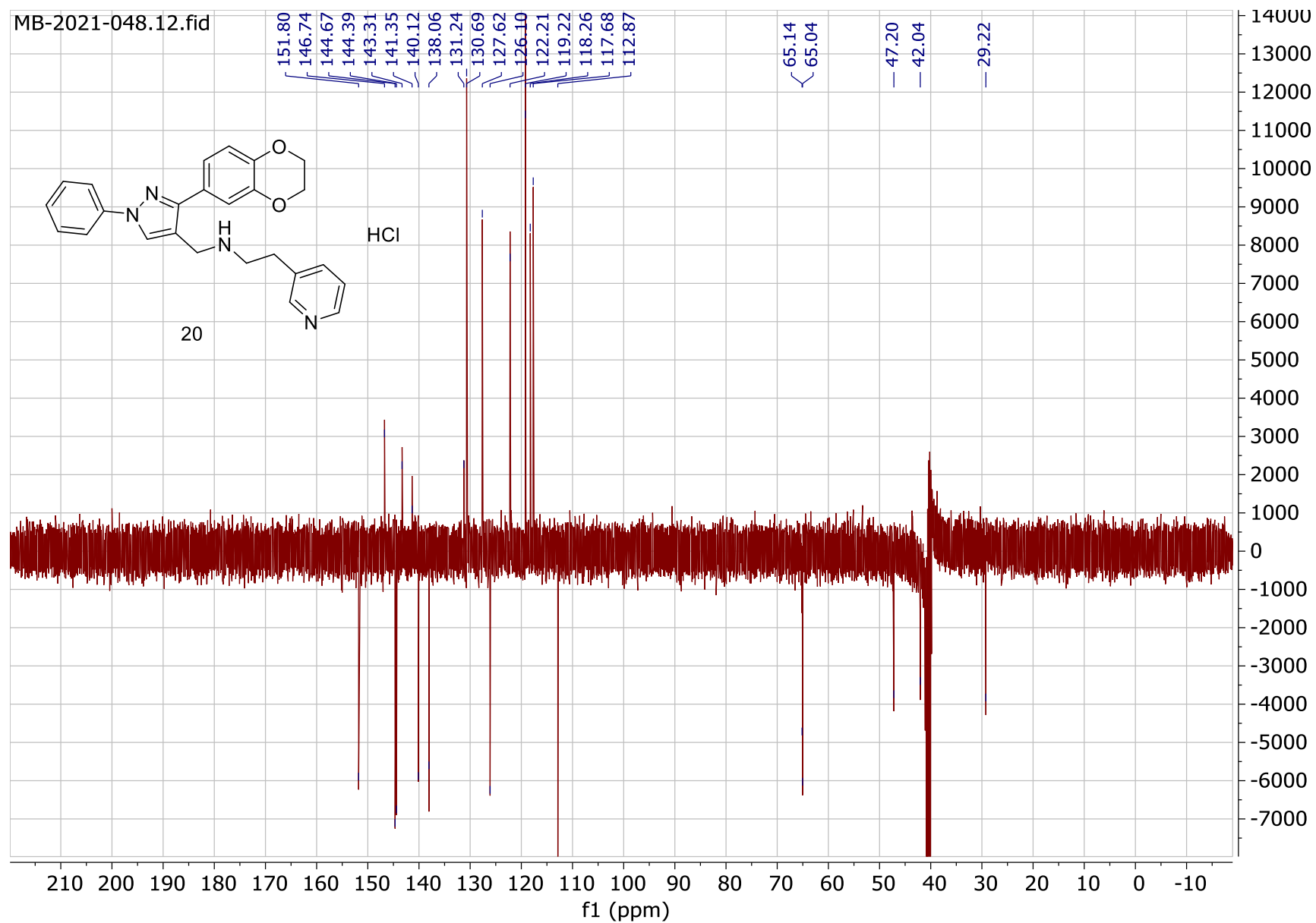
20

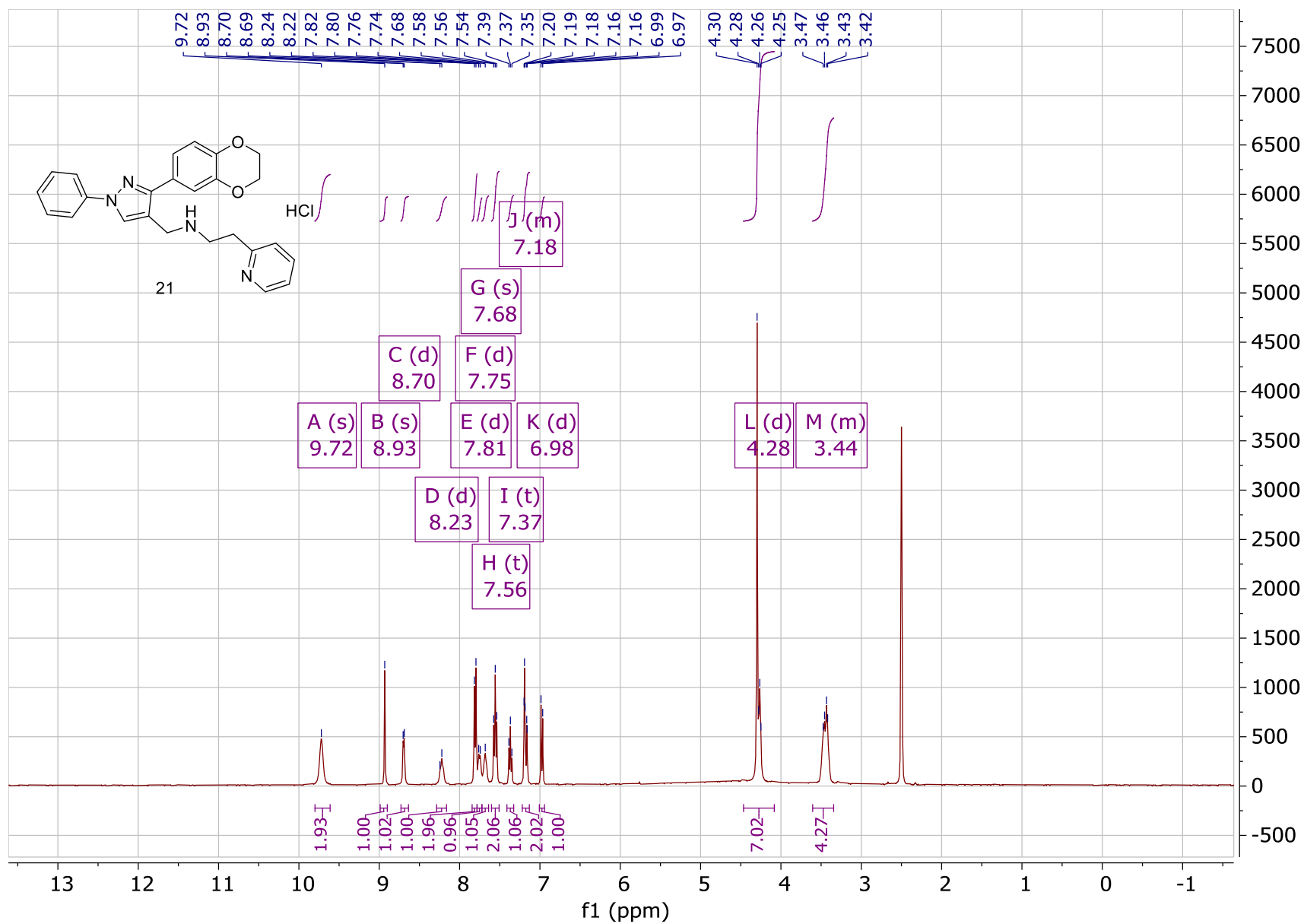
151.80
146.74
144.67
144.39
143.31
141.35
140.12
138.06
131.24
130.69
127.62
126.10
122.21
119.22
118.26
117.68
112.87

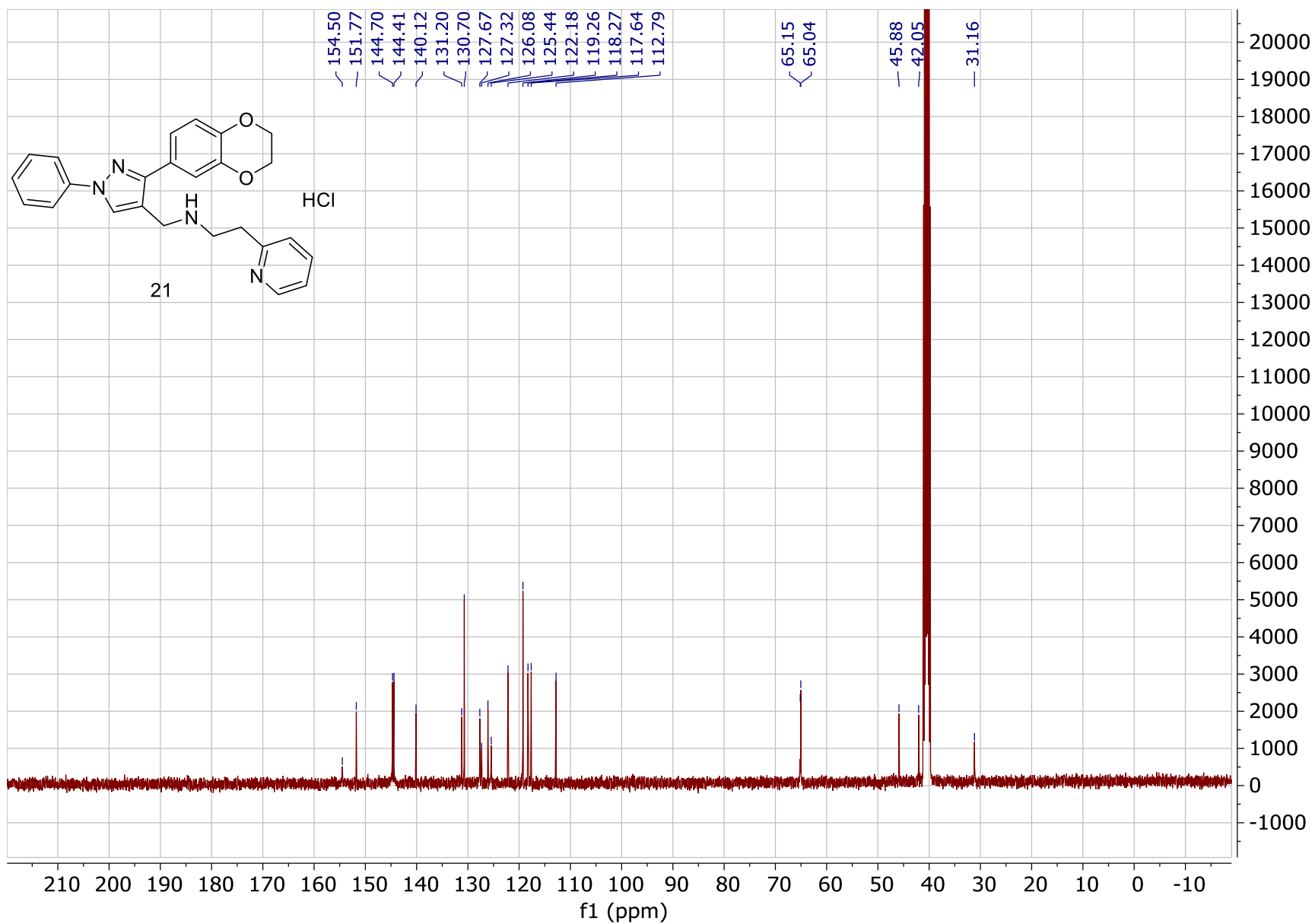
65.14
65.04

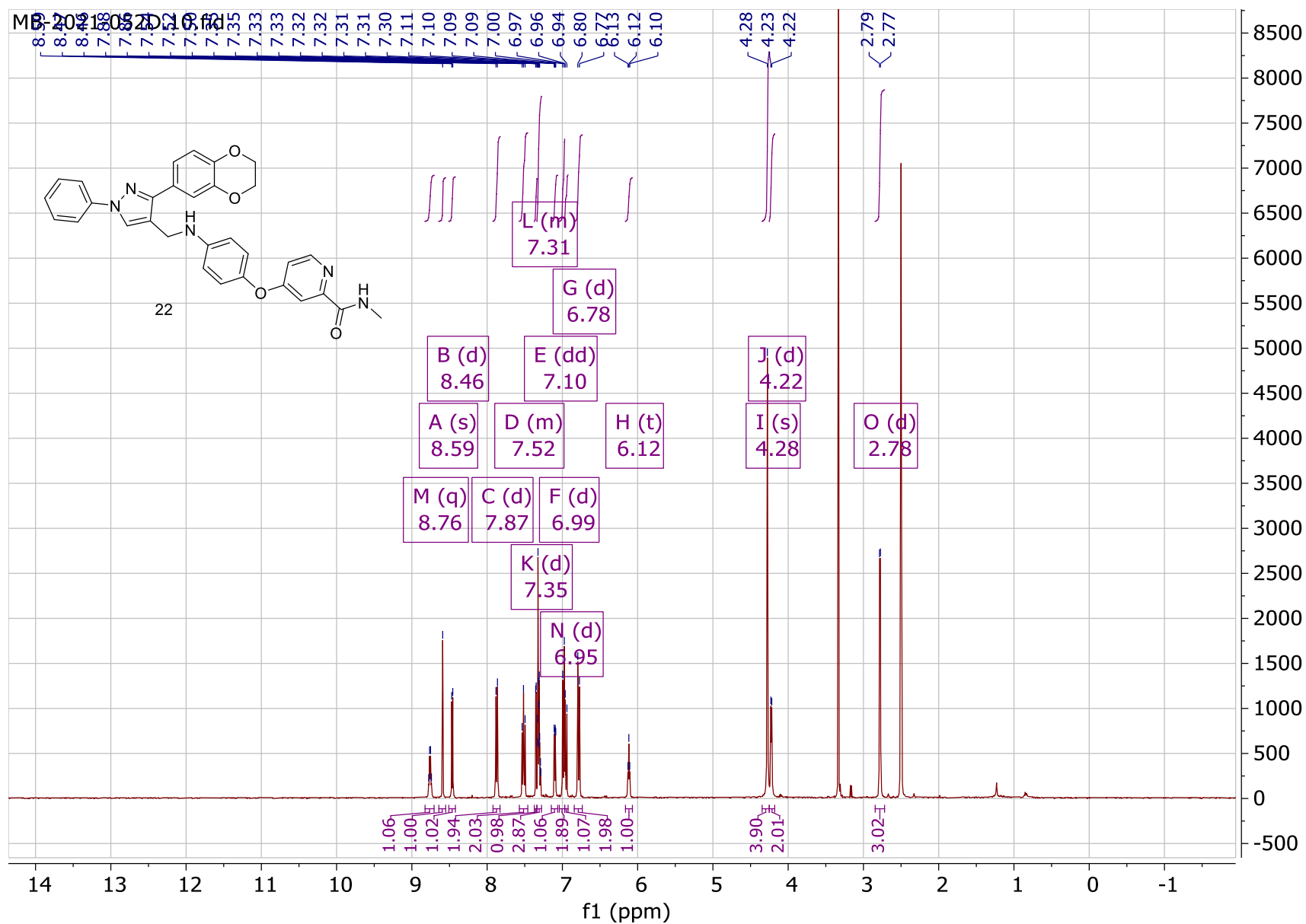
47.20
42.04

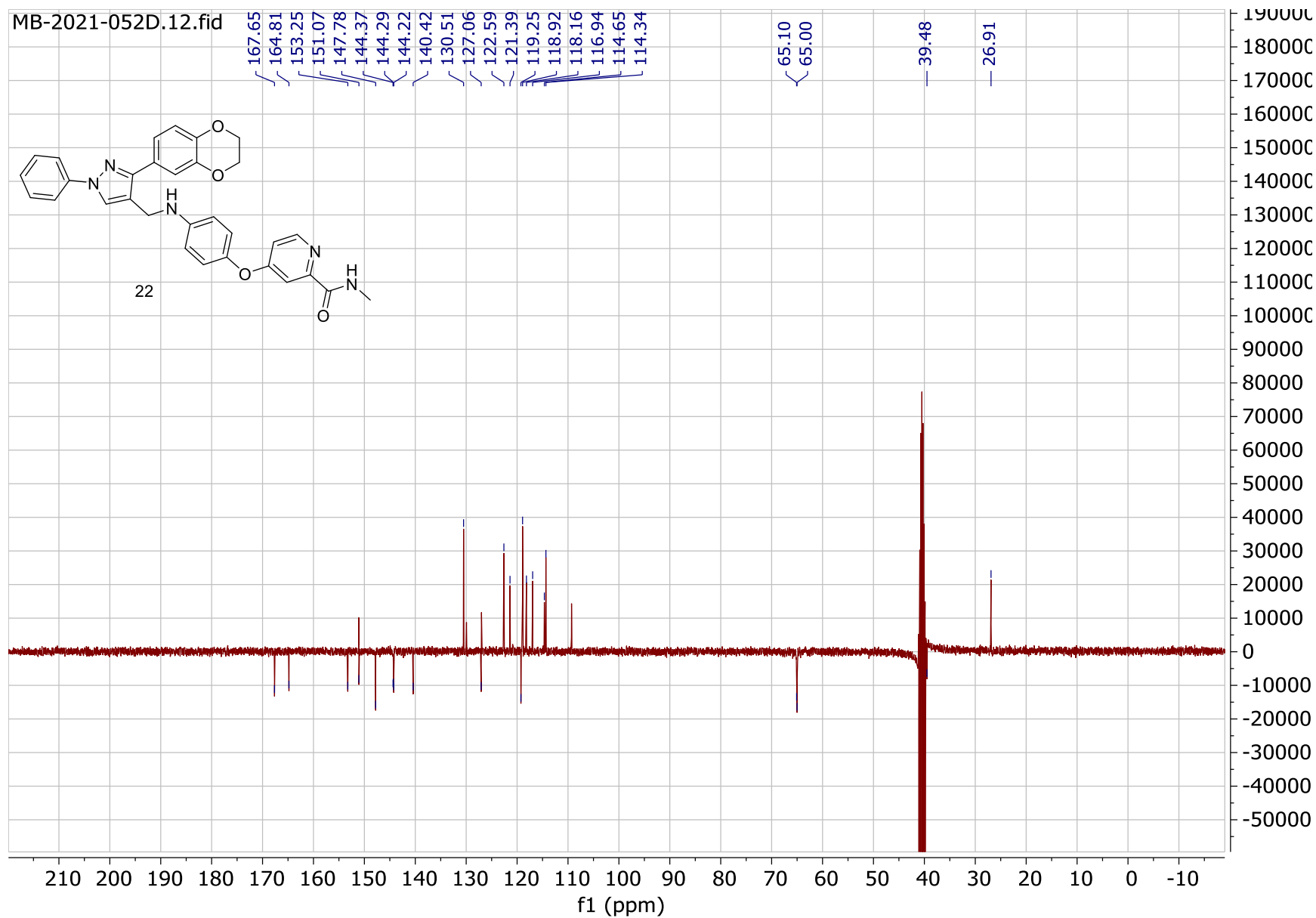
29.22

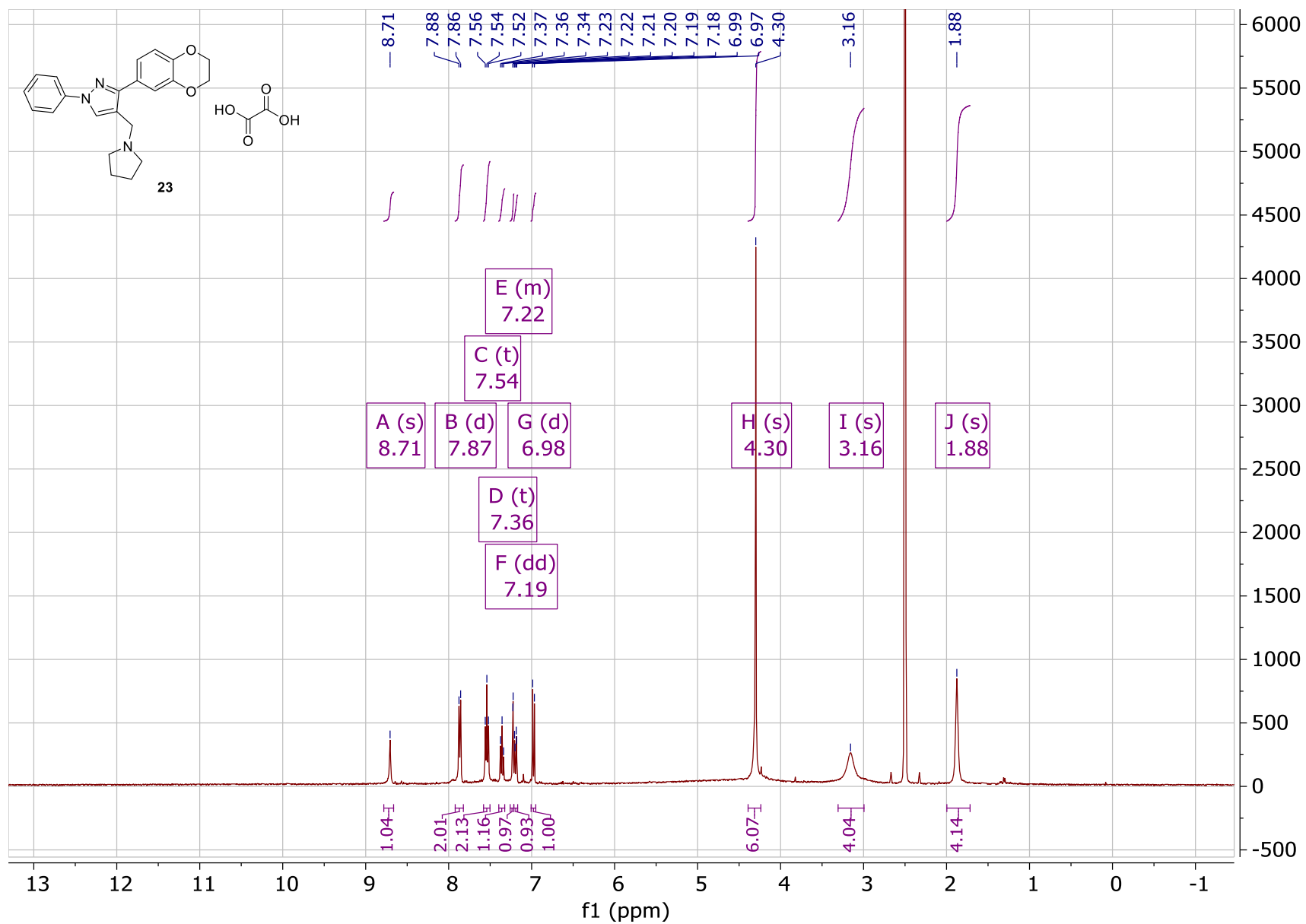


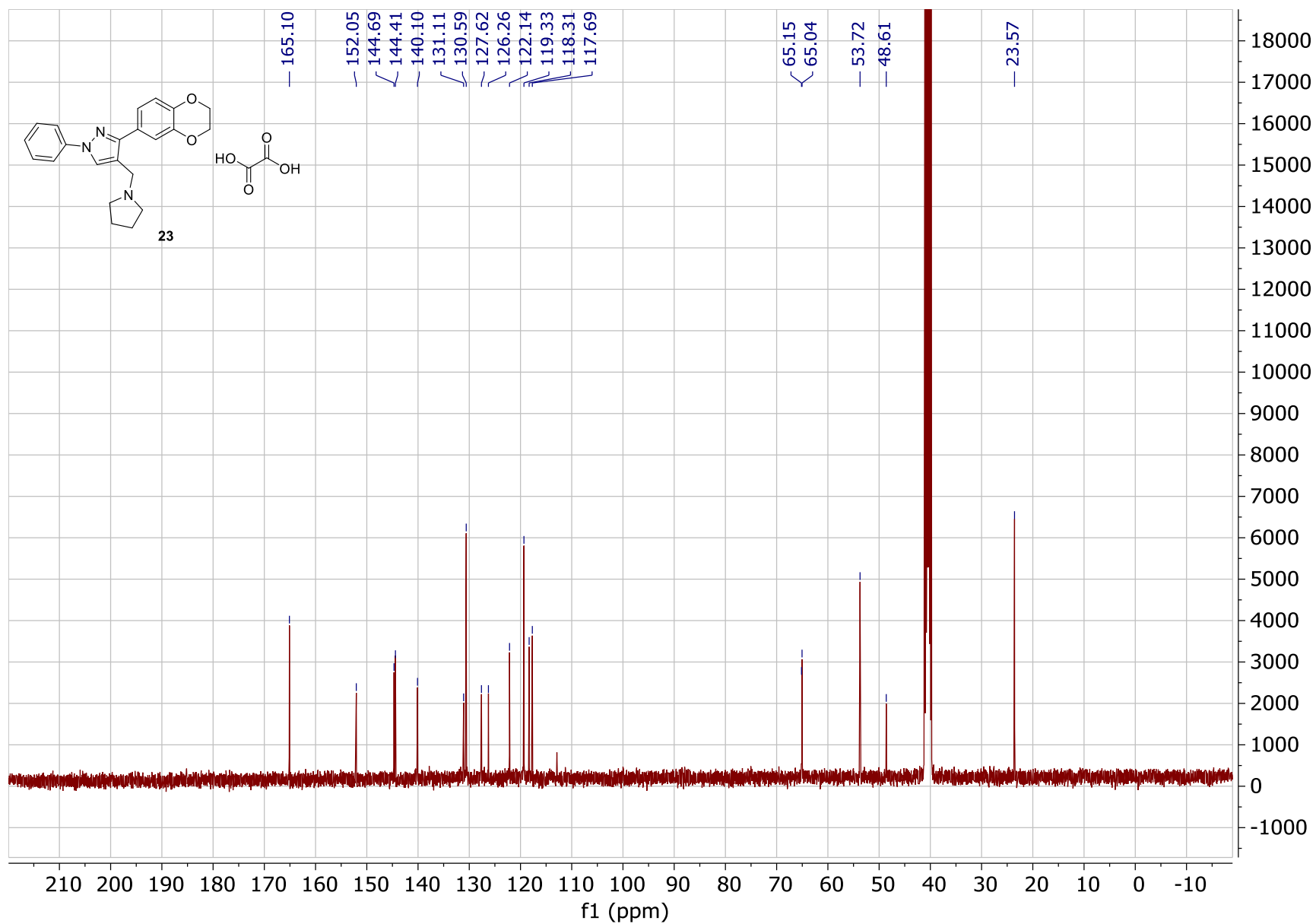




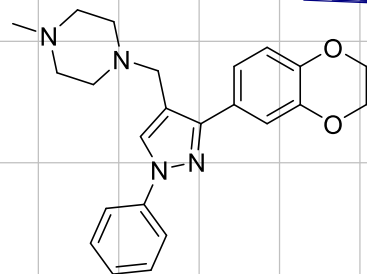




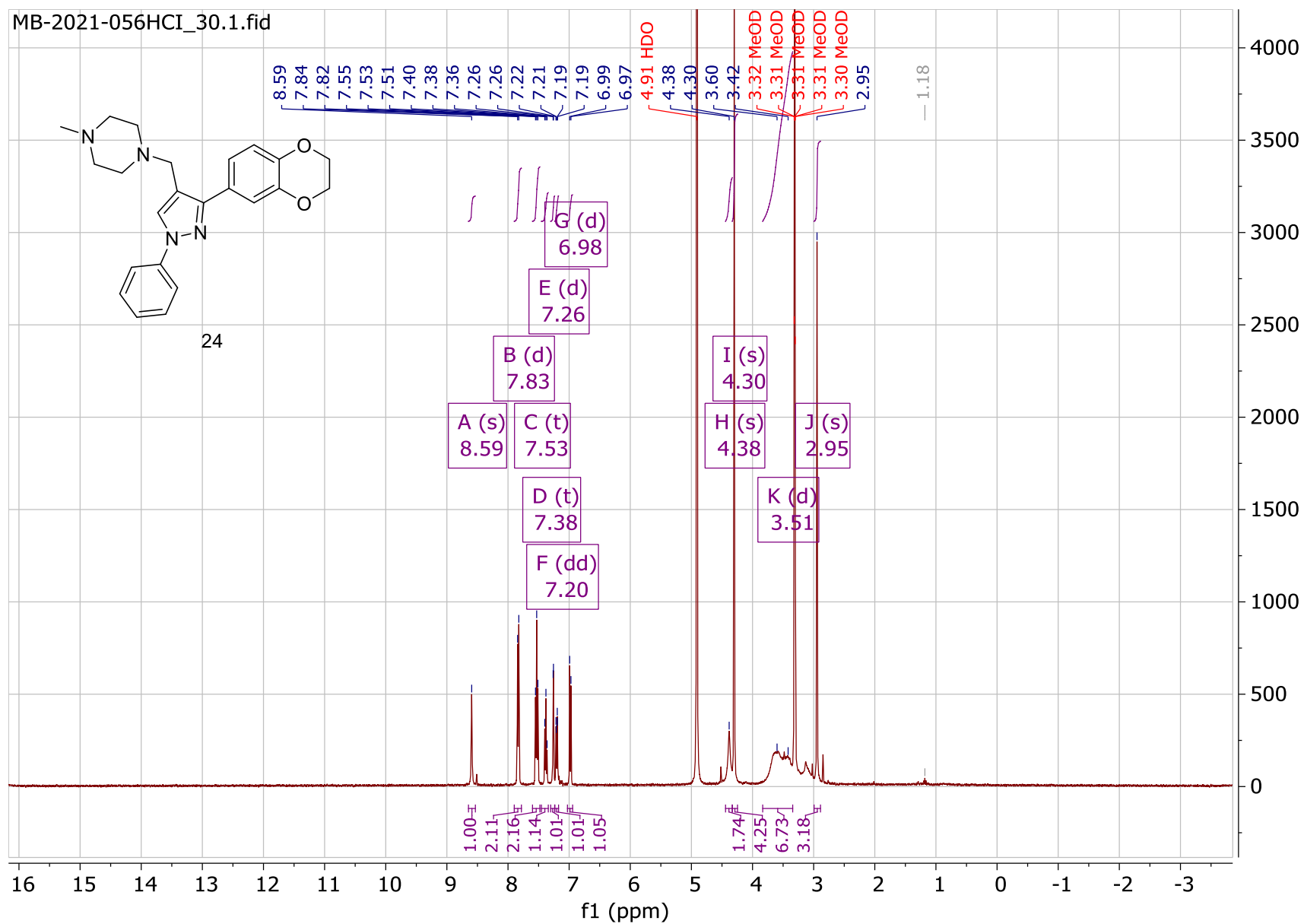




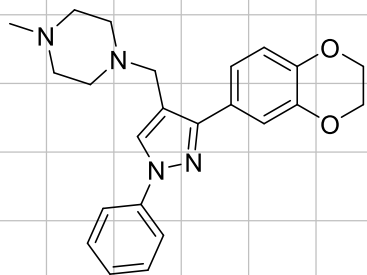
MB-2021-056HCl_30.1.fid



24



MB-2021-056HCl.31.fid

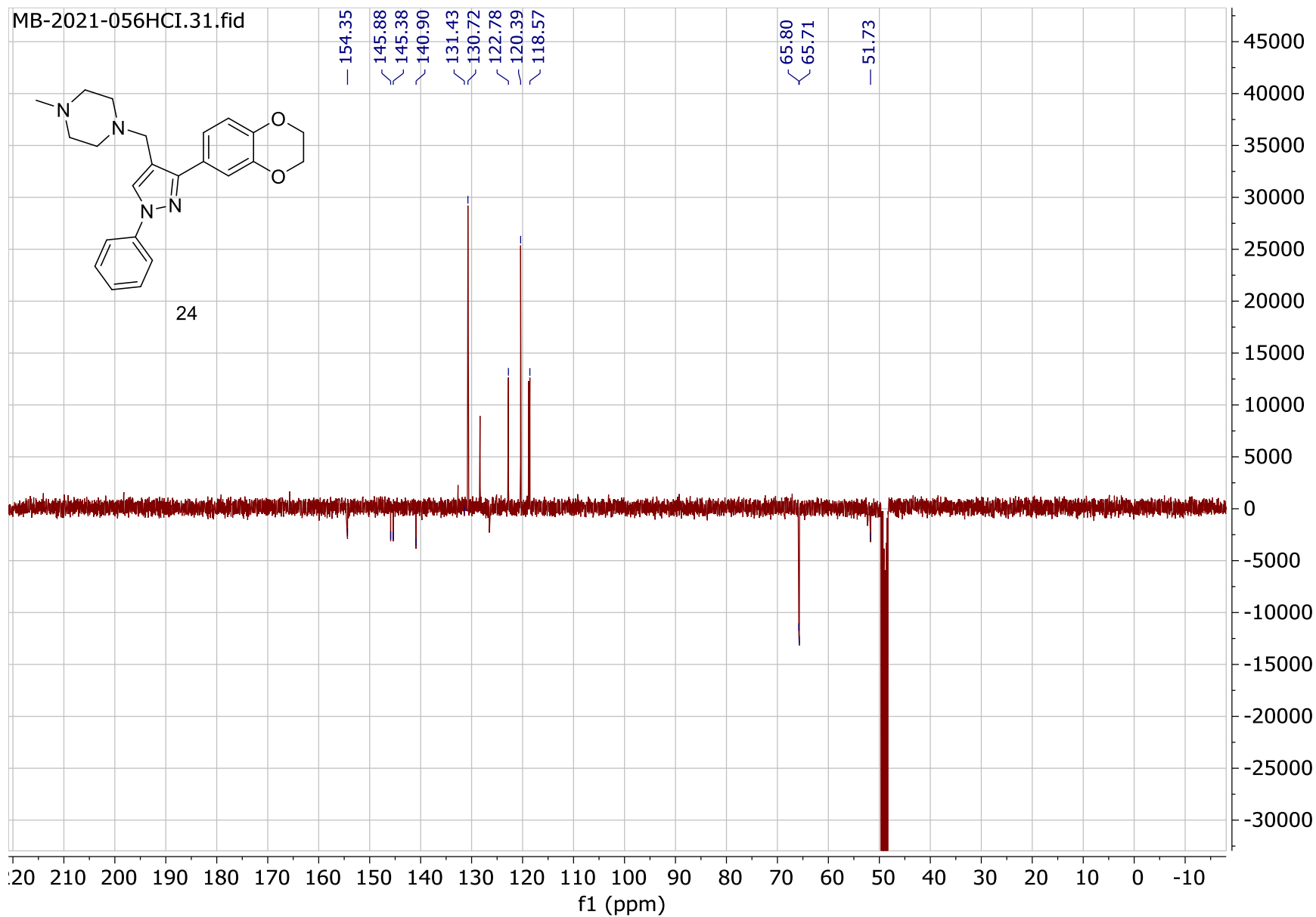


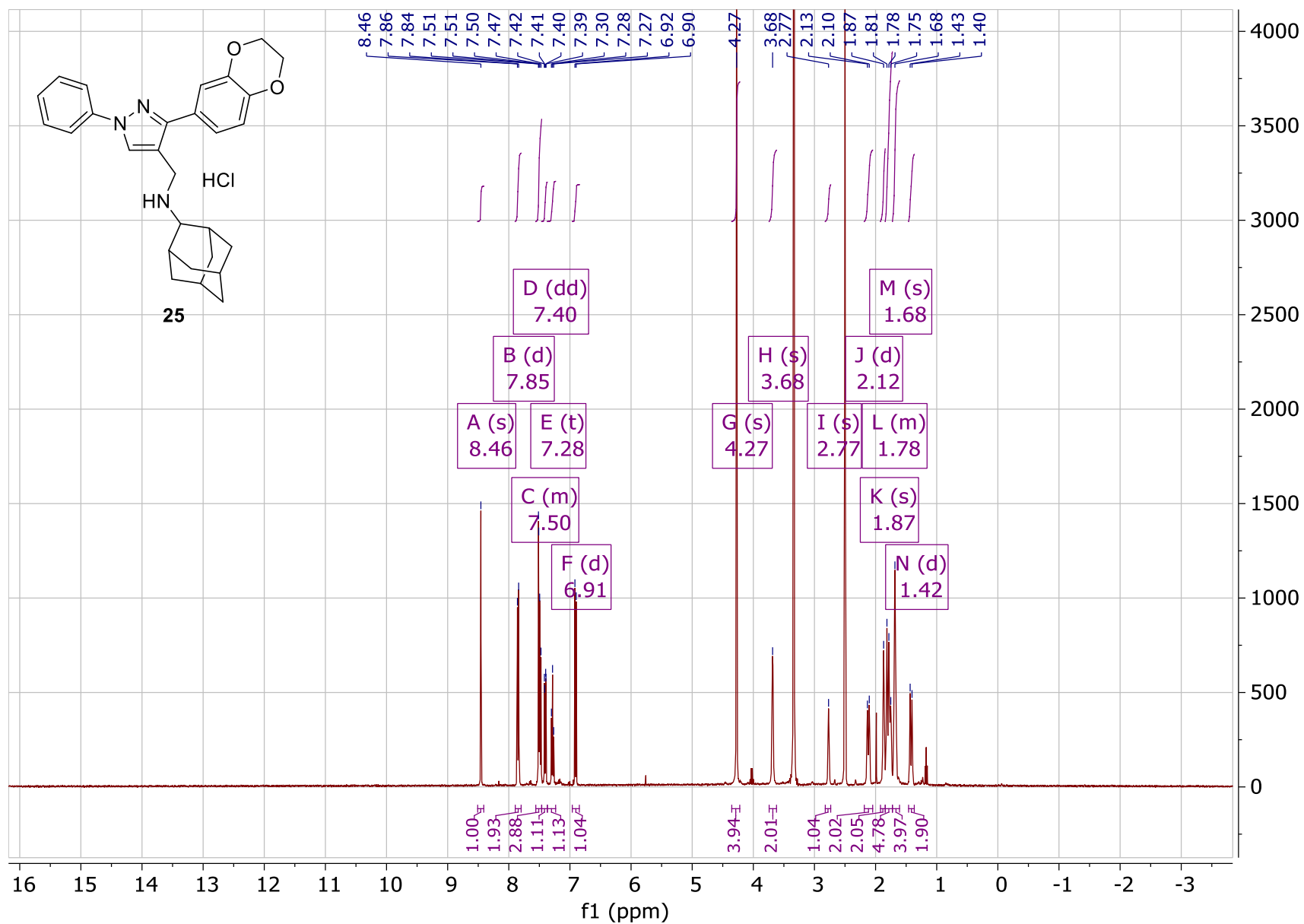
24

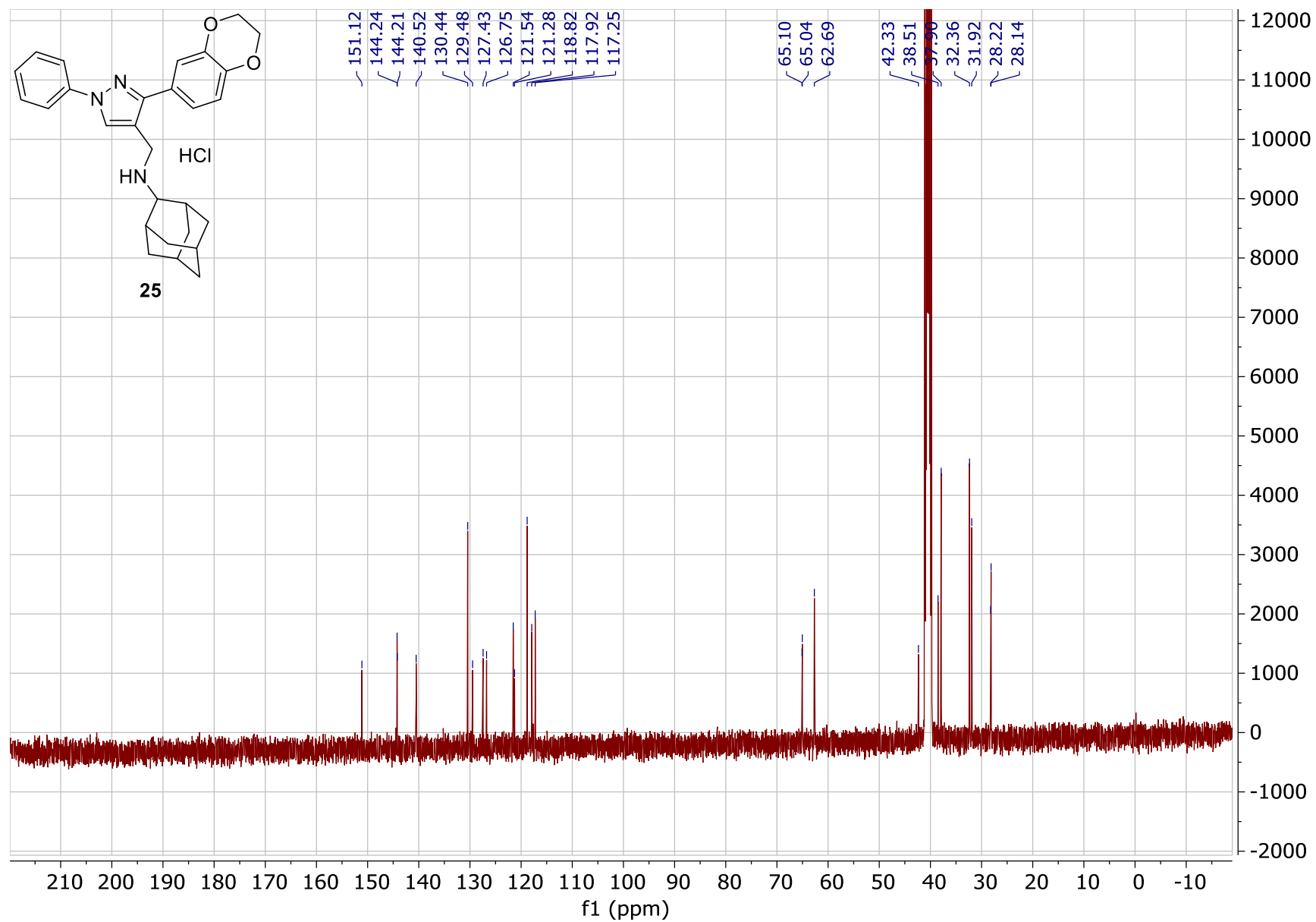
— 154.35
145.88
145.38
140.90
131.43
130.72
122.78
120.39
118.57

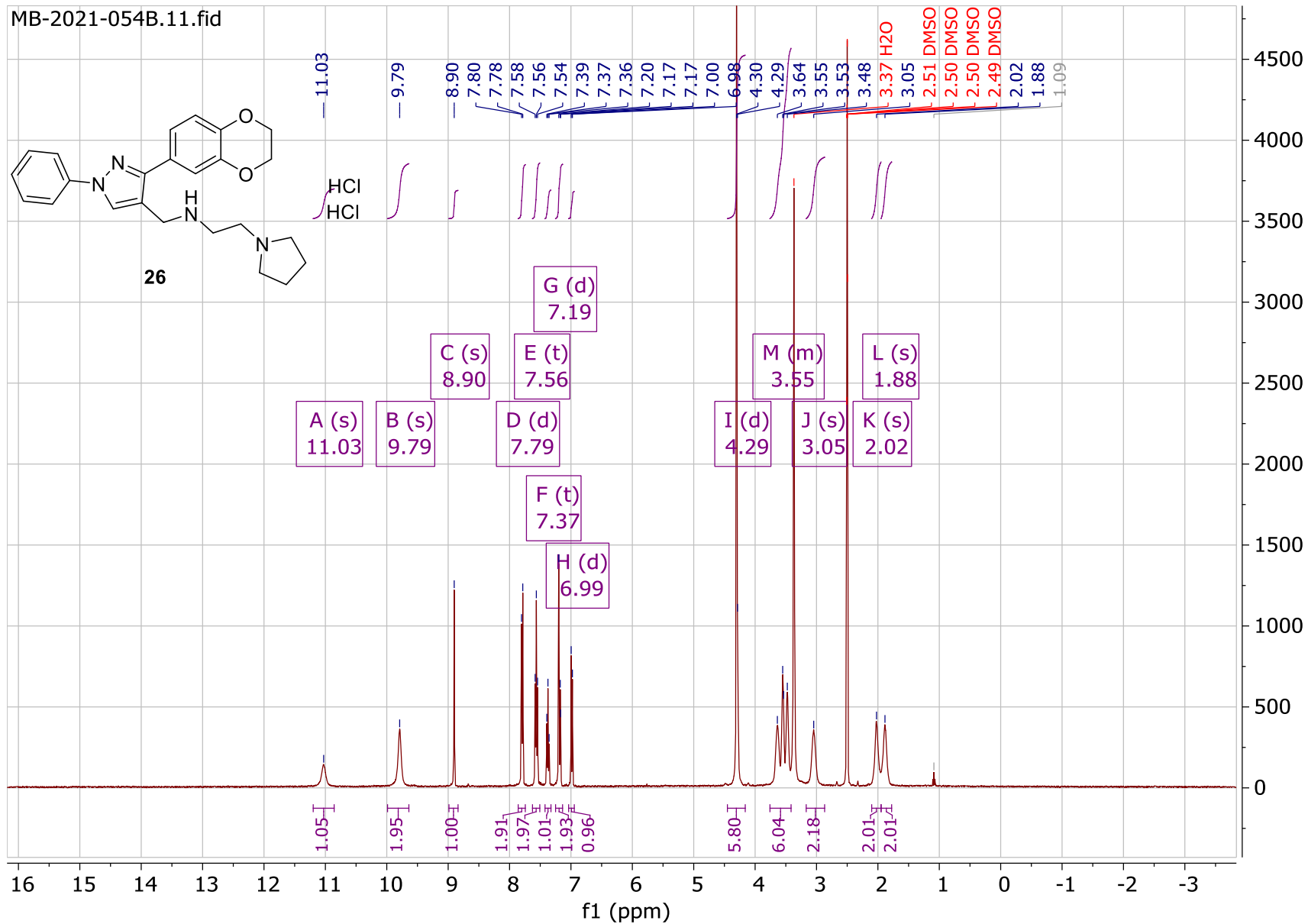
65.80
65.71

— 51.73

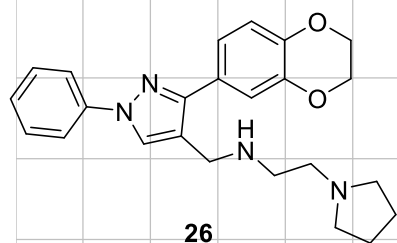








MB-2021-054B.12.fid



HCl
HCl

151.56
144.73
144.42
140.08
130.79
130.75
127.74
126.03
122.13
119.25
118.29
117.59
112.81

65.15
65.05

54.16
50.47

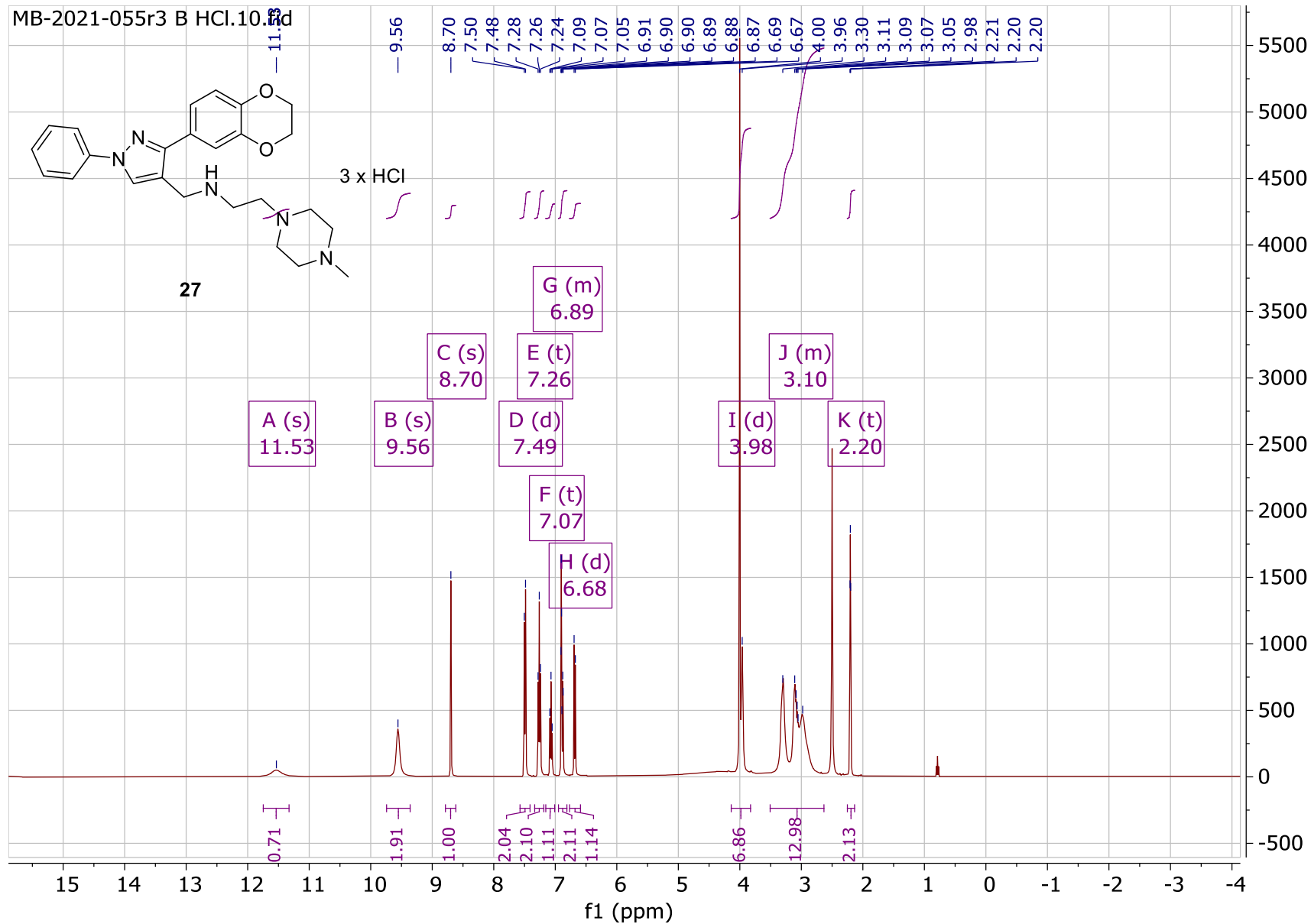
43.36
42.38

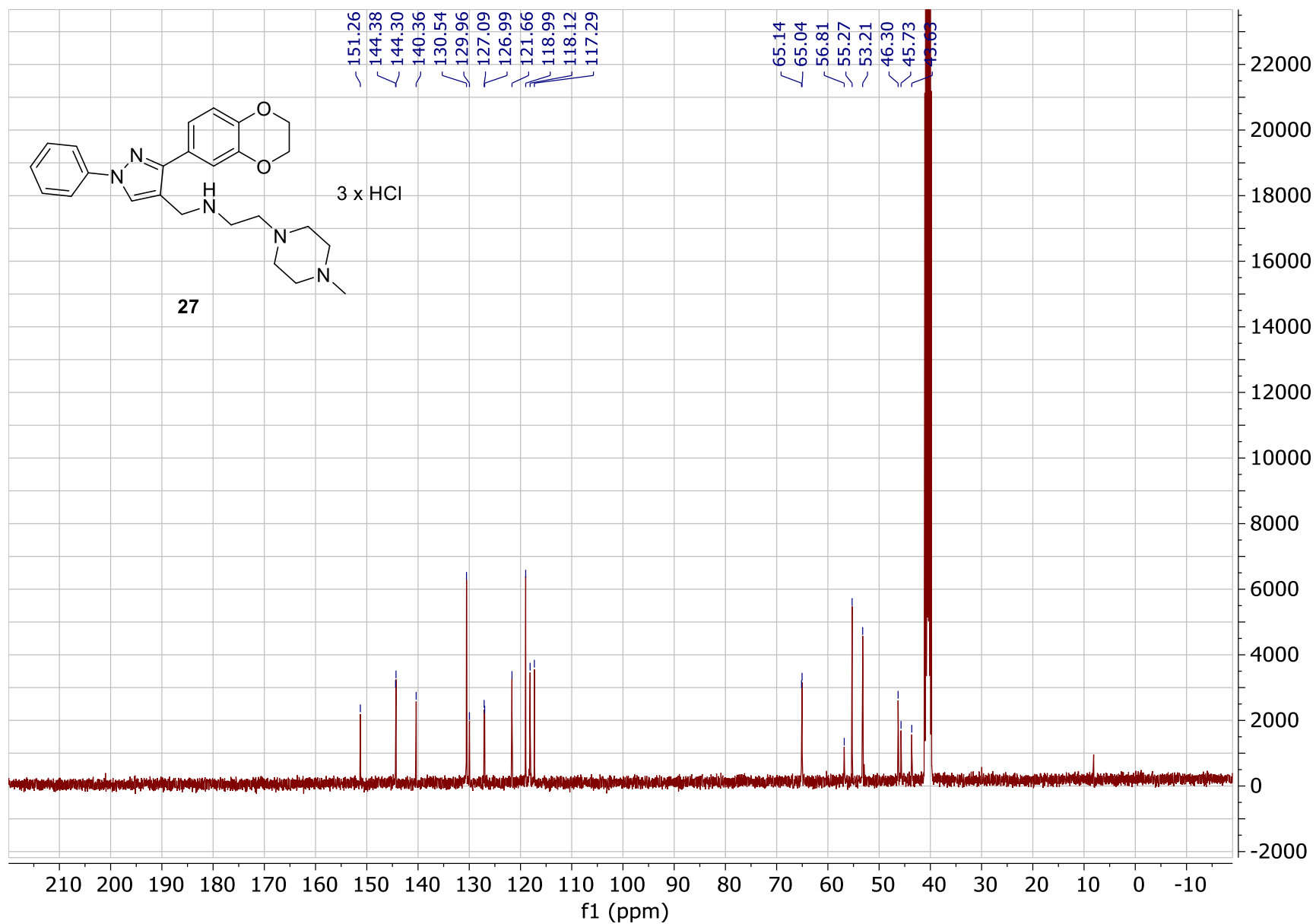
23.53

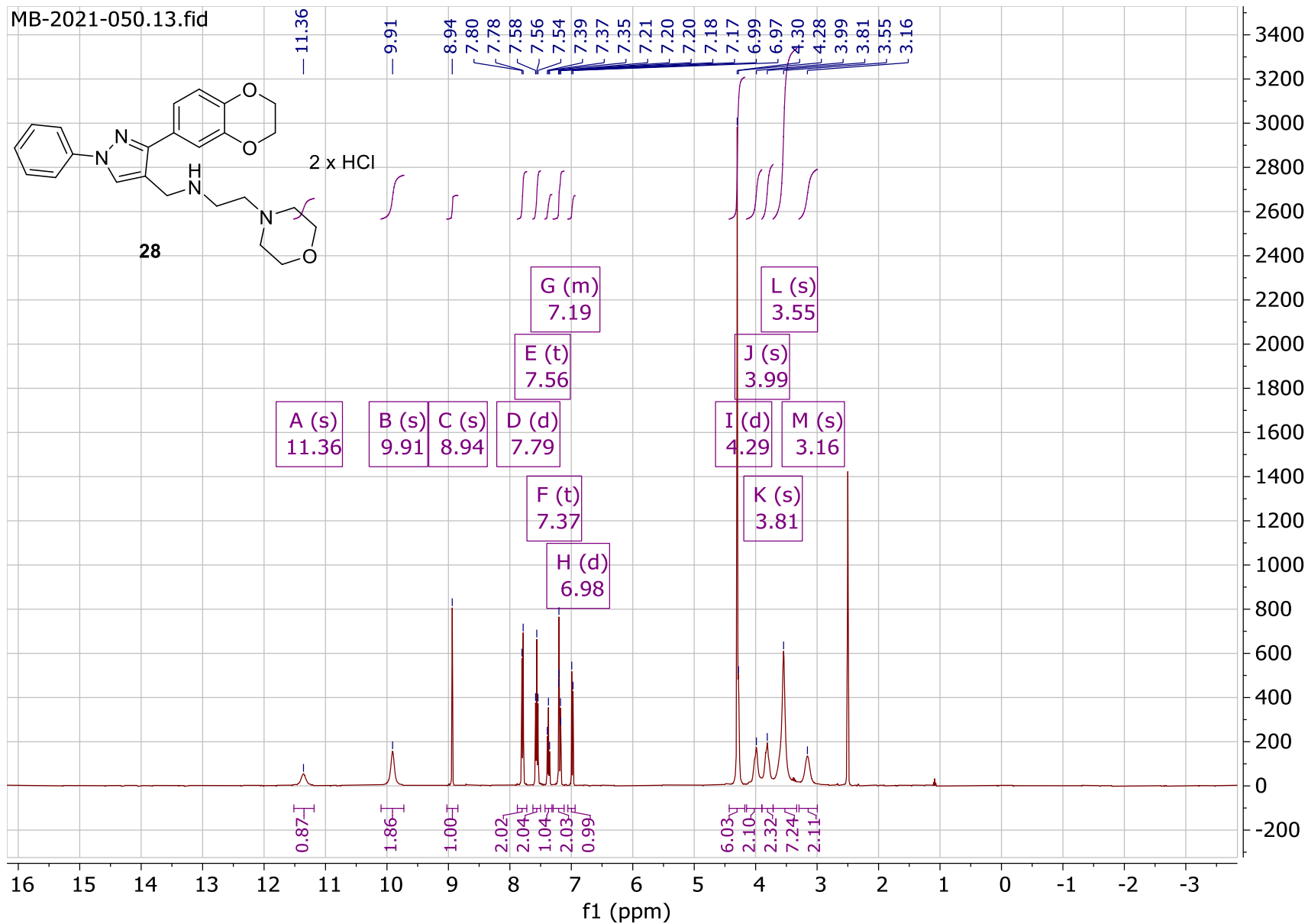
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

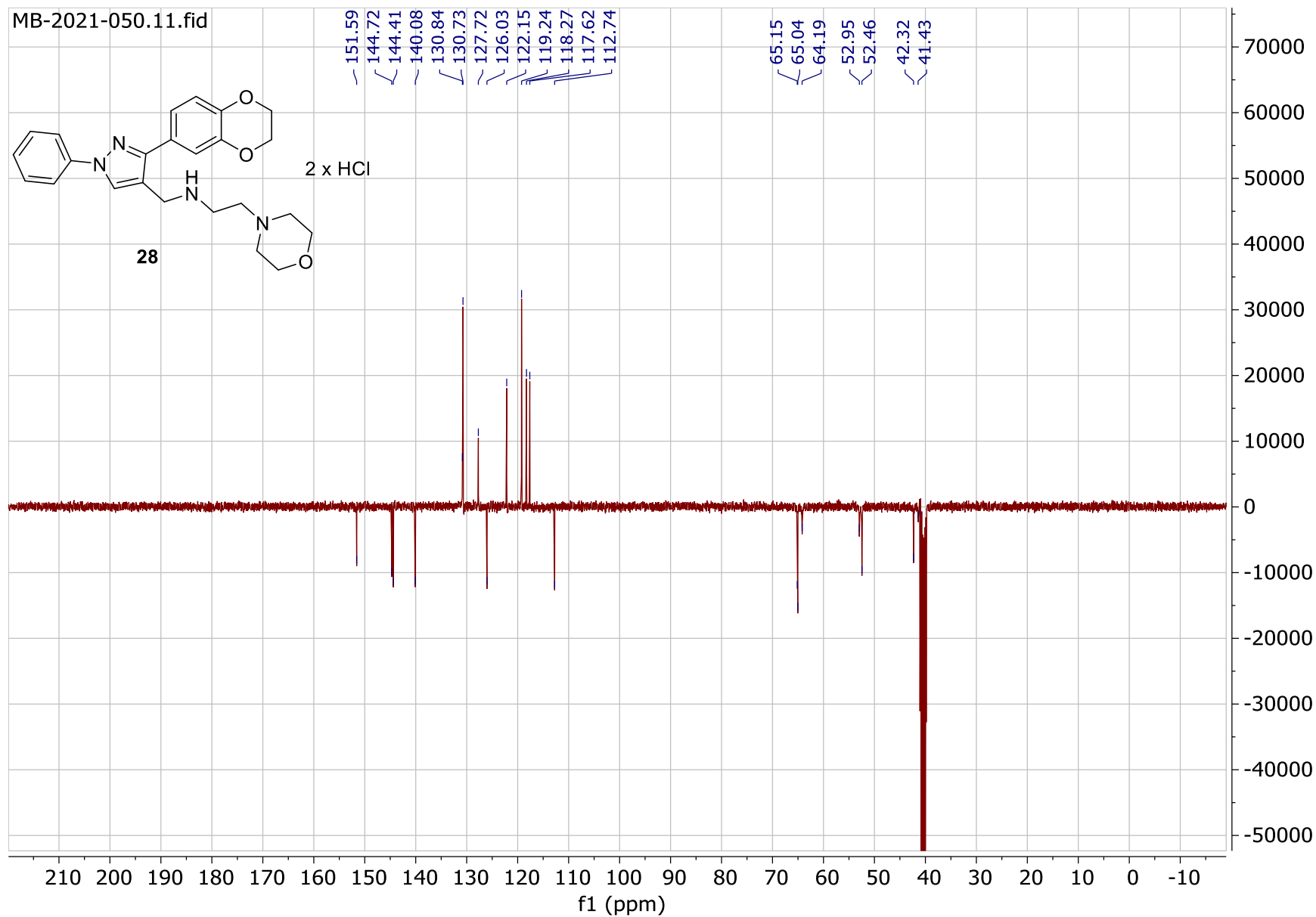
f1 (ppm)

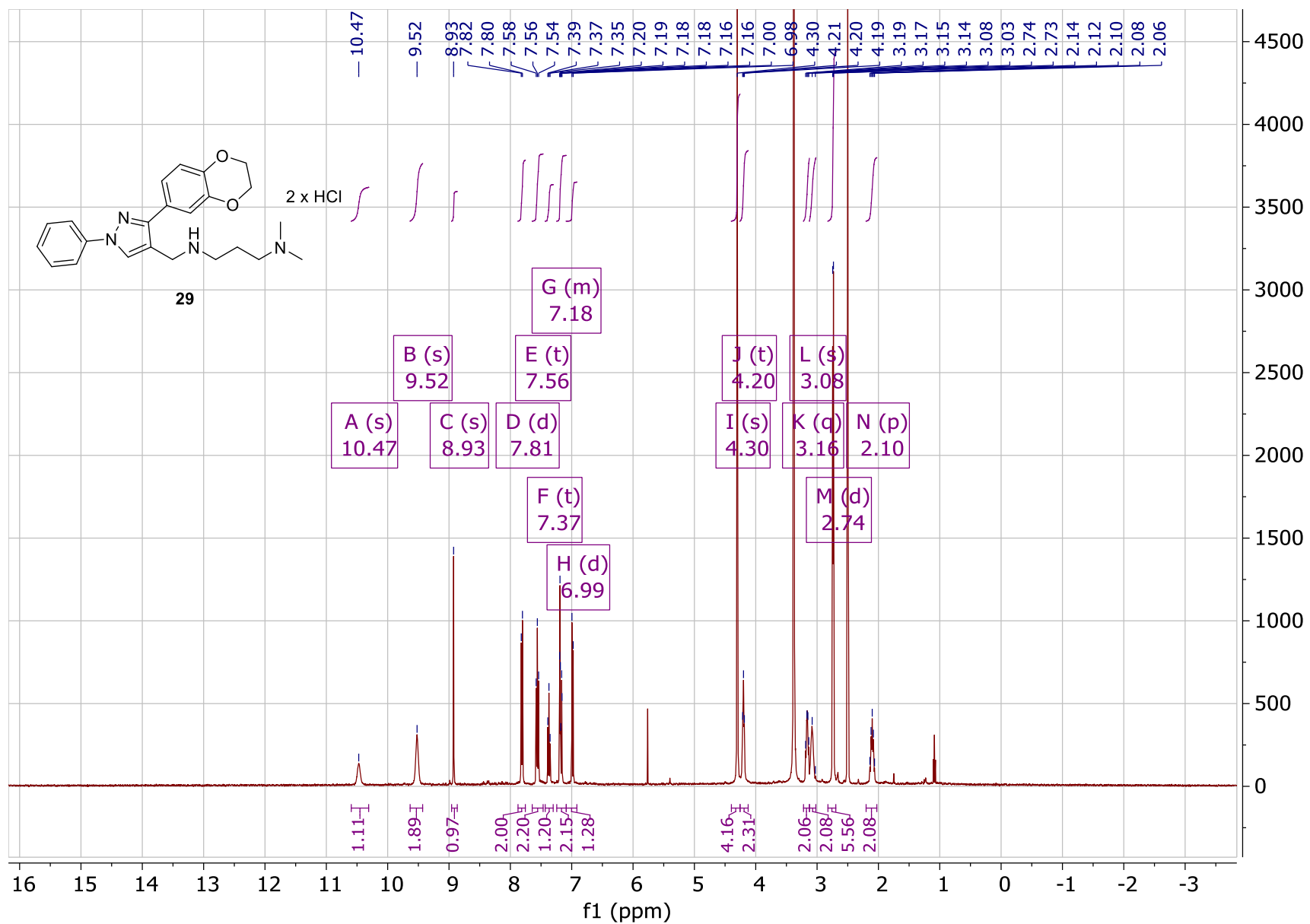


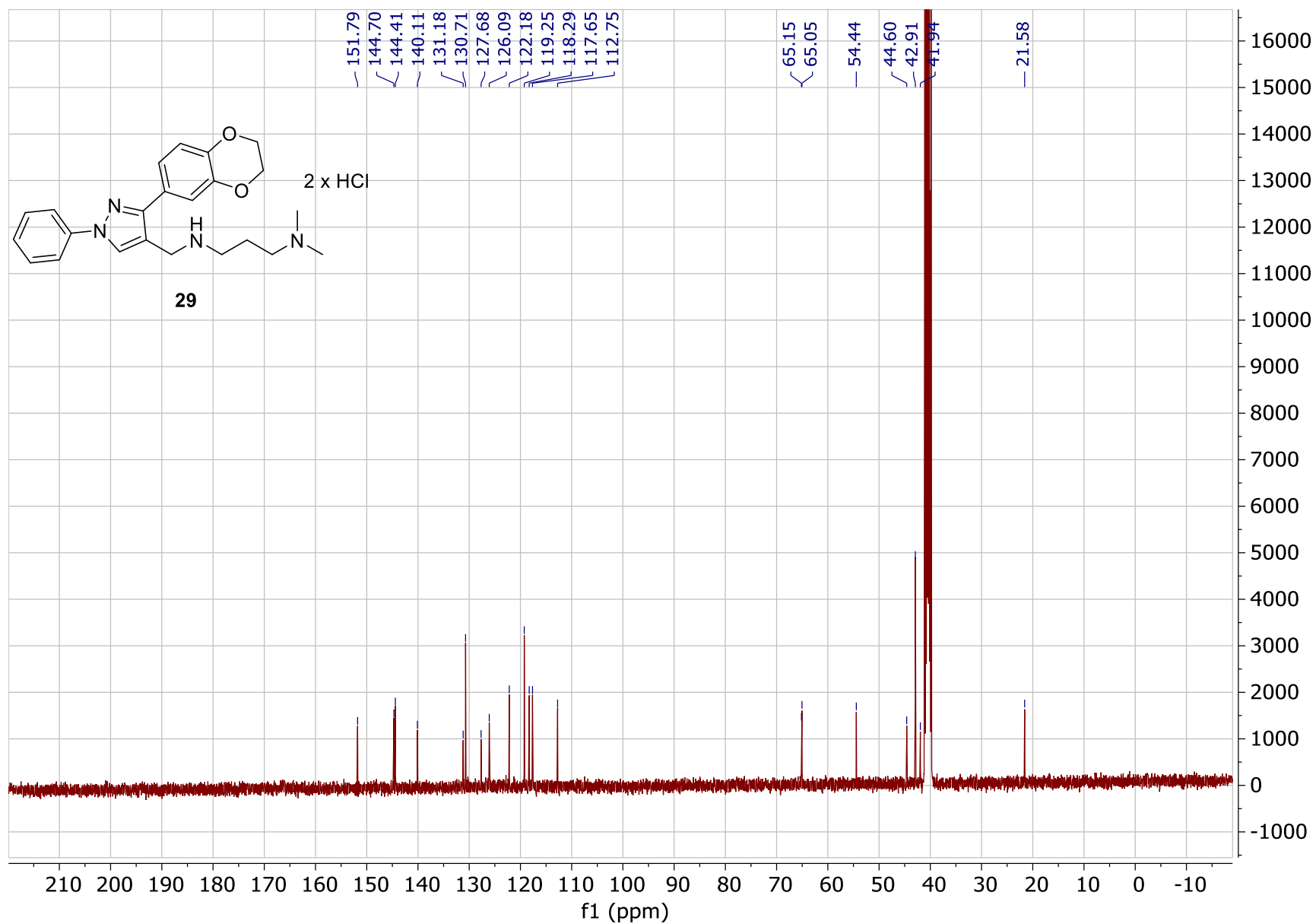


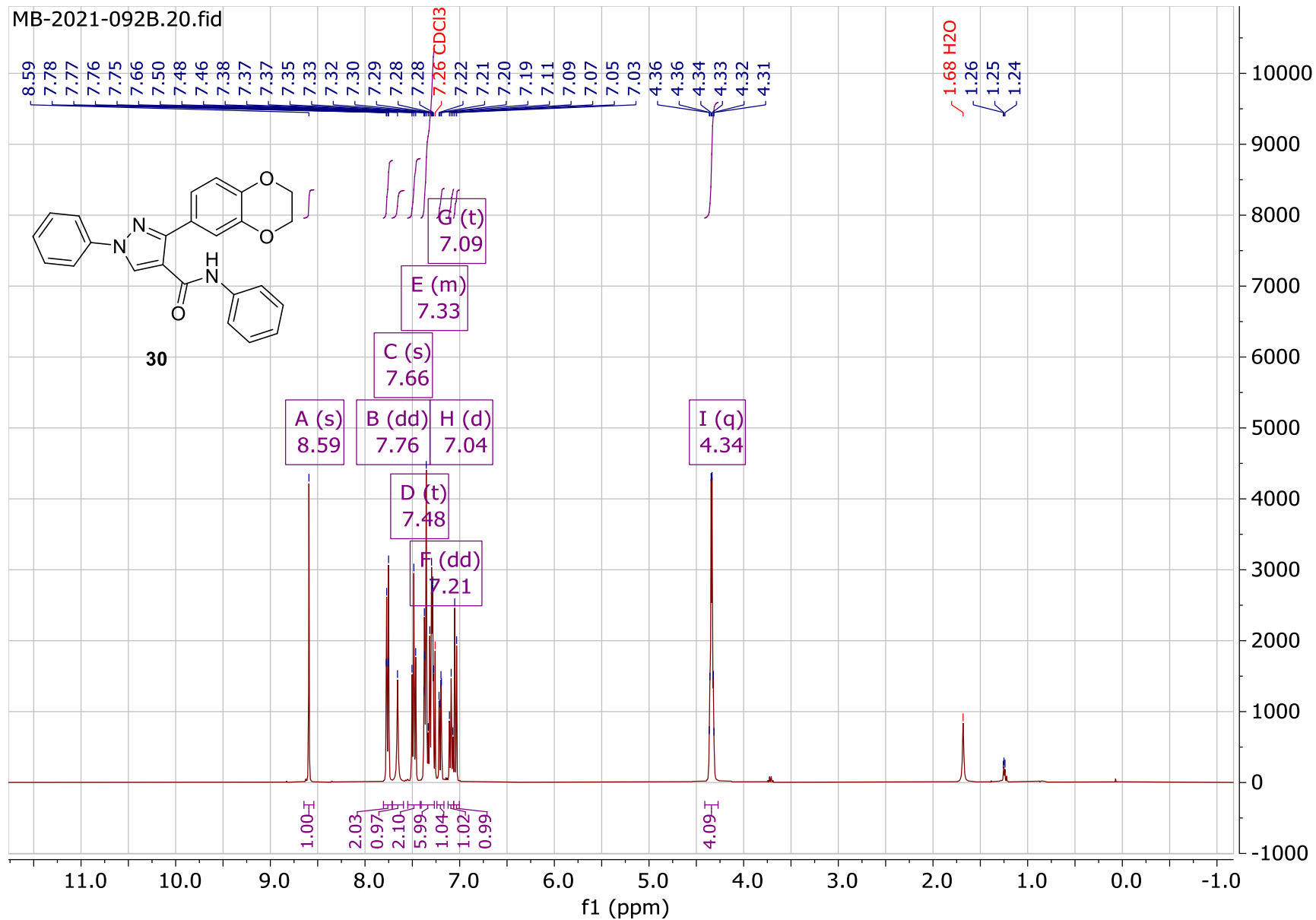


MB-2021-050.11.fid

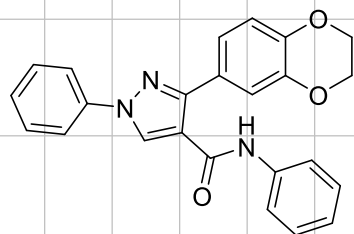








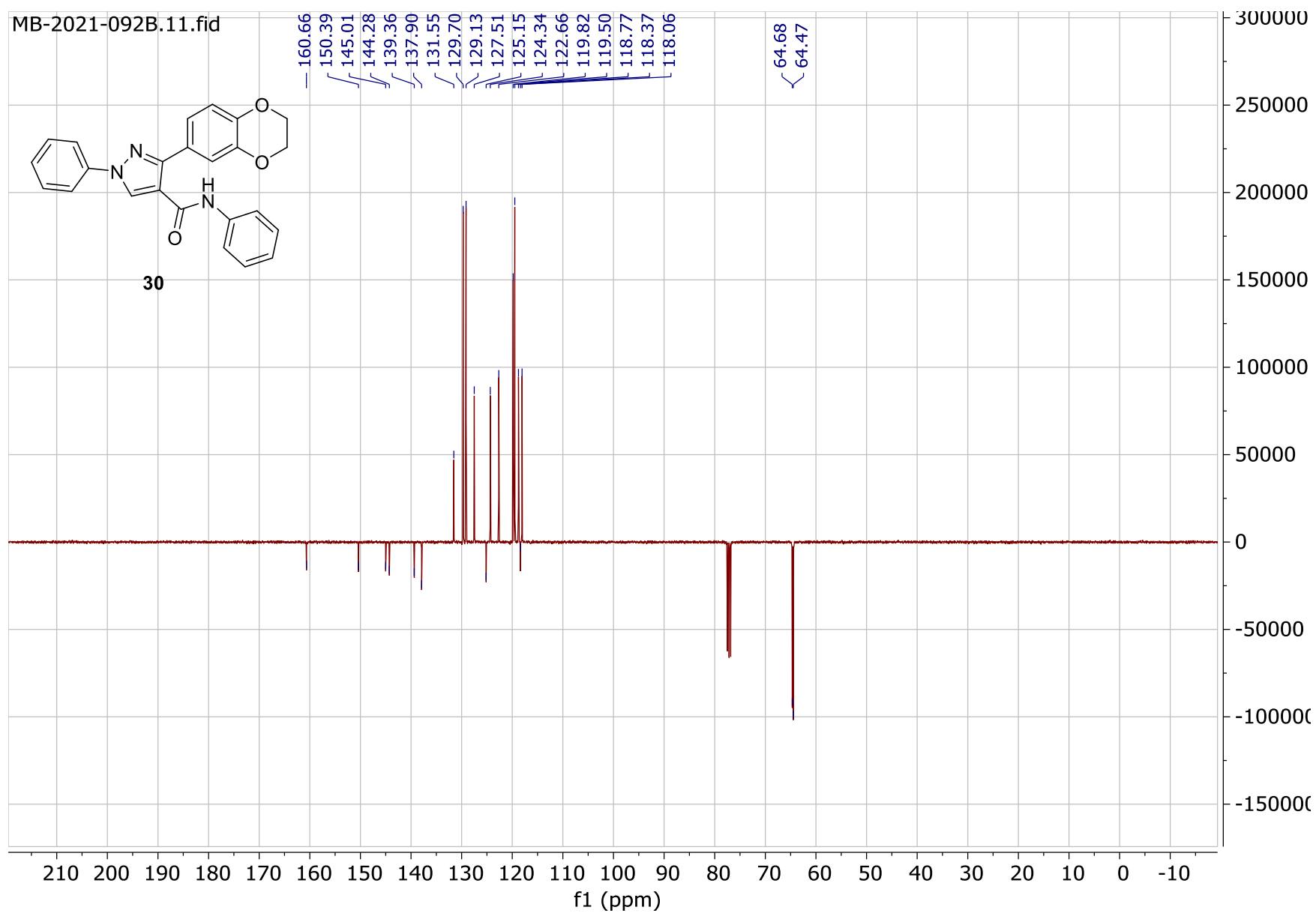
MB-2021-092B.11.fid

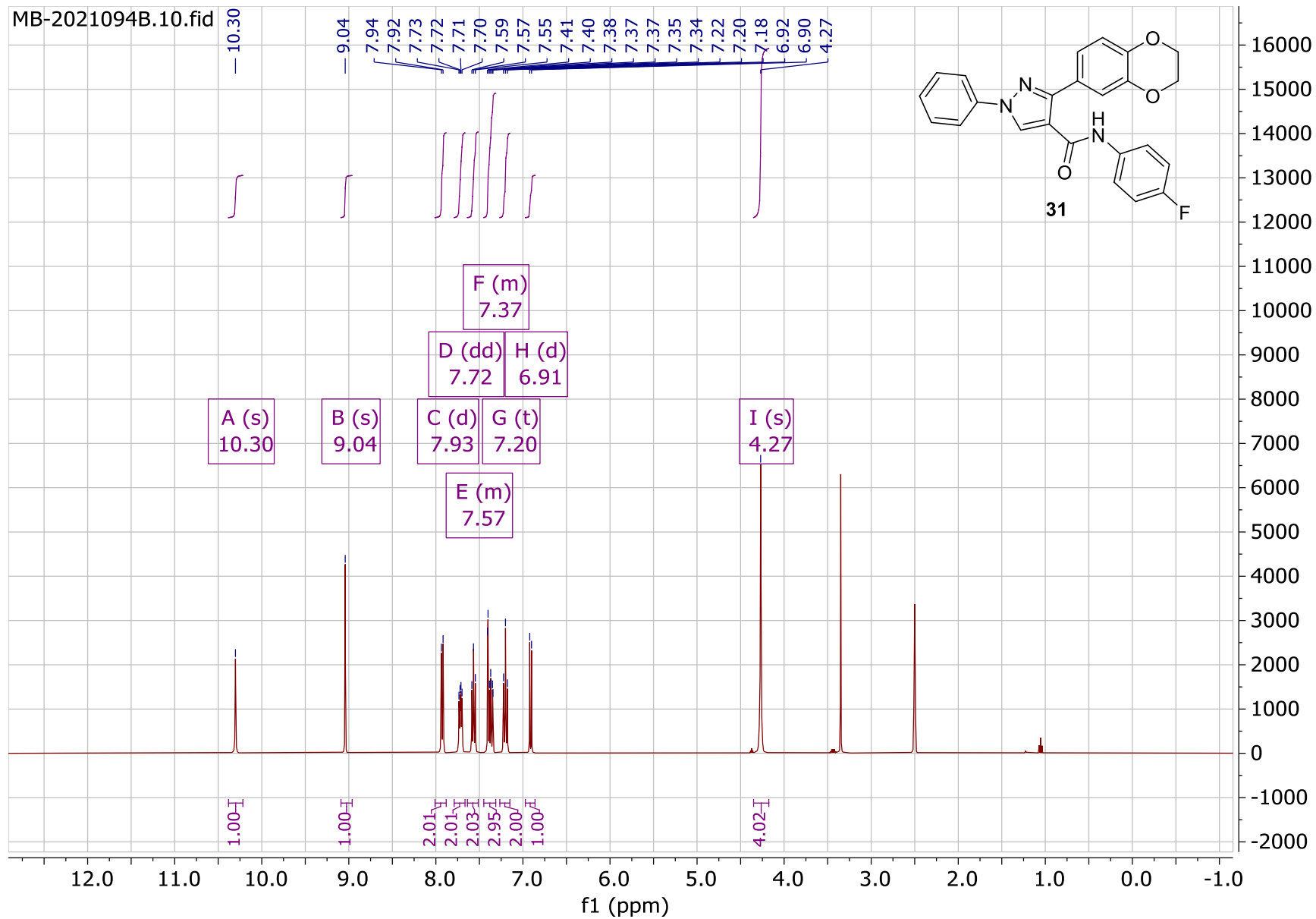


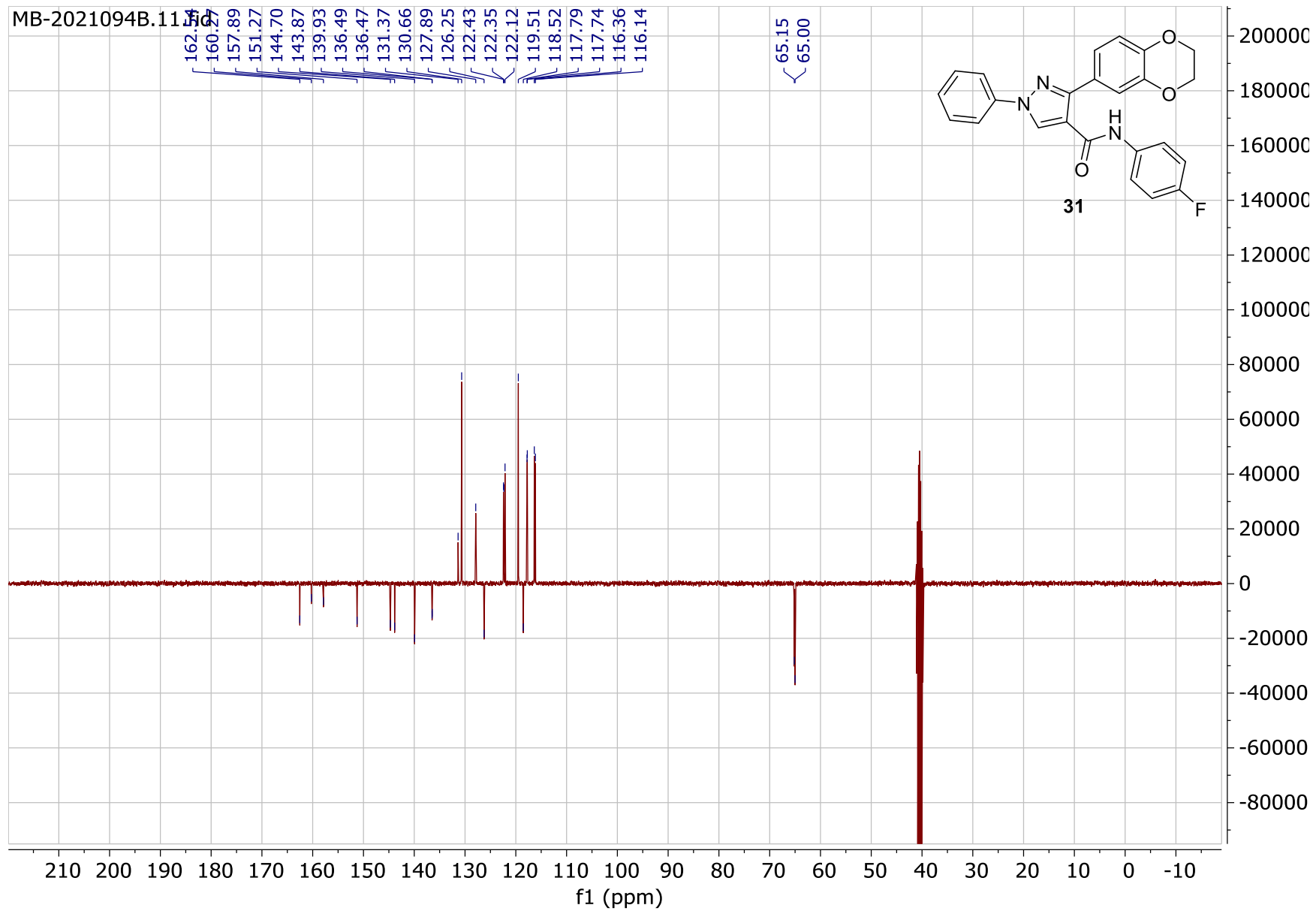
30

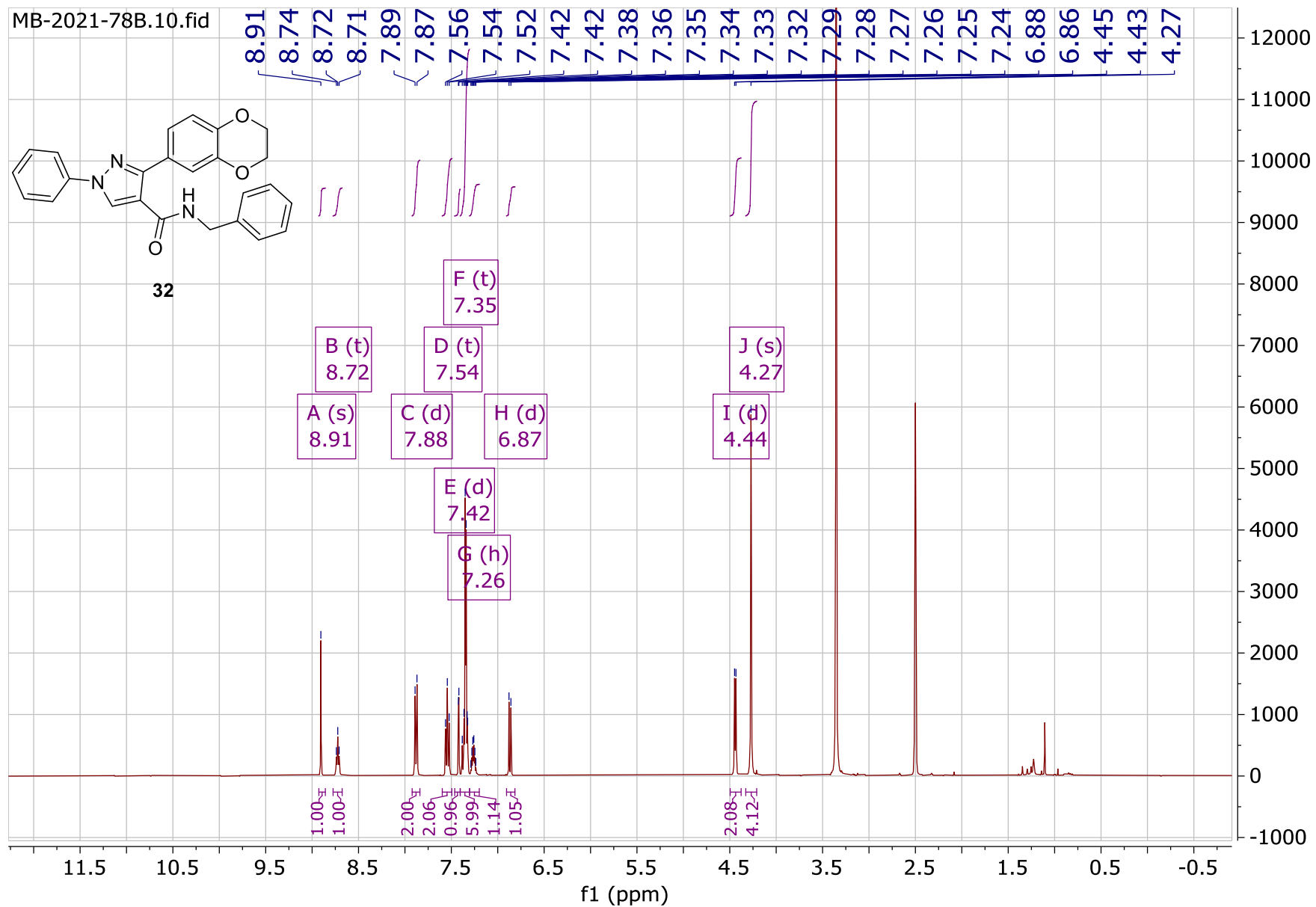
160.66
150.39
145.01
144.28
139.36
137.90
131.55
129.70
129.13
127.51
125.15
124.34
122.66
119.82
119.50
118.77
118.37
118.06

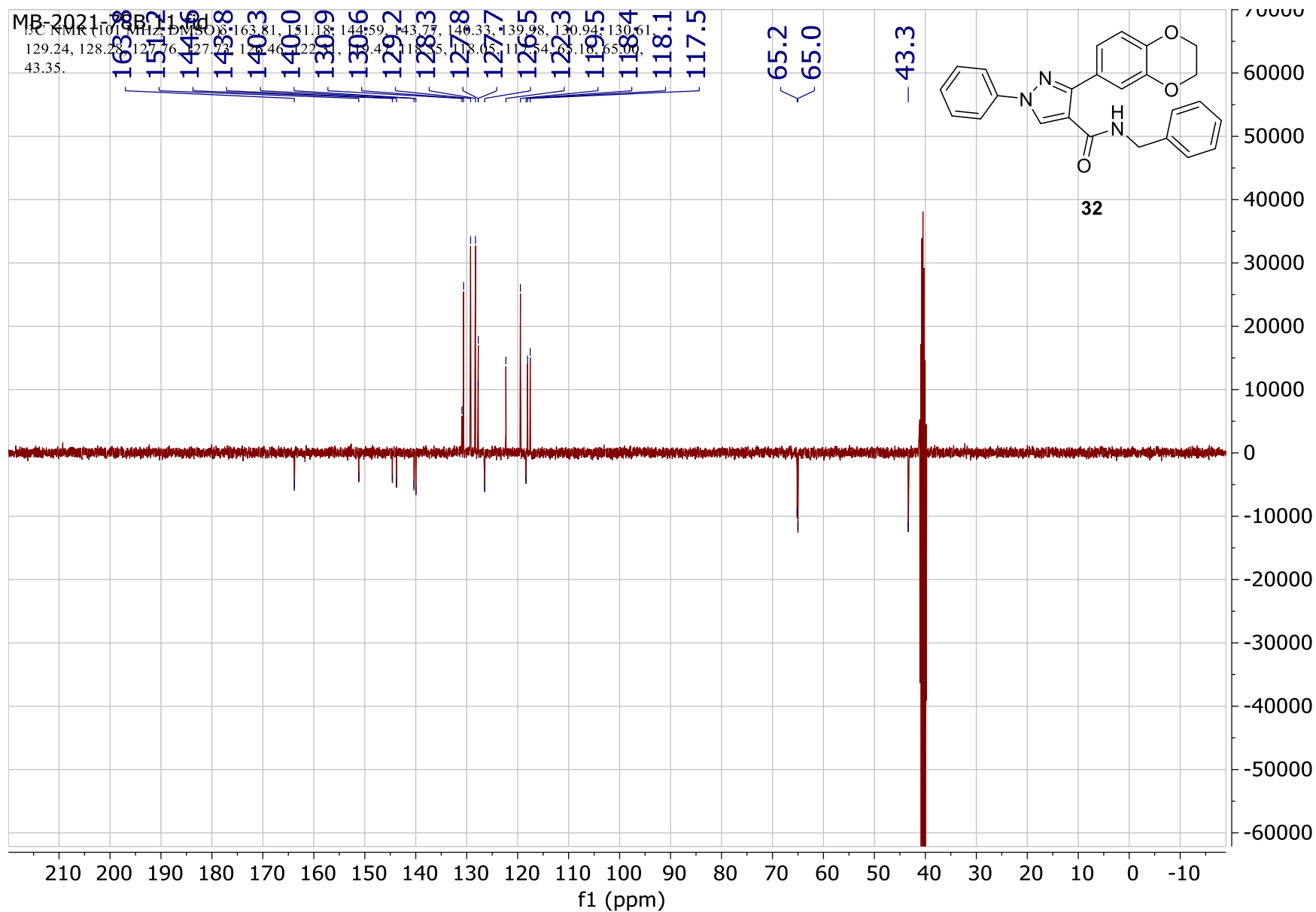
64.68
64.47



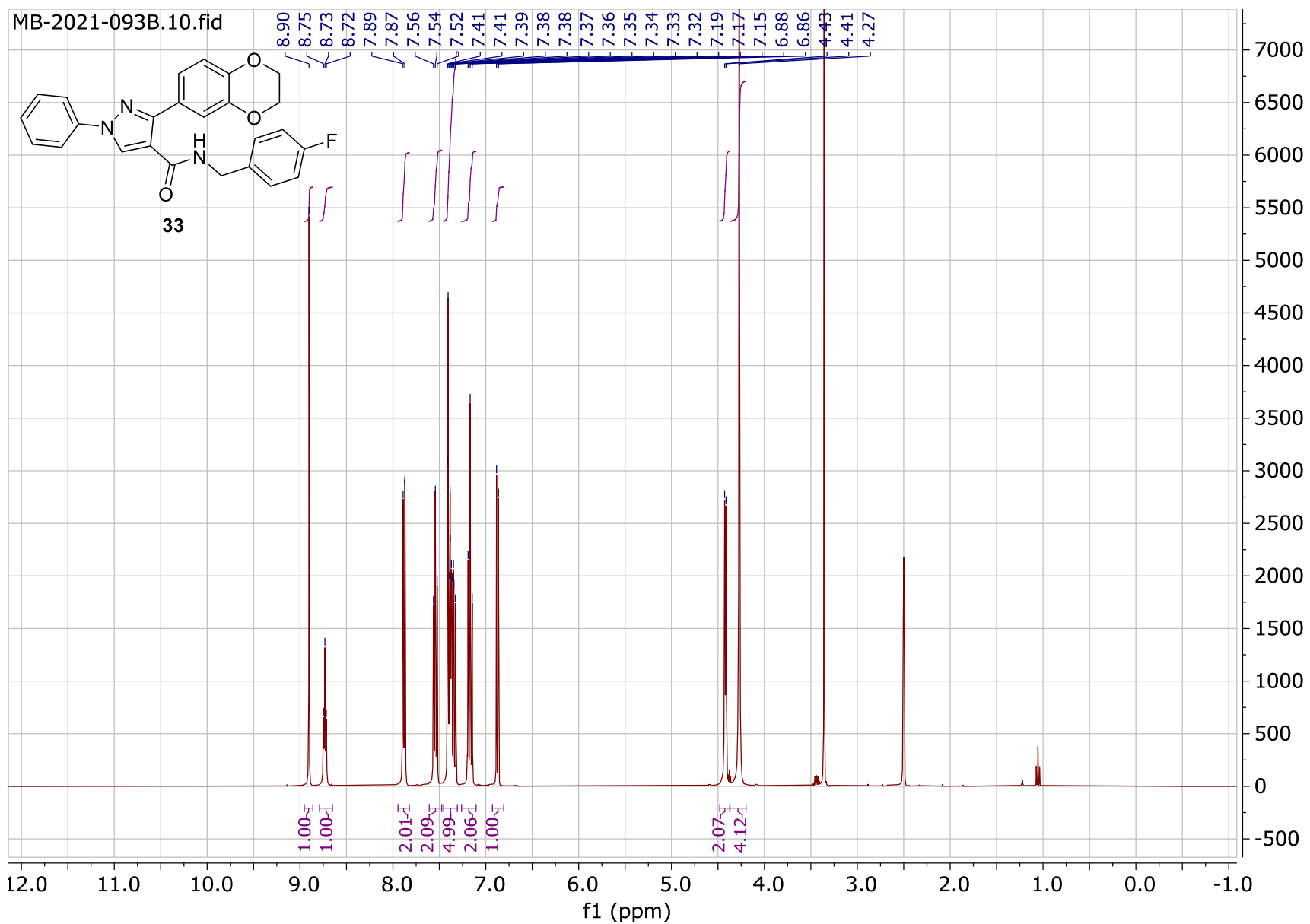


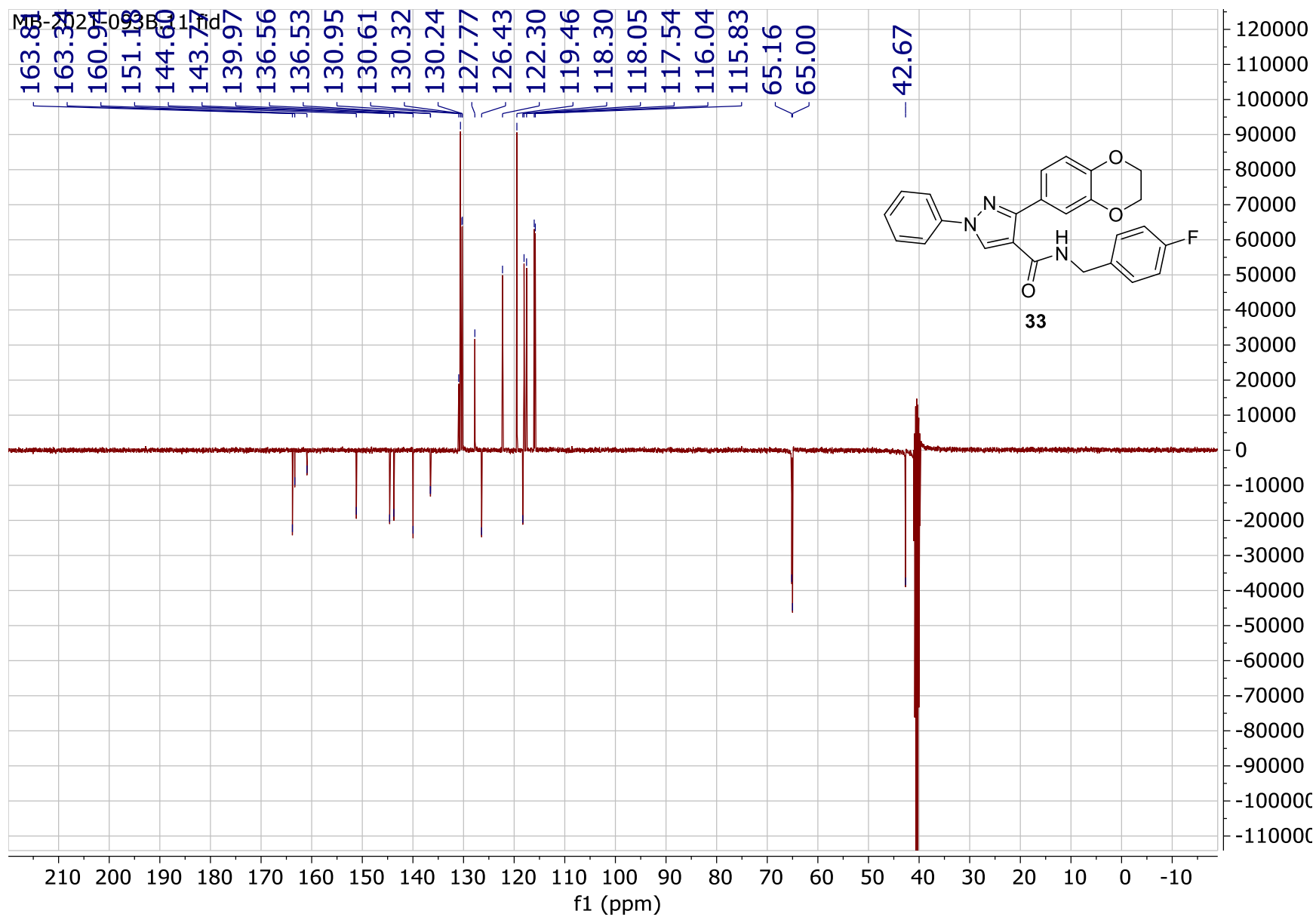


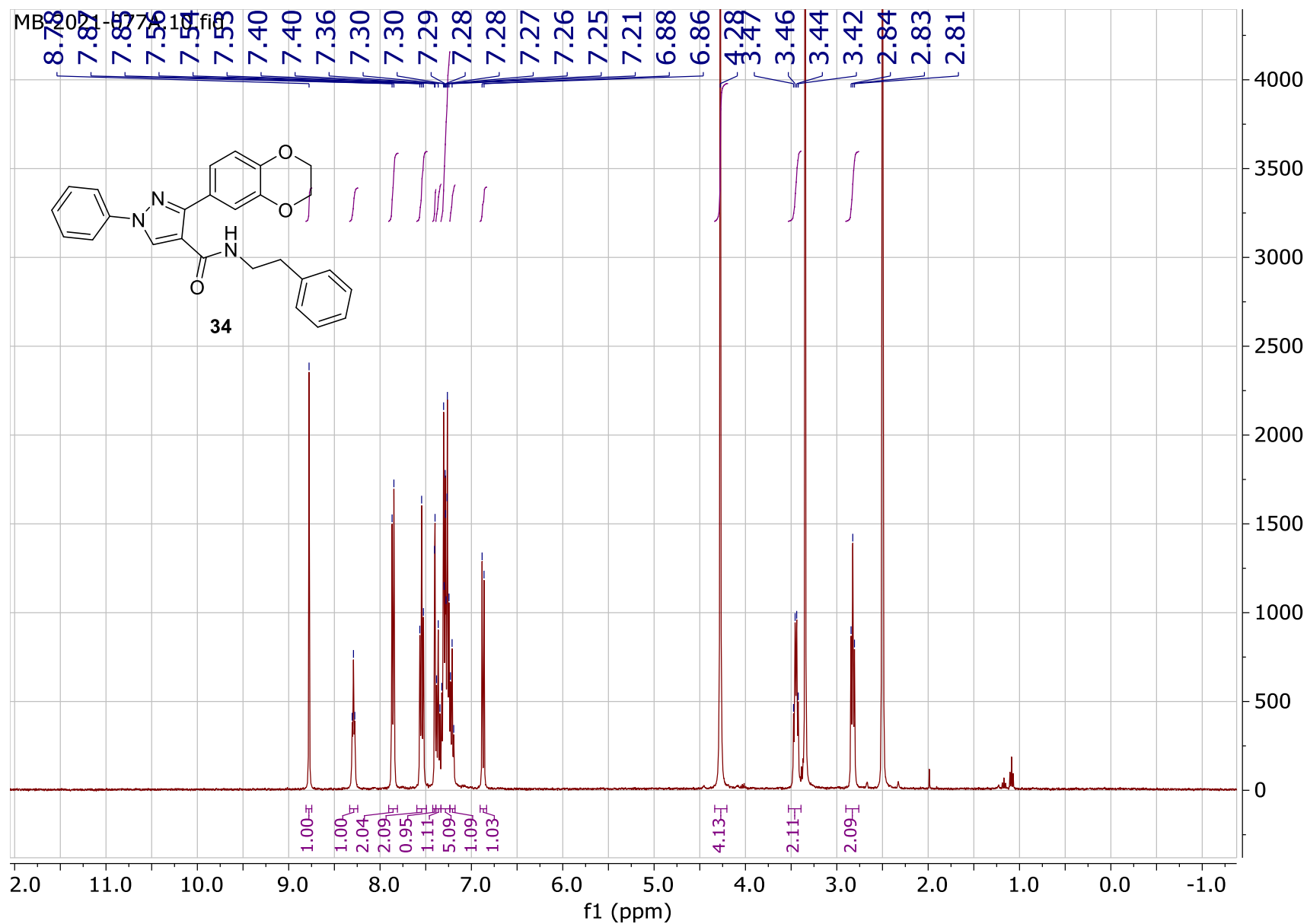


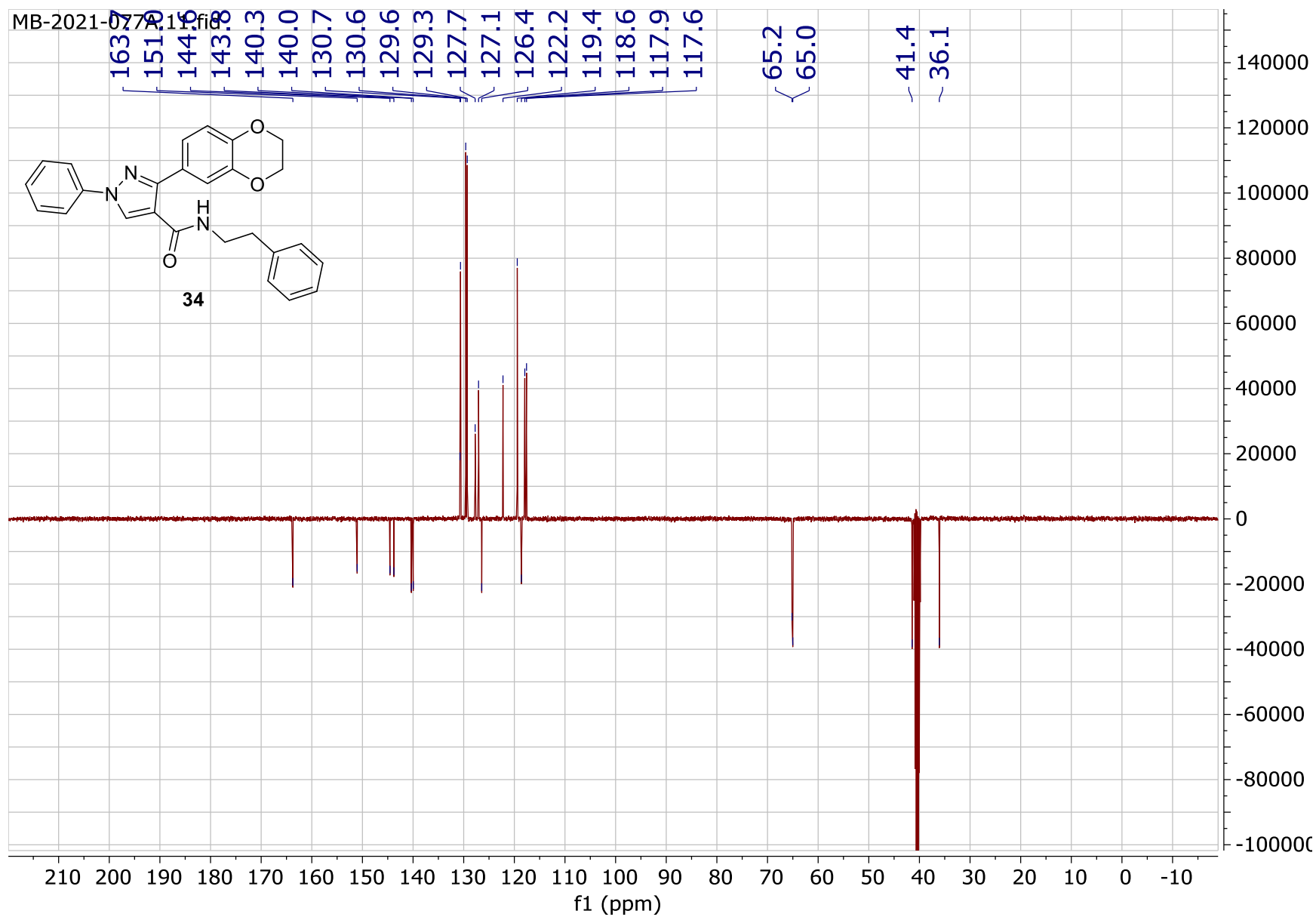


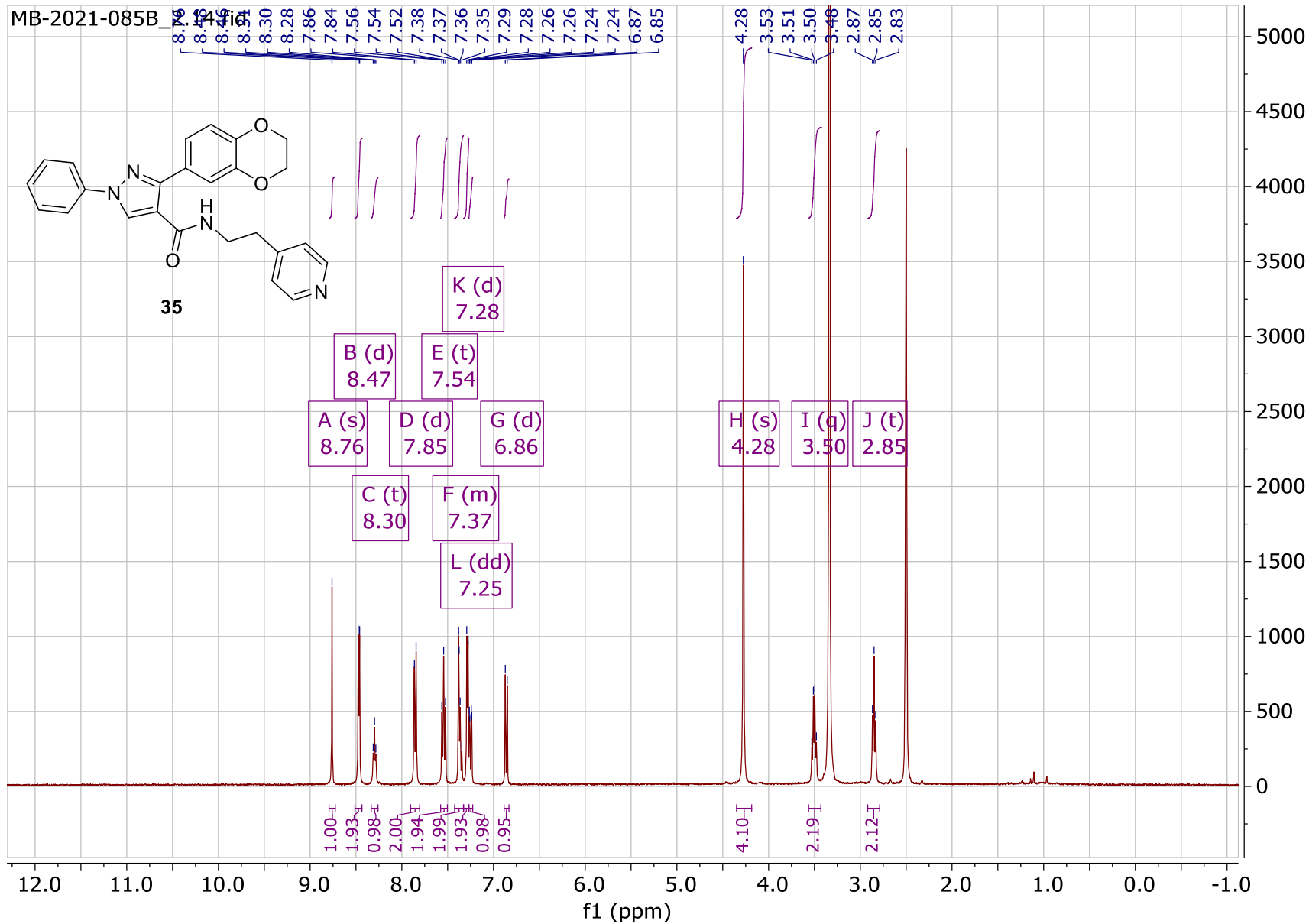
MB-2021-093B.10.fid



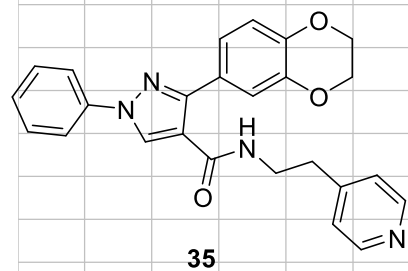








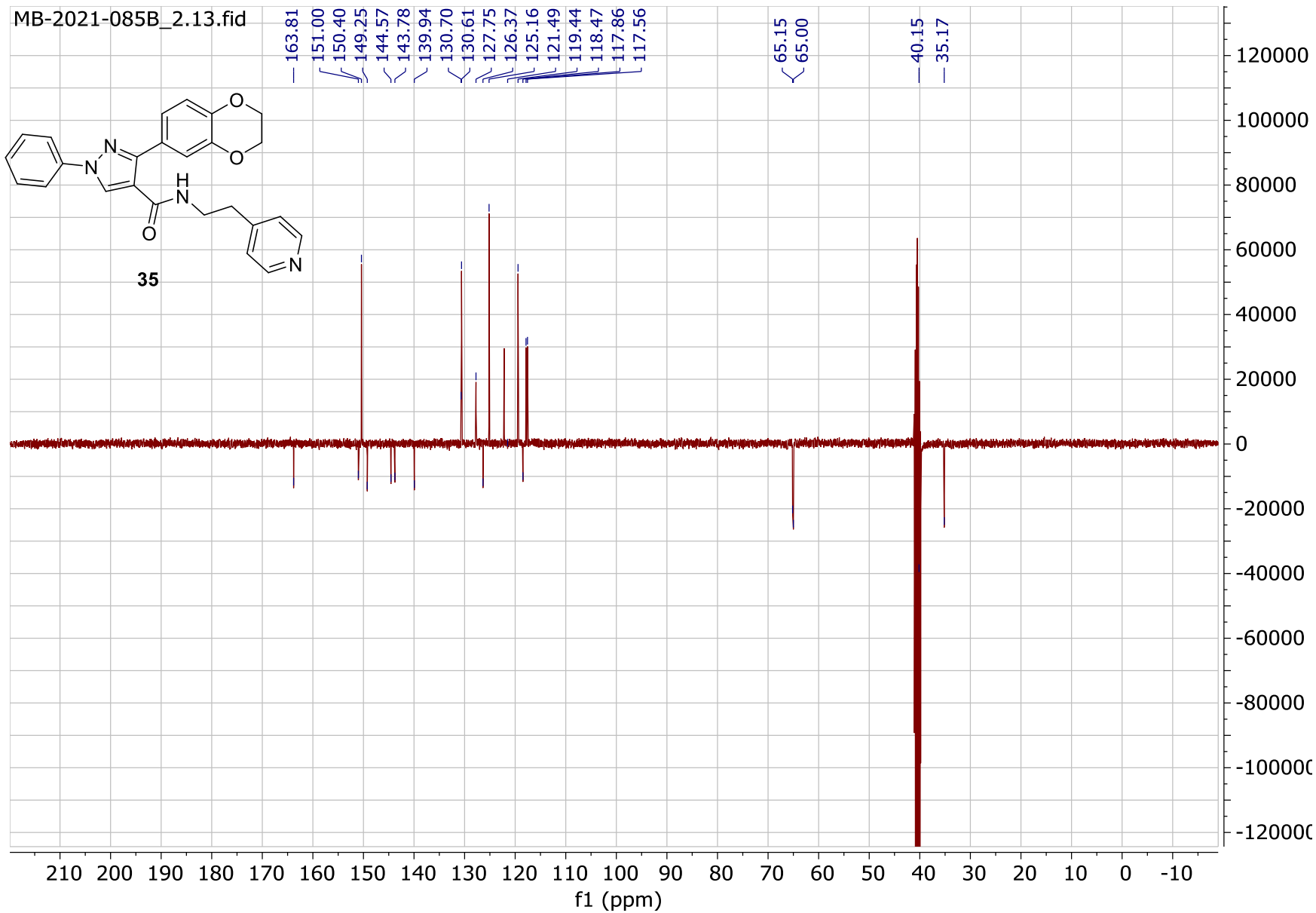
MB-2021-085B_2.13.fid

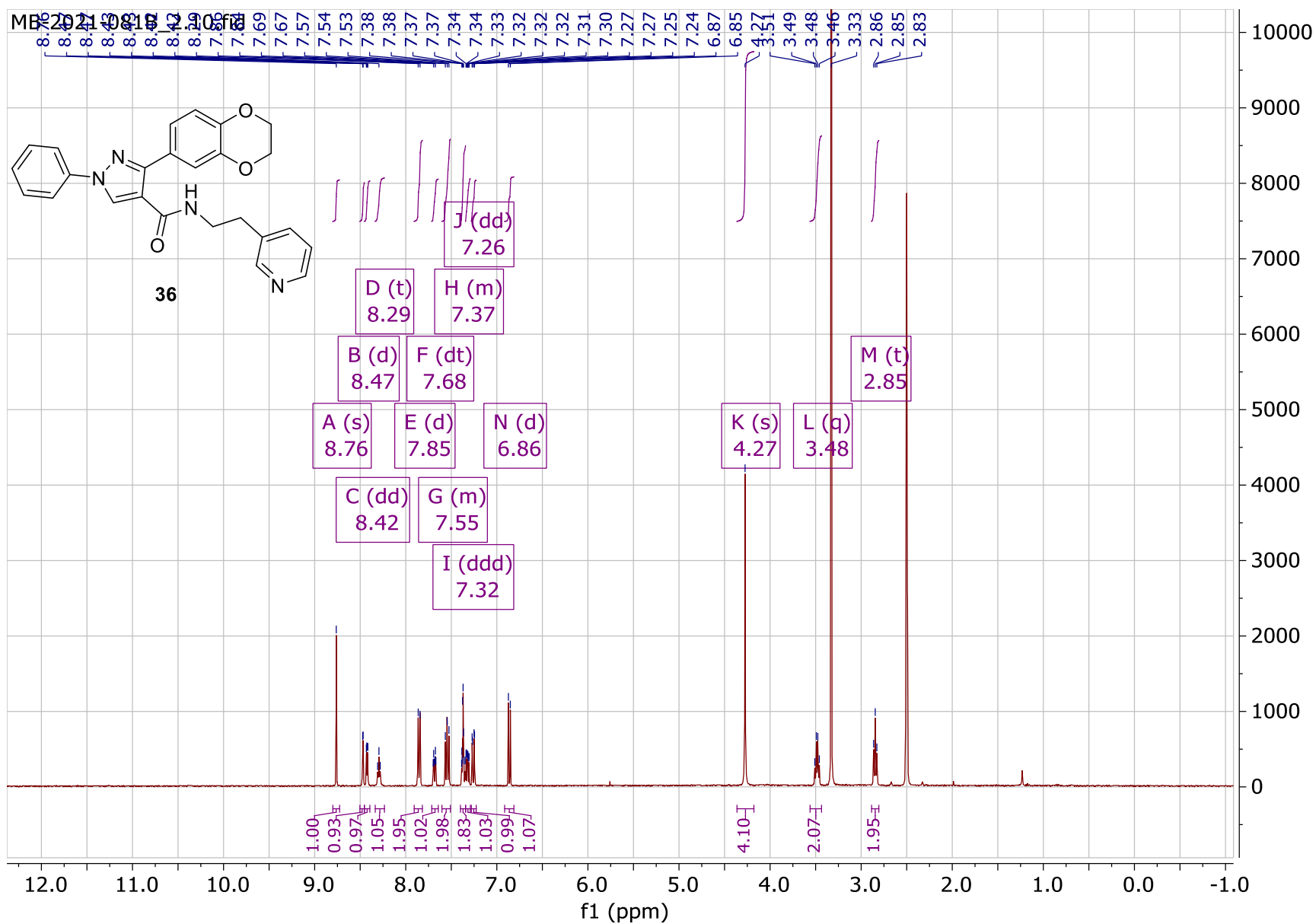


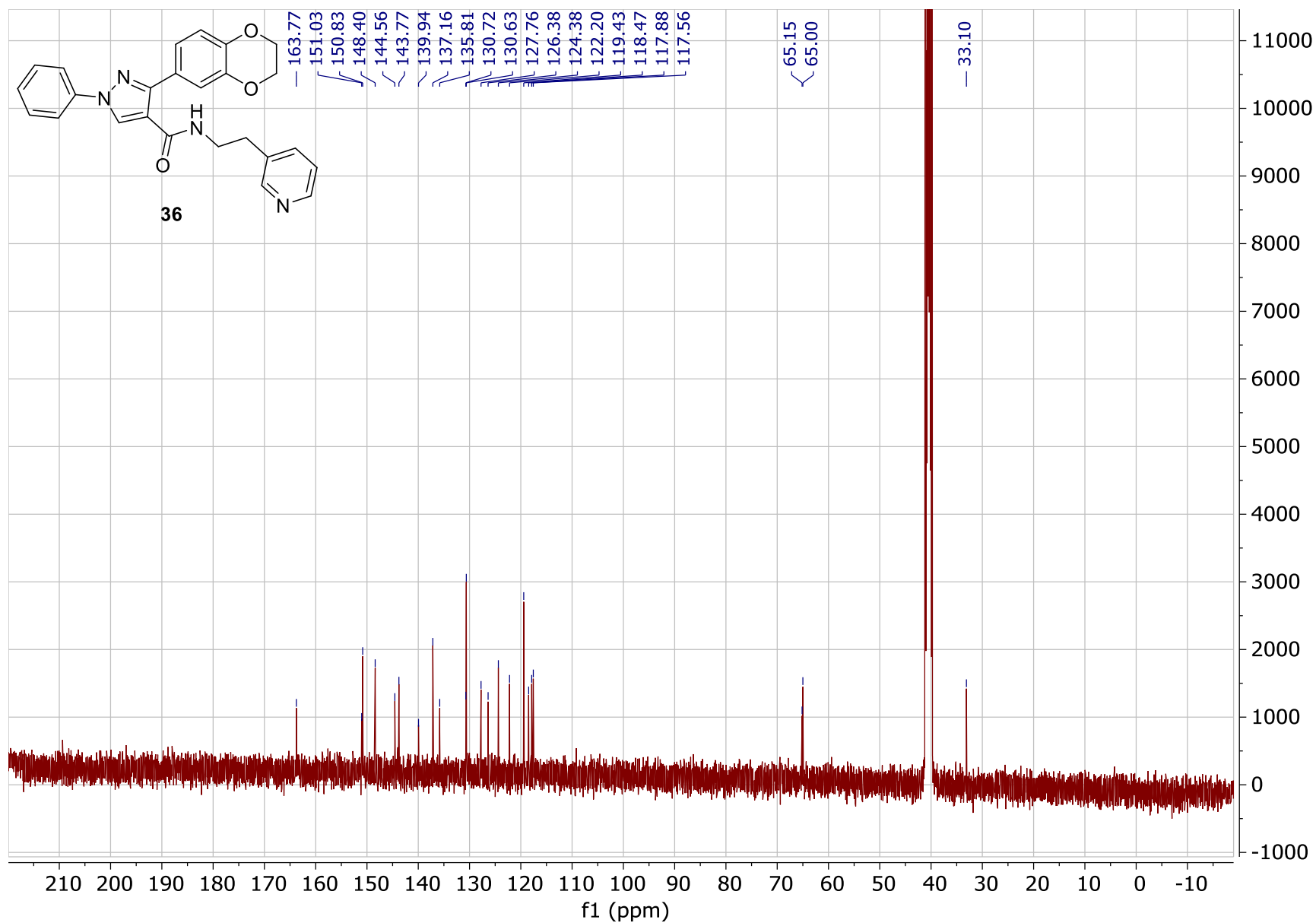
163.81
151.00
150.40
149.25
144.57
143.78
139.94
130.70
130.61
127.75
126.37
125.16
121.49
119.44
118.47
117.86
117.56

65.15
65.00

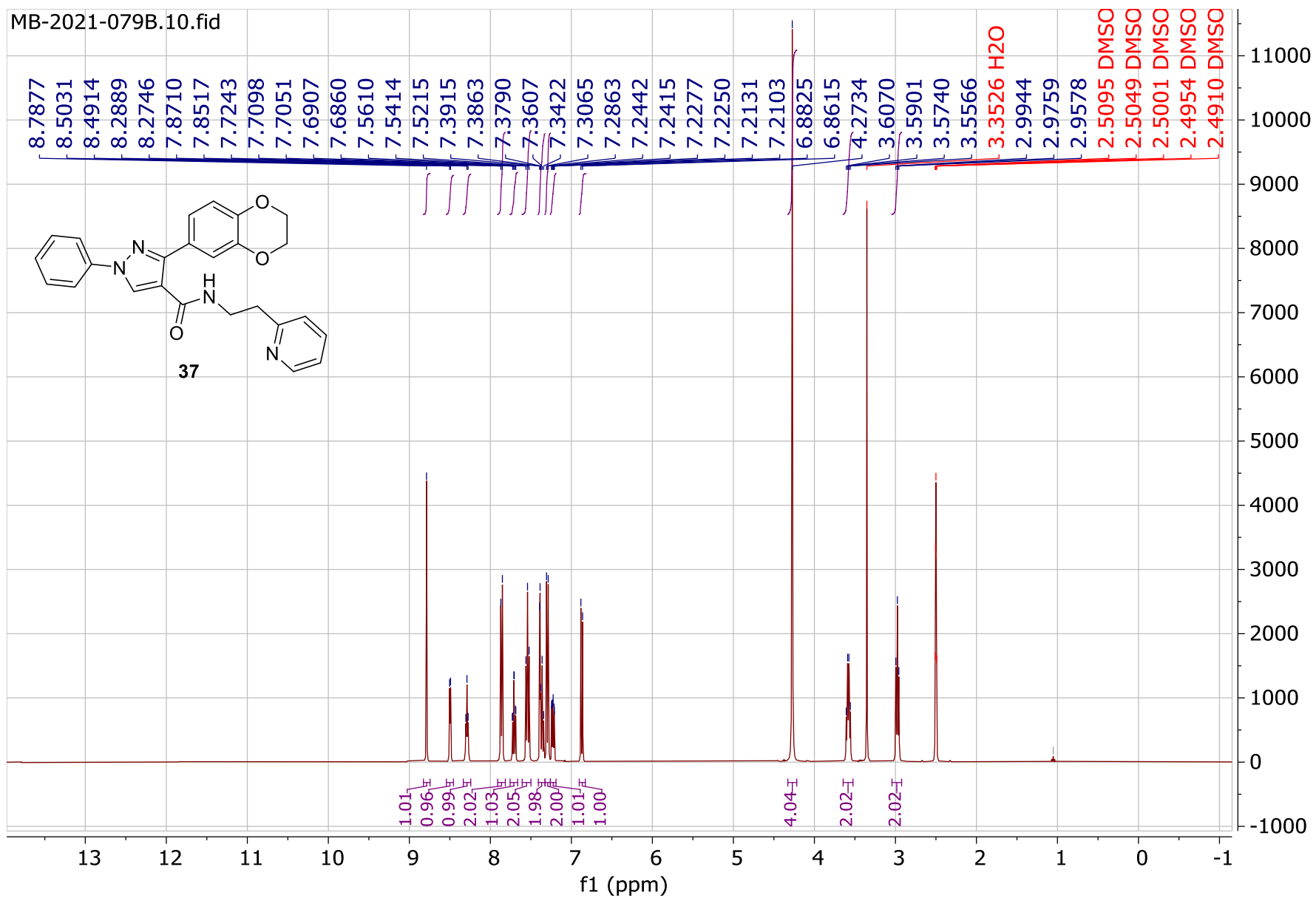
40.15
35.17

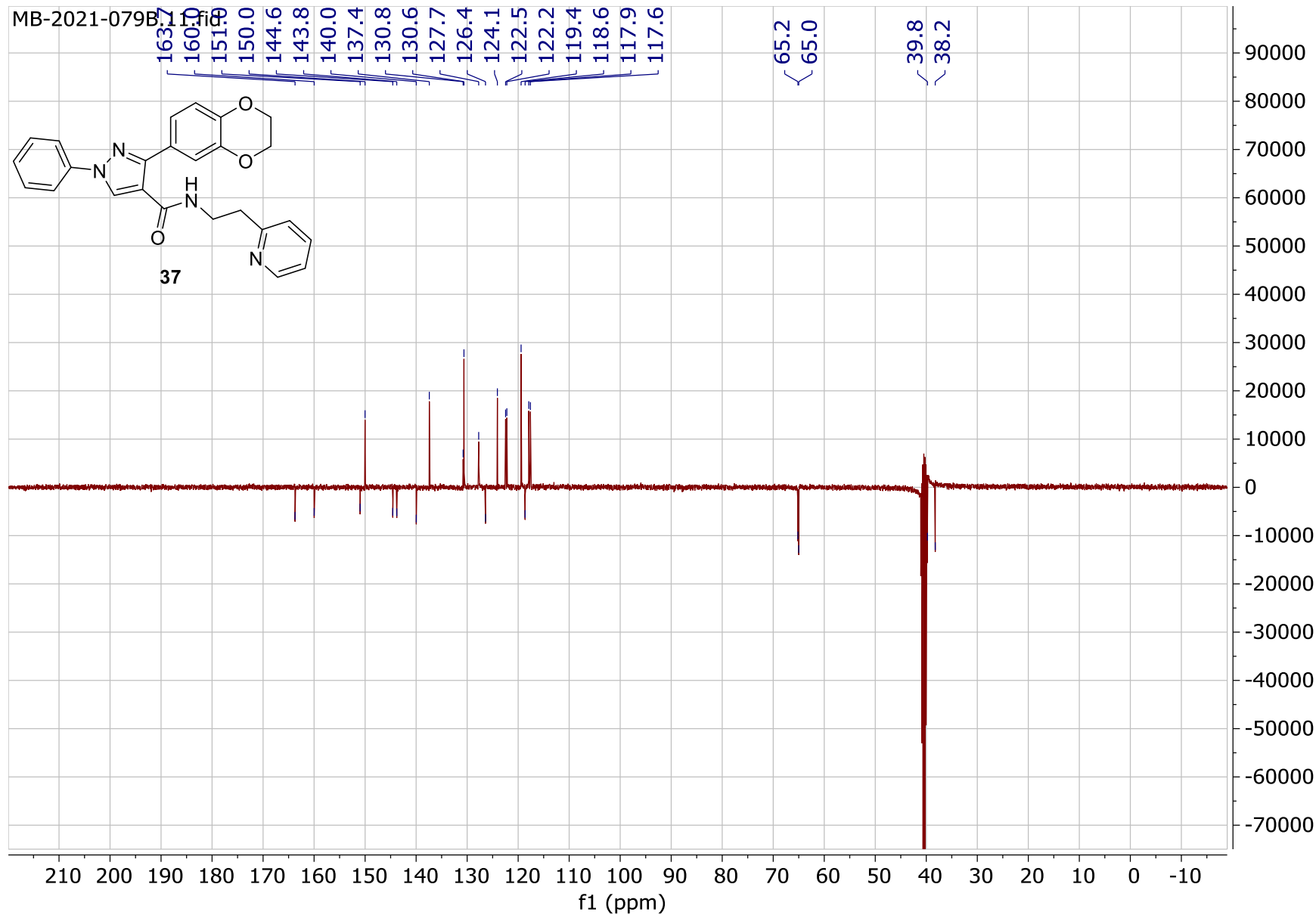


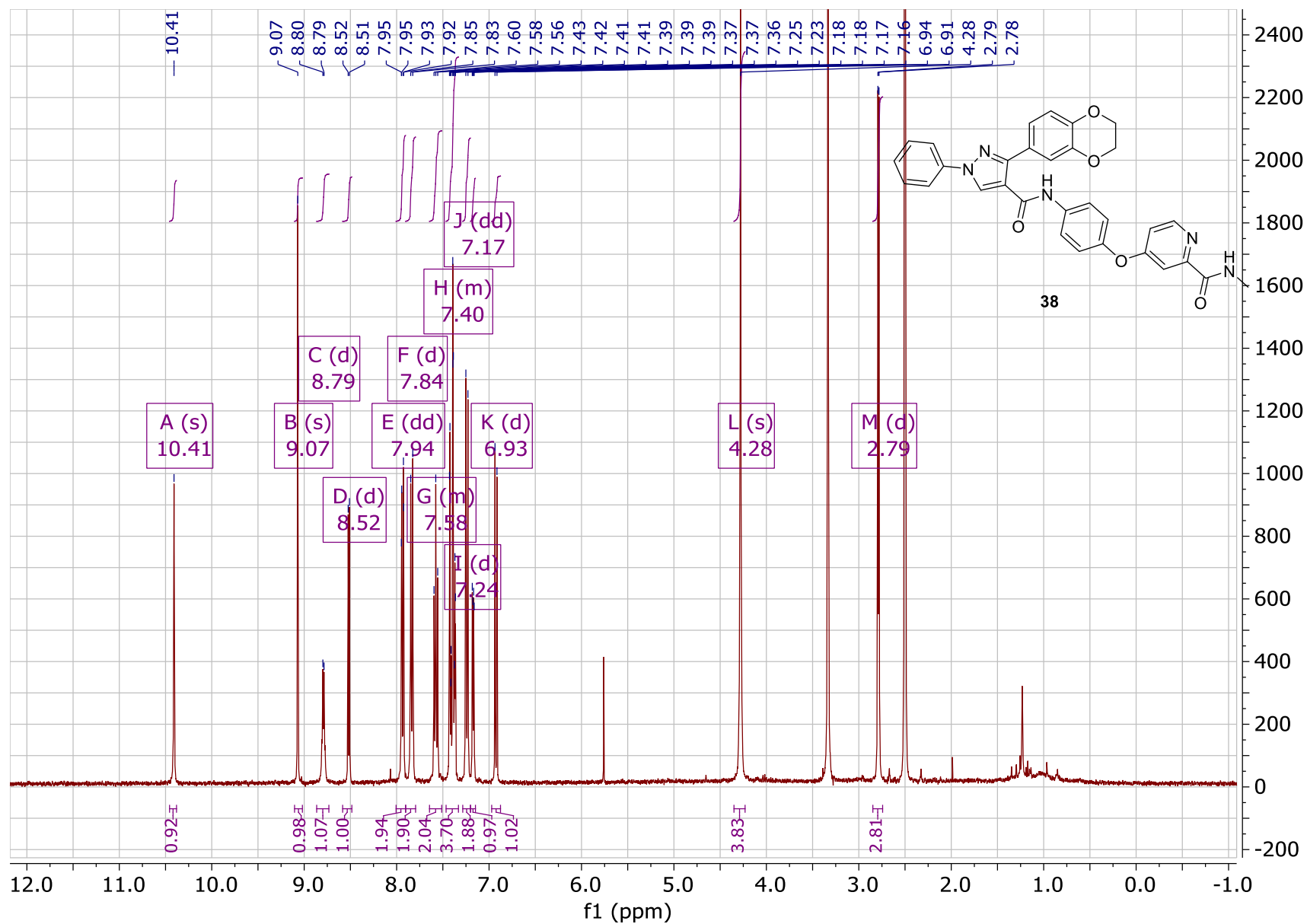


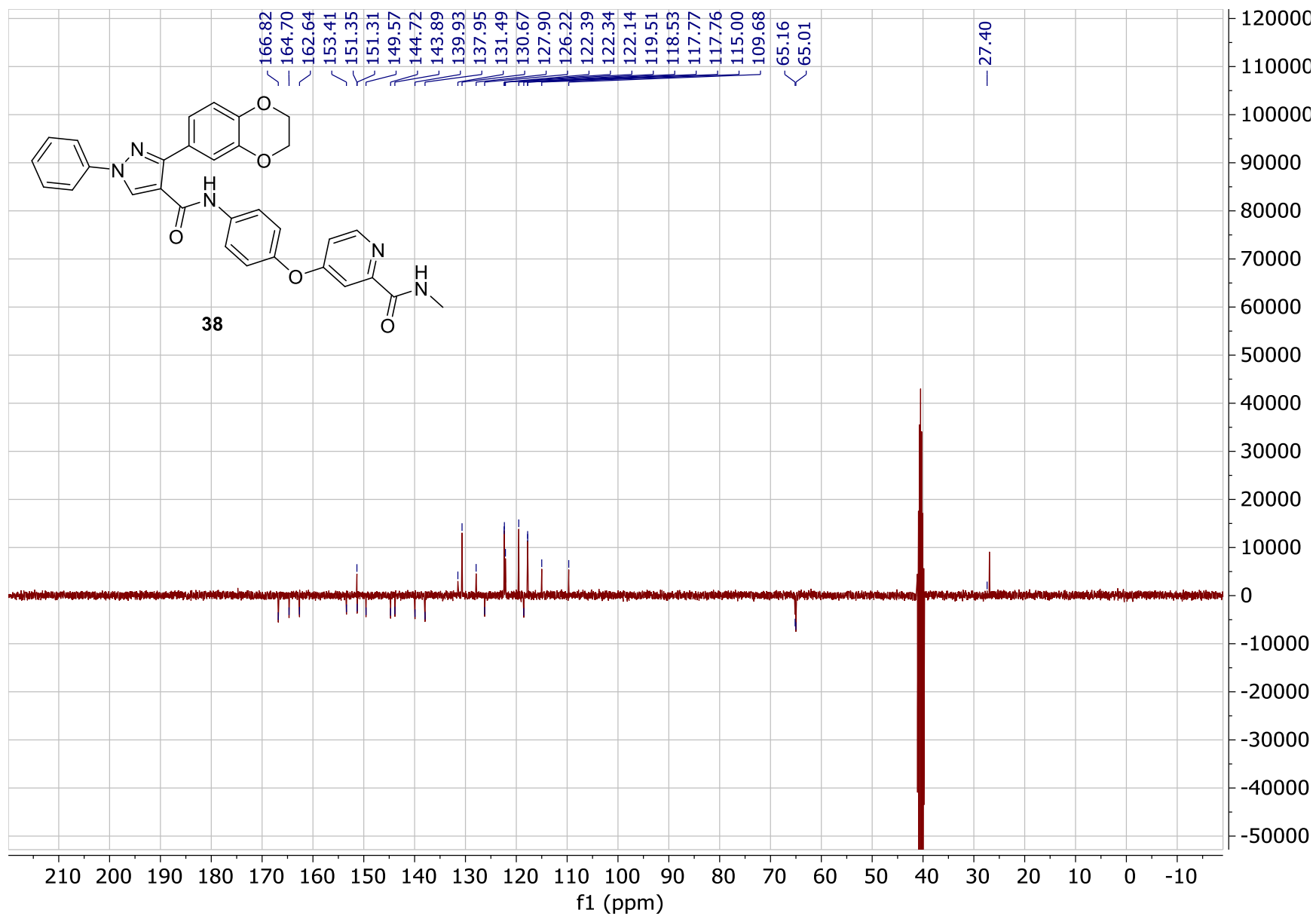


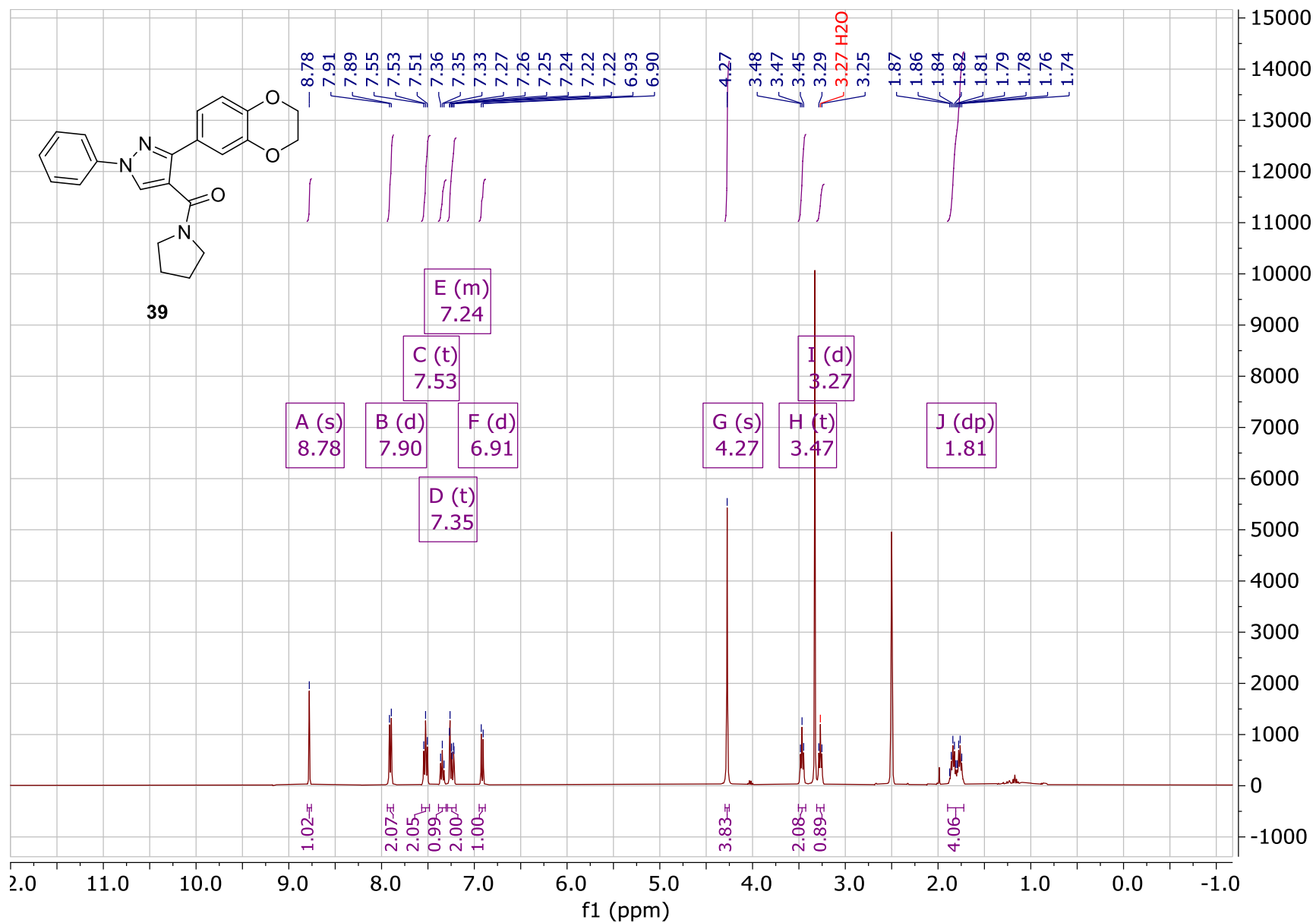
MB-2021-079B.10.fid

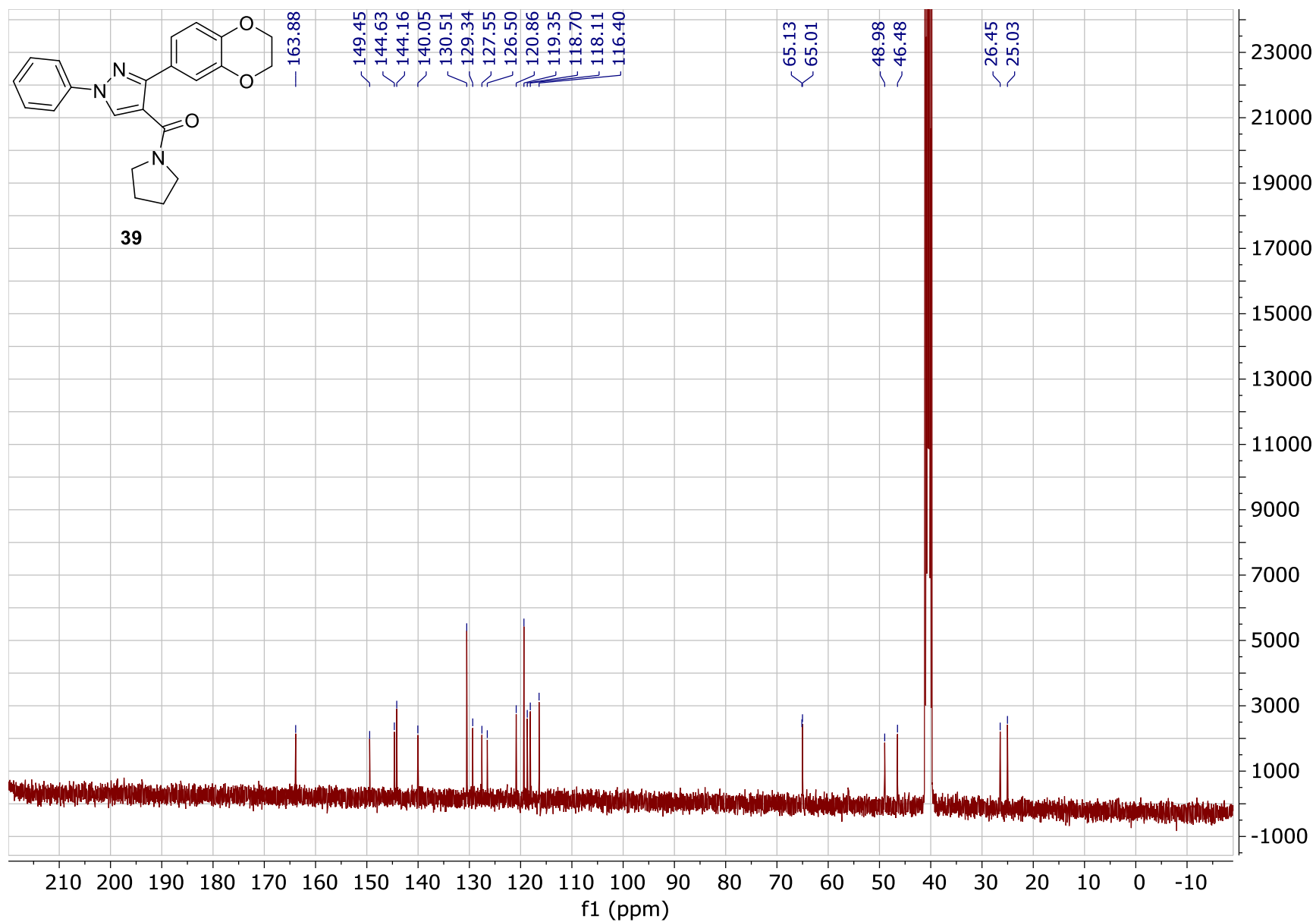


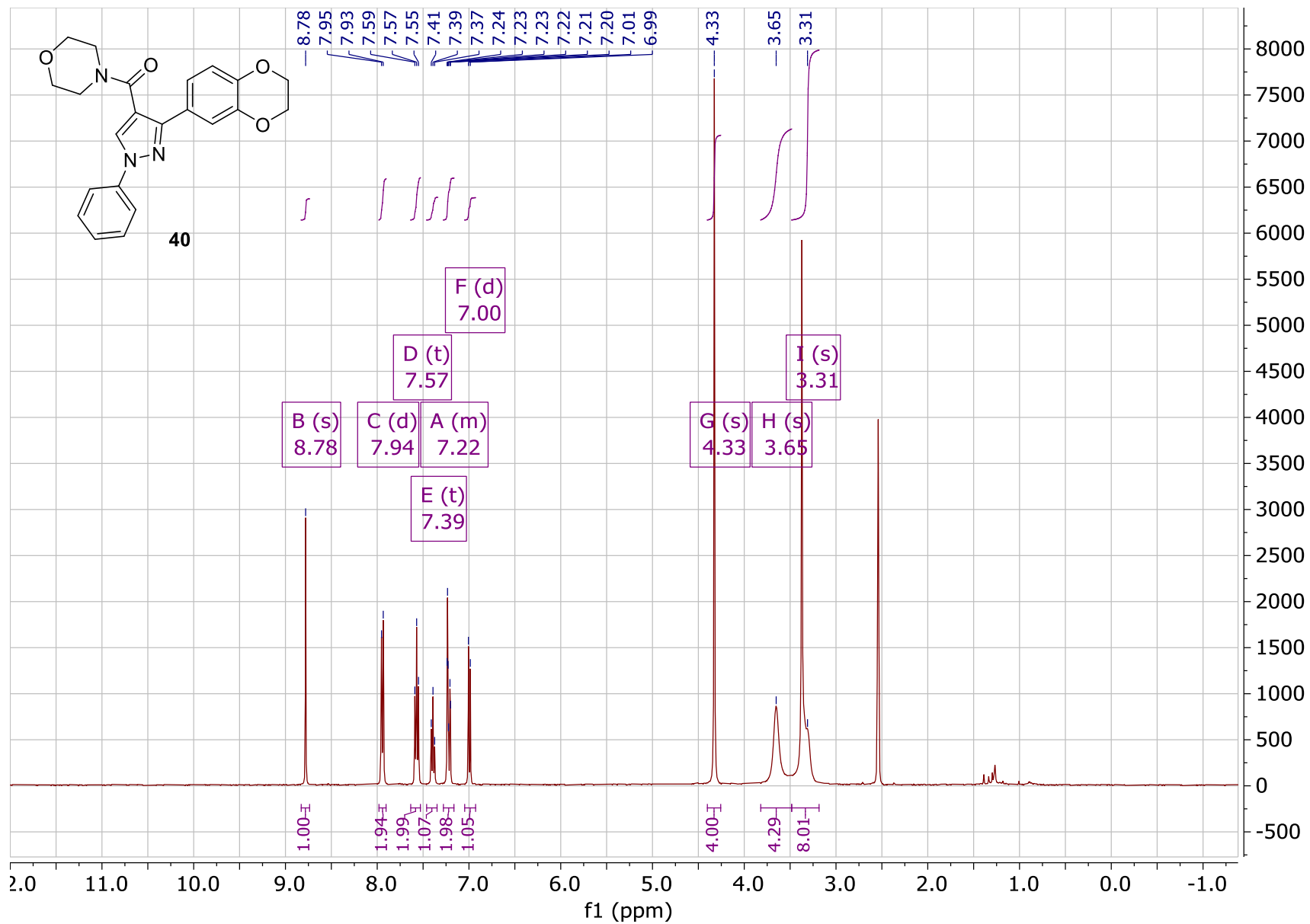


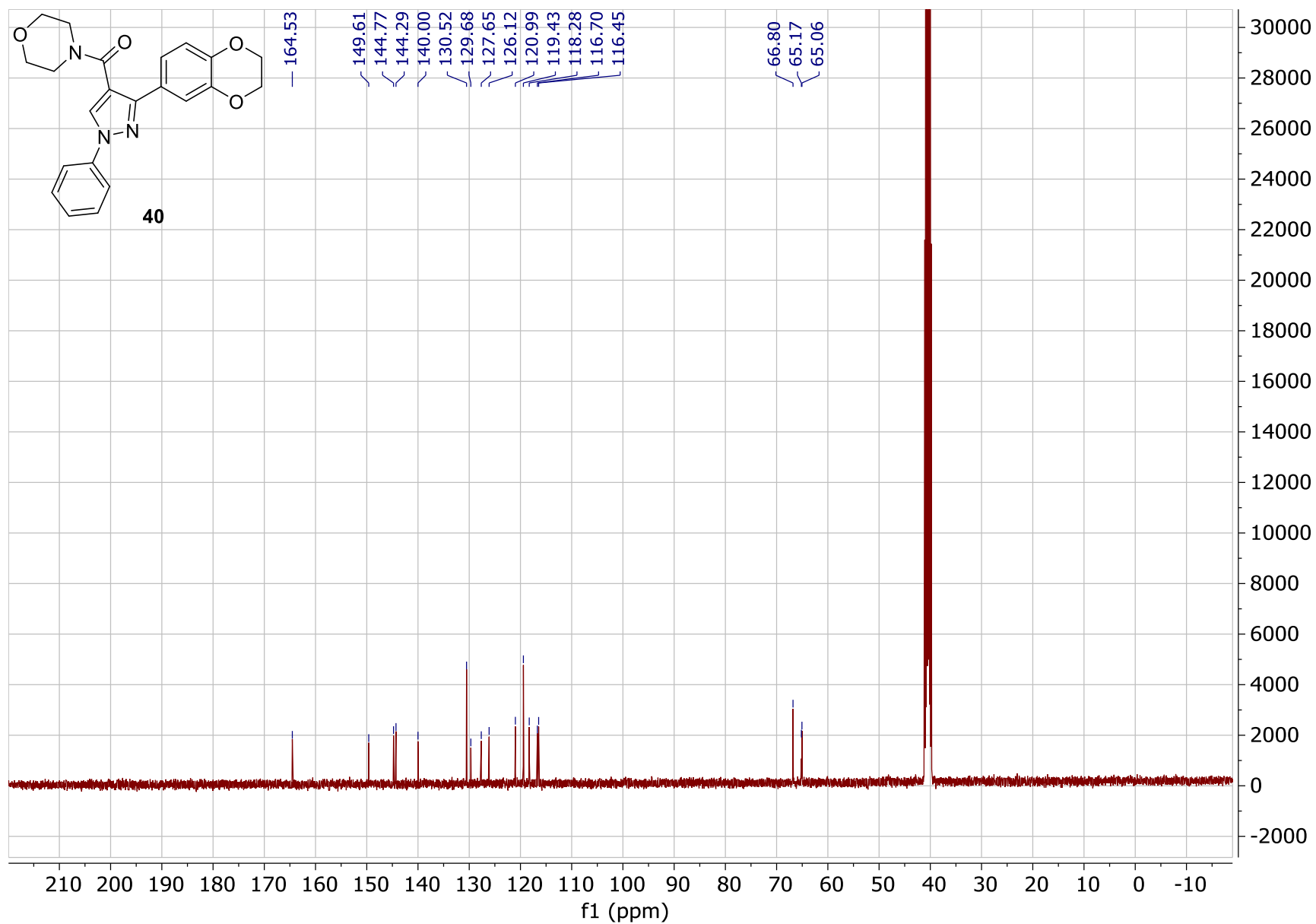




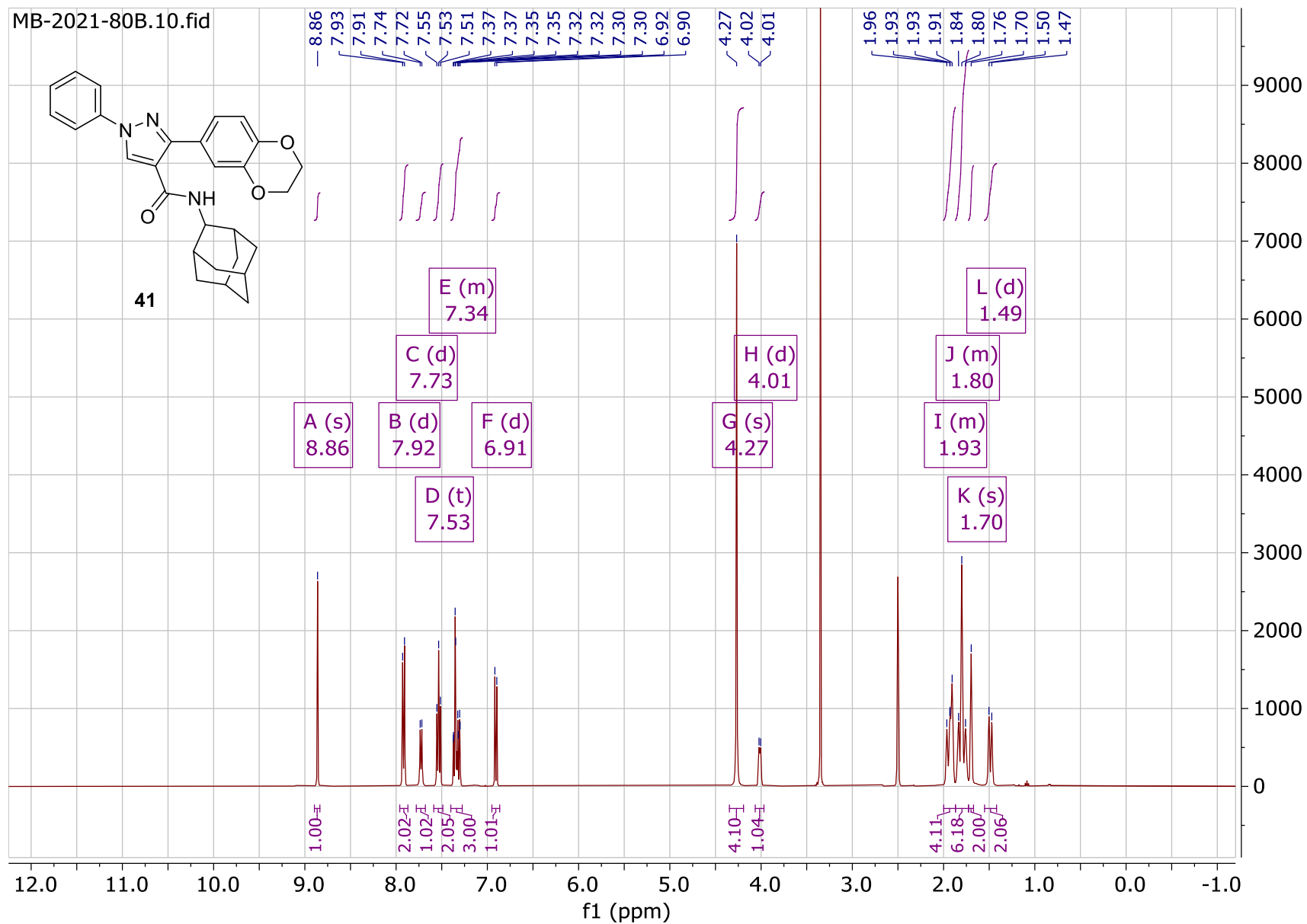
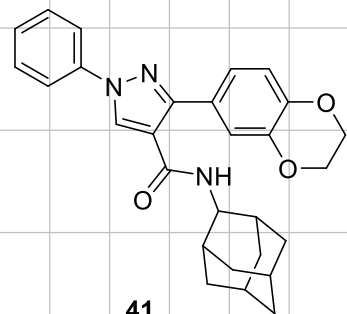


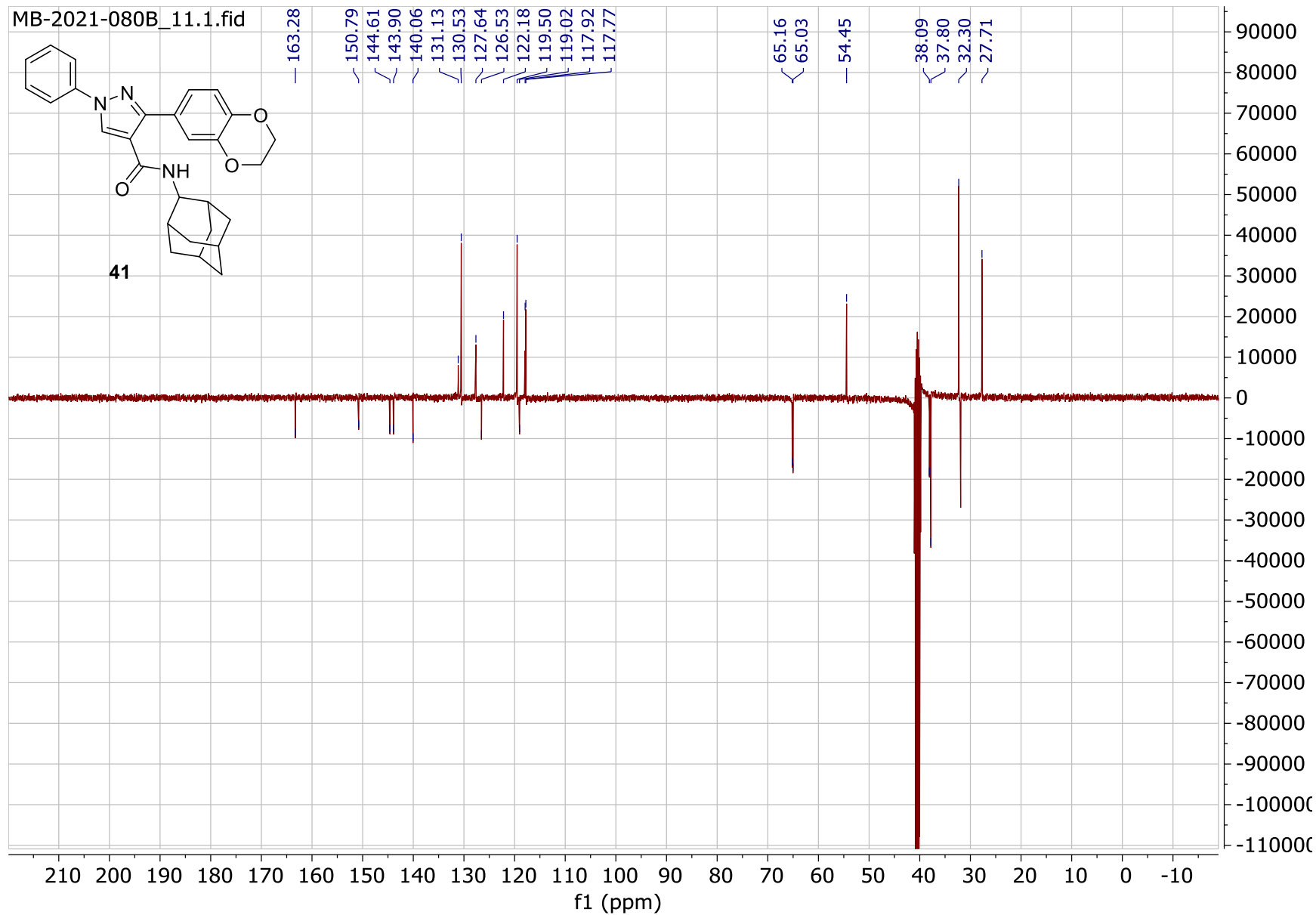




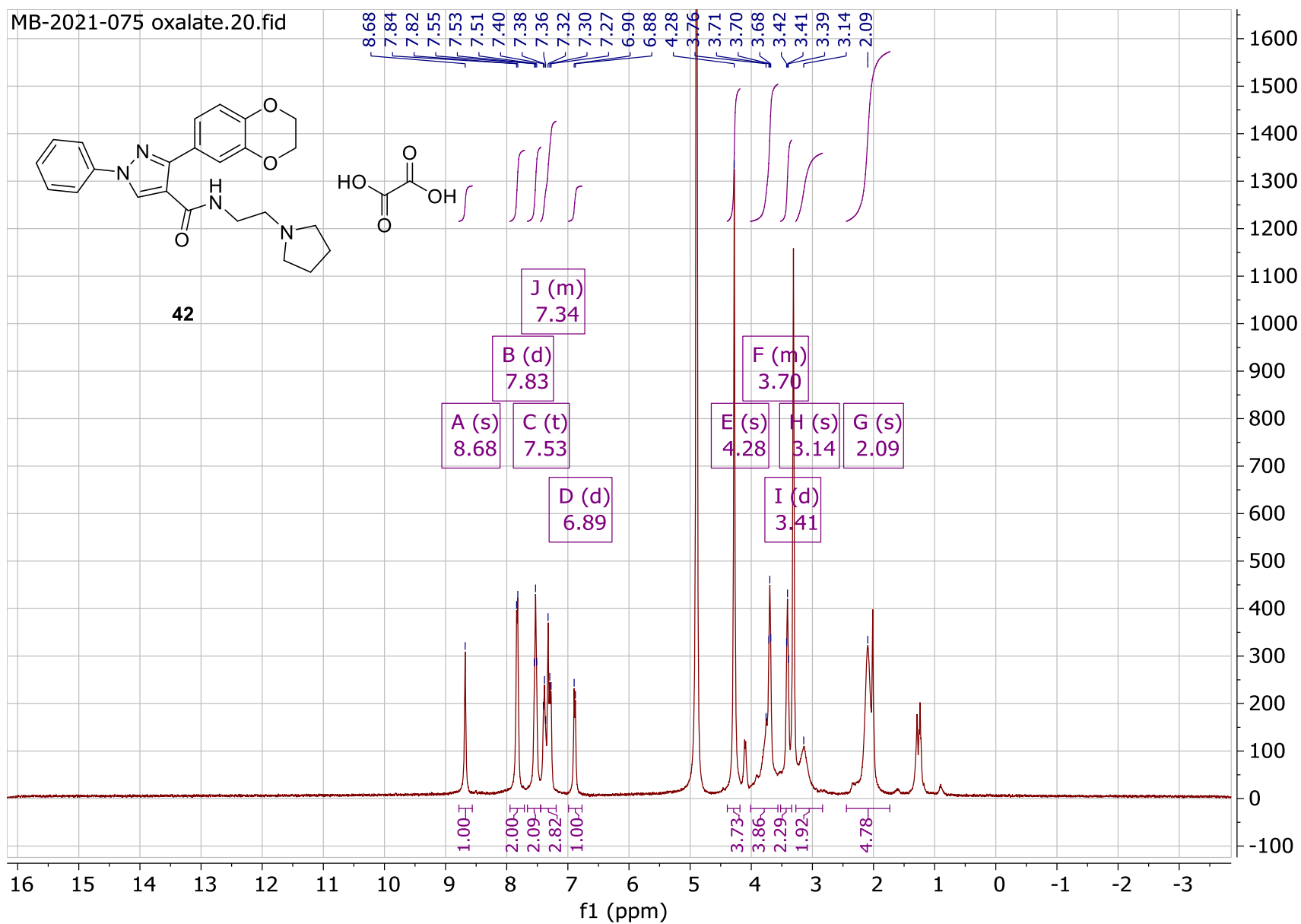


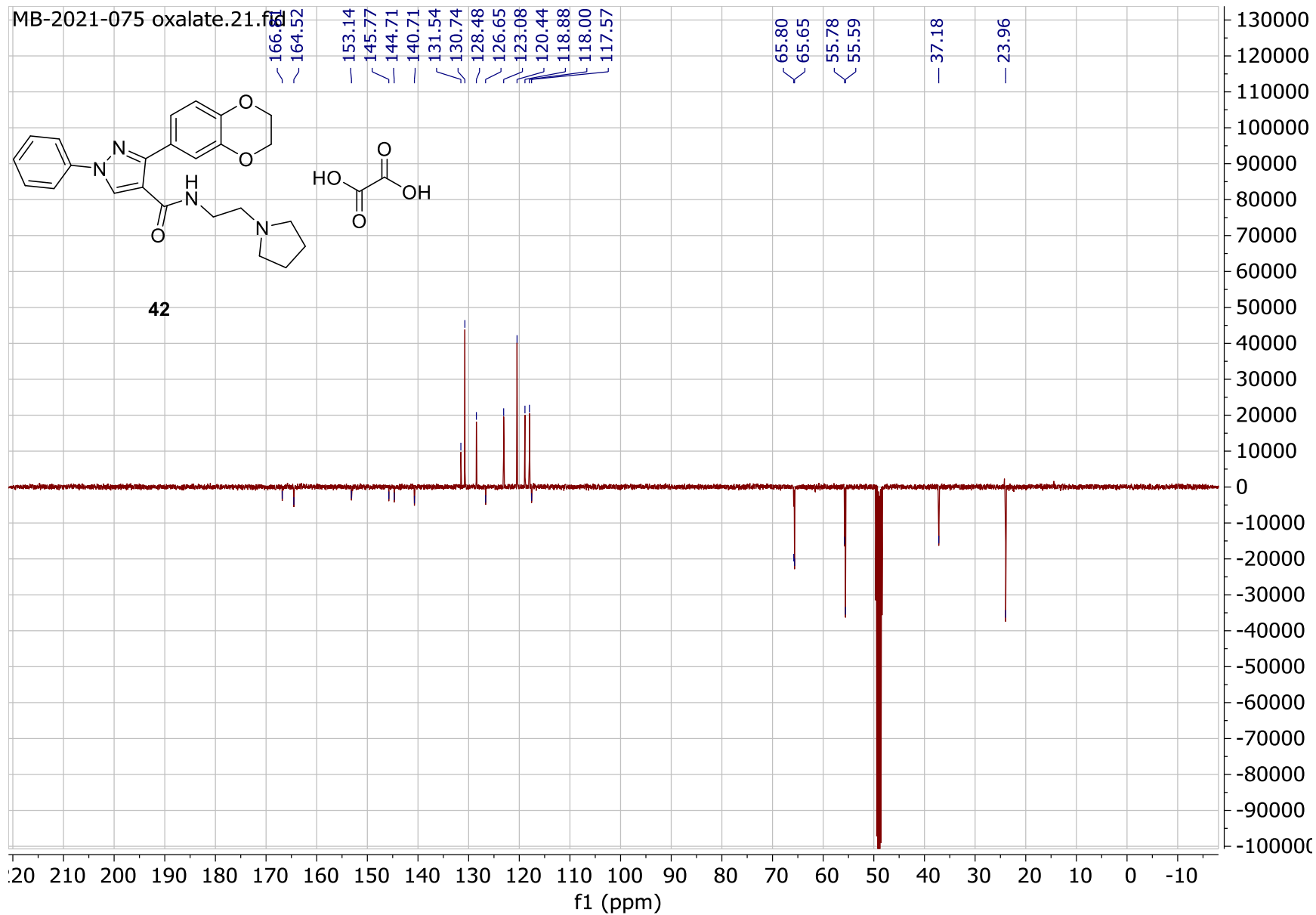
MB-2021-80B.10.fid



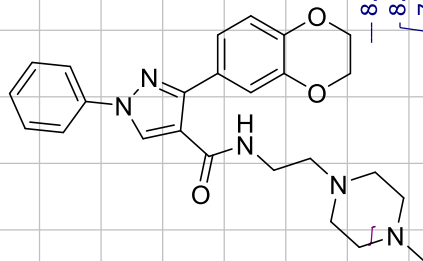


MB-2021-075 oxalate.20.fid

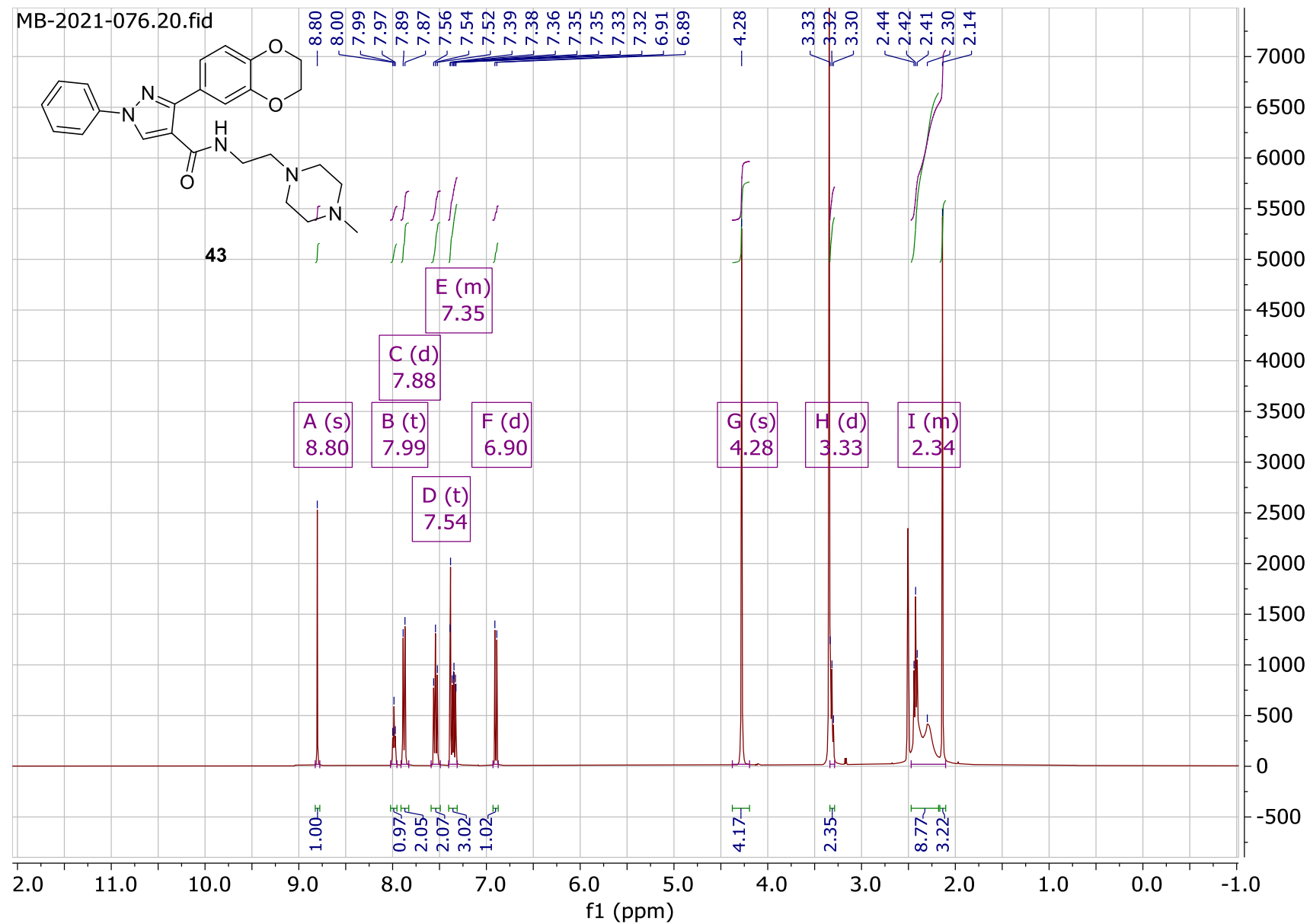


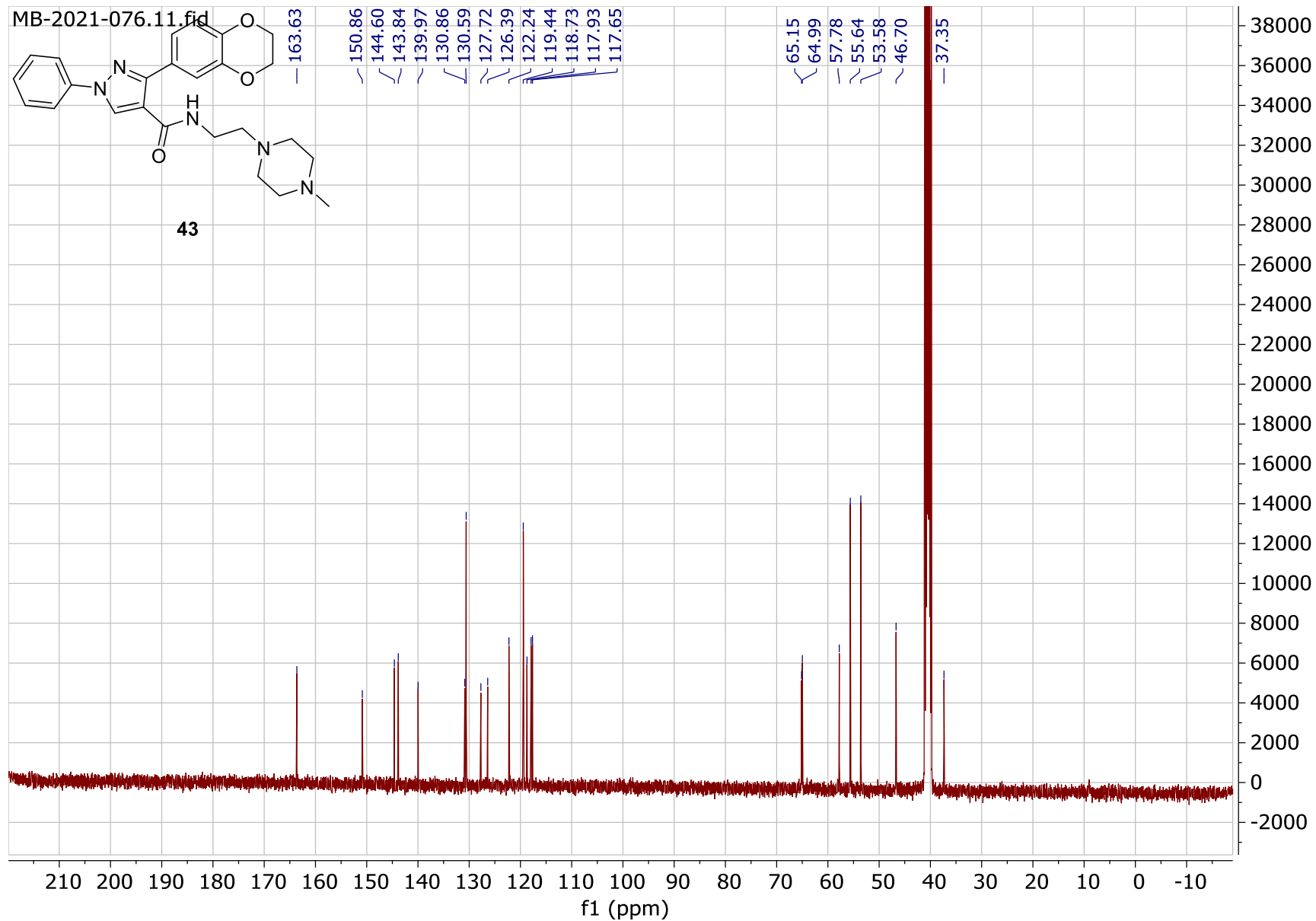


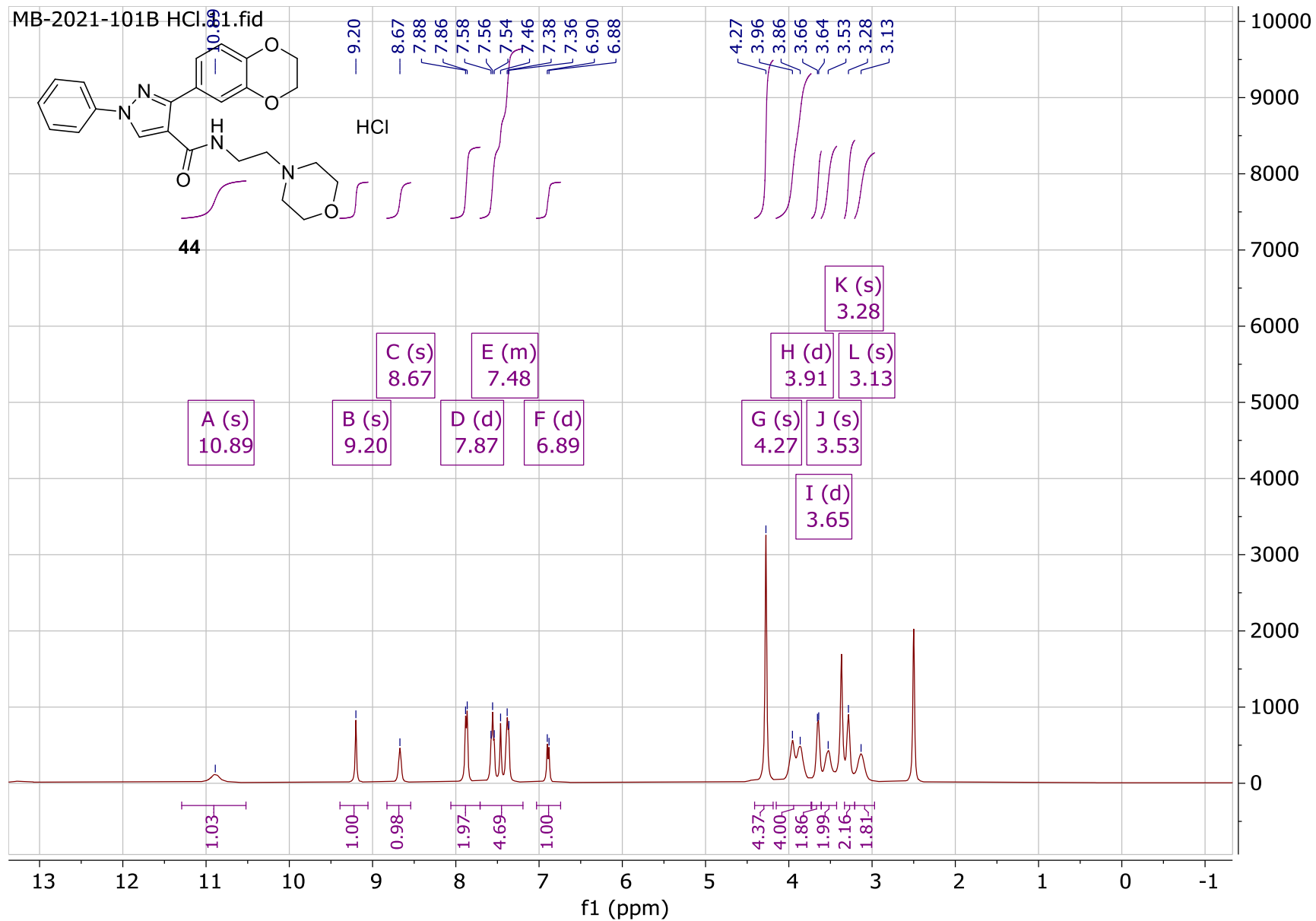
MB-2021-076.20.fid

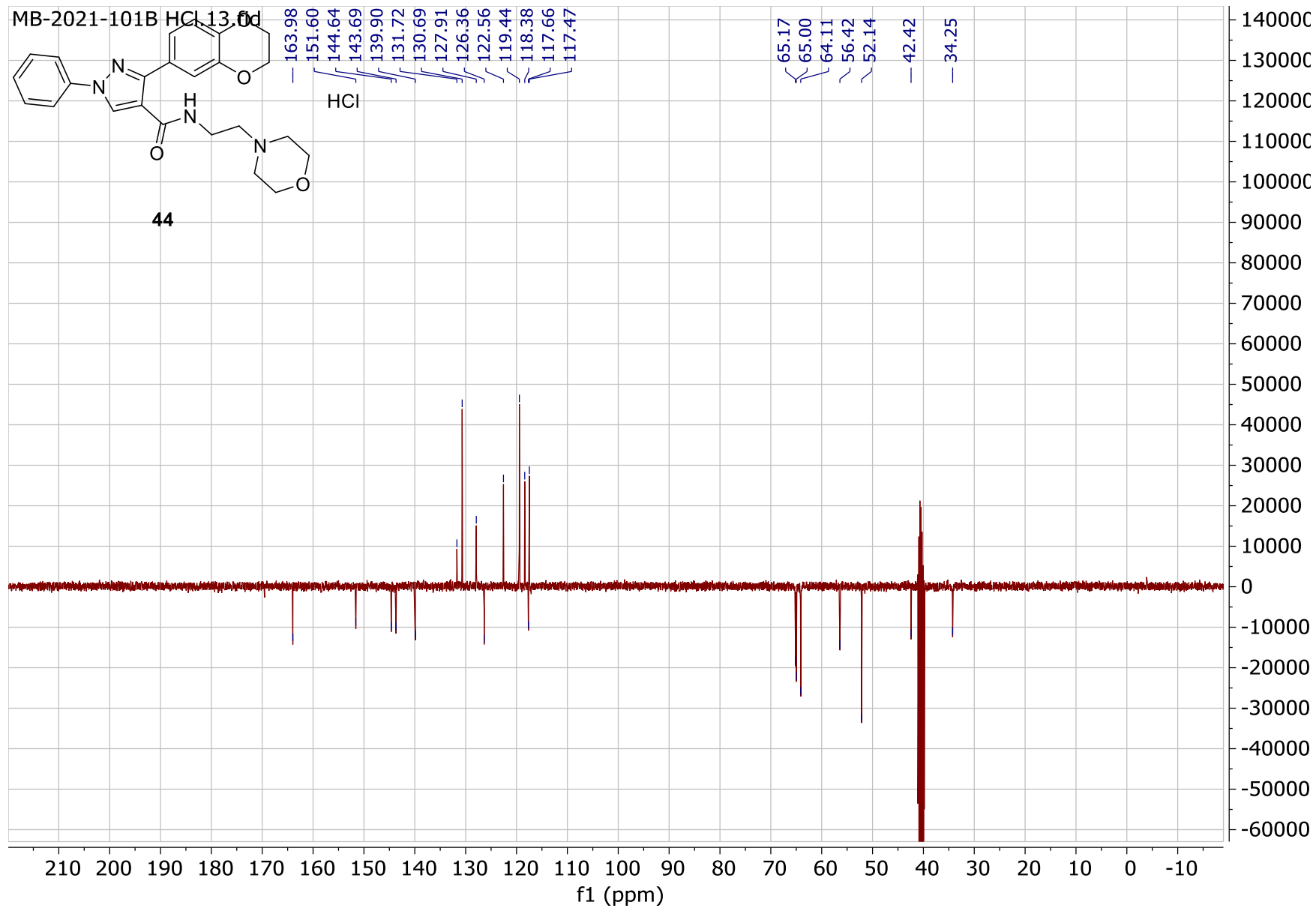


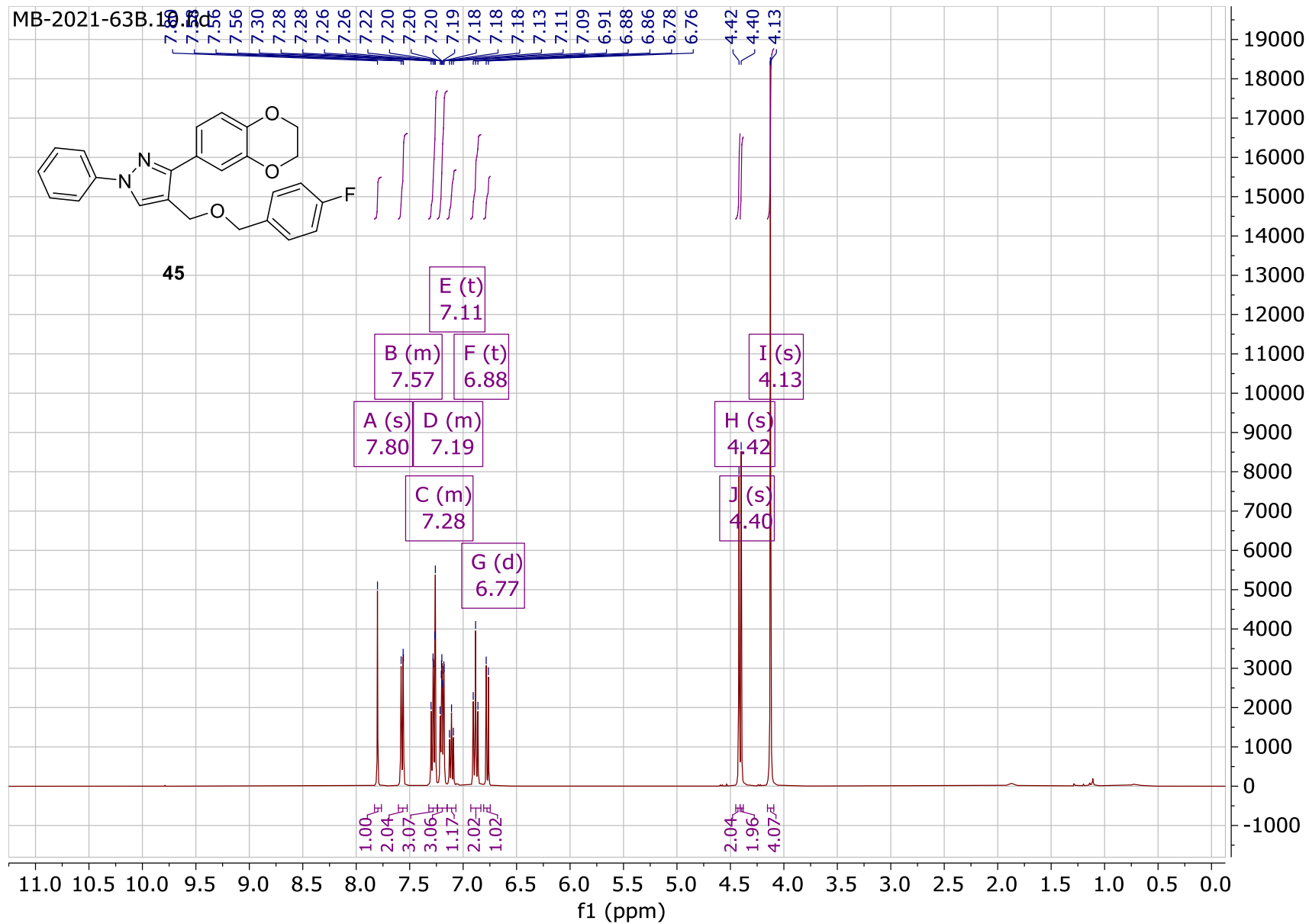
43

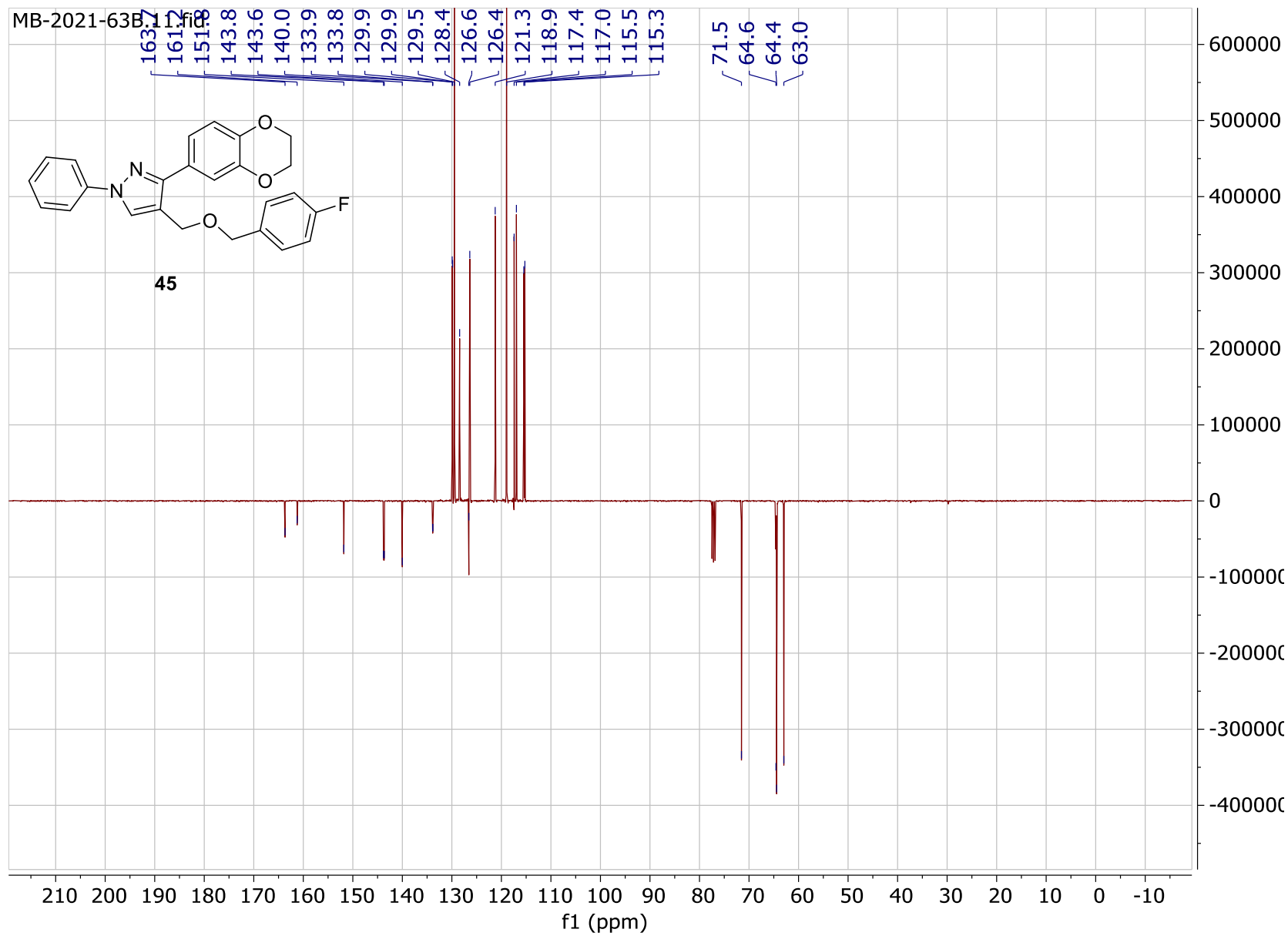


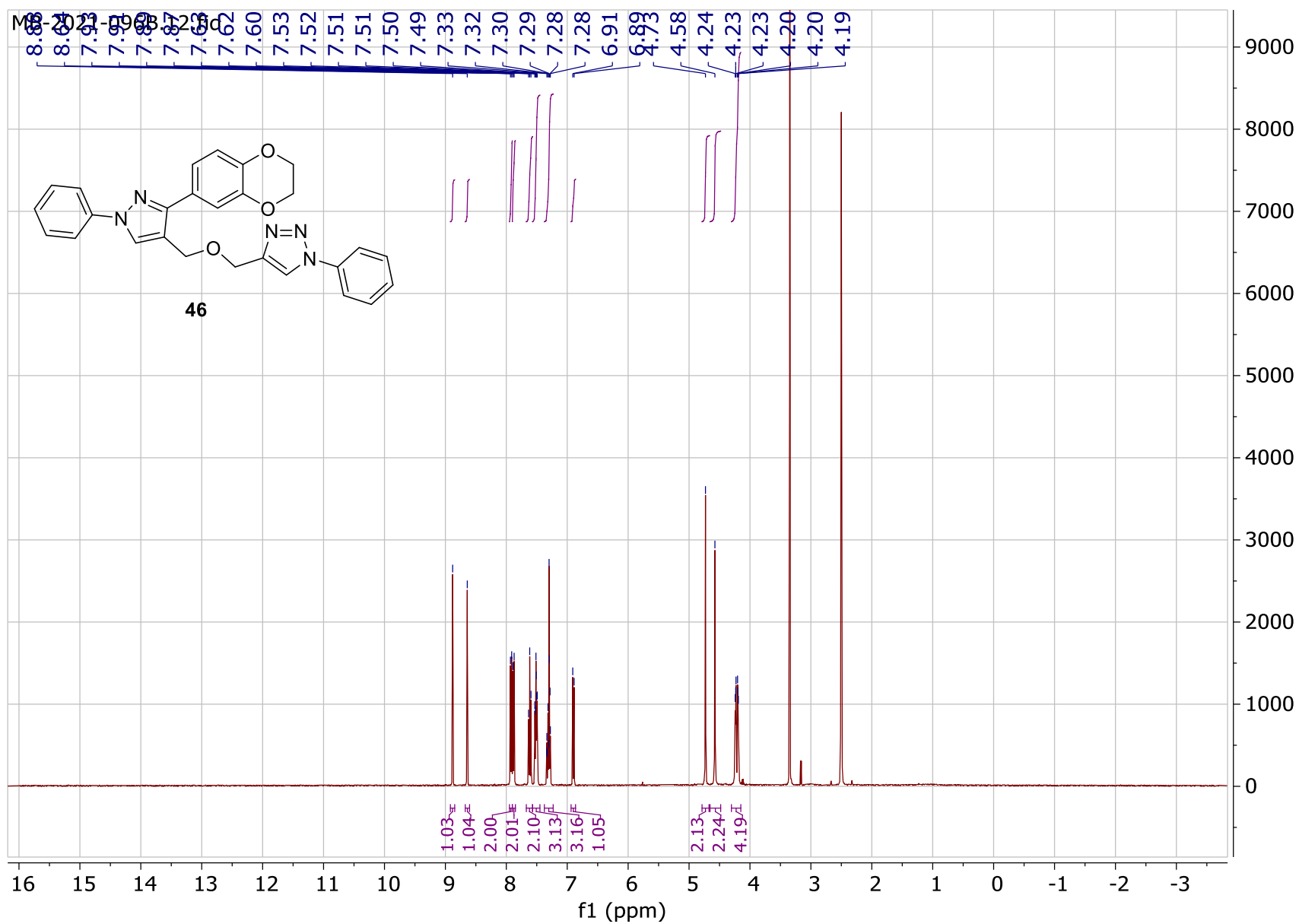




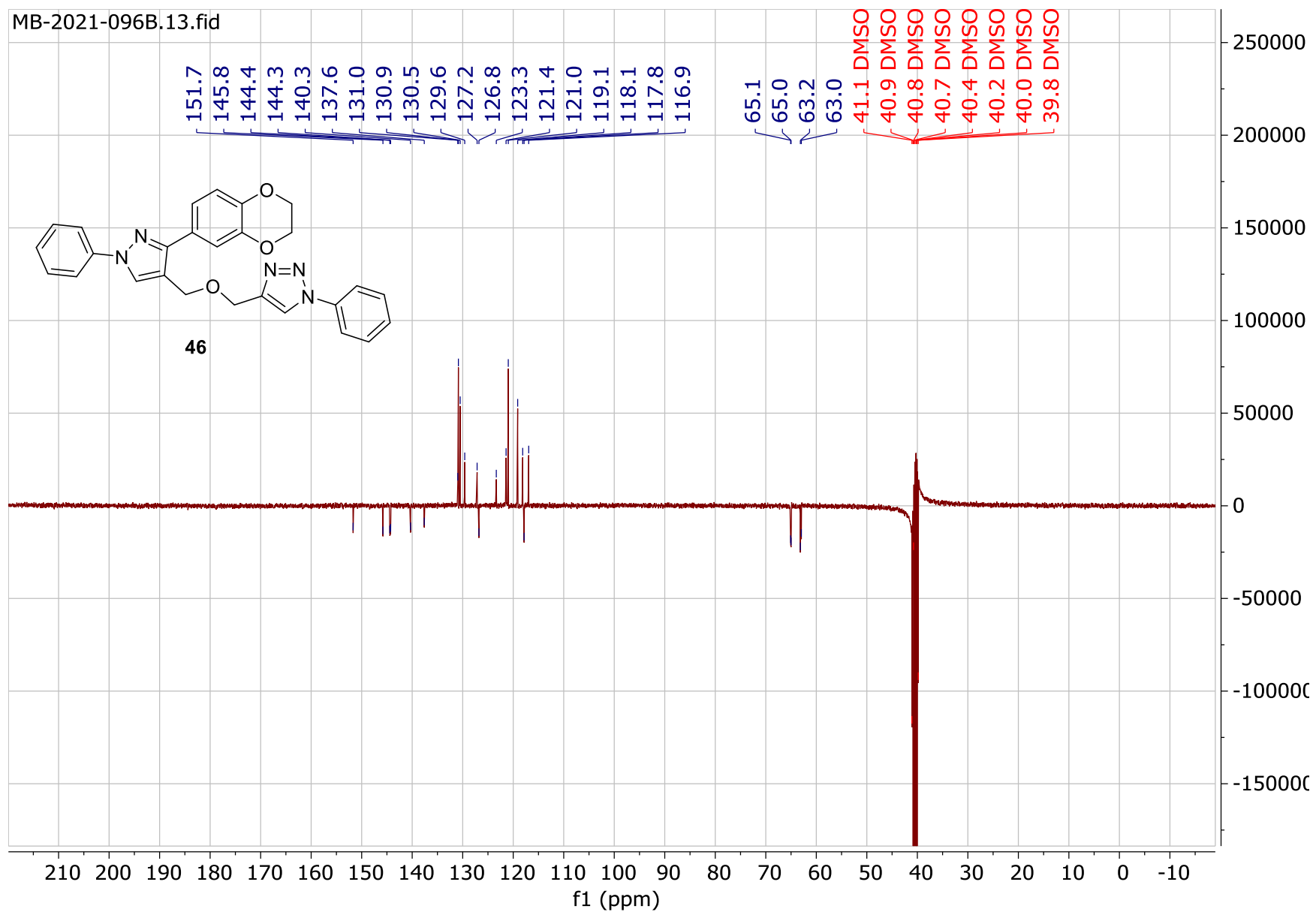


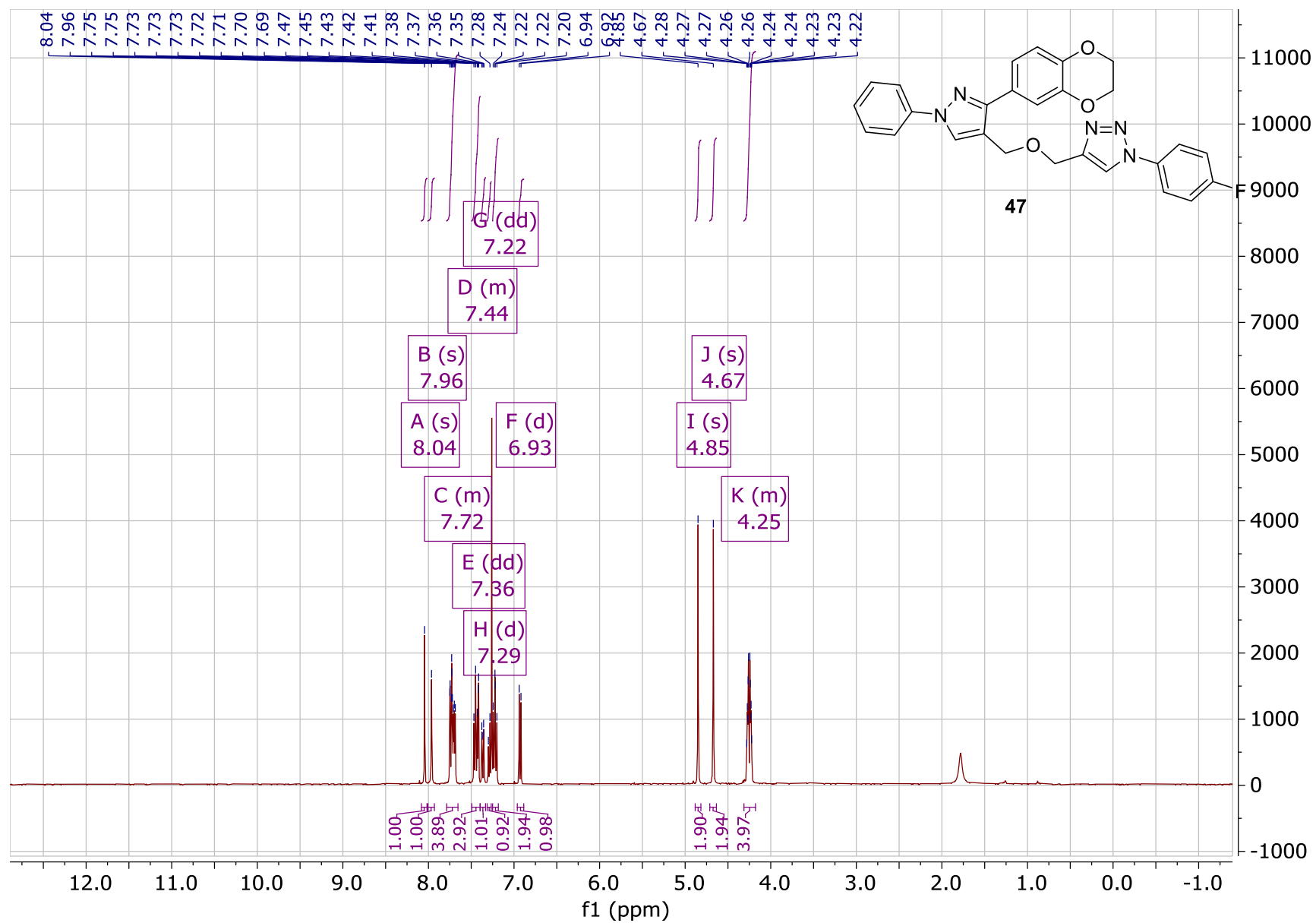


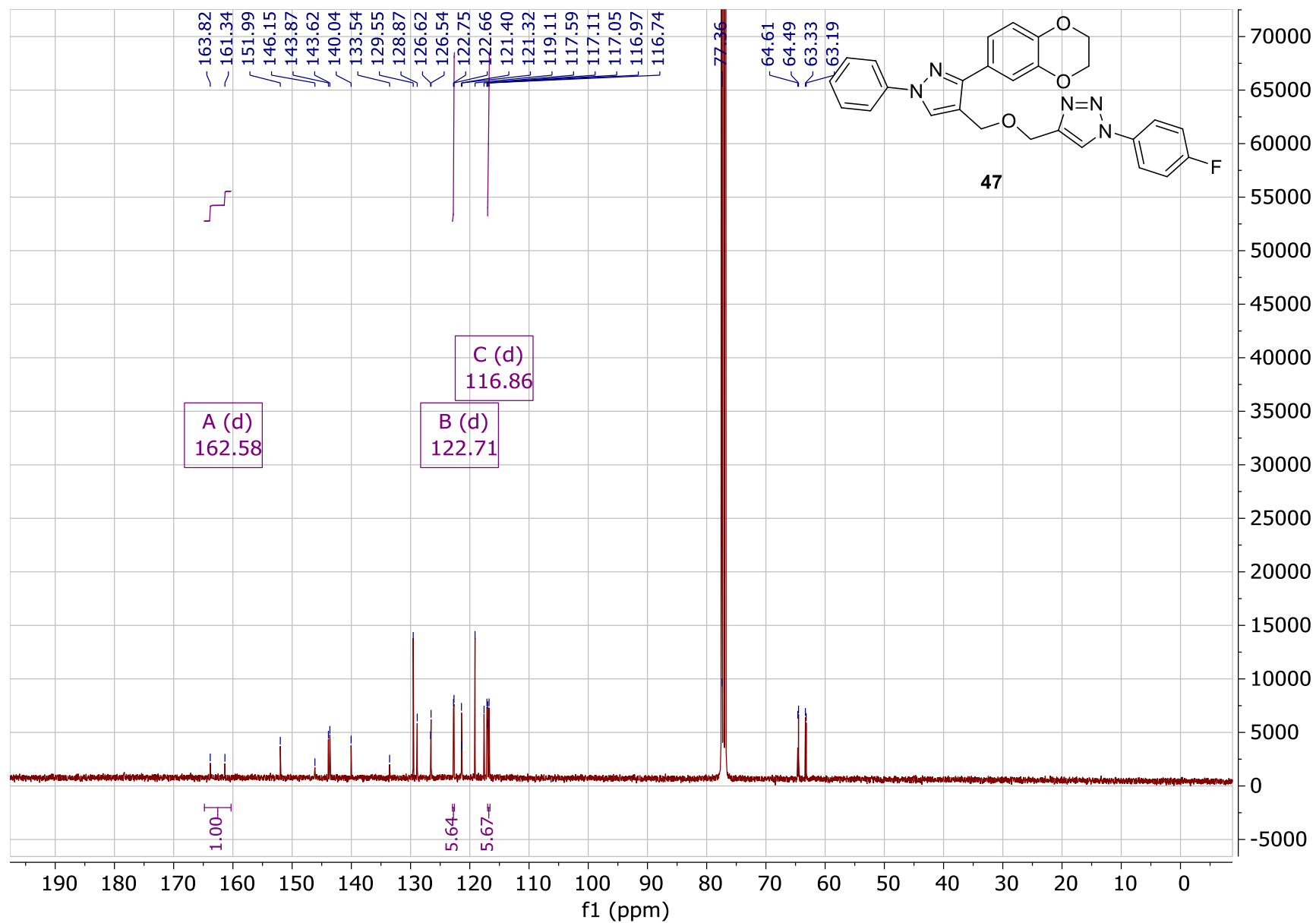




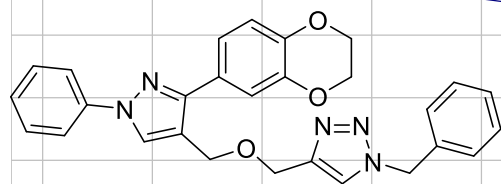
MB-2021-096B.13.fid



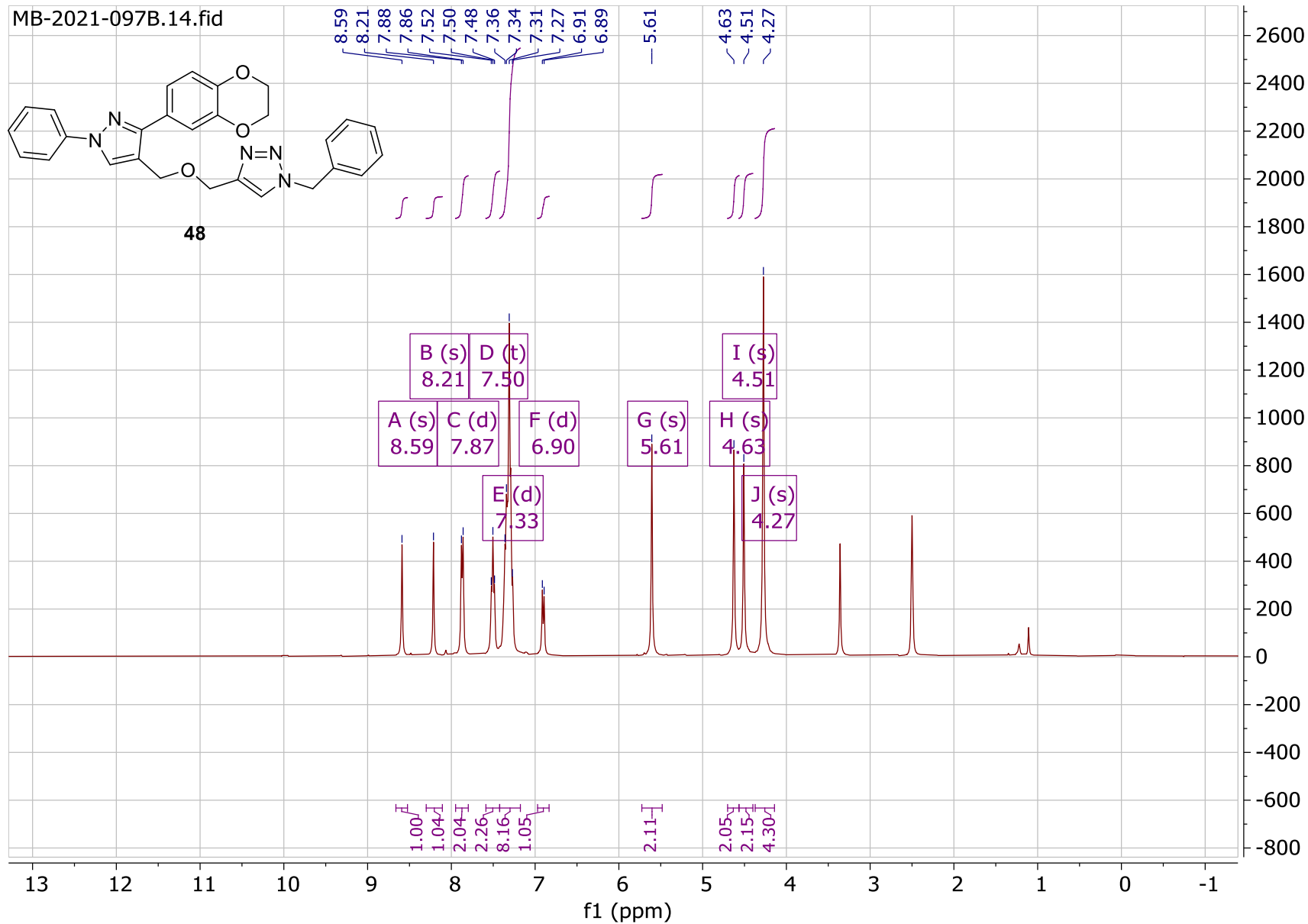


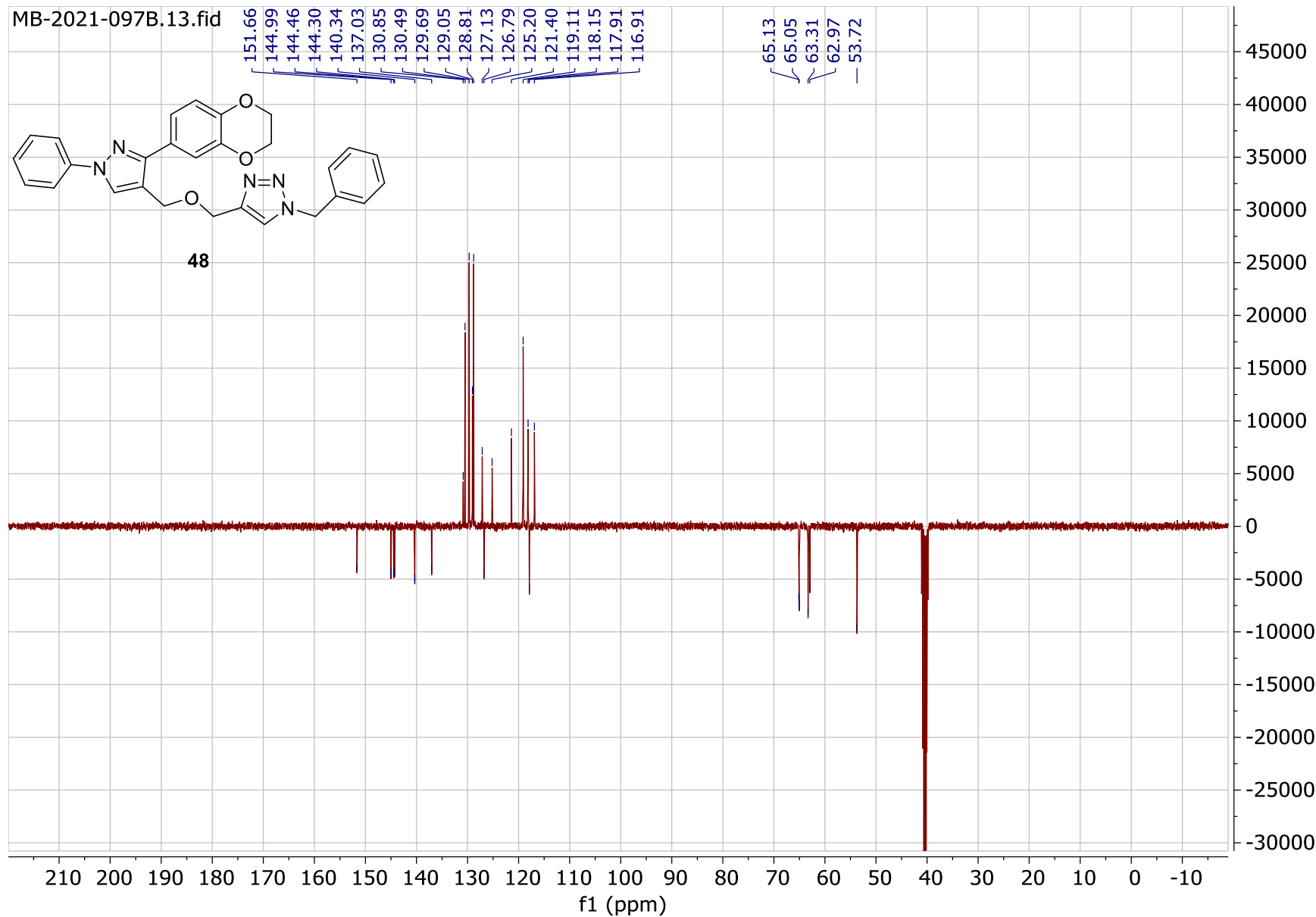


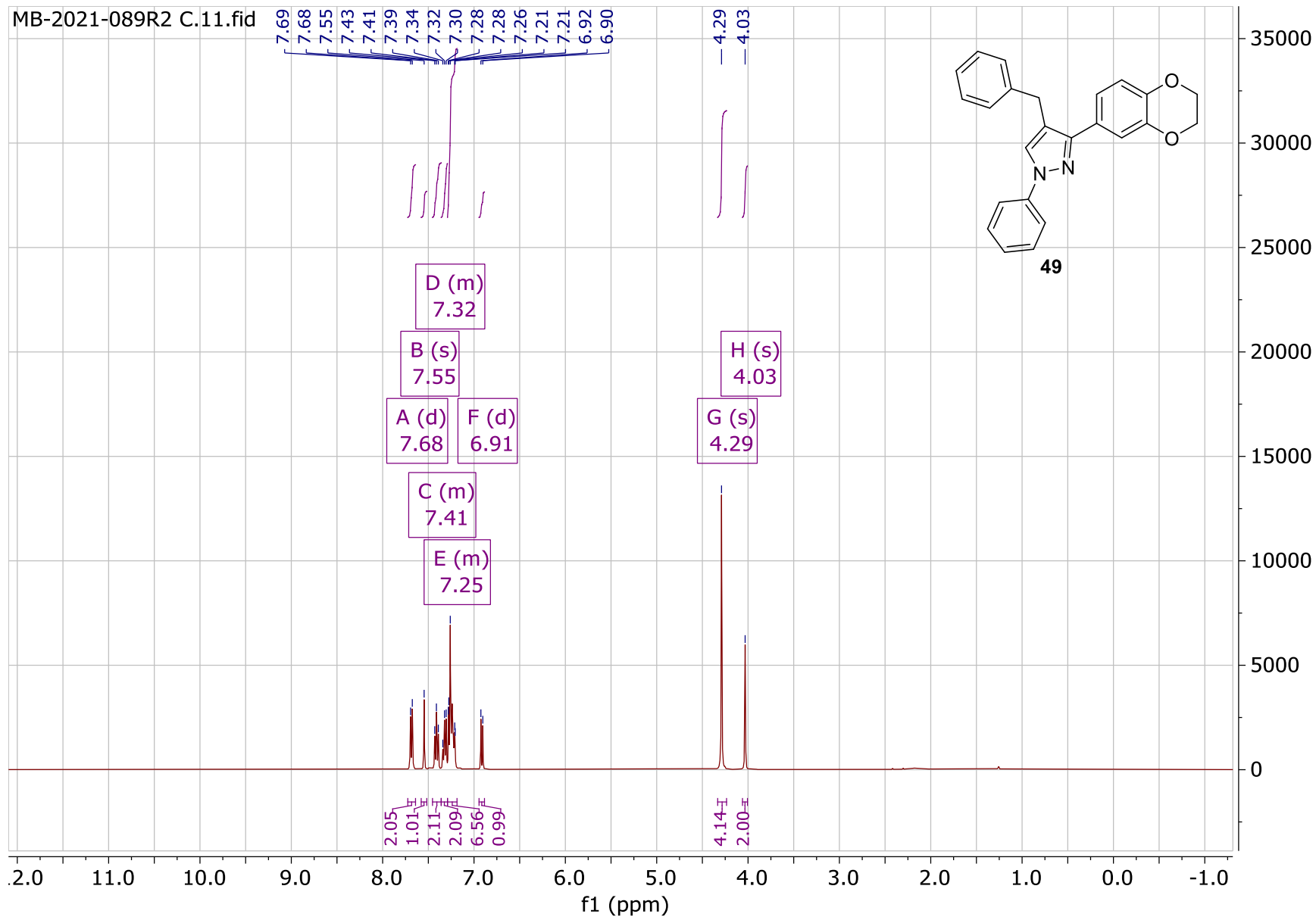
MB-2021-097B.14.fid



48



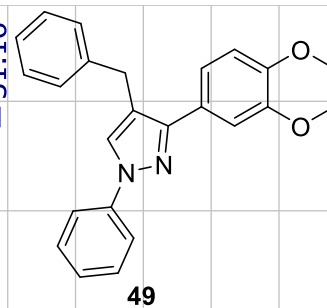




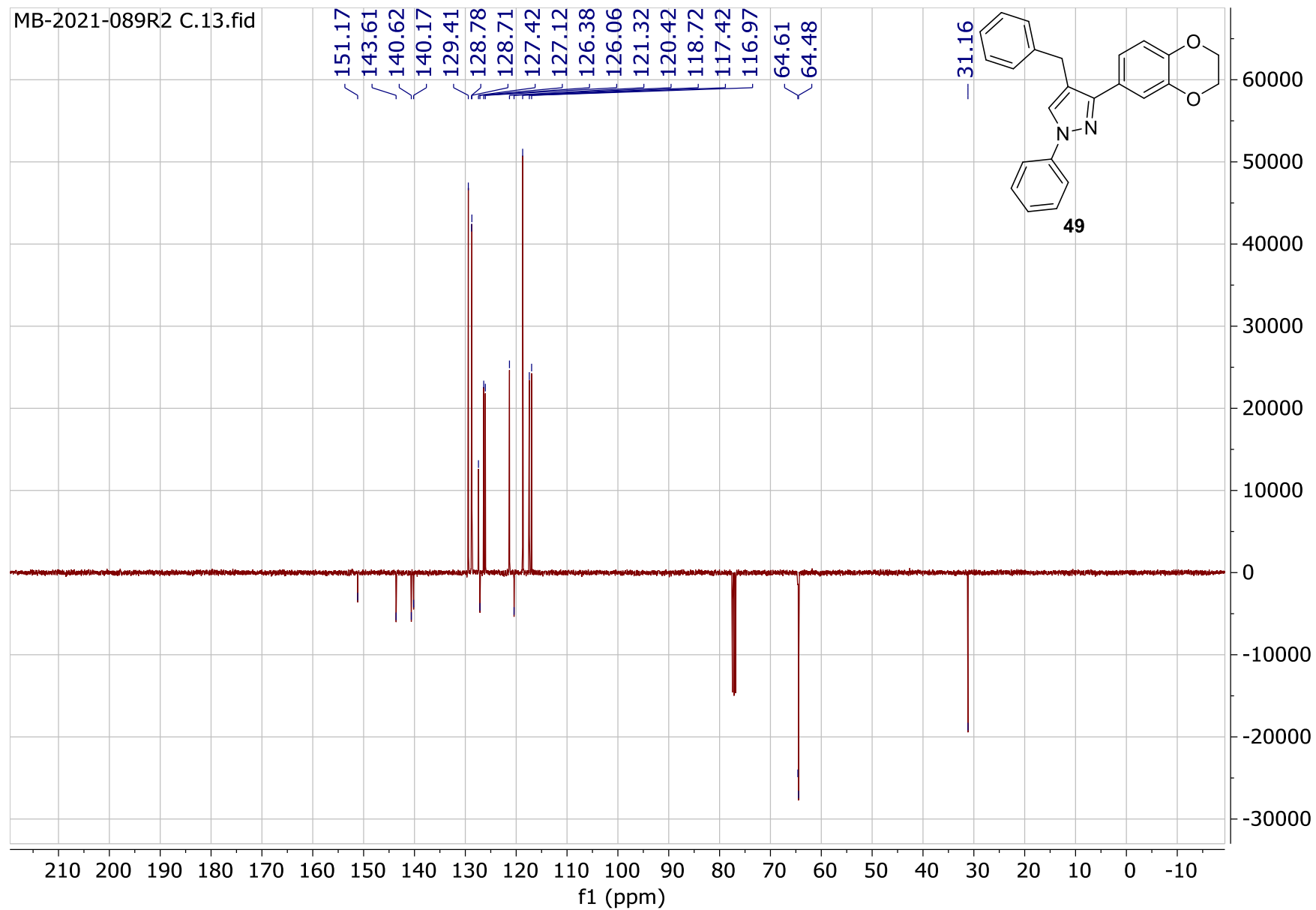
MB-2021-089R2 C.13.fid

151.17
143.61
140.62
140.17
129.41
128.78
128.71
127.42
127.12
126.38
126.06
121.32
120.42
118.72
117.42
116.97
64.61
64.48

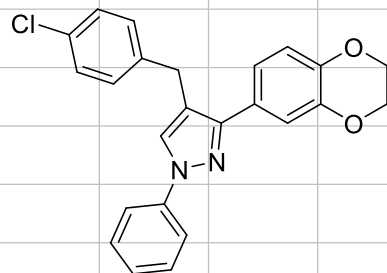
31.16



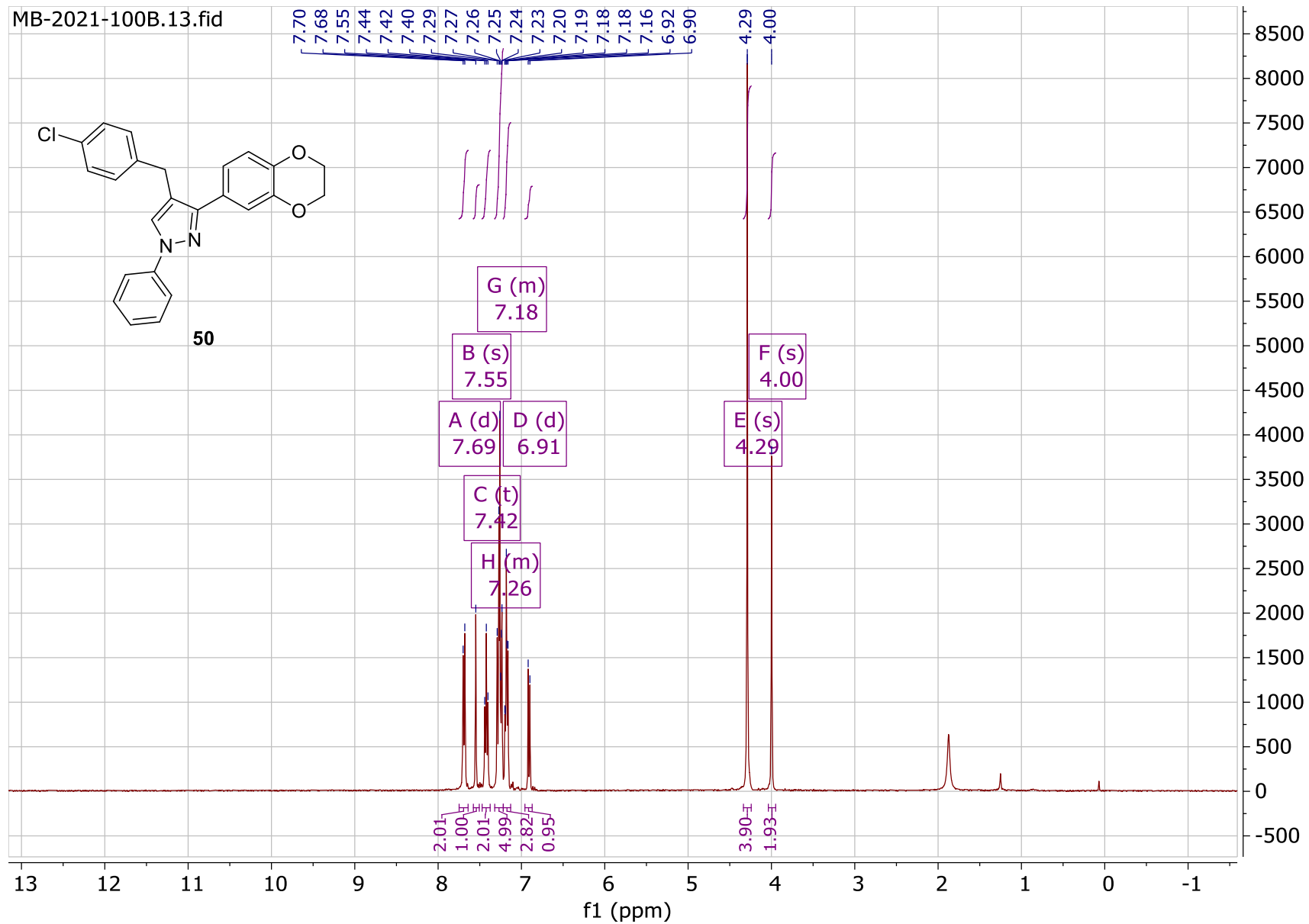
49

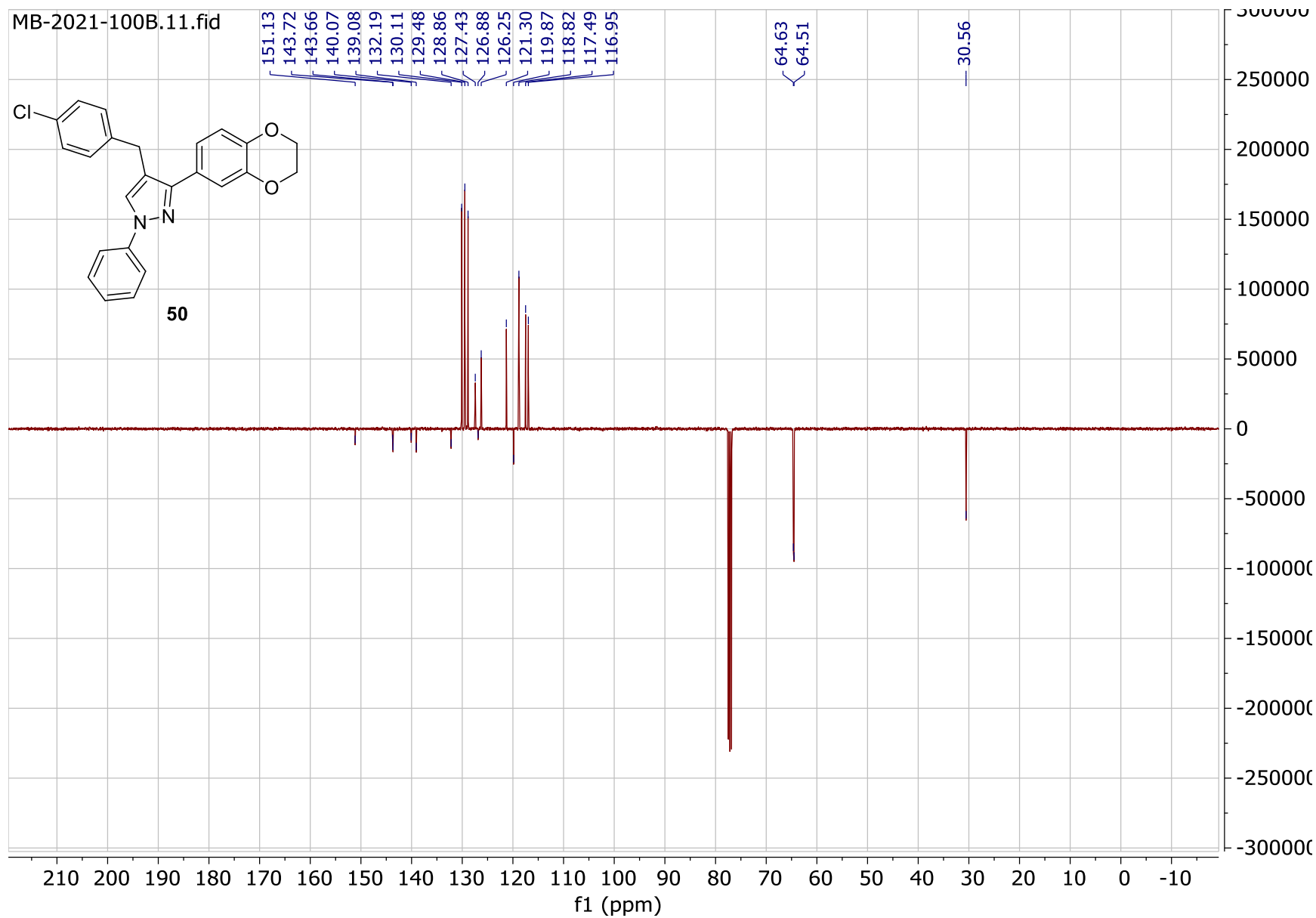


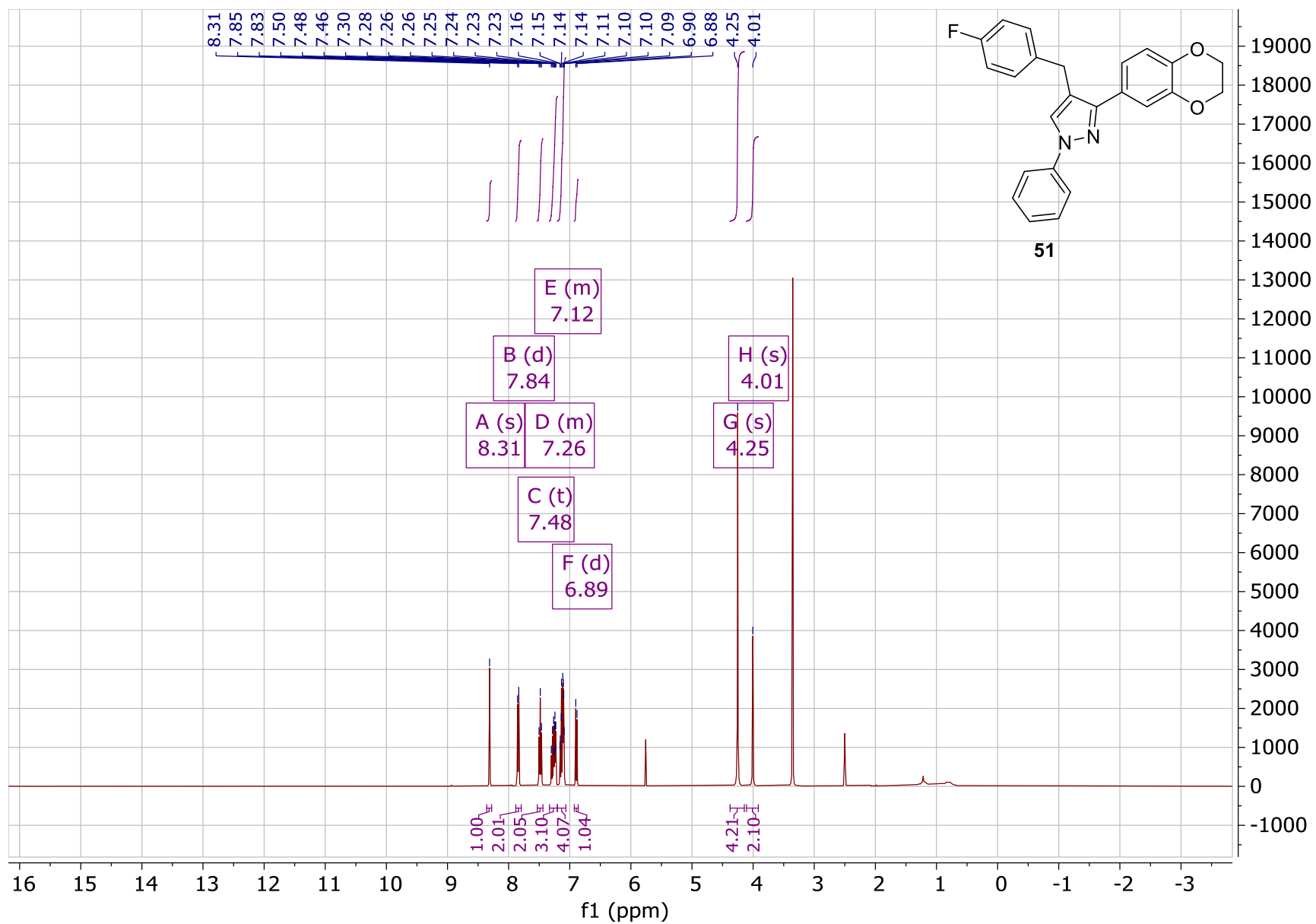
MB-2021-100B.13.fid

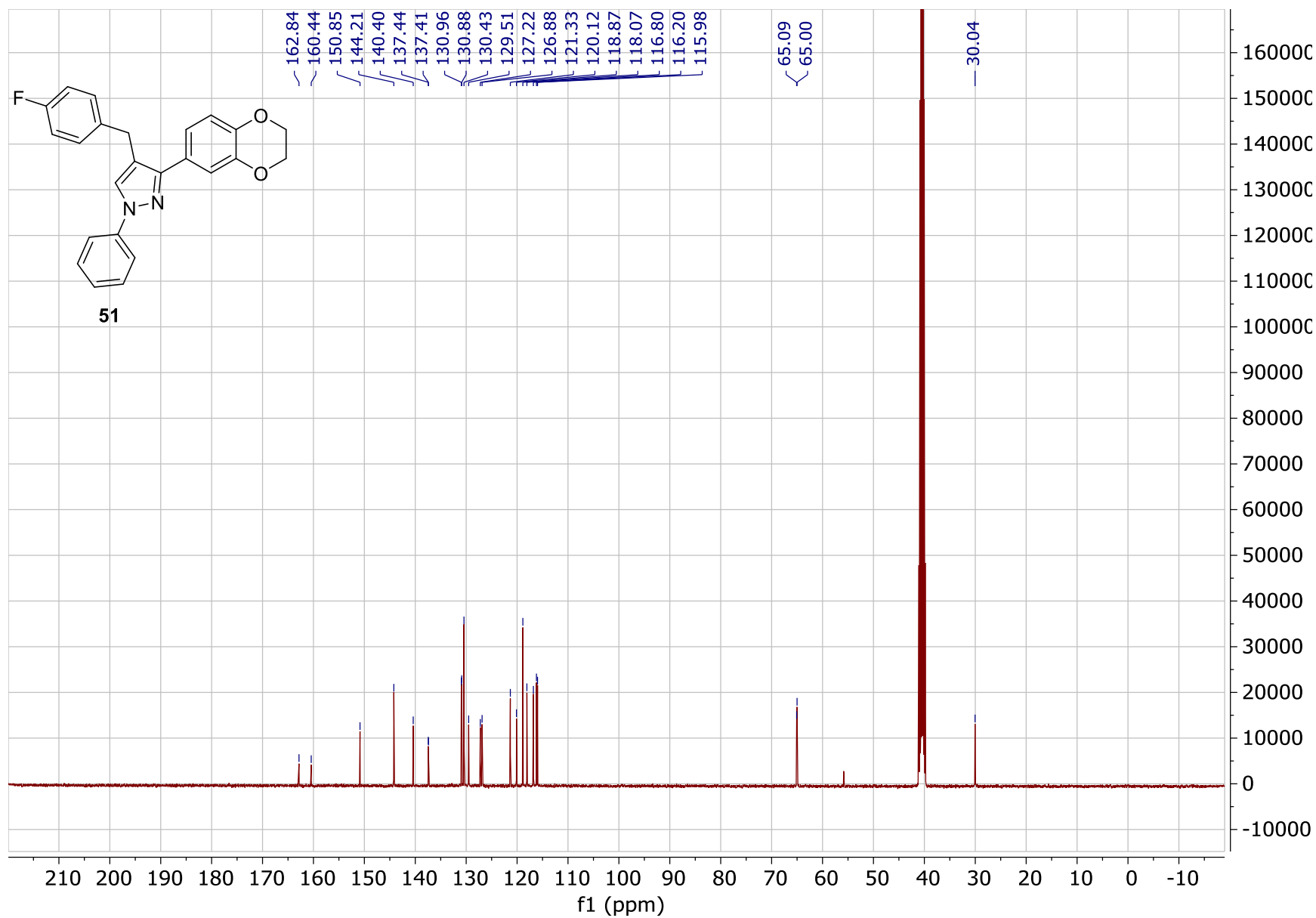


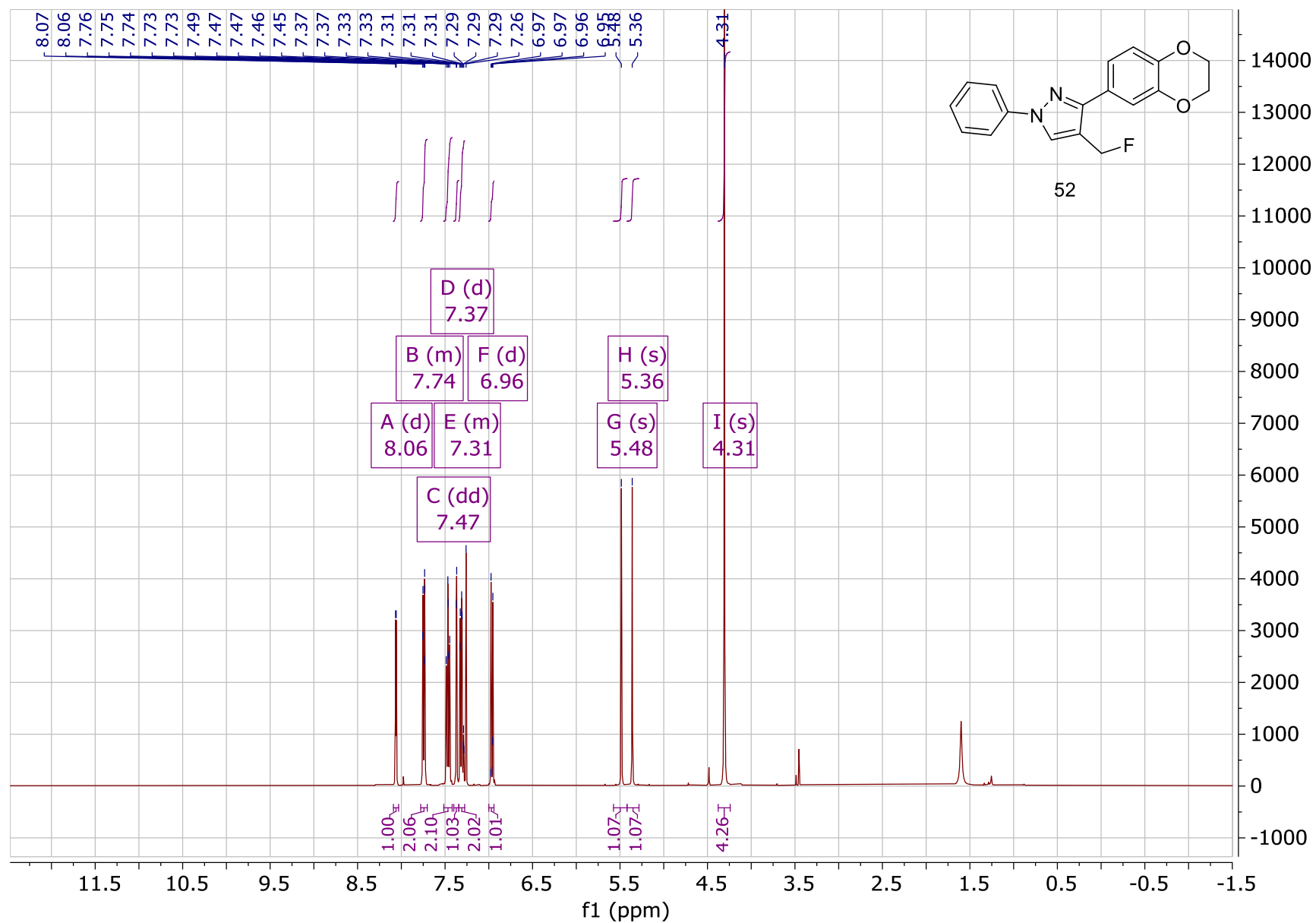
50

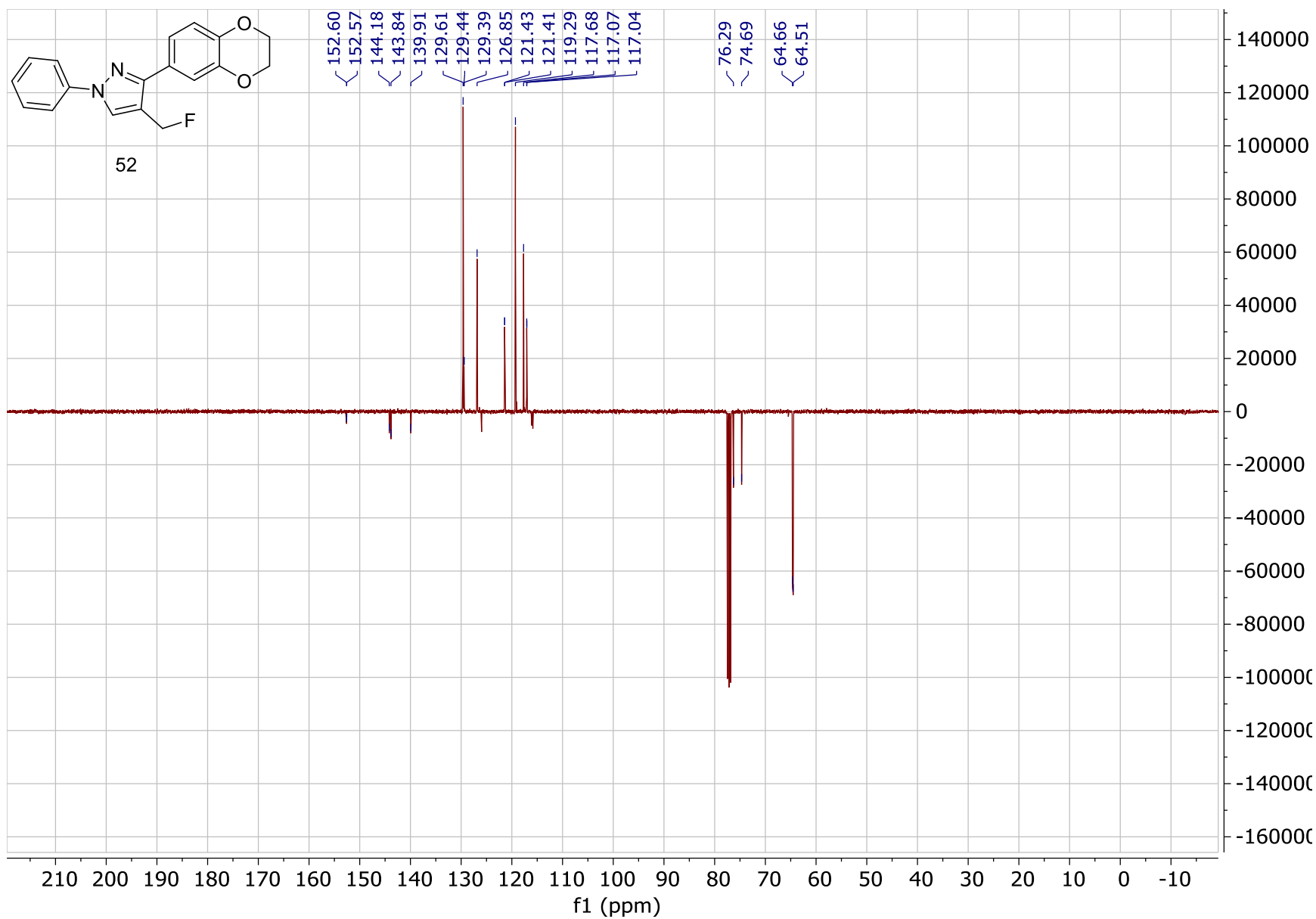


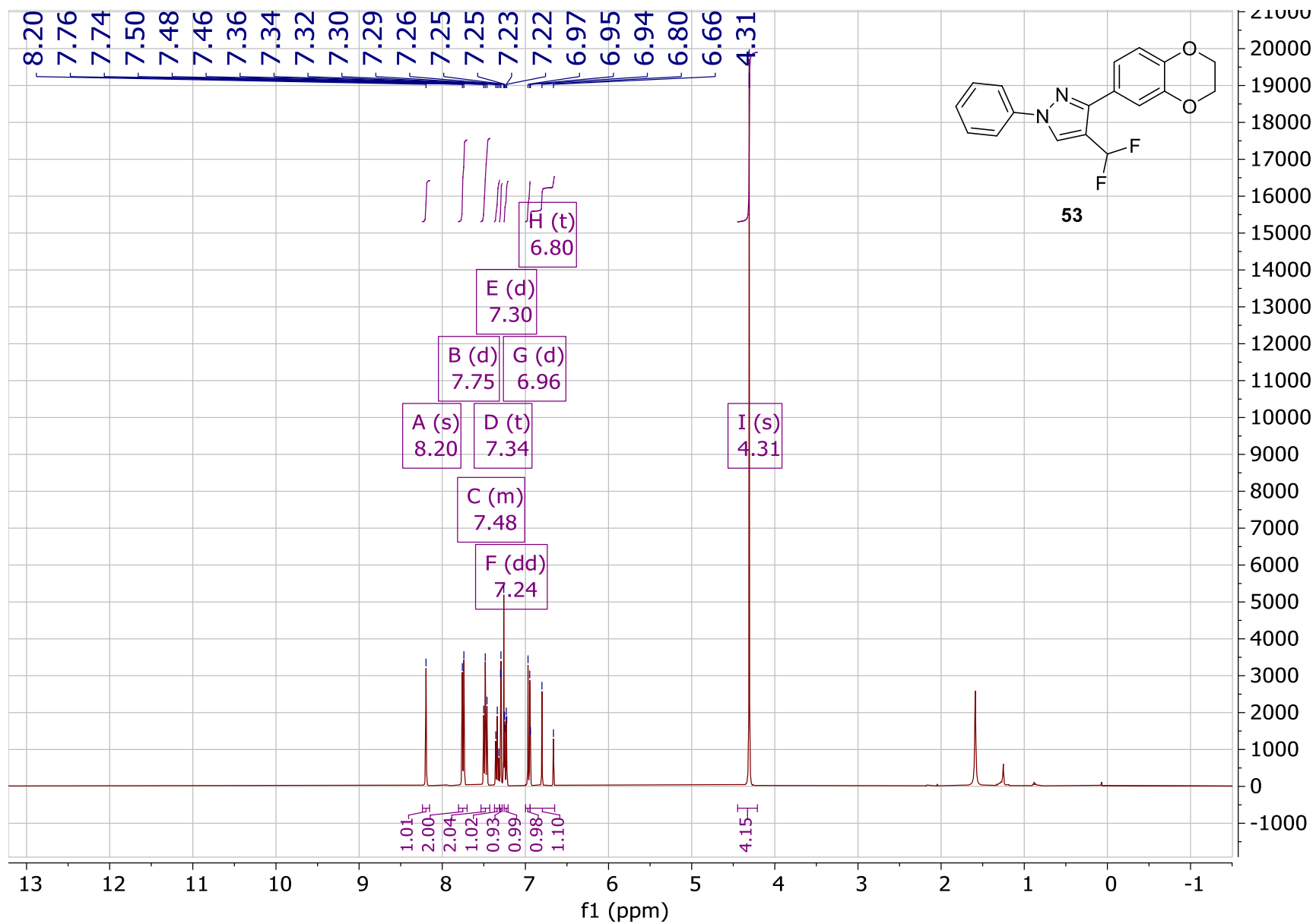


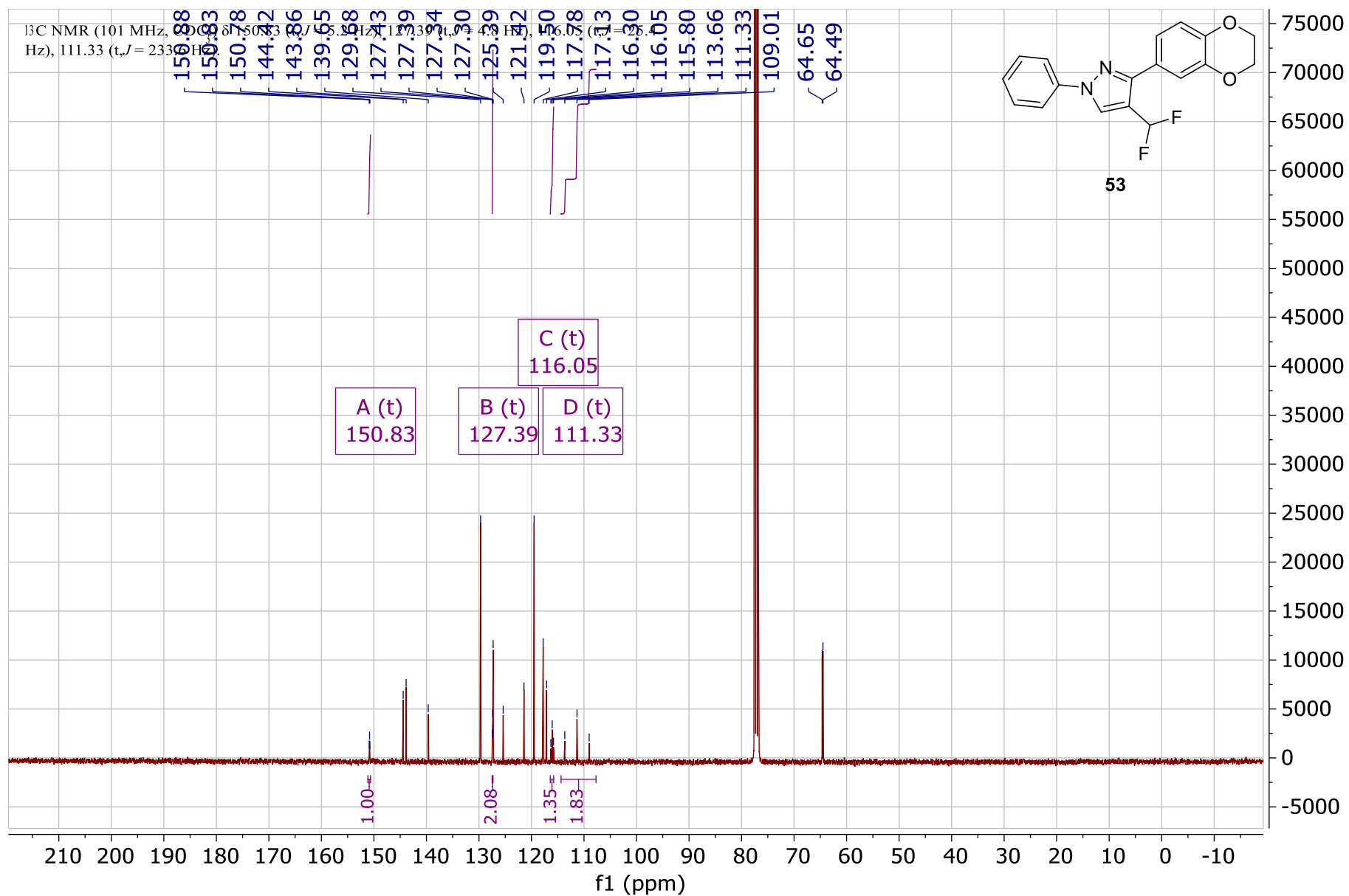


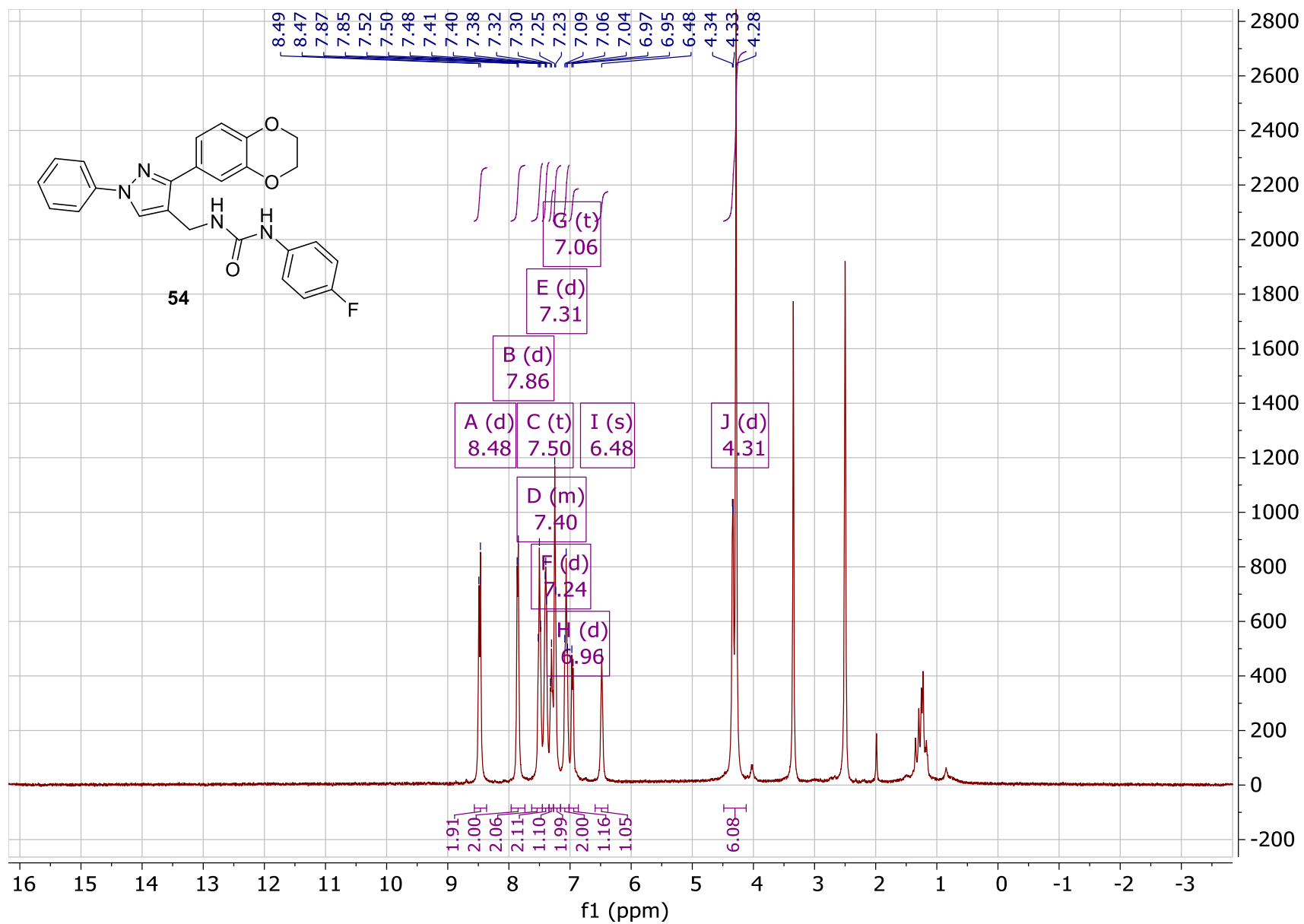


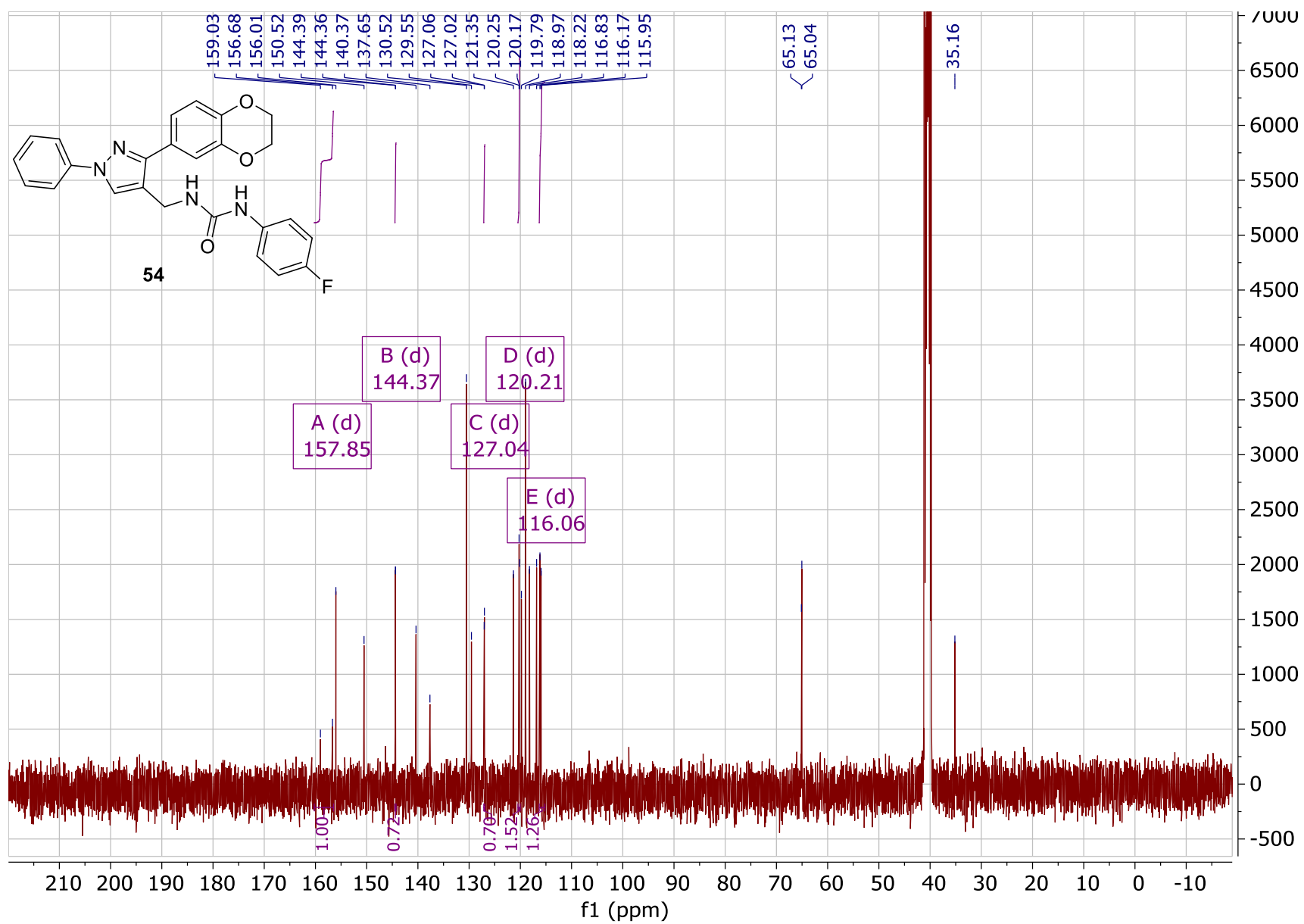




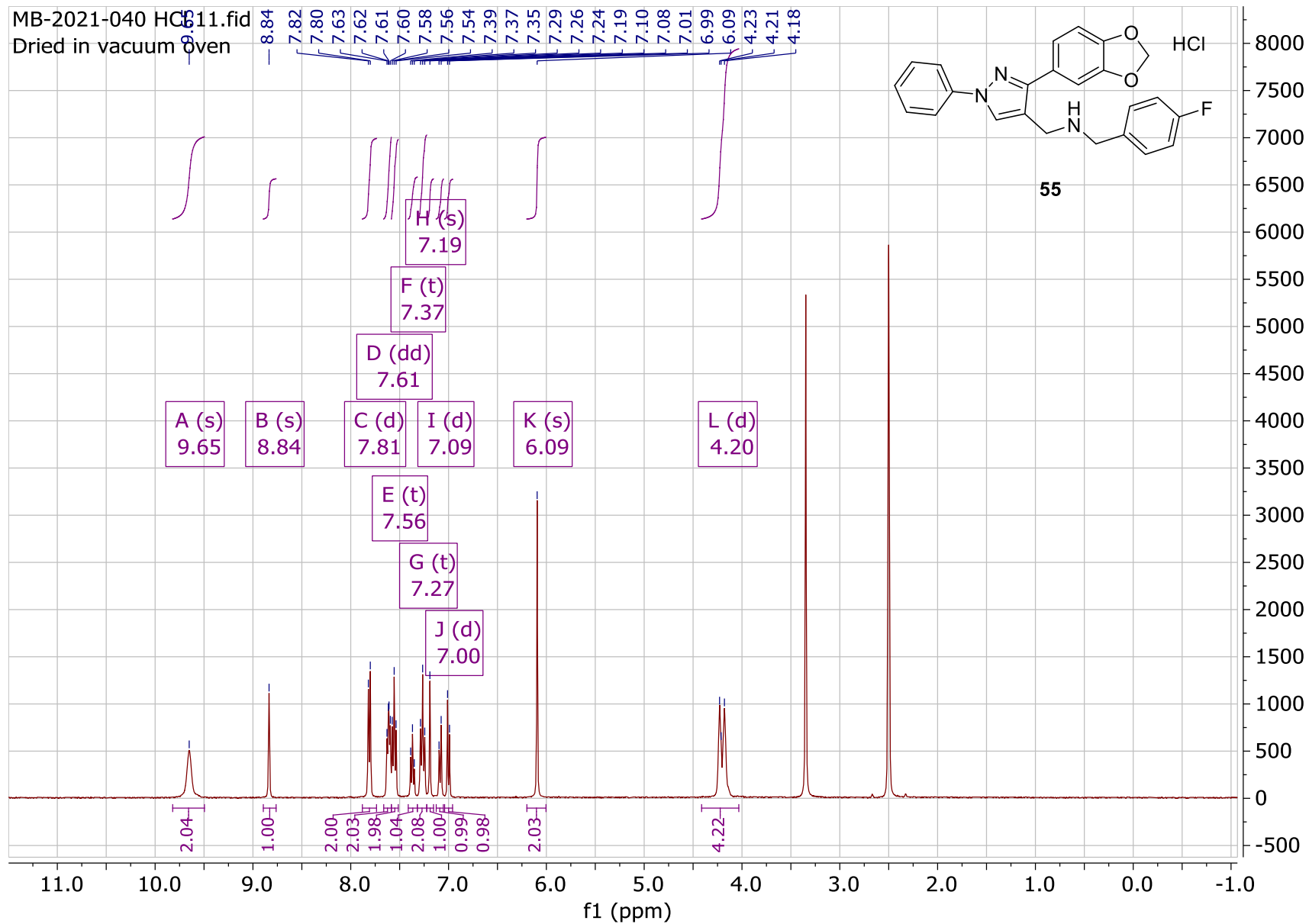




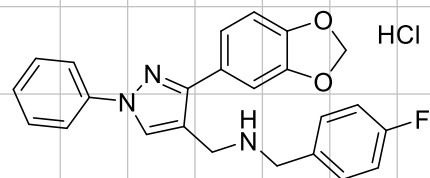




MB-2021-040 HCl
Dried in vacuum oven



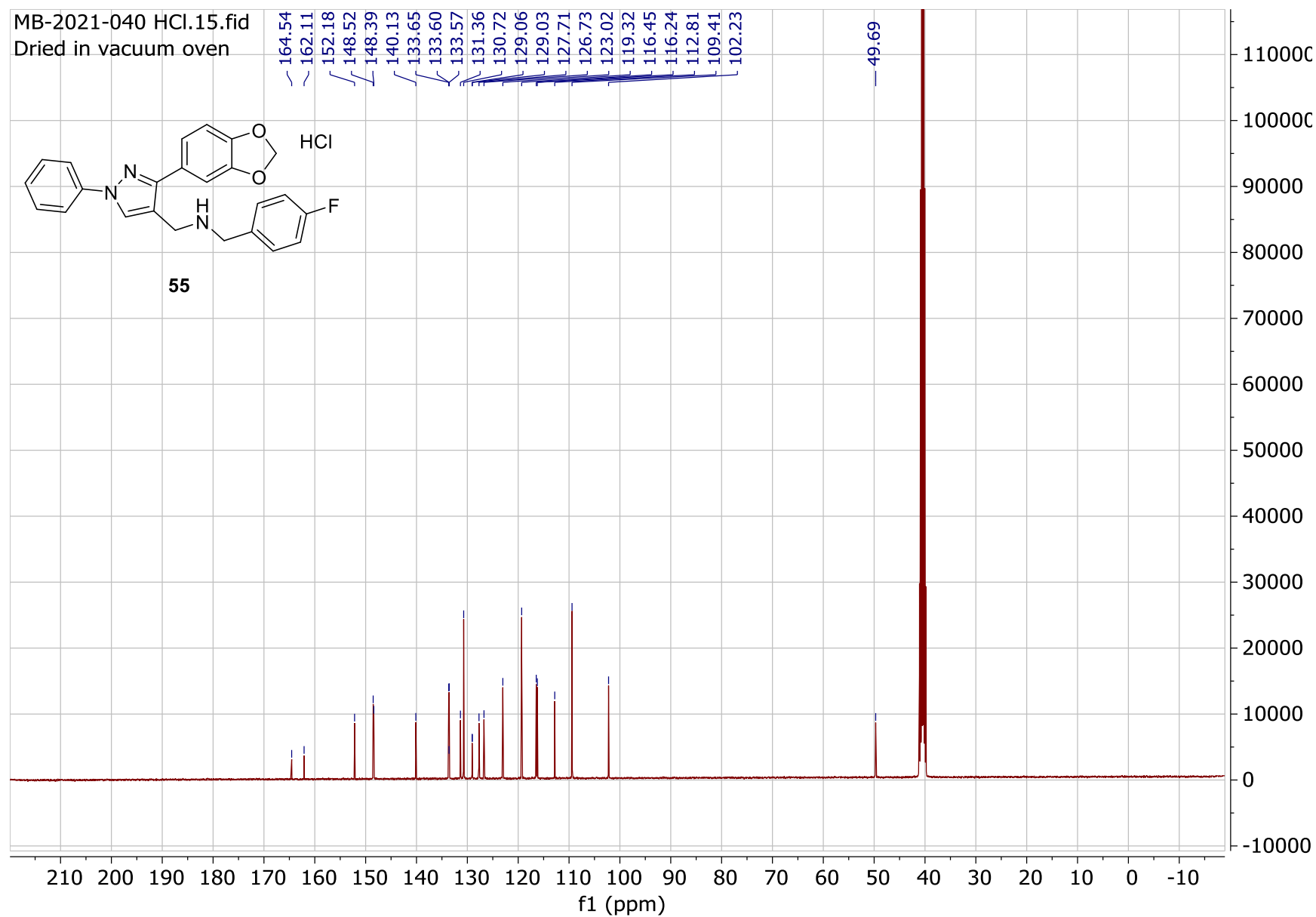
MB-2021-040 HCl.15.fid
Dried in vacuum oven



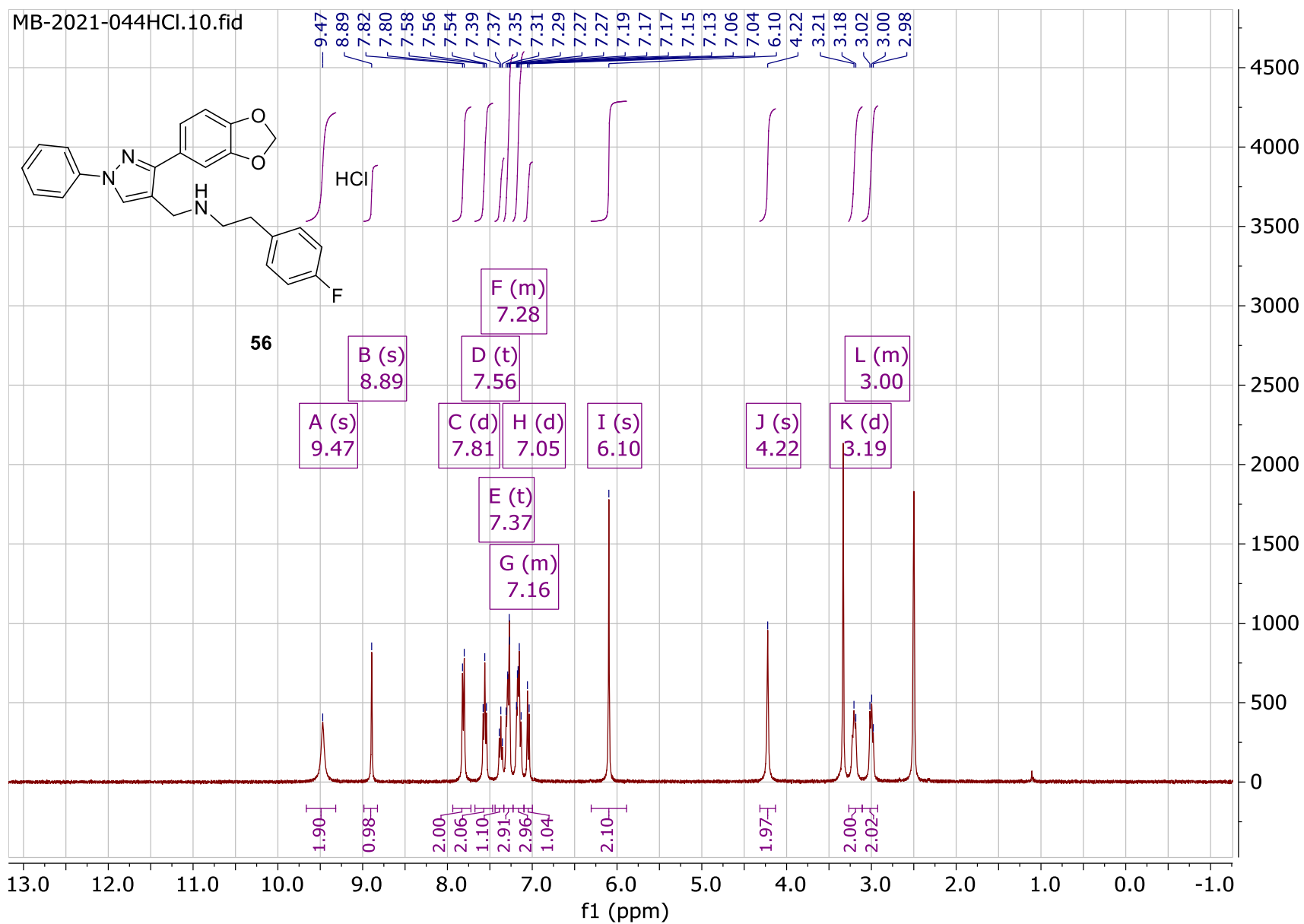
55

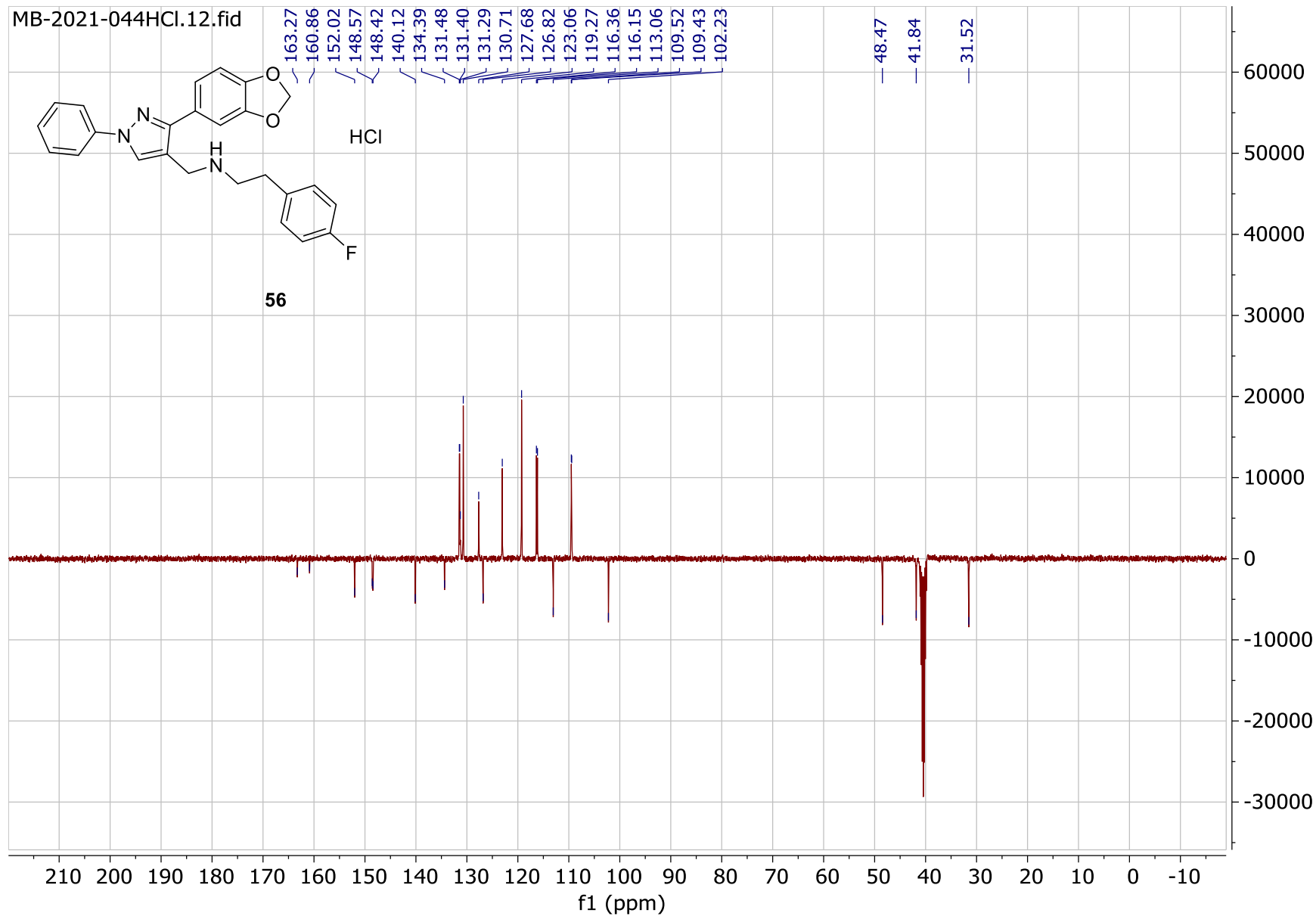
164.54
162.11
152.18
148.52
148.39
140.13
133.65
133.60
133.57
131.36
130.72
129.06
129.03
127.71
126.73
123.02
119.32
116.45
116.24
112.81
109.41
102.23

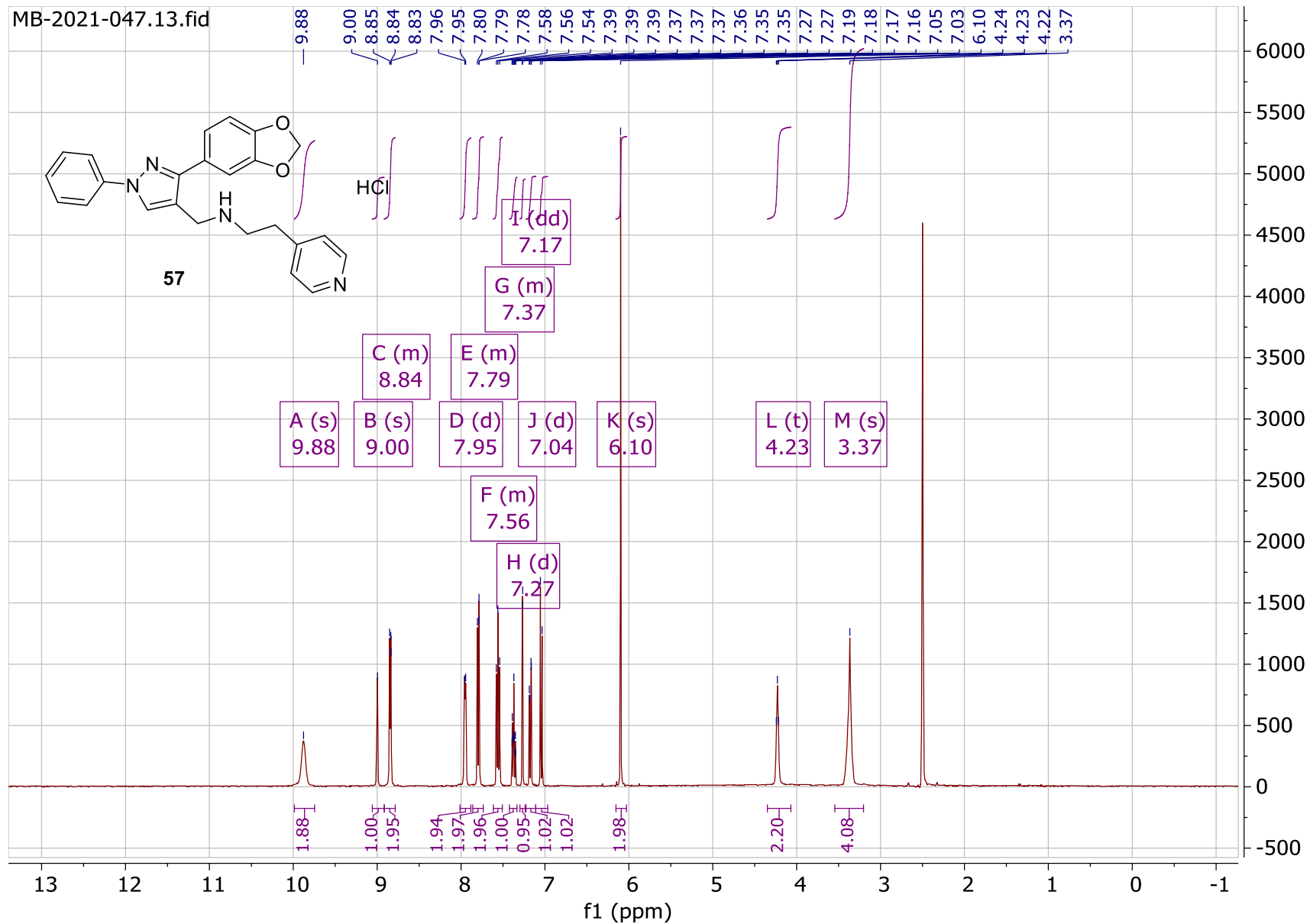
49.69

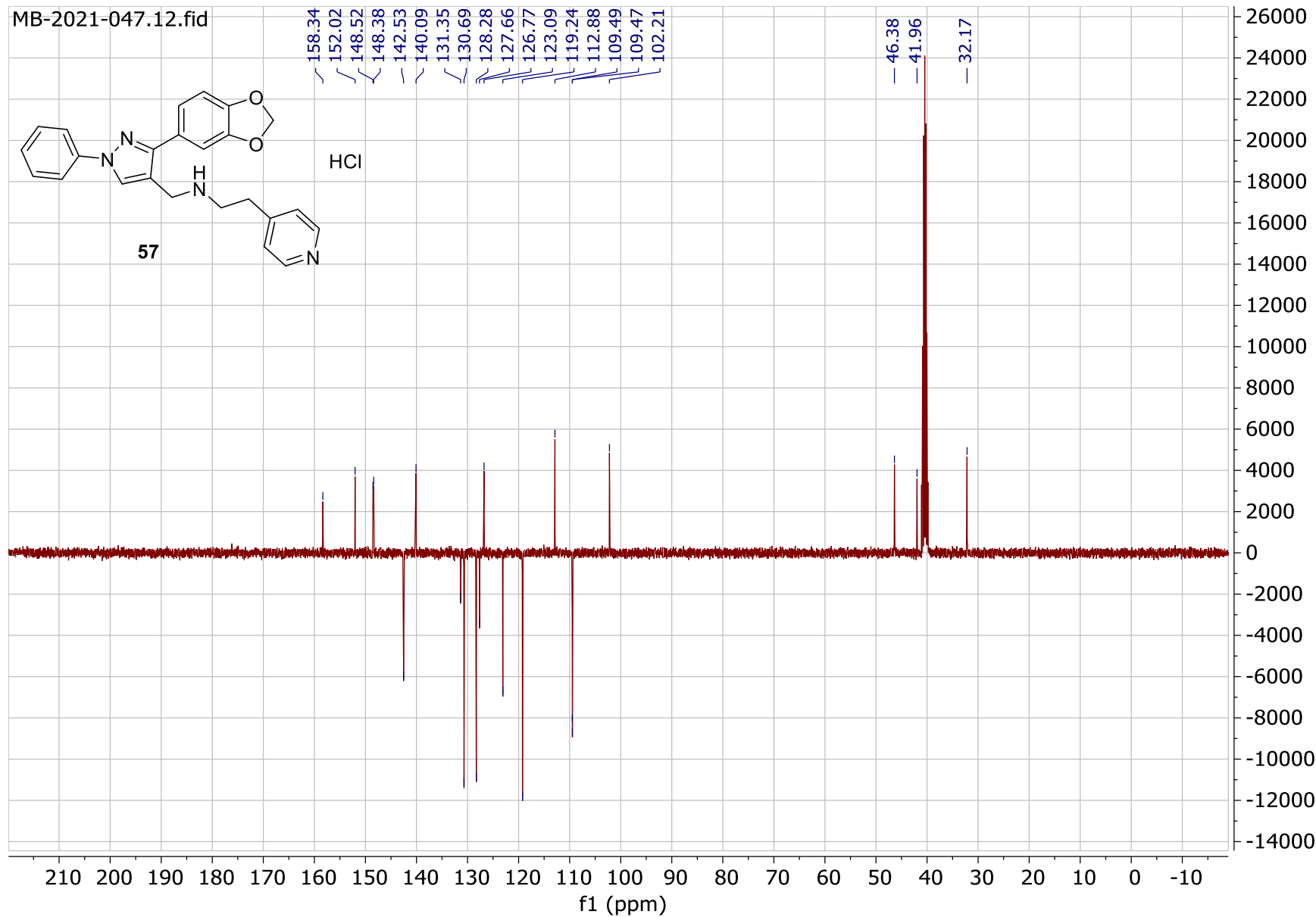


MB-2021-044HCl.10.fid

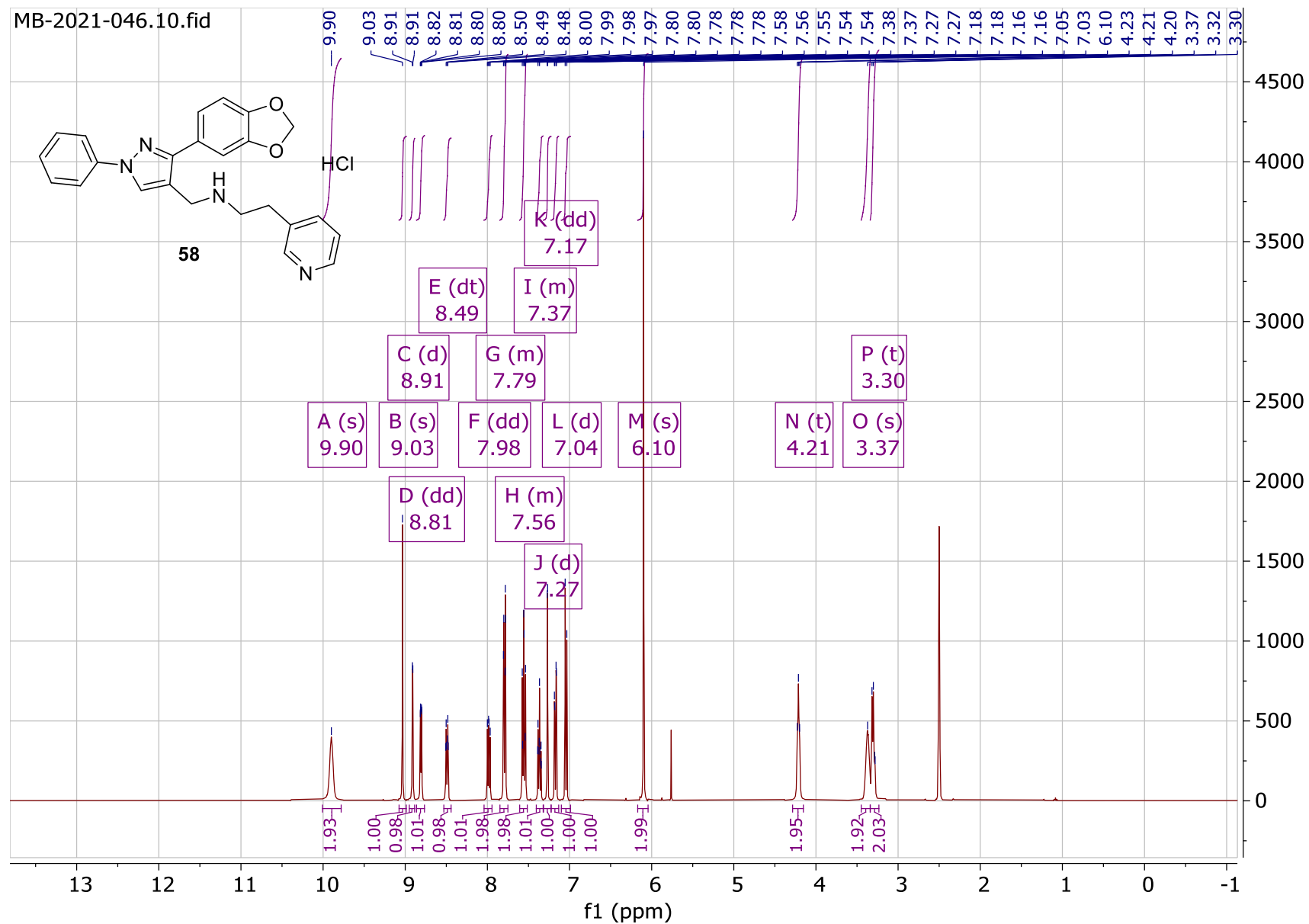
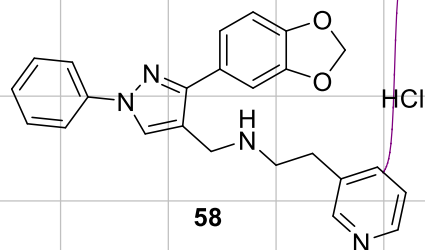




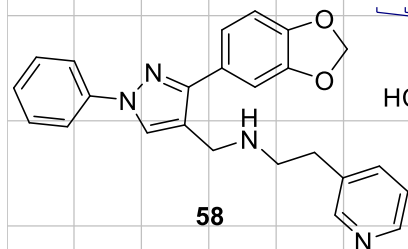




MB-2021-046.10.fid



MB-2021-046.12.fid



152.02
148.54
148.40
146.47
143.55
141.61
140.09
137.92
131.32
130.69
127.68
127.53
126.76
123.06
119.25
112.87
109.49
109.43
102.21

47.19
41.98
29.22

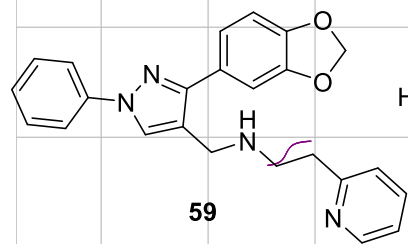
50000
40000
30000
20000
10000
0
-10000
-20000
-30000
-40000

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

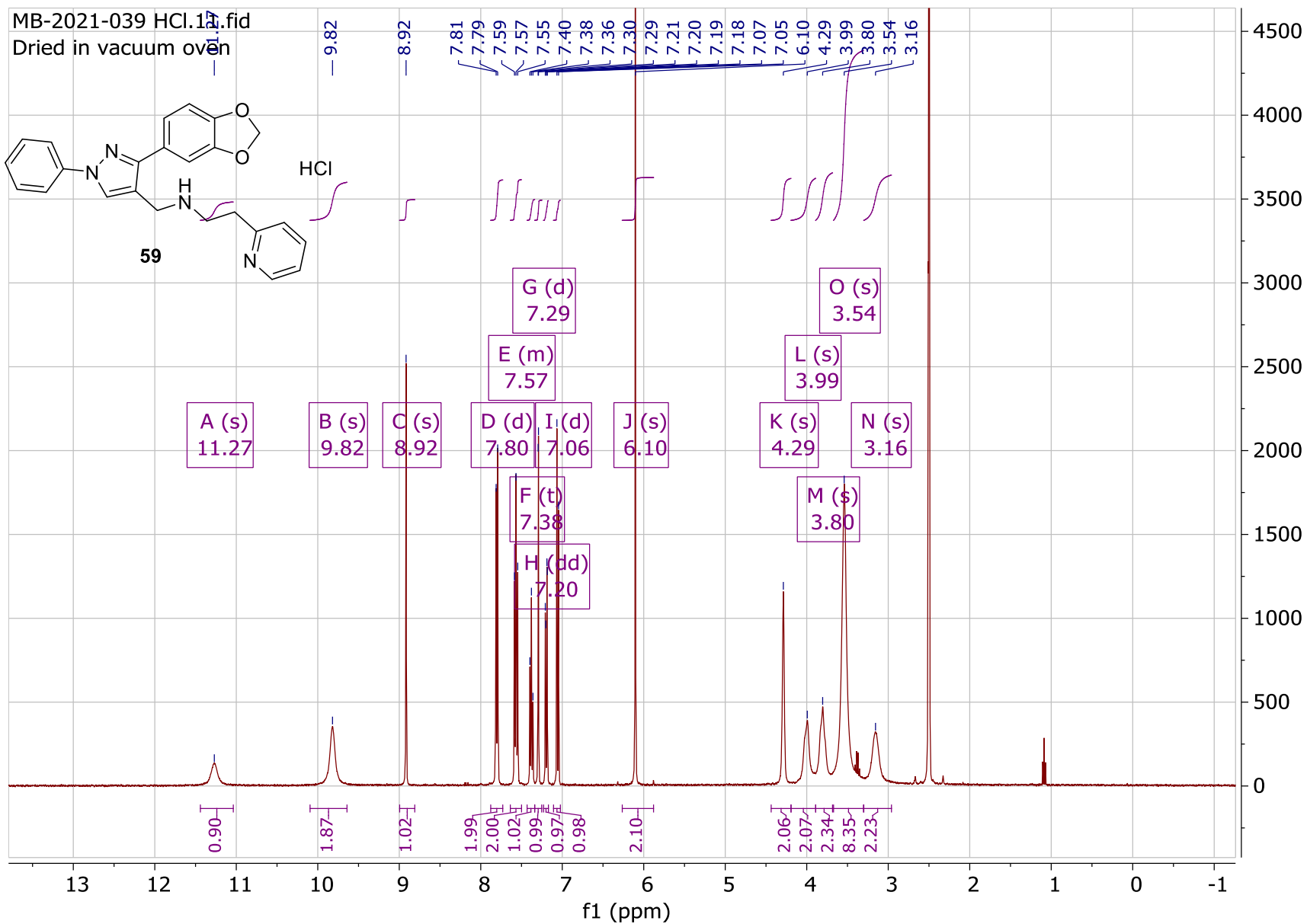
MB-2021-039 HCl.12.fid

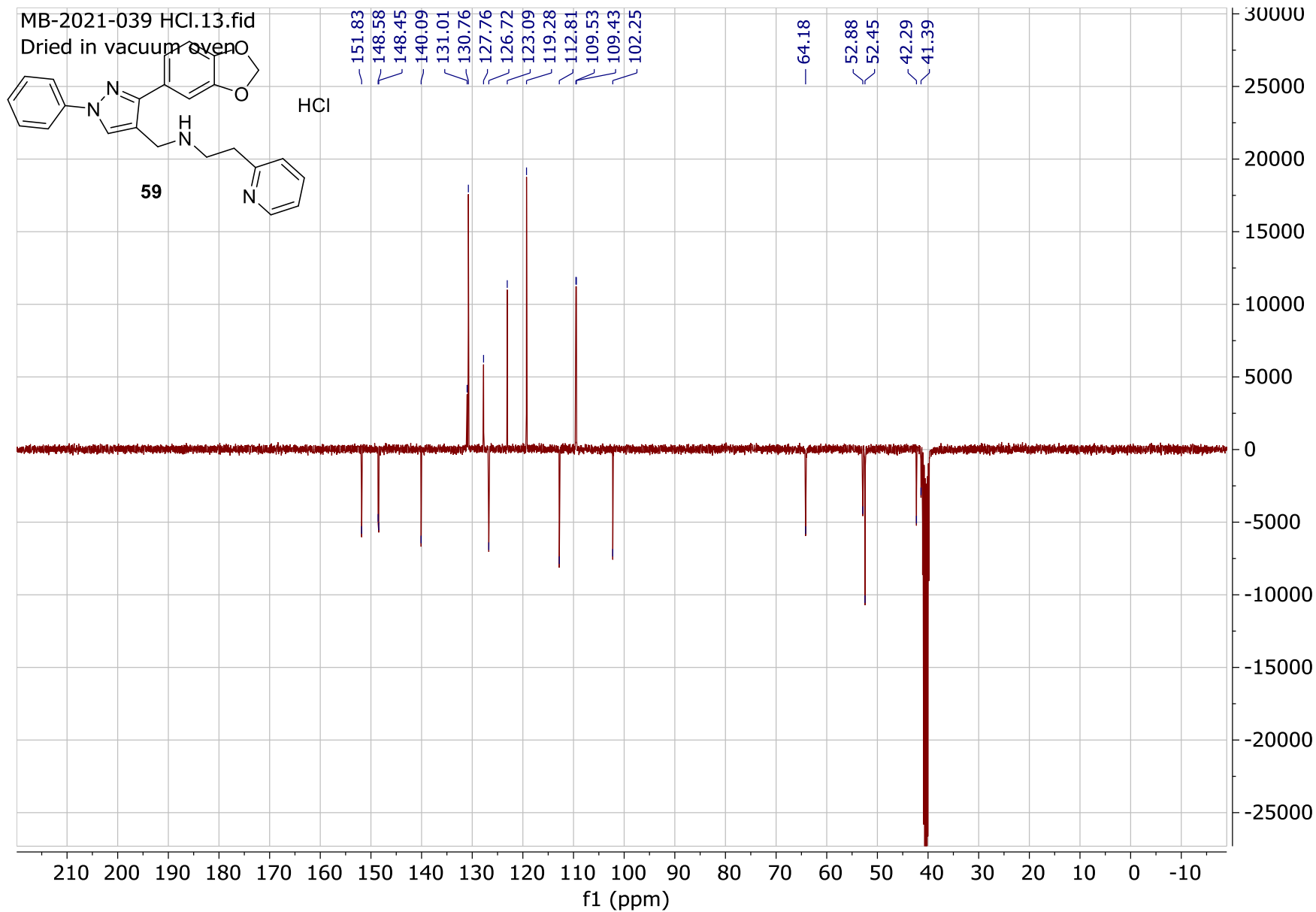
Dried in vacuum oven

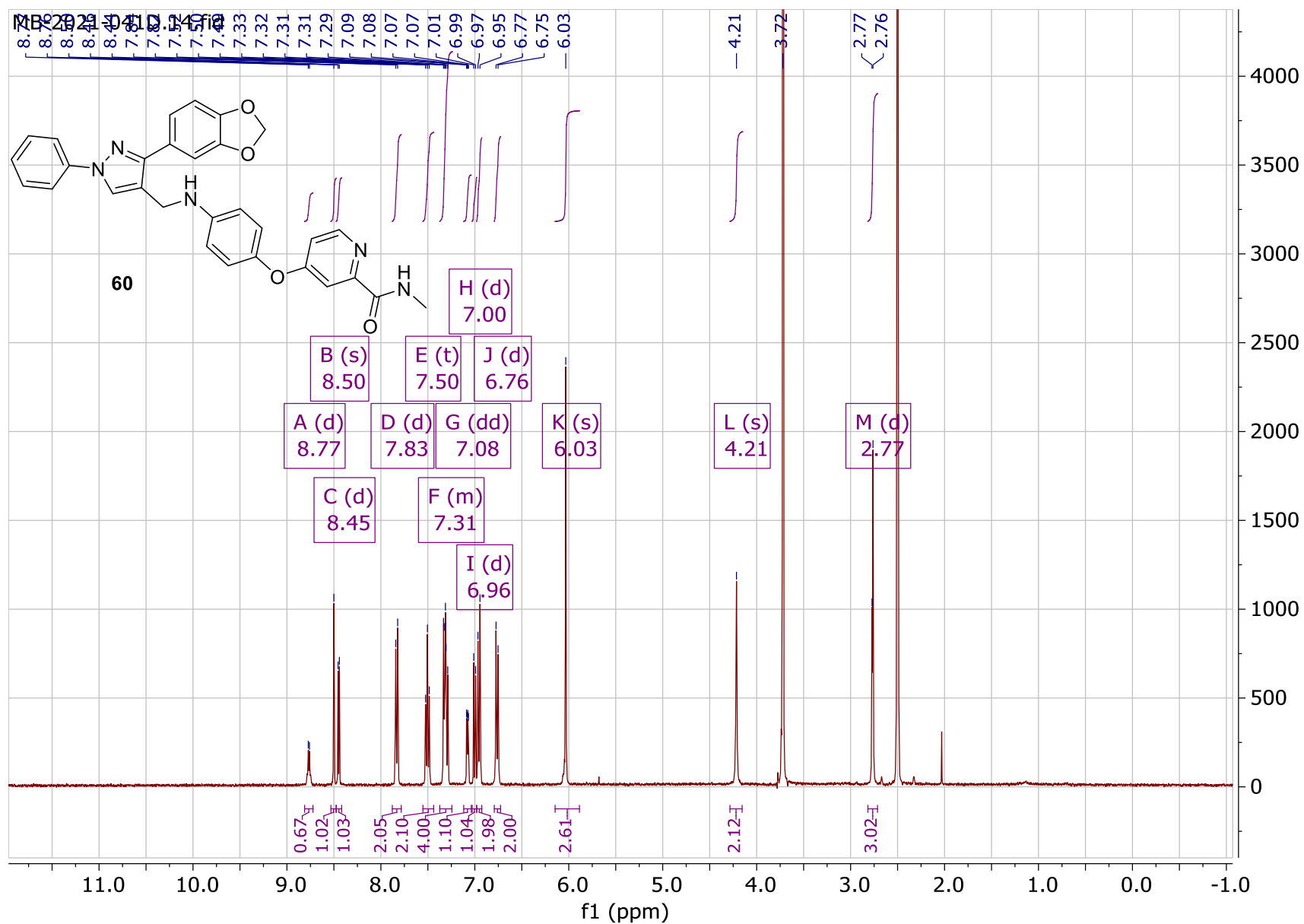


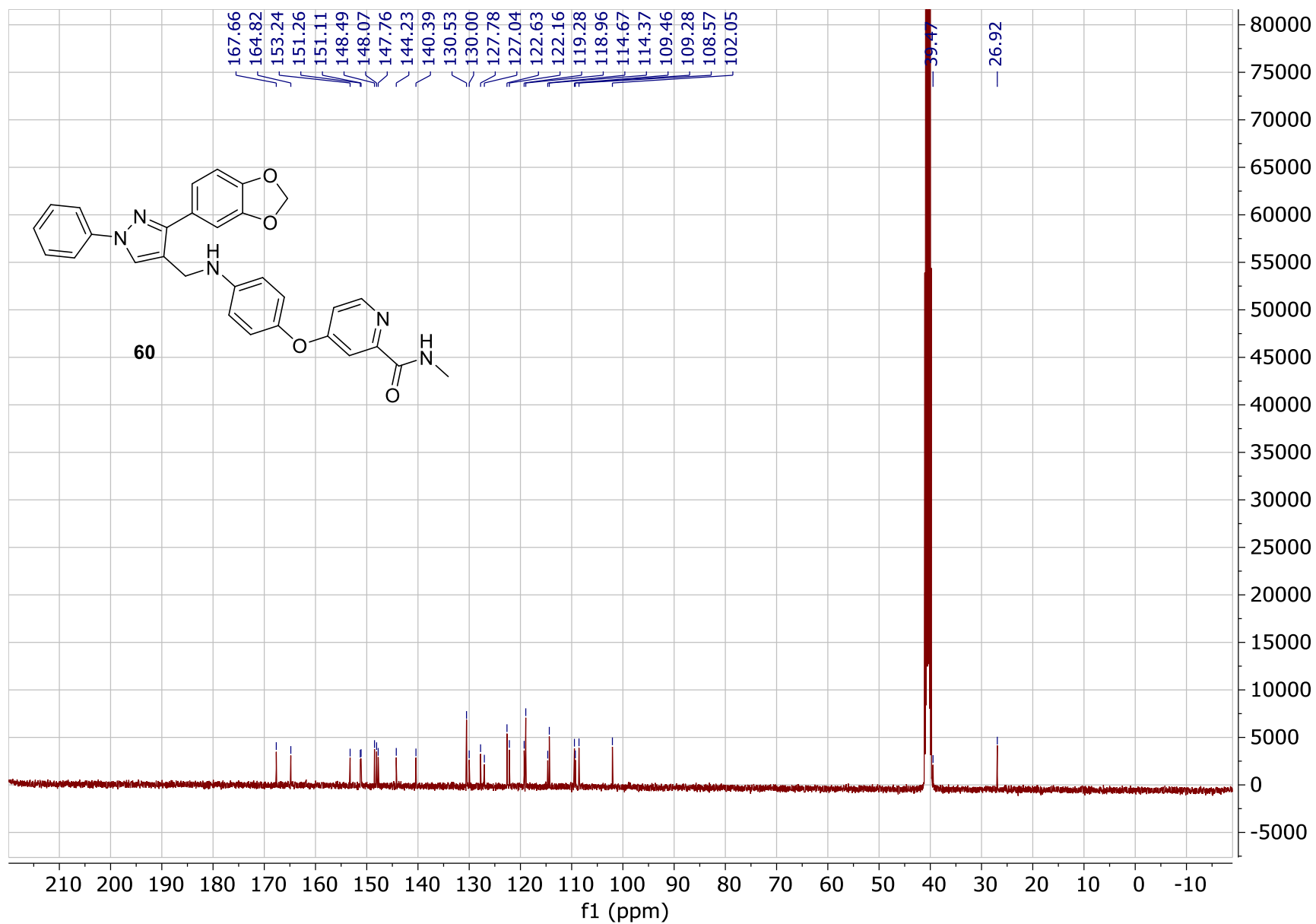
HCl

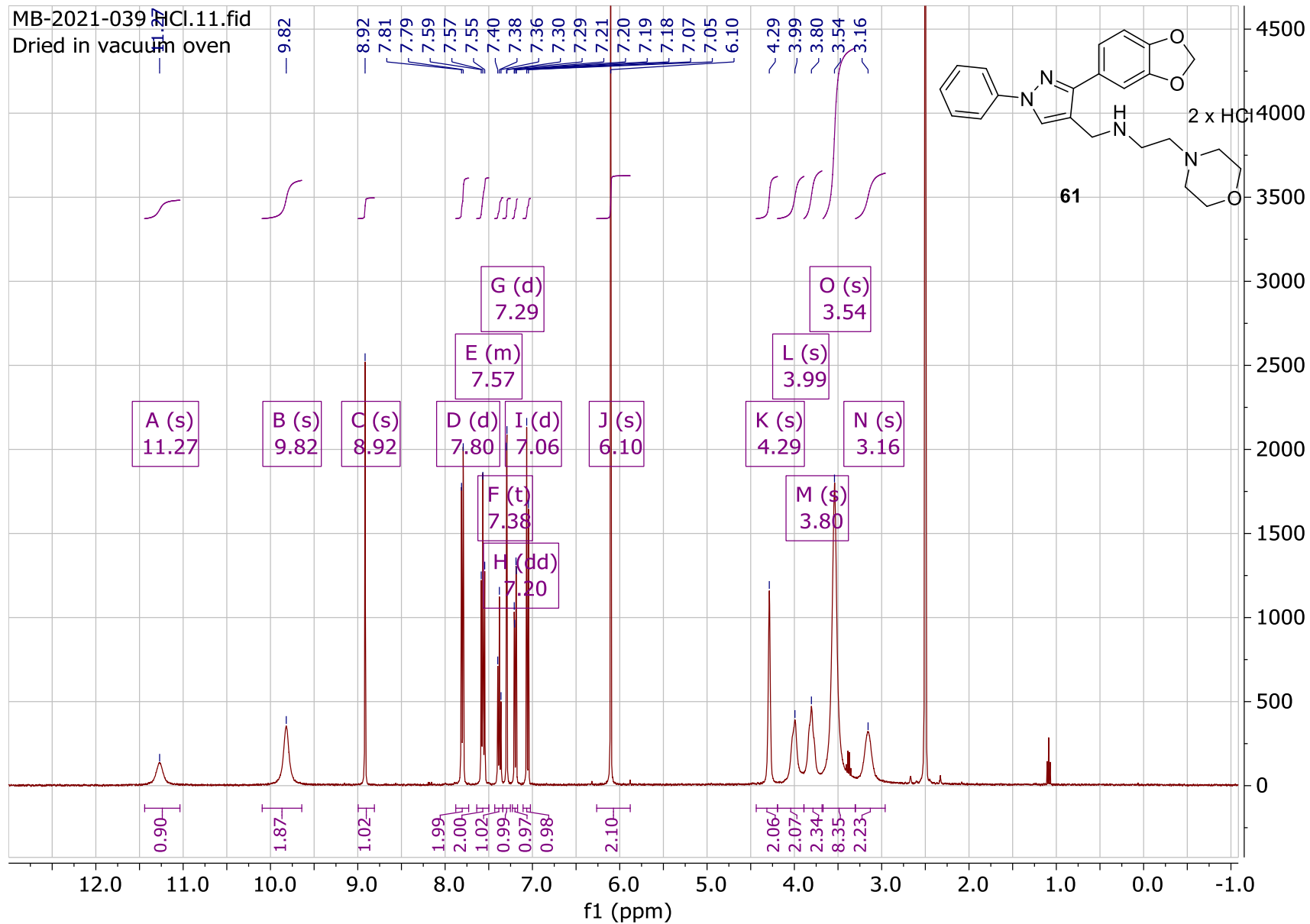
59



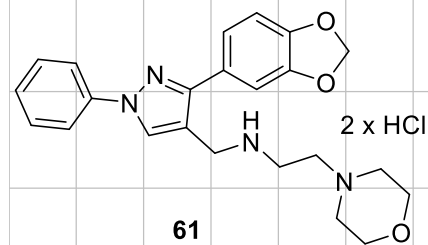








MB-2021-039 HCl.13.fid
Dried in vacuum oven

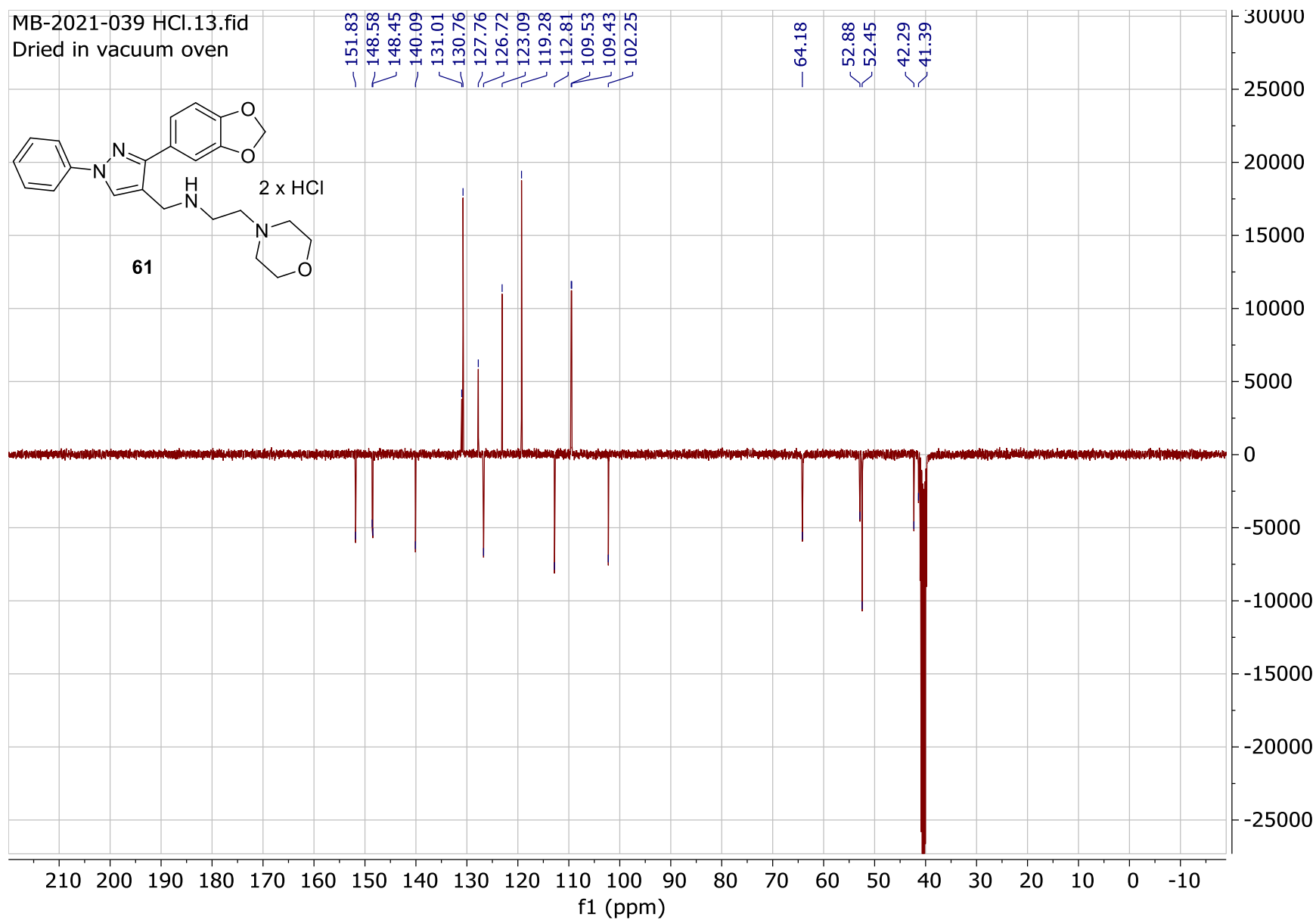


151.83
148.58
148.45
140.09
131.01
130.76
127.76
126.72
123.09
119.28
112.81
109.53
109.43
102.25

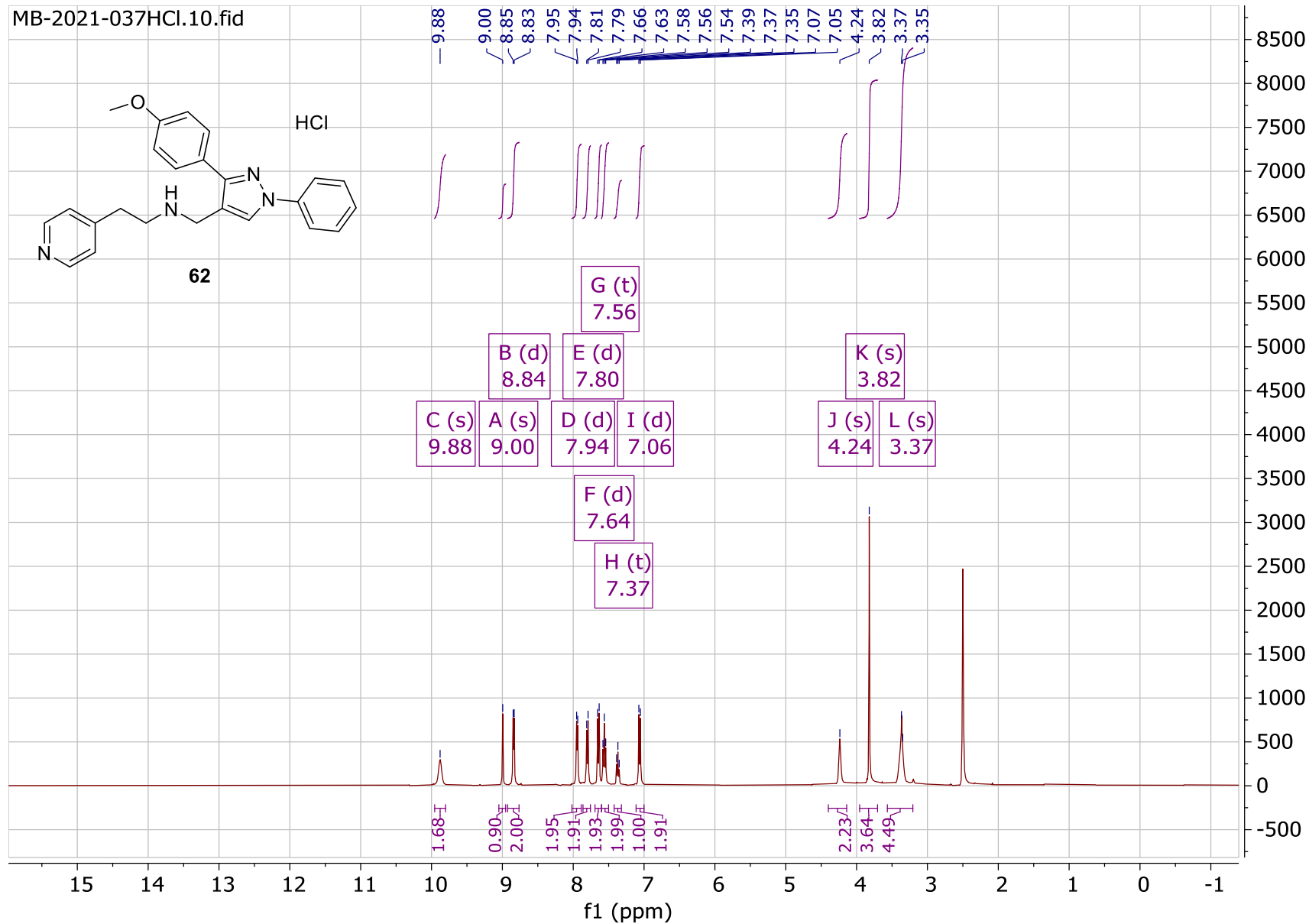
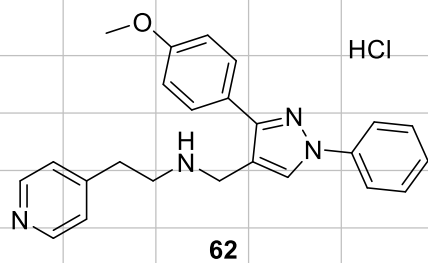
64.18

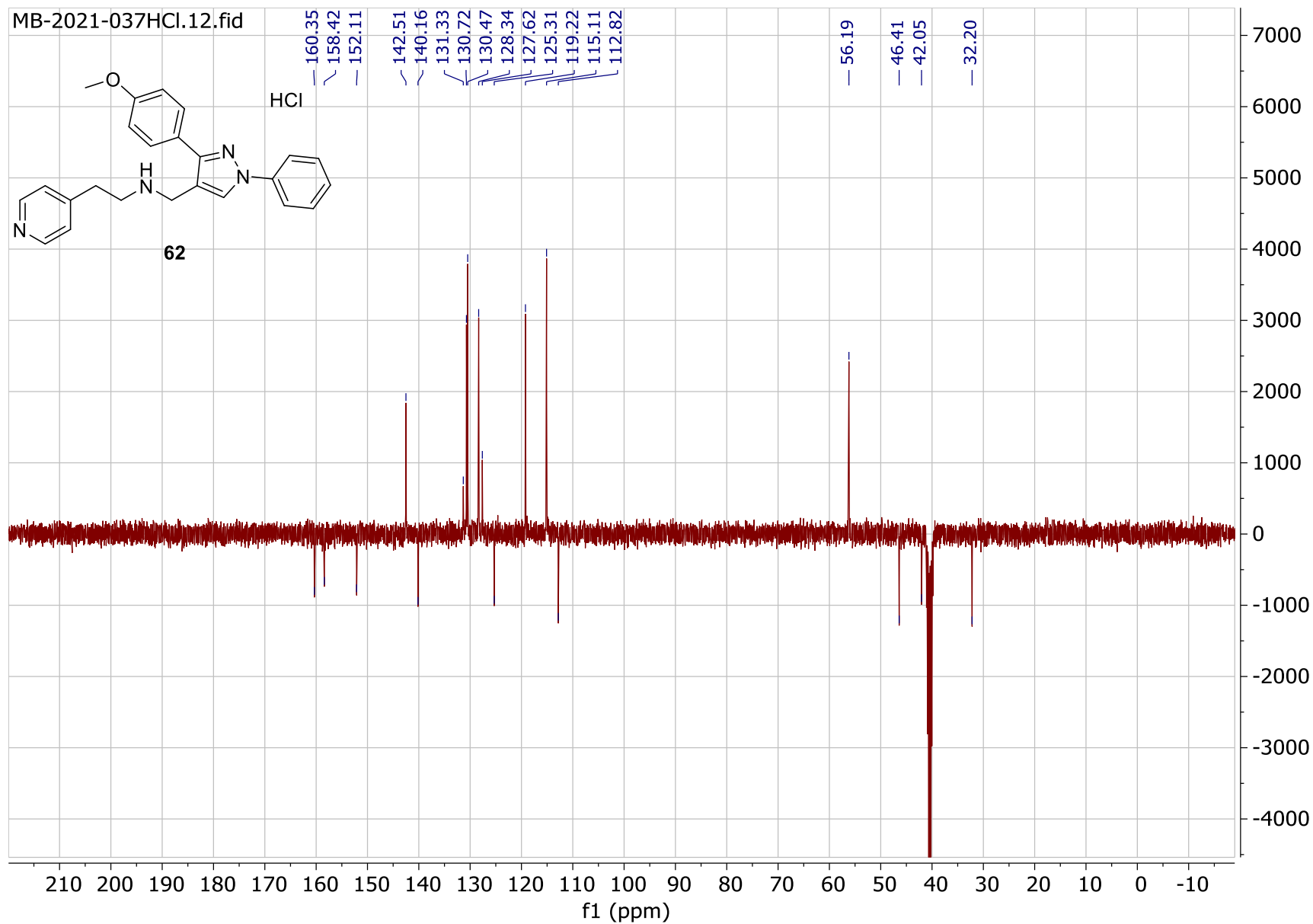
52.88
52.45

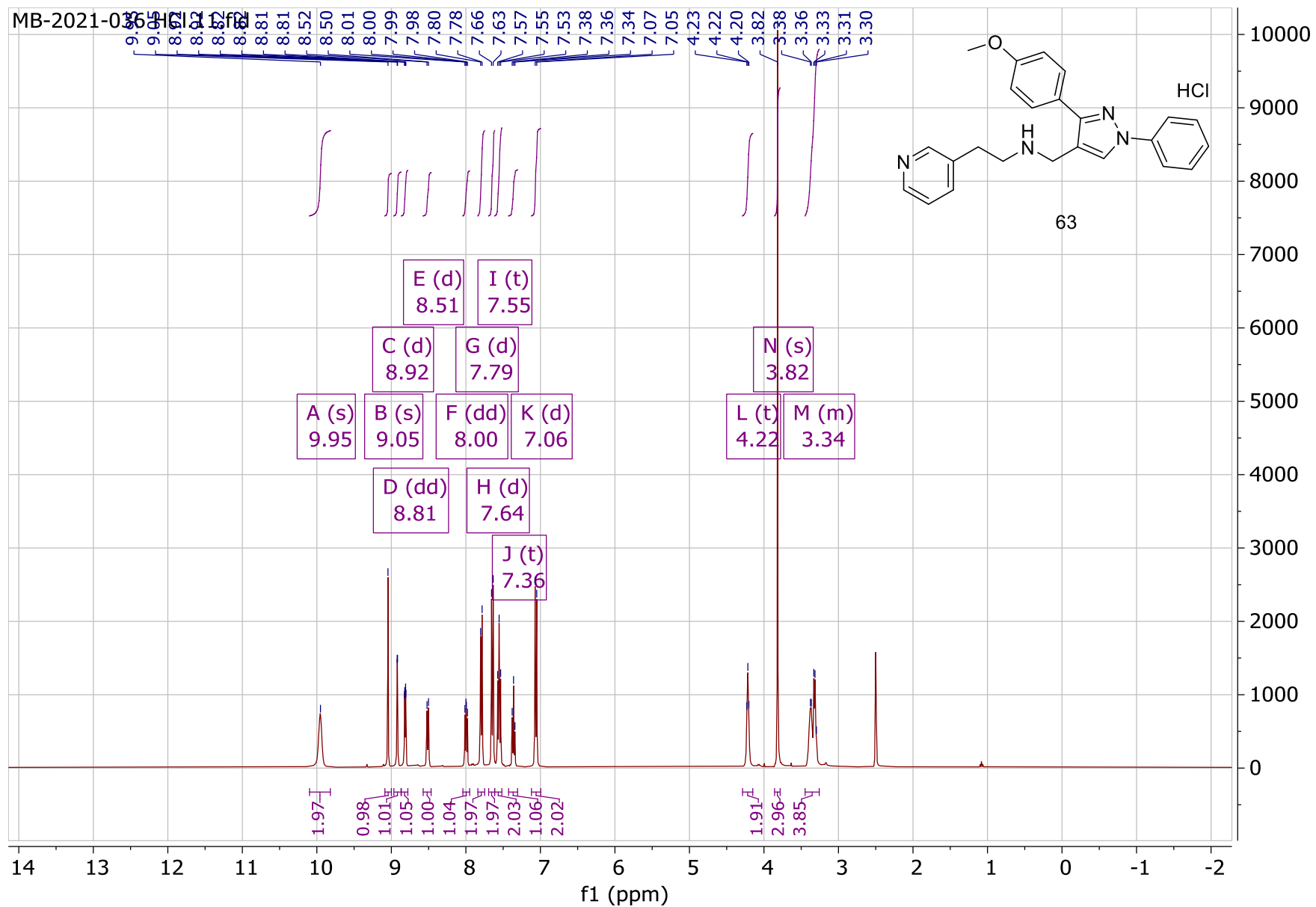
42.29
41.39

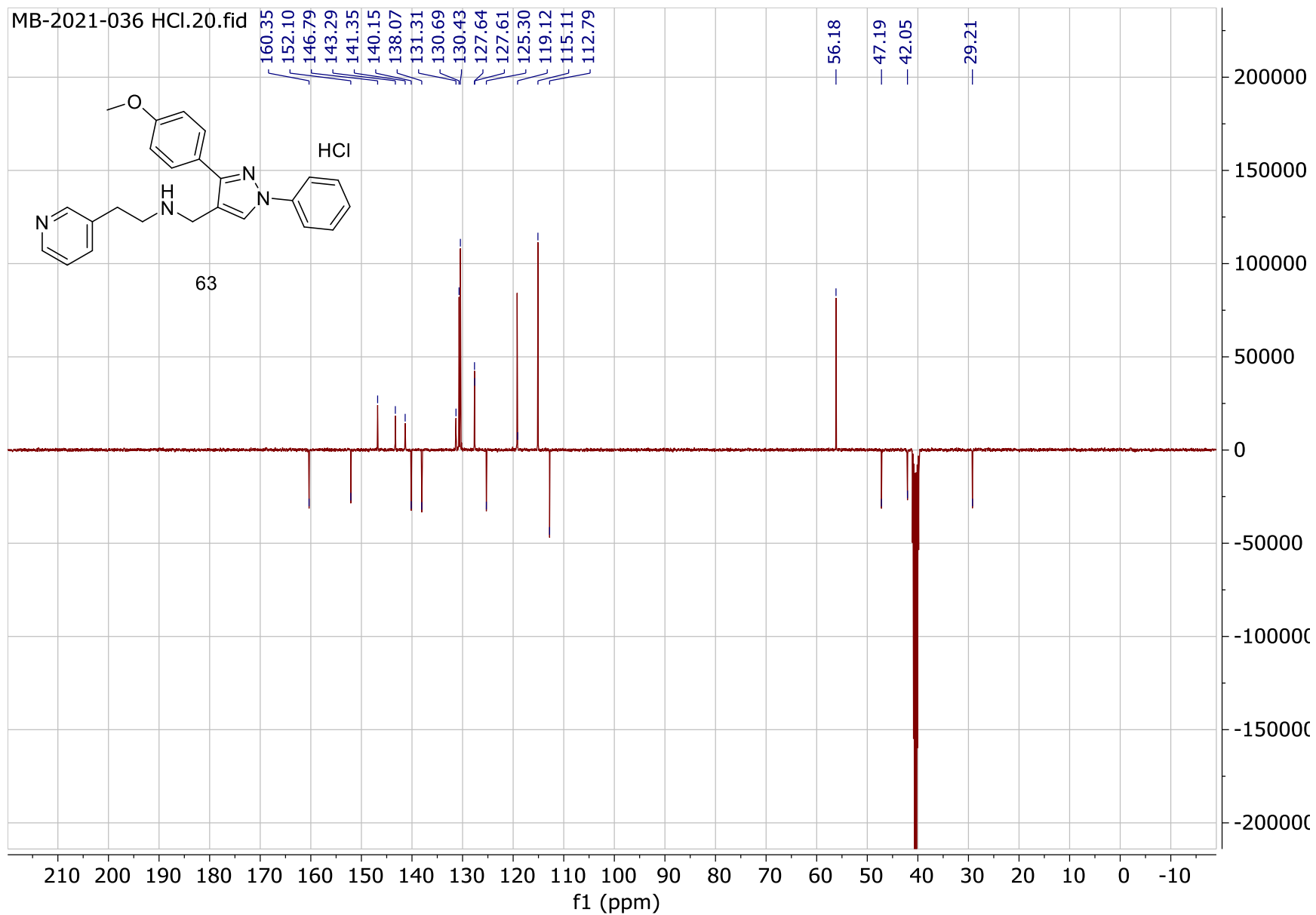


MB-2021-037HCl.10.fid

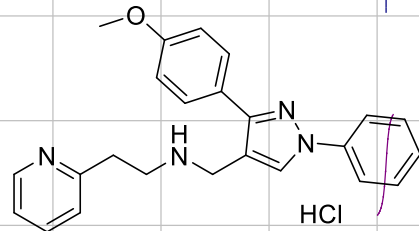




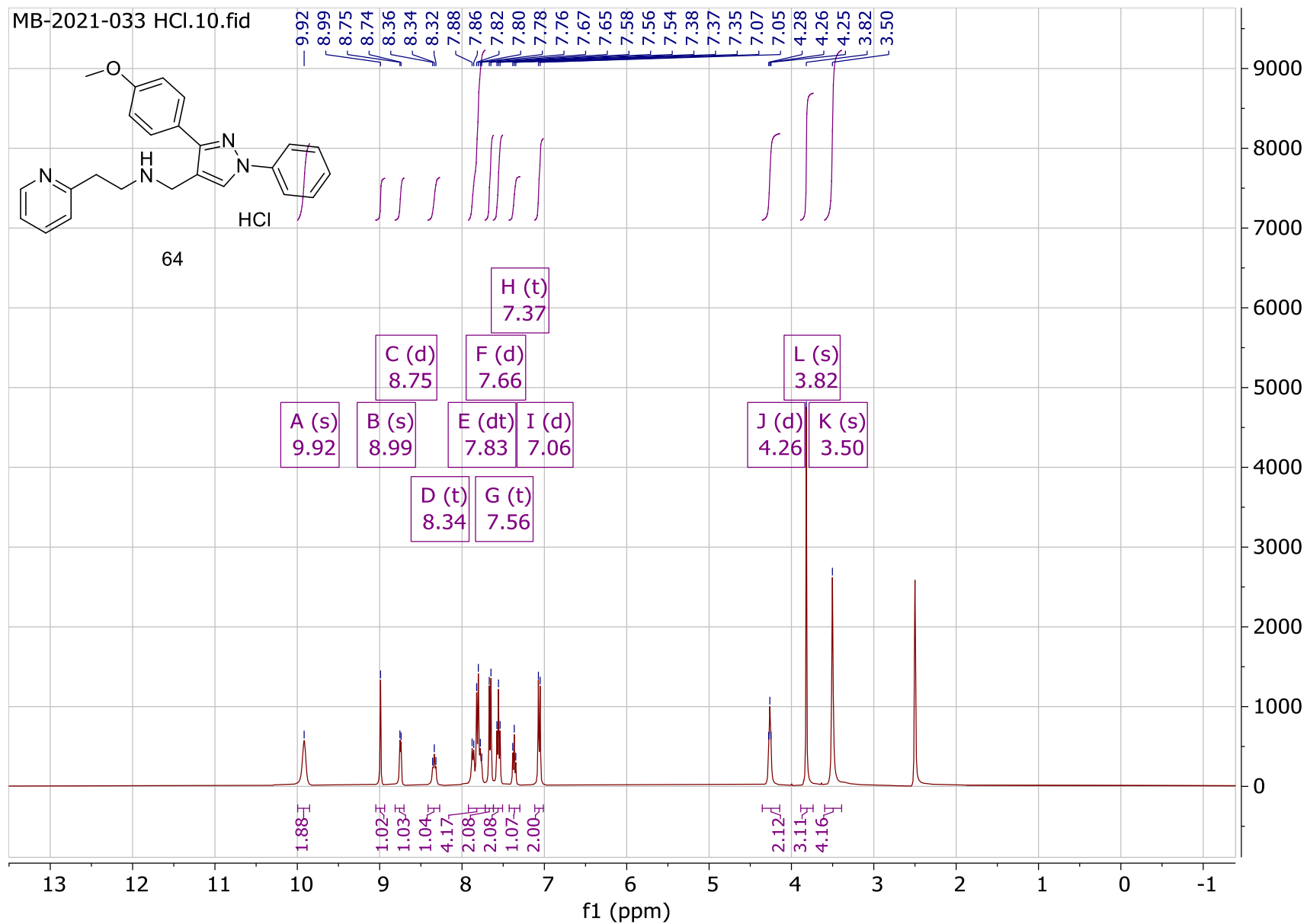




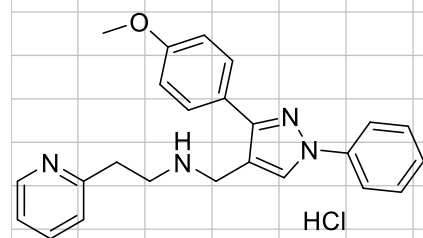
MB-2021-033 HCl.10.fid



64



MB-2021-033 HCl.13.fid



64

160.37
154.37
152.07
144.58
140.16
131.27
130.73
130.42
127.66
127.45
125.56
125.29
119.26
115.13
112.75

56.19

45.87

42.10

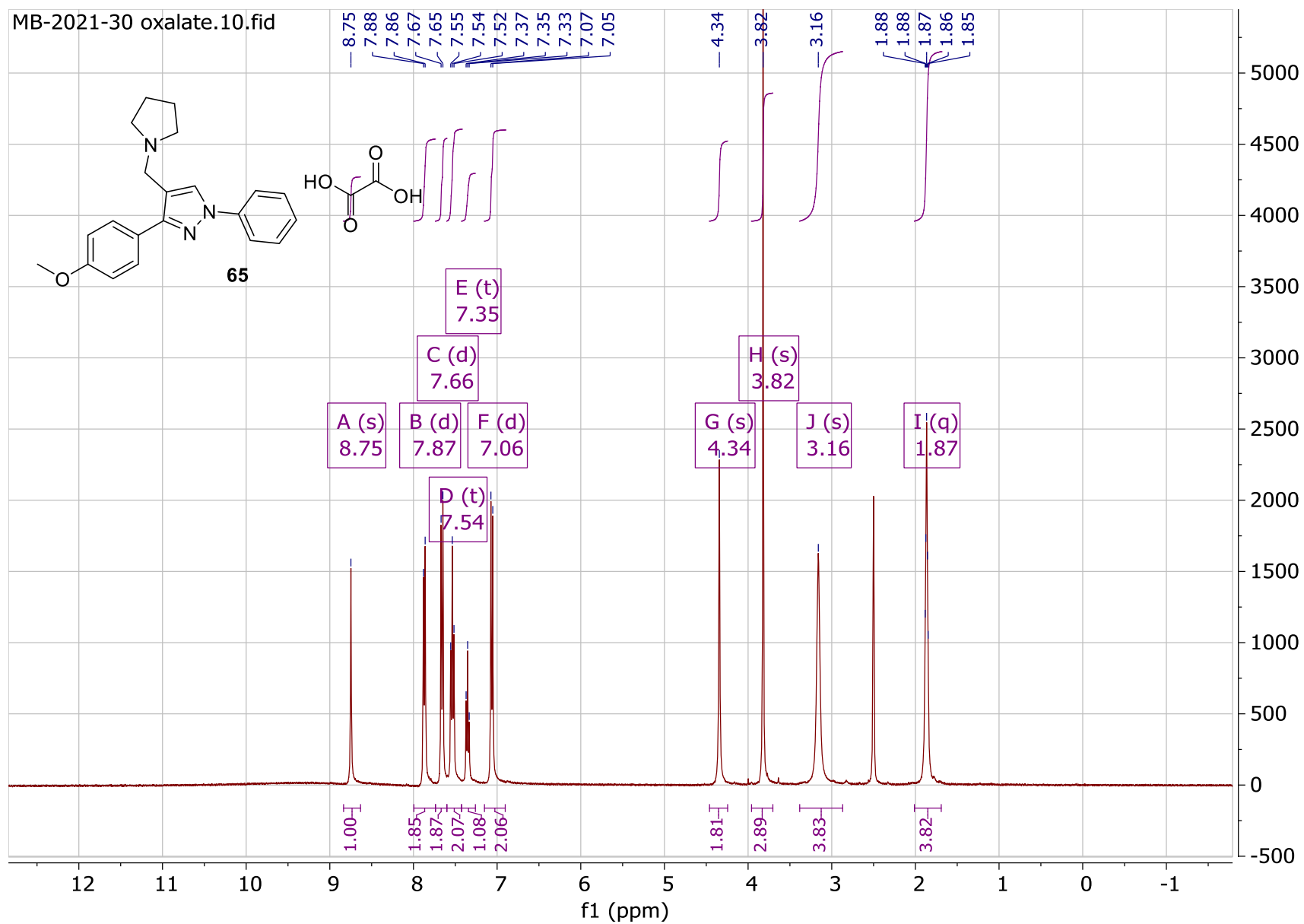
31.08

140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
-20000
-30000
-40000
-50000
-60000
-70000
-80000
-90000
-100000

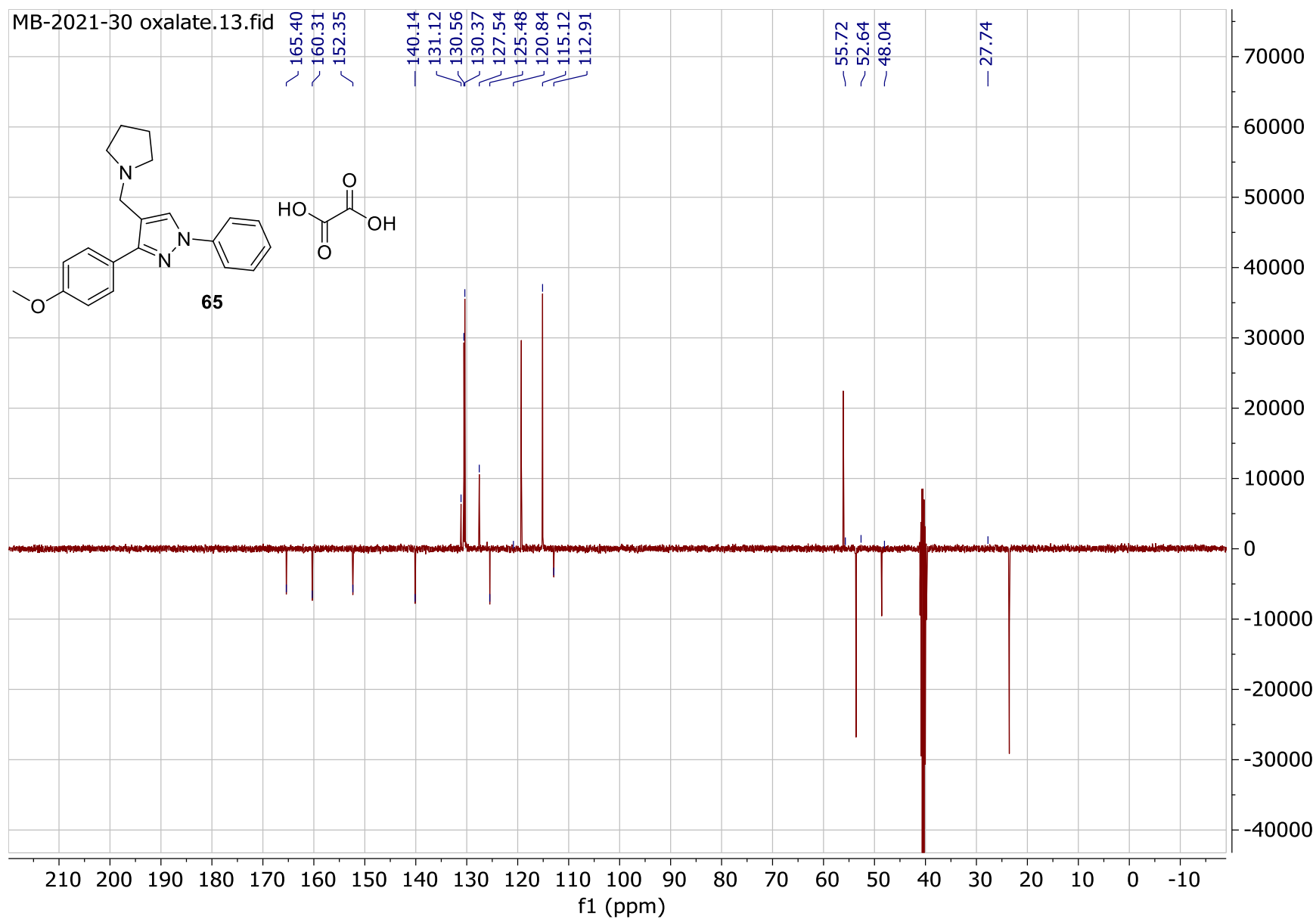
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

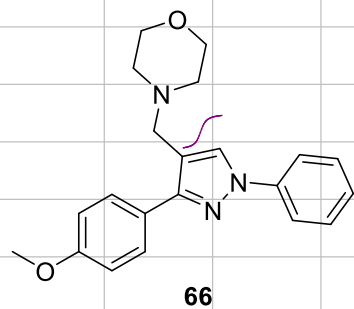
MB-2021-30 oxalate.10.fid



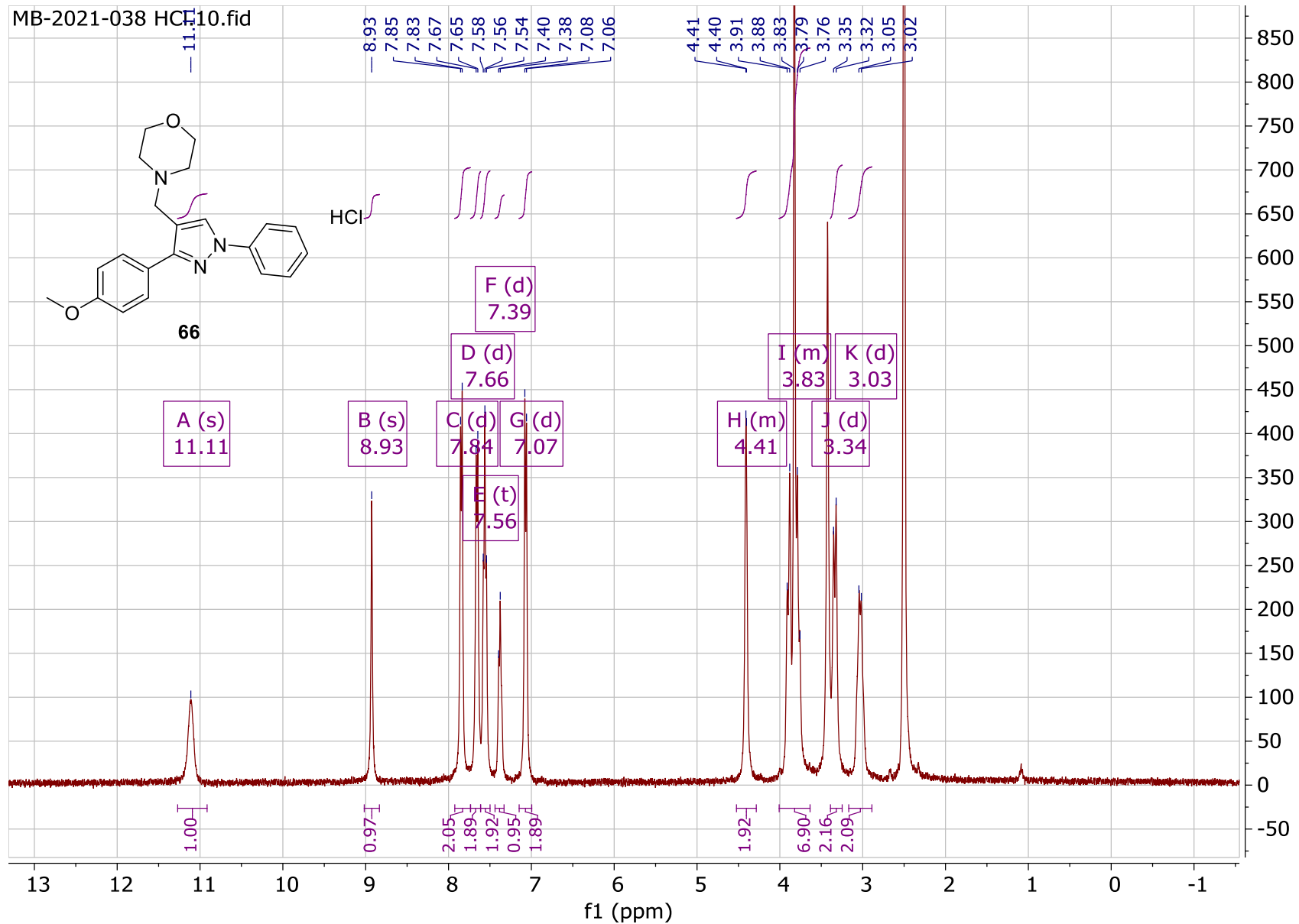
MB-2021-30 oxalate.13.fid

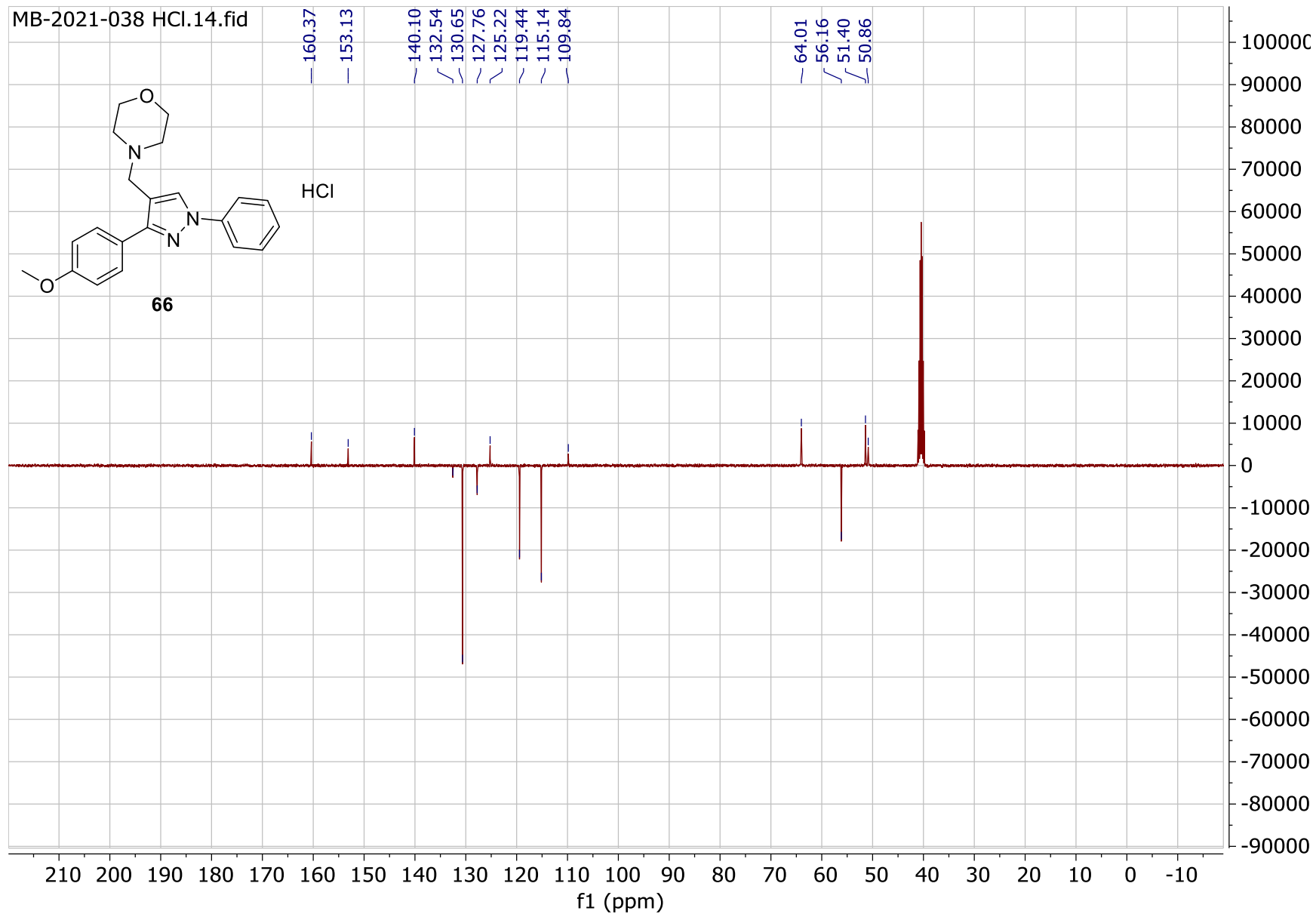


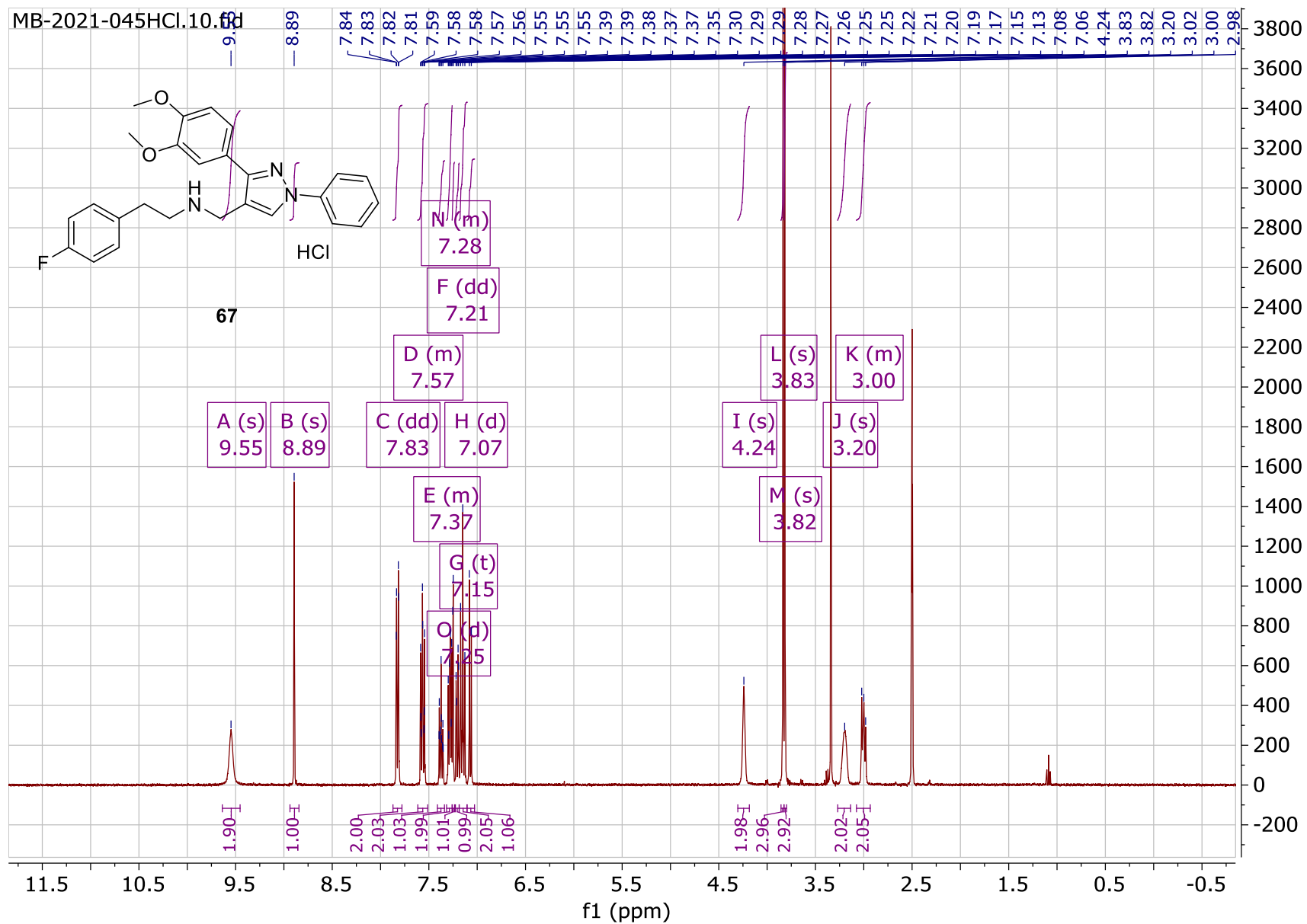
MB-2021-038 HCl 10.fid

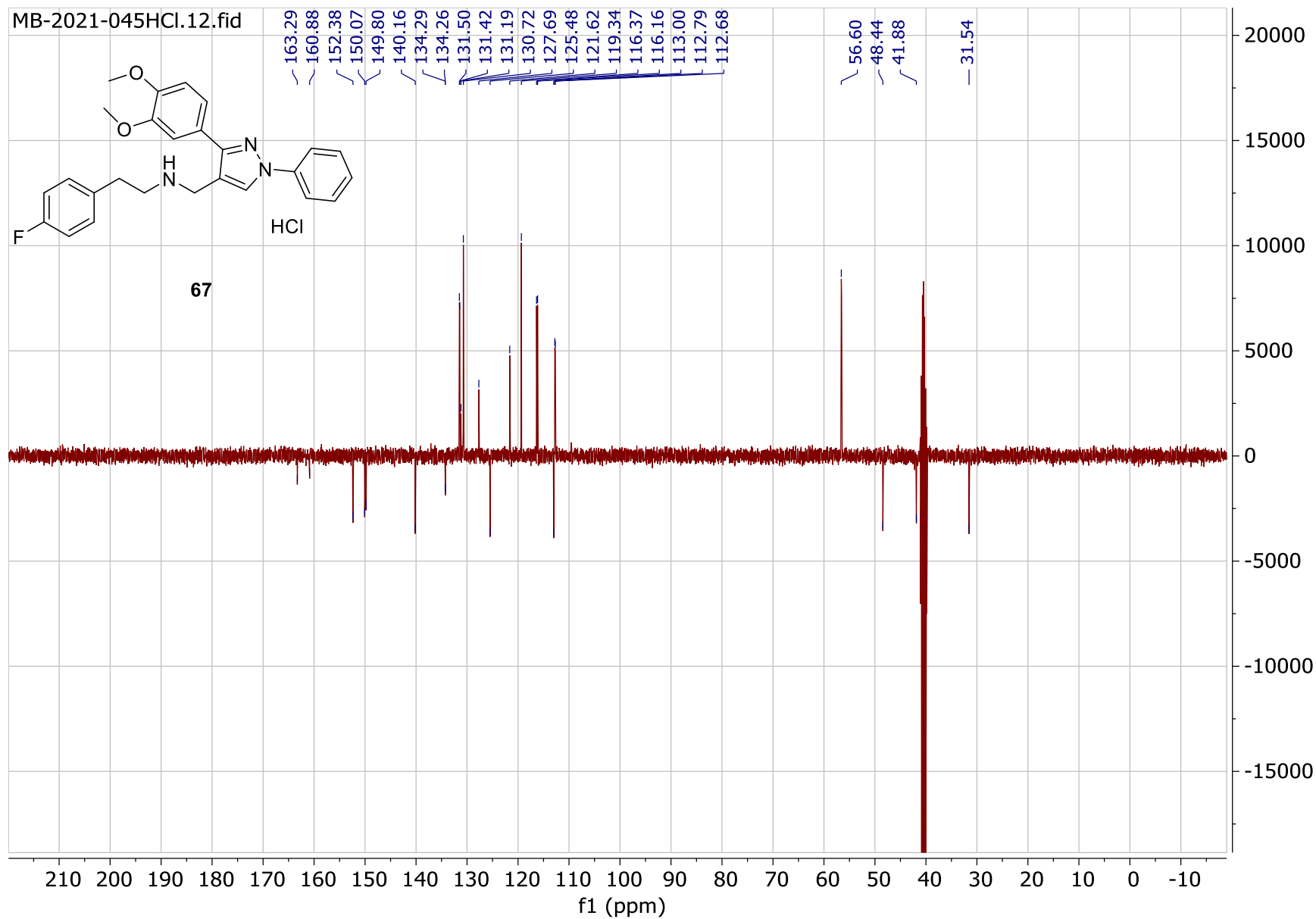


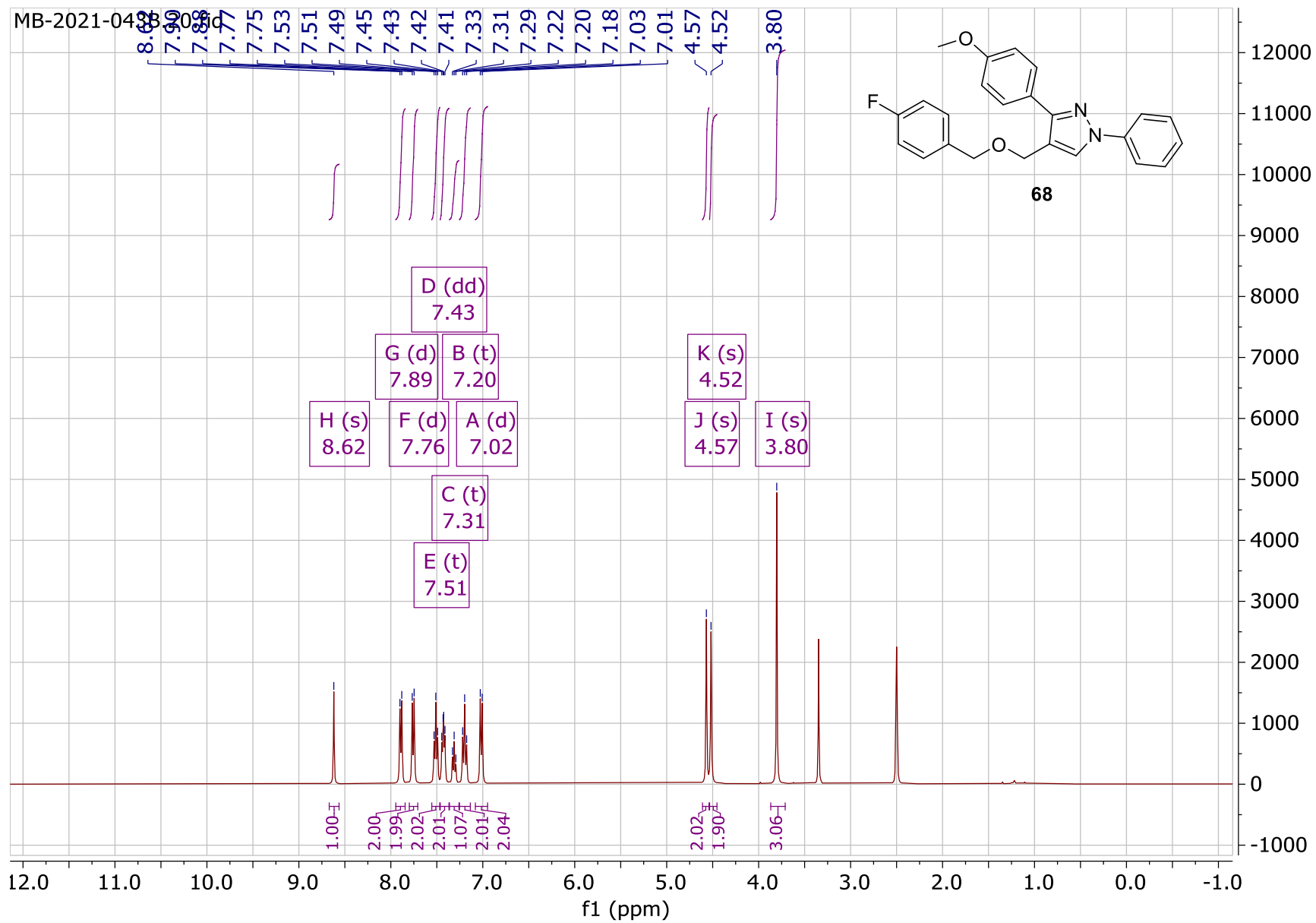
HCl

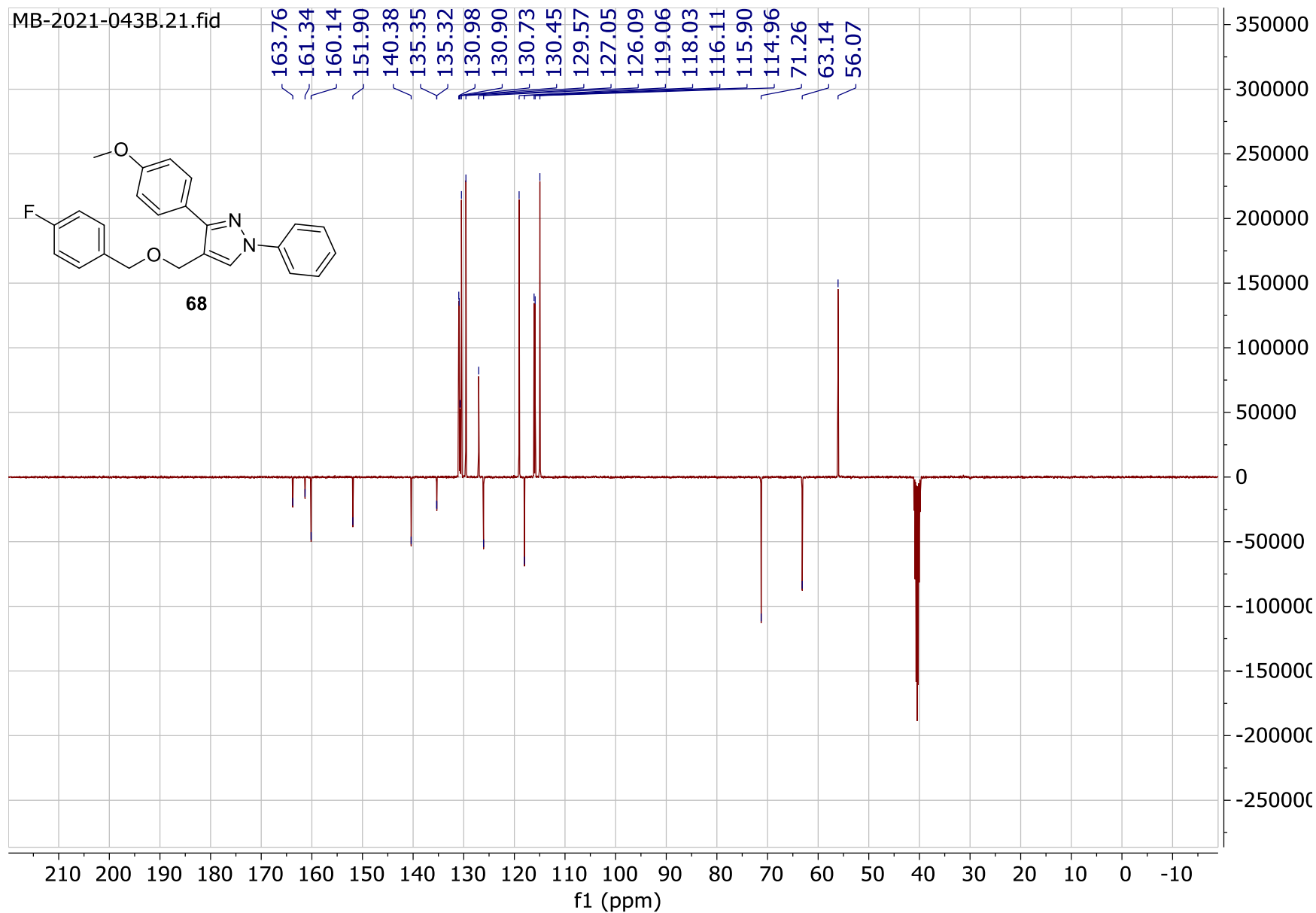




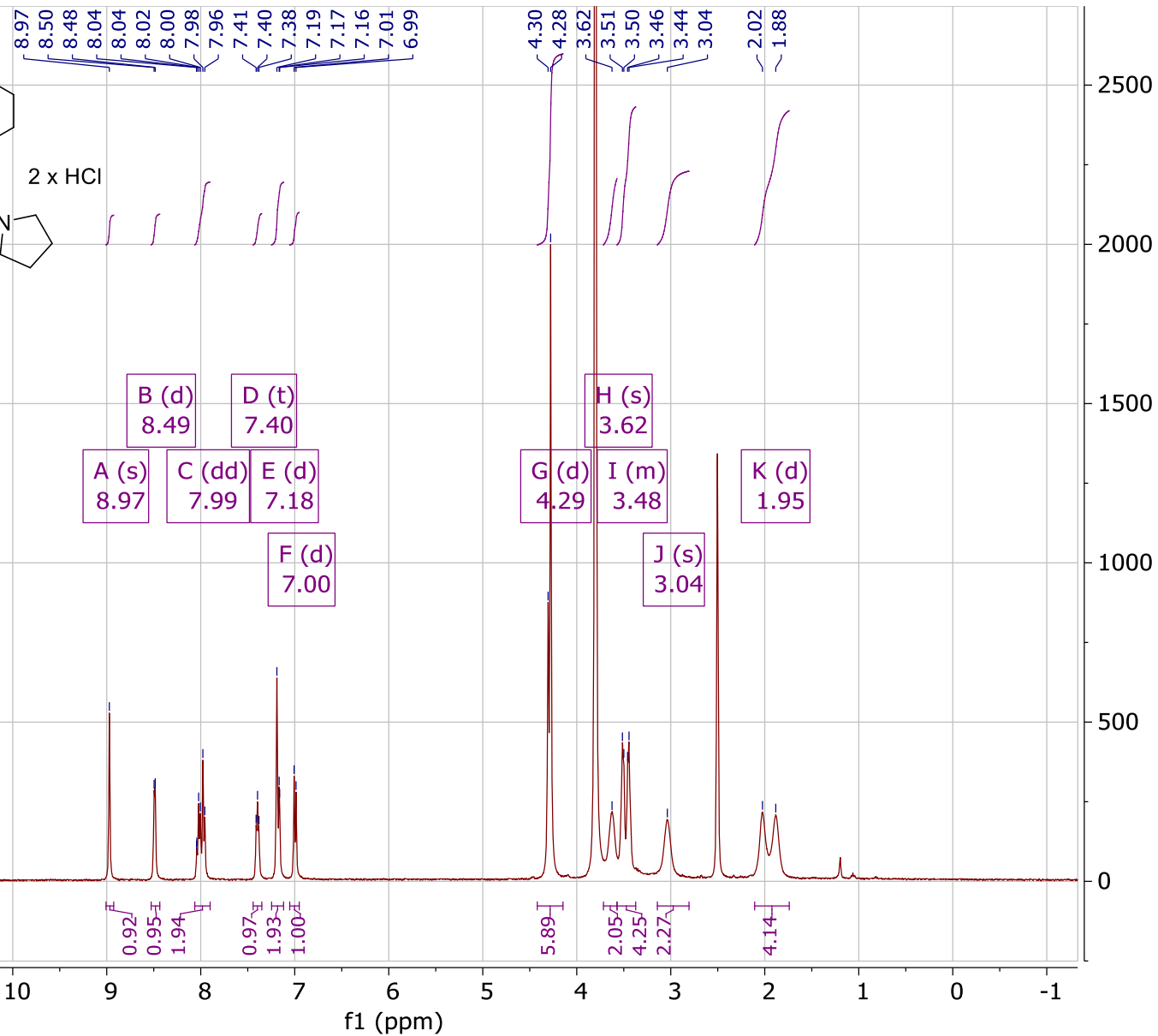
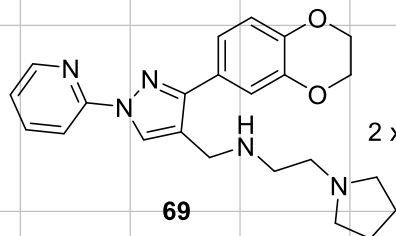


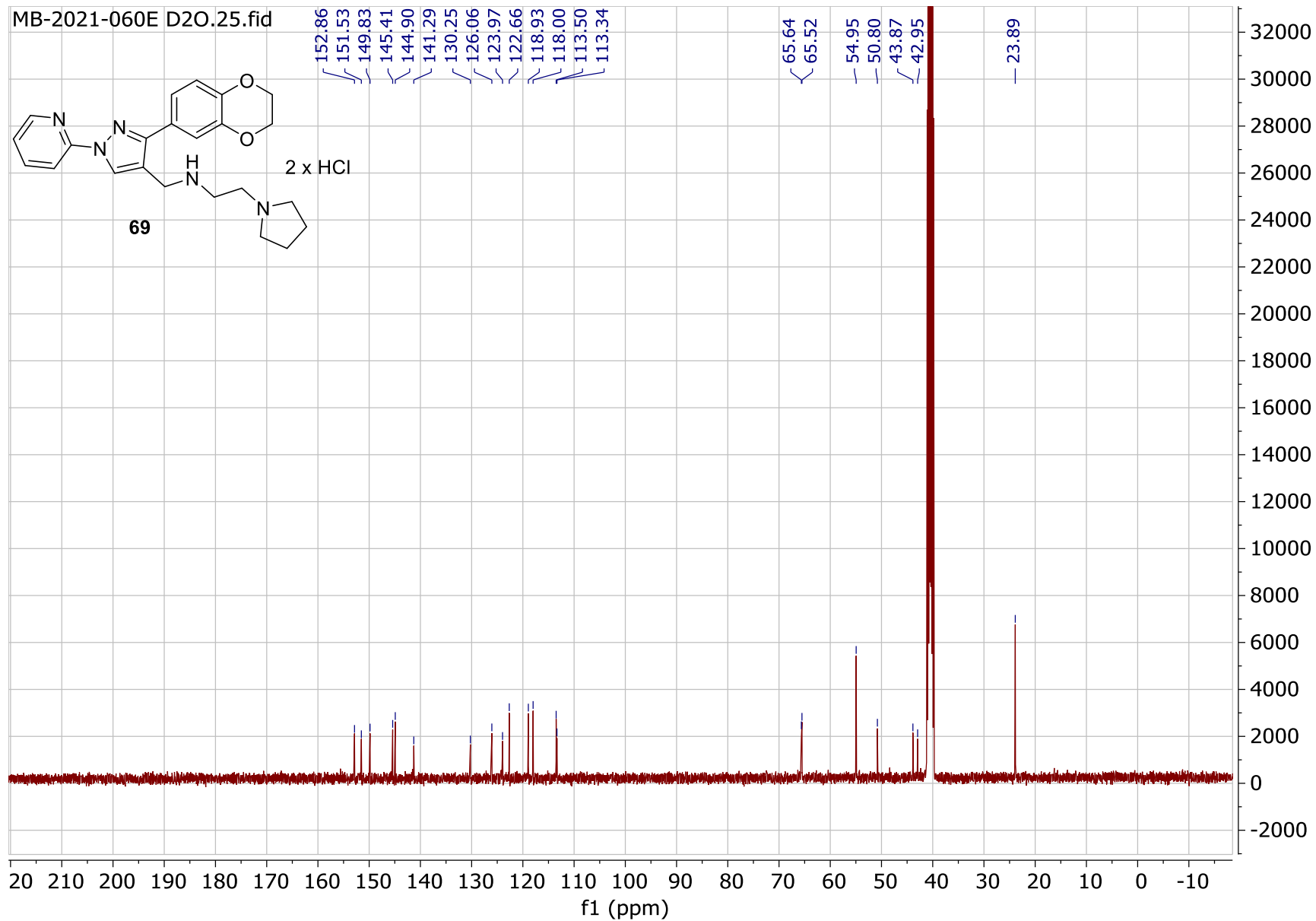






MB-2021-060E D2O.23.fid

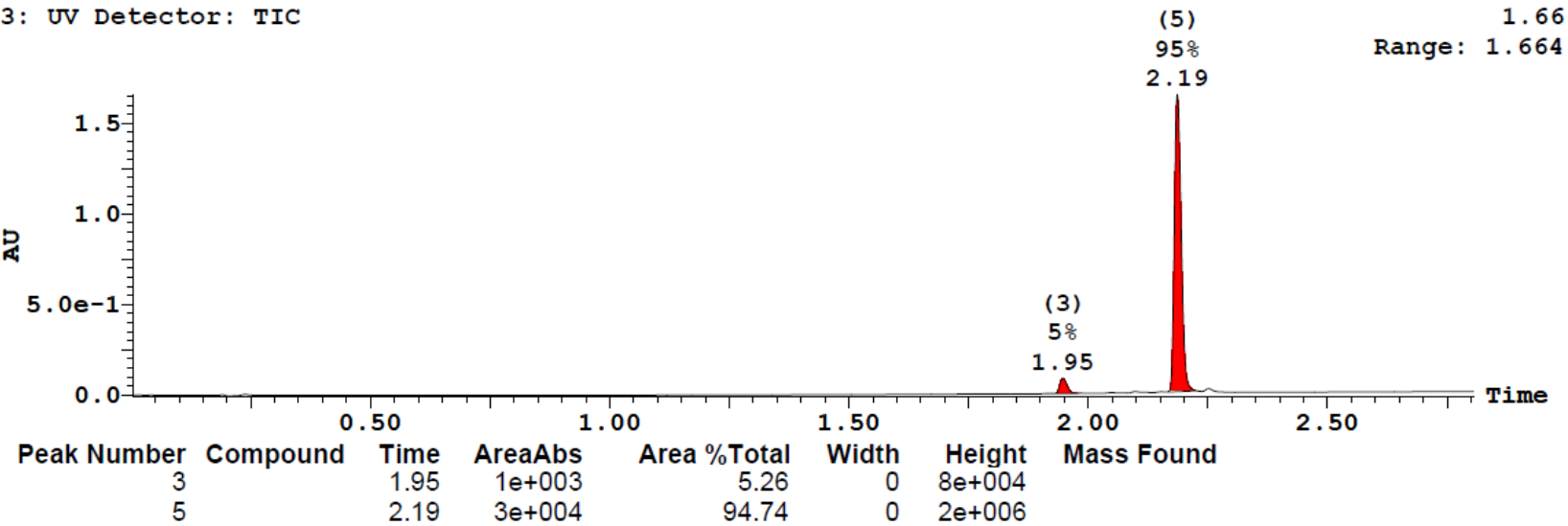




2. UPLC and HRMS spectra of the studied samples

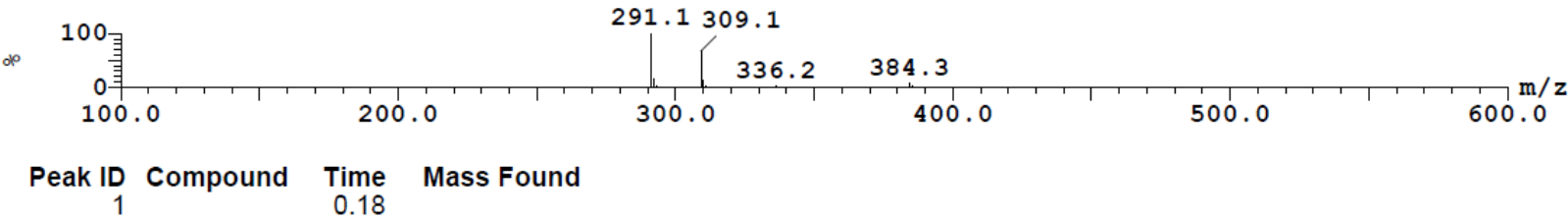
2.1 *N*-((3-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-1-phenyl-1*H*-pyrazol-4-yl)methyl)aniline (13)

3: UV Detector: TIC



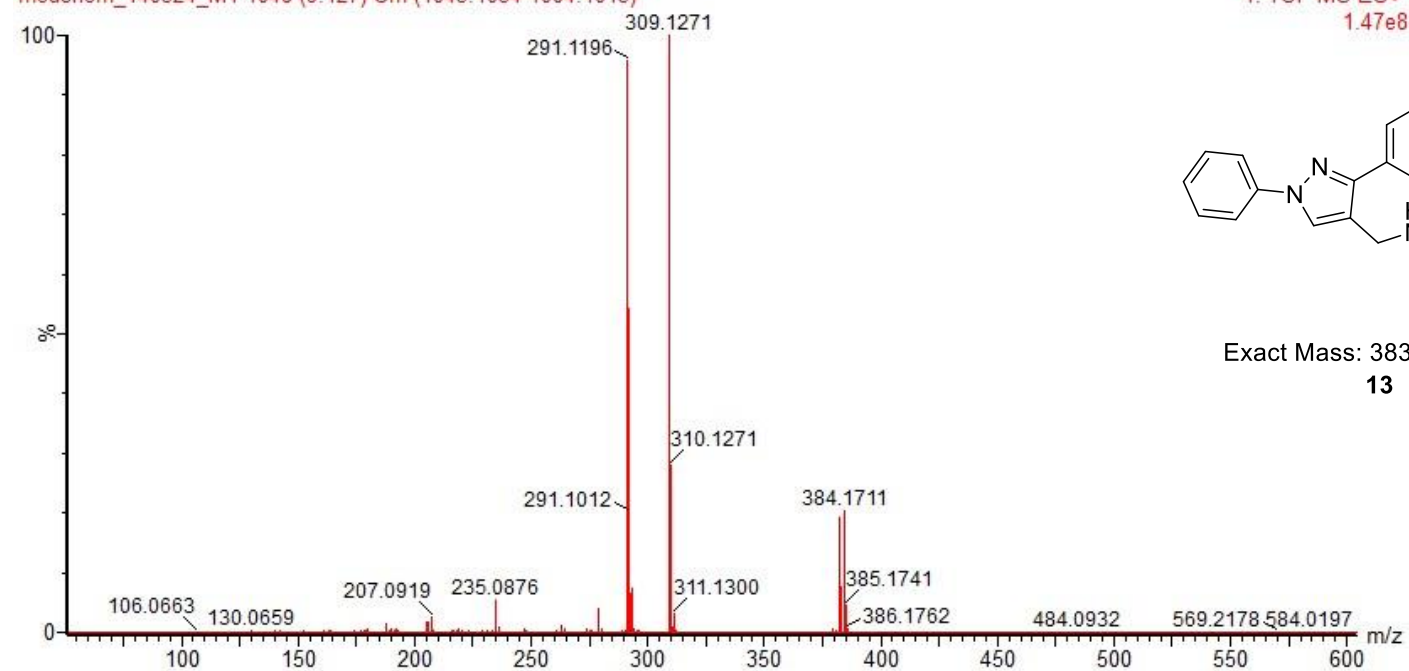
5: (Time: 2.19) Combine (871:879-(860:864+896:900))

1:MS ES+
6.0e+006

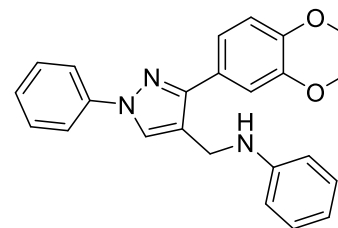


13UAMC5403

medchem_140324_M1 1048 (9.127) Cm (1043:1054-1004:1015)



1: TOF MS ES+
1.47e8

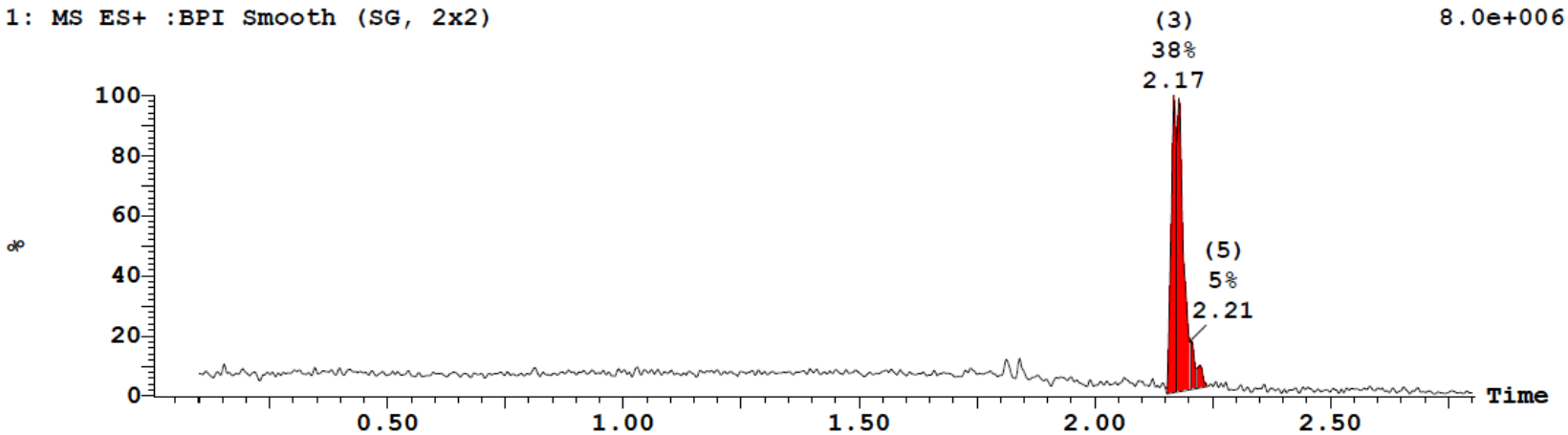


Exact Mass: 383,1634
13

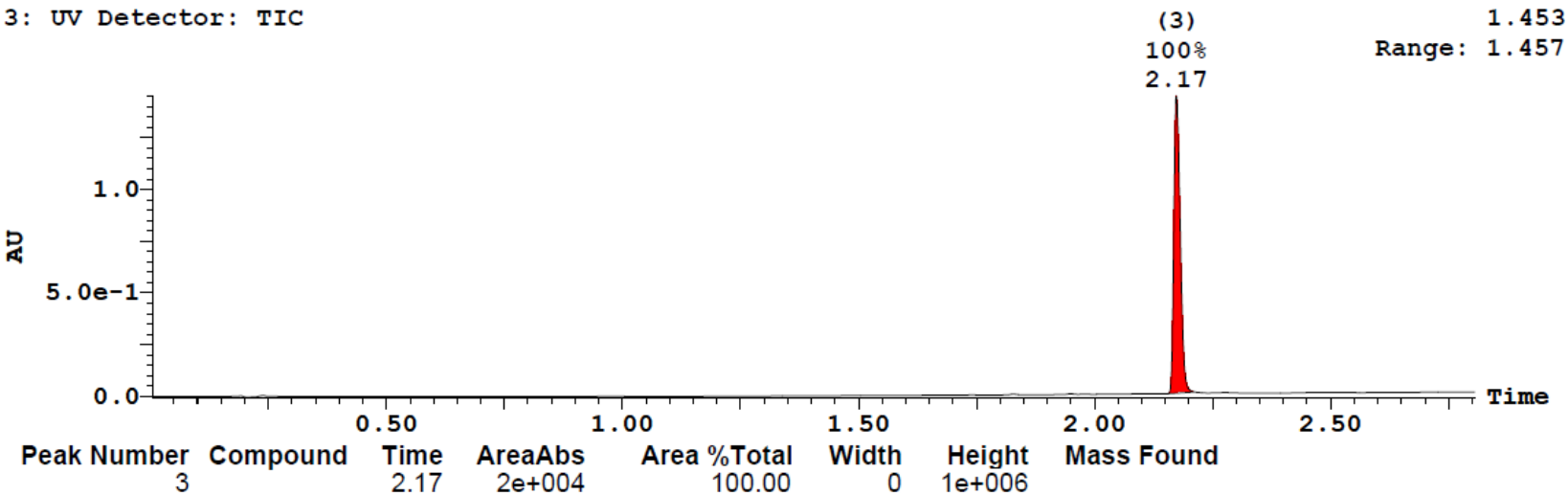
2.2 N-((3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-1-phenyl-1H-pyrazol-4-yl)methyl)-4-fluoroaniline (14)

Sample 1 Vial 1:57 ID UAMC-5435 File UAMC-5435 Date 13-Apr-2023 Time 17:49:49 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

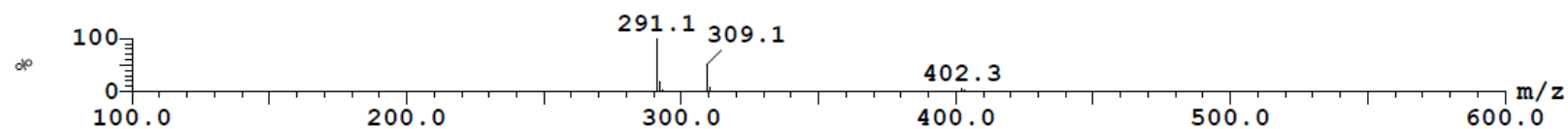


3: UV Detector: TIC



3: (Time: 2.17) Combine (866:874-(855:859+890:894))

1: MS ES+
6.7e+006

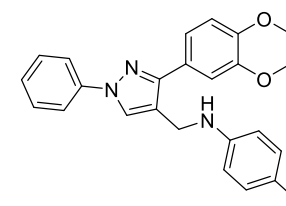
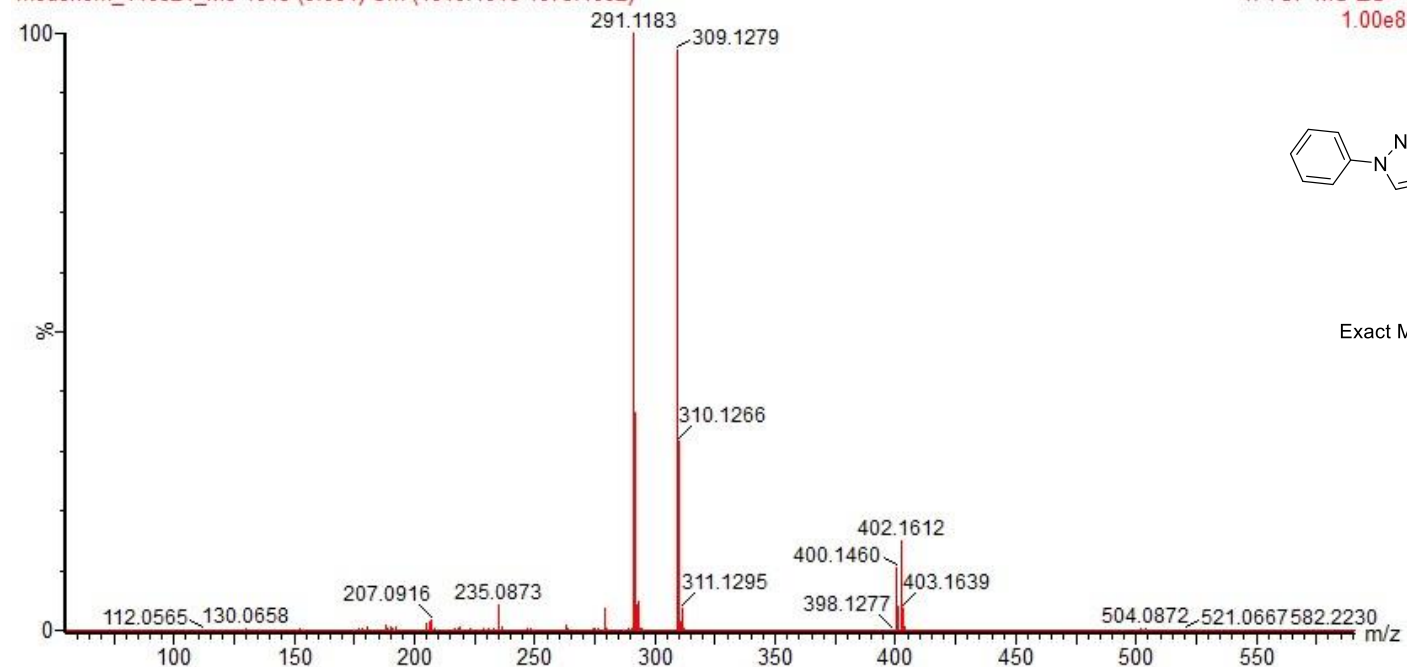


Peak ID	Compound	Time	Mass Found
4		2.18	

14UAMC5435

medchem_140324_M3 1043 (9.084) Cm (1040:1046-1075:1092)

1: TOF MS ES+
1.00e8

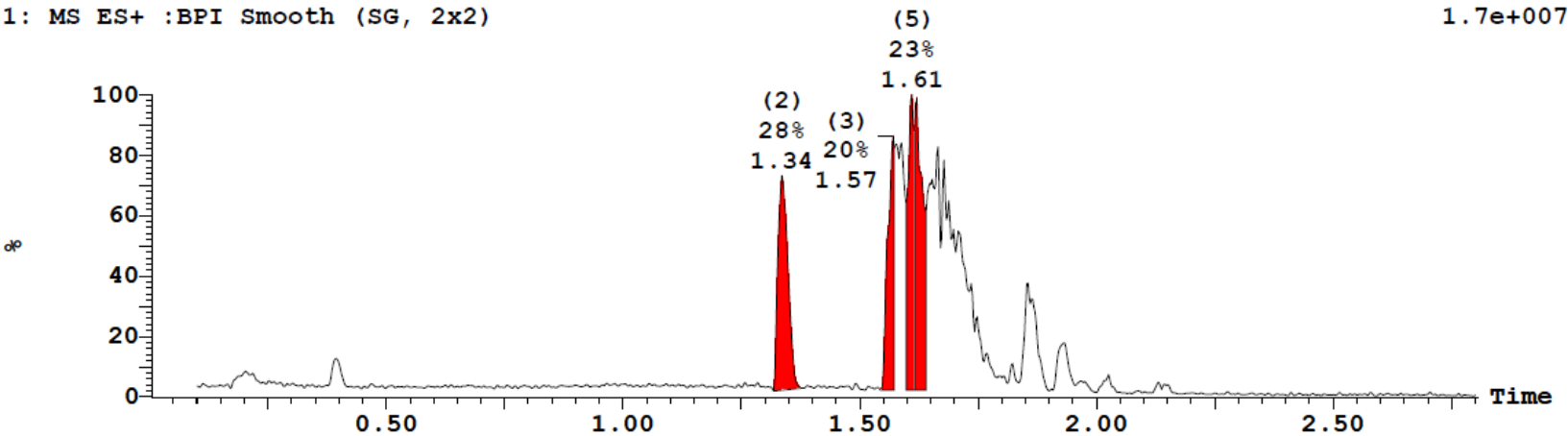


14

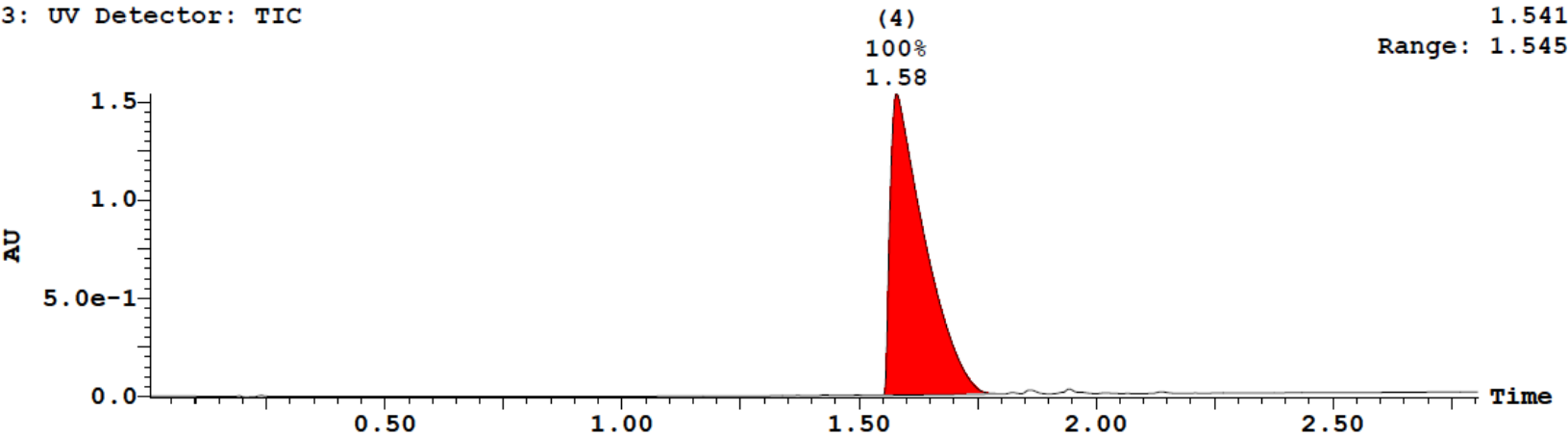
Exact Mass: 401,1540

2.3 N-((3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-1-phenyl-1H-pyrazol-4-yl)methyl)-2-phenylethan-1-amine hydrochloride (17)

1: MS ES+ :BPI Smooth (SG, 2x2) 1.7e+007



3: UV Detector: TIC 1.541
Range: 1.545

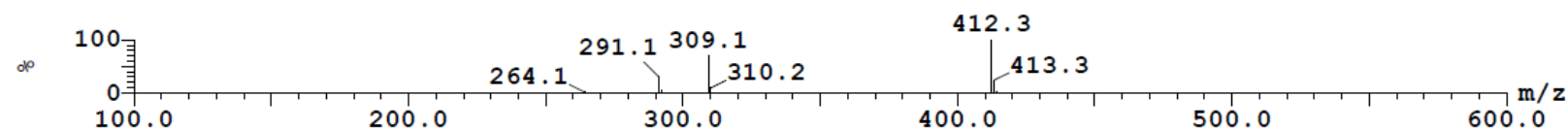


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
4		1.58	1e+005	100.00	0	2e+006	

Peak ID	Compound	Time	Mass Found
4		1.58	

4: (Time: 1.58) Combine (628:636-(610:614+727:731))

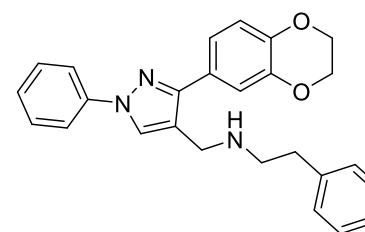
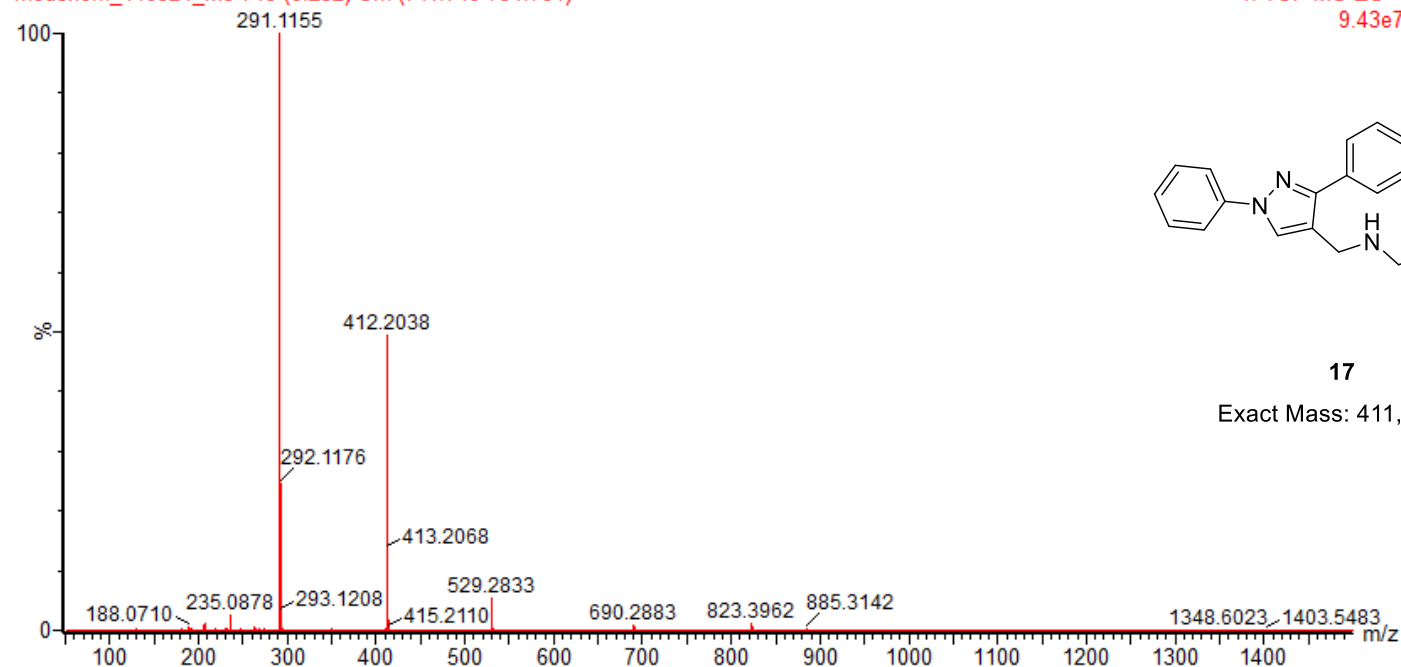
1:MS ES+
1.3e+007



17UAMC5404

medchem_140324_M5 715 (6.232) Cm (711:719-754:784)

1: TOF MS ES+
9.43e7



17

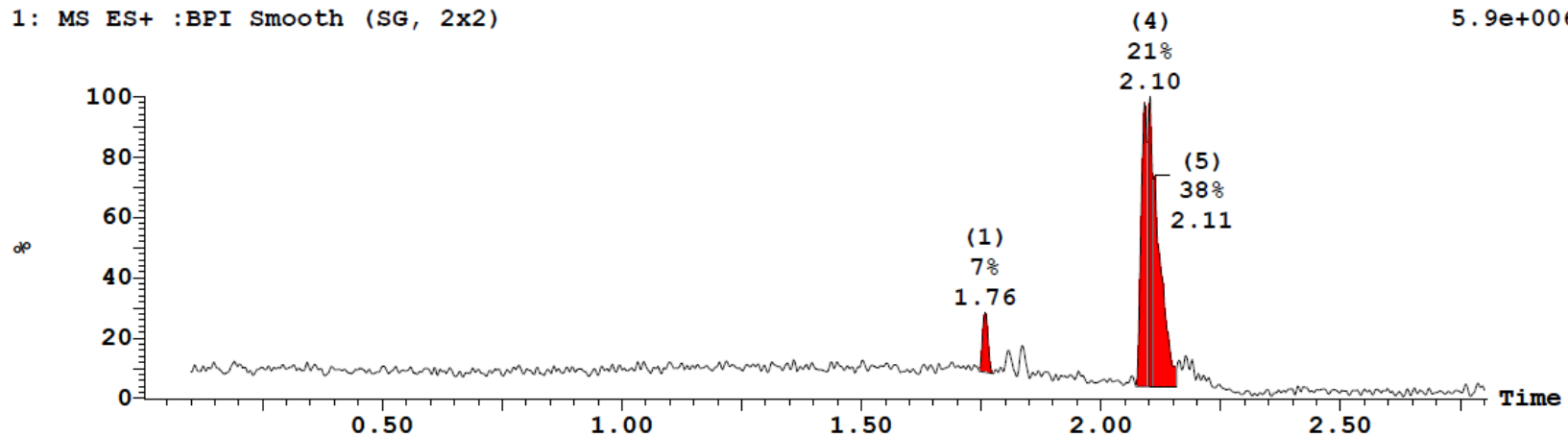
Exact Mass: 411,1947

2.4 4-(4-(((3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-1-phenyl-1H-pyrazol-4-yl)methyl)amino)phenoxy)-N-methylpicolinamide (22)

Sample 1 Vial 2:37 ID UAMC-5410 File UAMC-5410 Date 12-Apr-2023 Time 13:17:45 Description

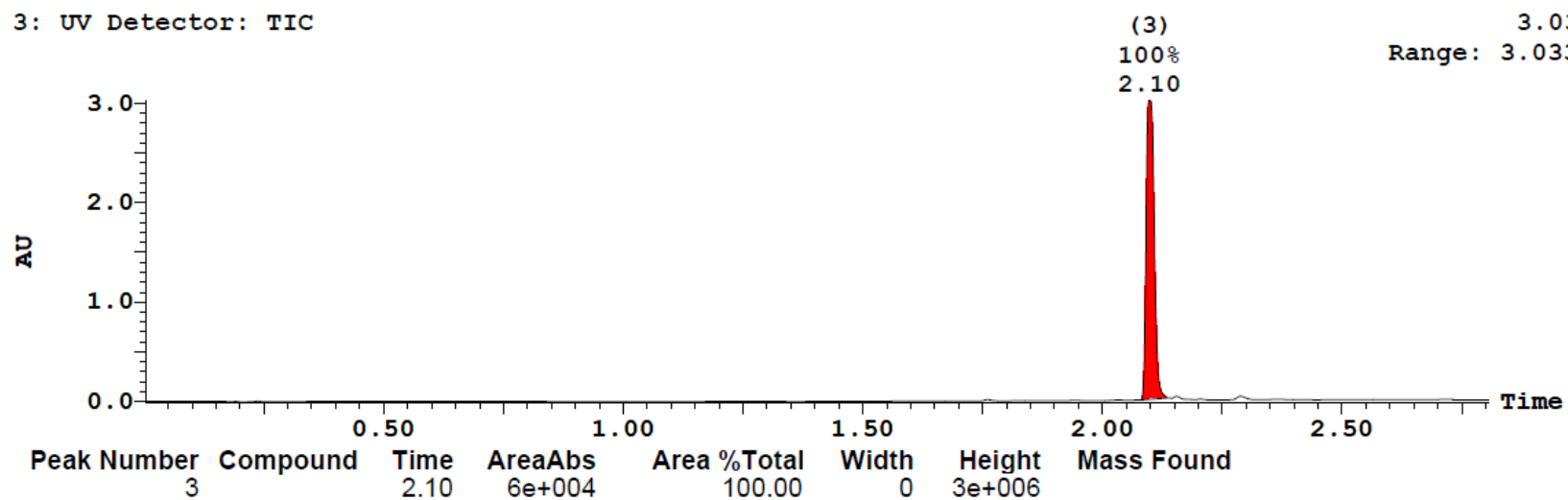
1: MS ES+ :BPI Smooth (SG, 2x2)

5.9e+006



3: UV Detector: TIC

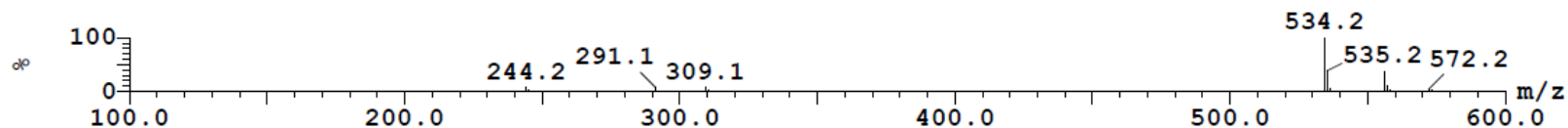
3.03
Range: 3.033



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
3		2.10	6e+004	100.00	0	3e+006	

Peak ID Compound Time Mass Found
3 2.09
3: (Time: 2.10) Combine (836:844-(824:828+861:865))

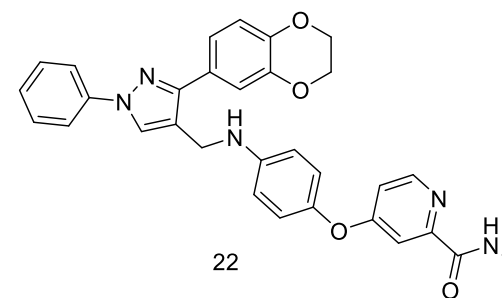
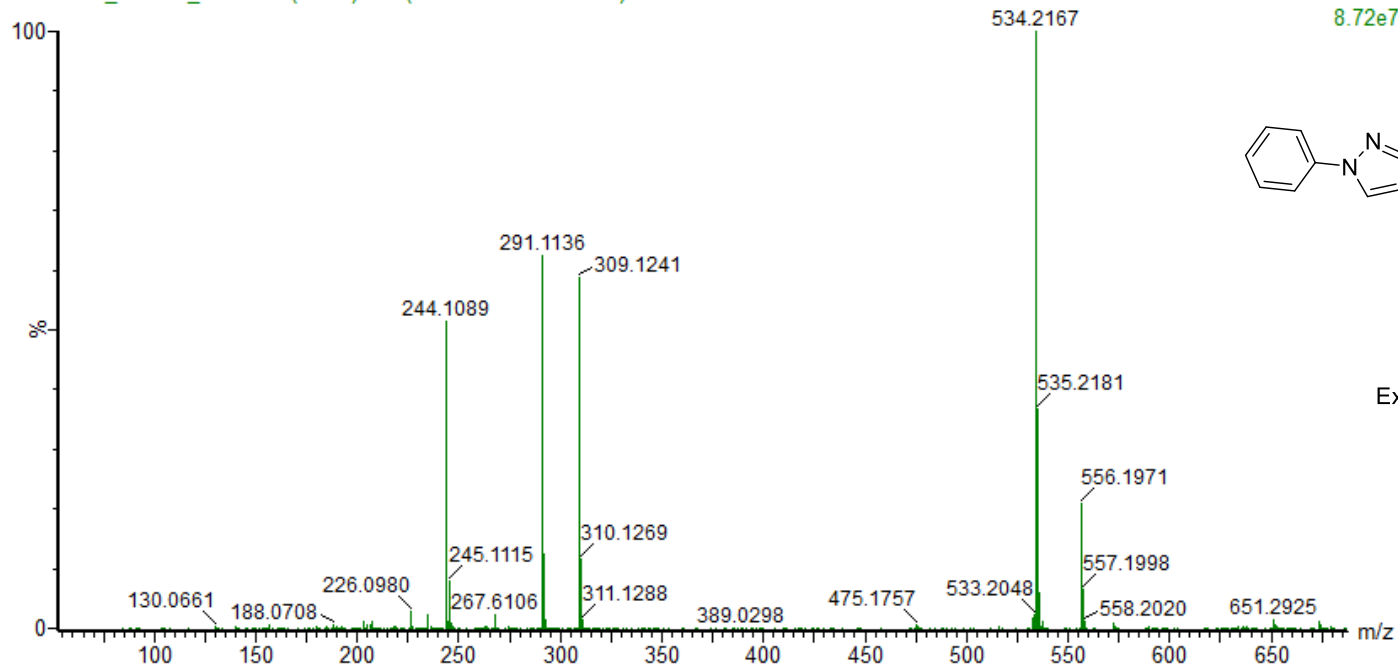
1:MS ES+
4.9e+006



22UAMC5410

medchem_140324_M7 1009 (8.786) Cm (1007:1014-1096:1168)

1: TOF MS ES+
8.72e7



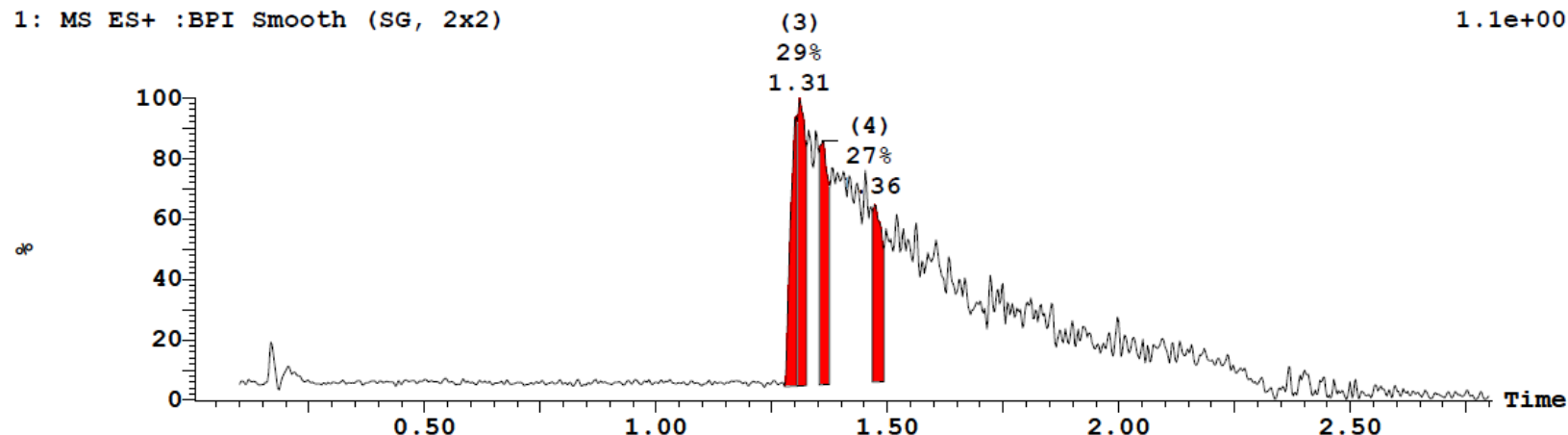
Exact Mass: 533,2063

2.5 *N*-((3-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-1-phenyl-1*H*-pyrazol-4-yl)methyl)-2-(pyrrolidin-1-yl)ethan-1-amine dihydrochloride (26)

Sample 1 Vial 2:74 ID MB-2021-054B CHK File MB-2021-054B CHK Date 22-Feb-2023 Time 10:17:46 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

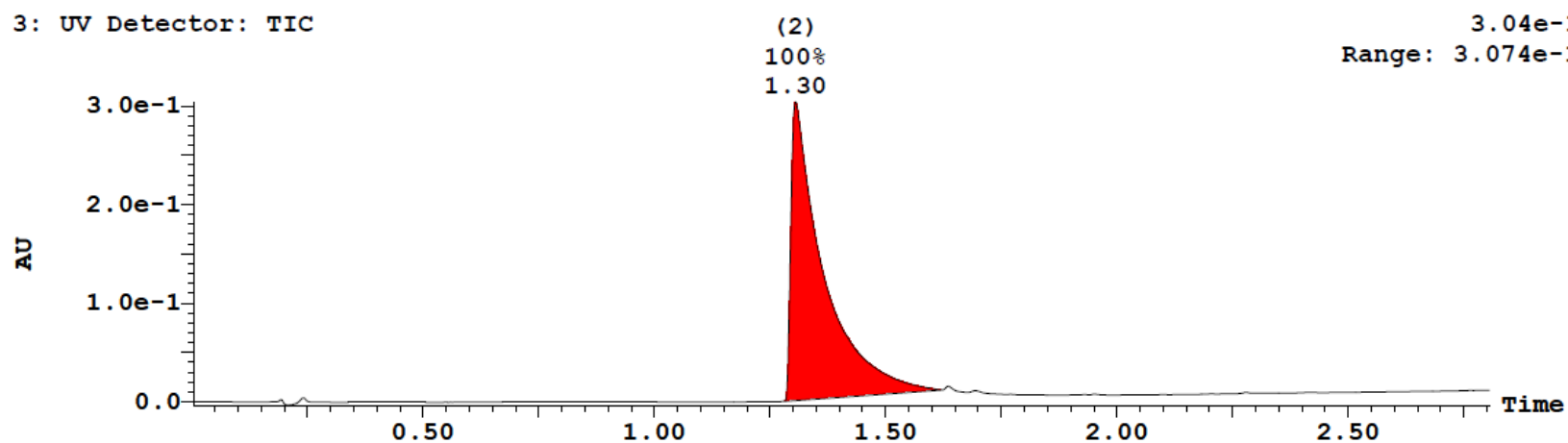
1.1e+007



3: UV Detector: TIC

3.04e-1

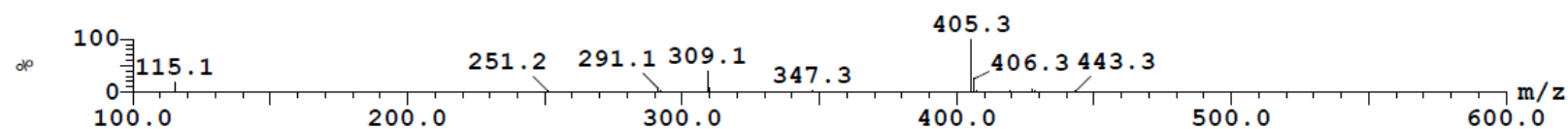
Range: 3.074e-1



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
2		1.30	2e+004	100.00	0	3e+005	

2: (Time: 1.30) Combine (519:527- (504:508+654:658))

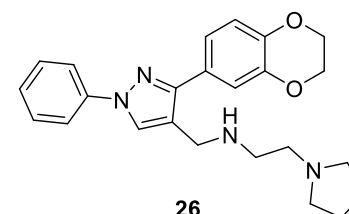
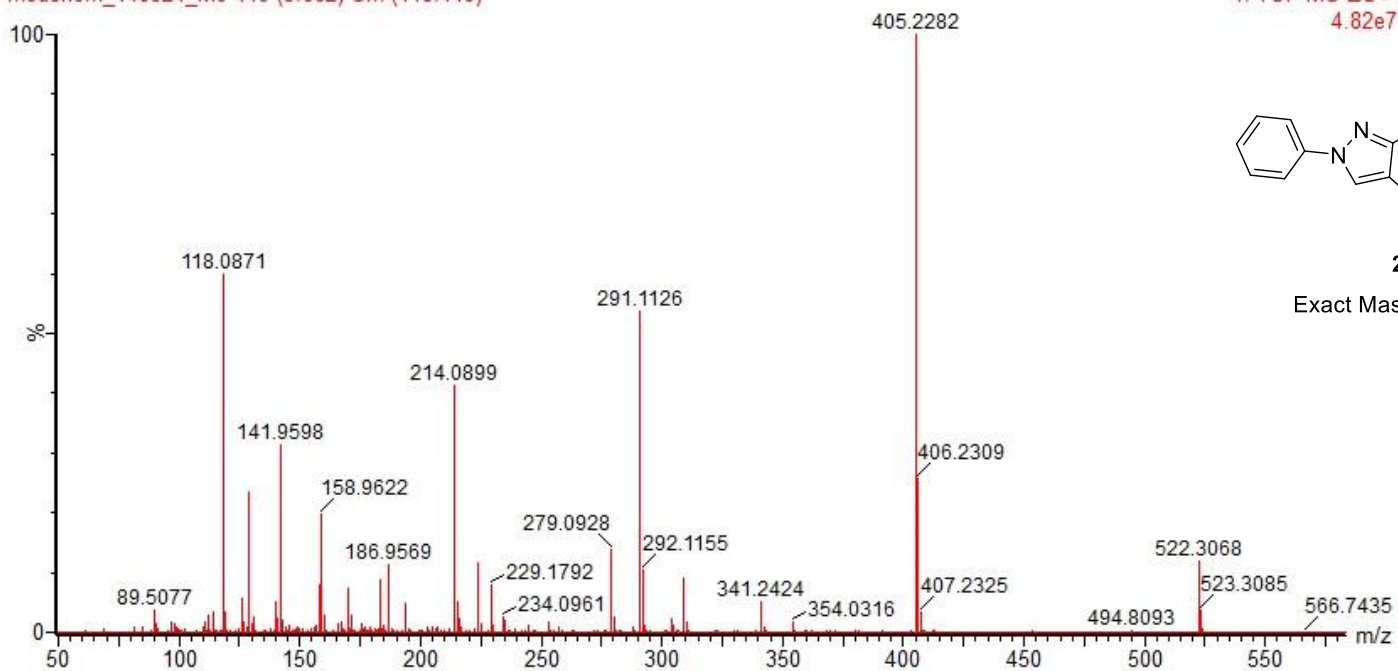
1: MS ES+
7.4e+006



26UAMC5295

medchem_140324_M9 419 (3.662) Cm (418.449)

1: TOF MS ES+
4.82e7



26

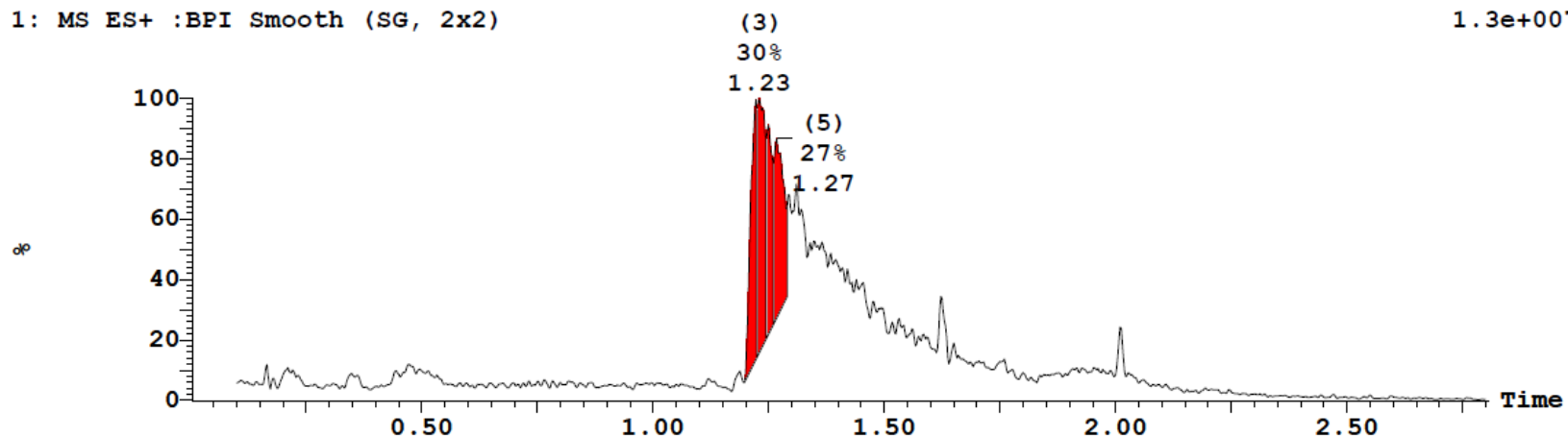
Exact Mass: 404,2212

2.6 *N*¹-((3-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-1-phenyl-1*H*-pyrazol-4-yl)methyl)-*N*³,*N*³-dimethylpropane-1,3-diamine dihydrochloride (29)

Sample 1 Vial 2:8 ID MB-2023-019 HCI File MB-2023-019 HCI Date 17-Feb-2023 Time 14:19:41 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

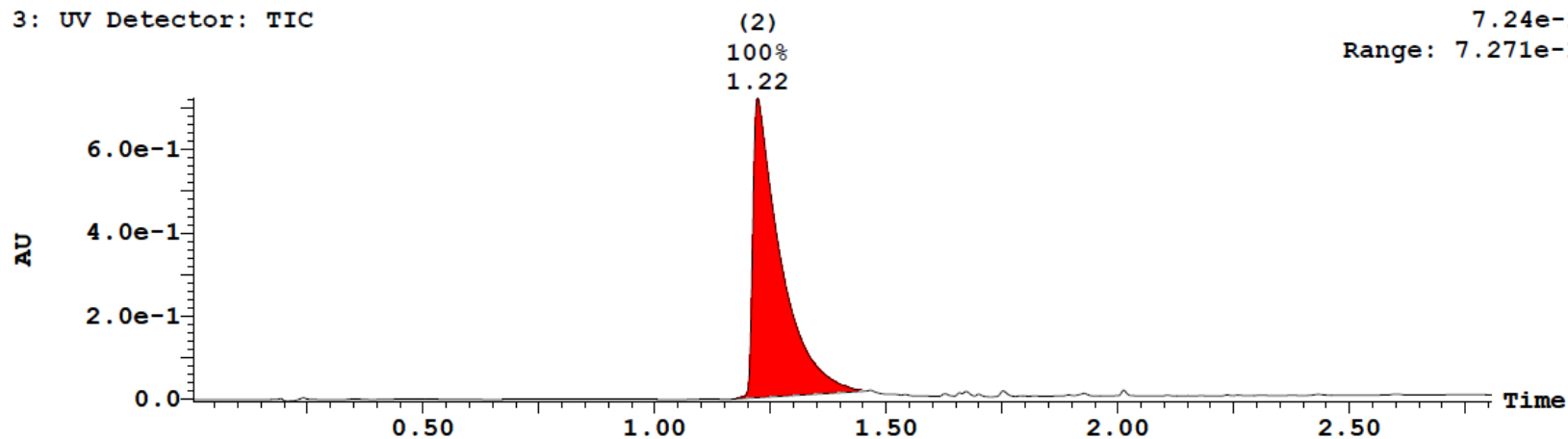
1.3e+007



3: UV Detector: TIC

7.24e-1

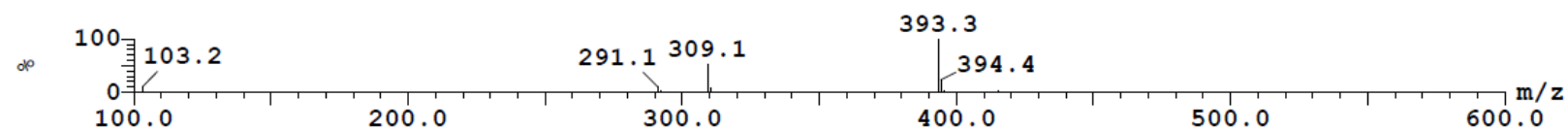
Range: 7.271e-1



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
2		1.22	5e+004	100.00	0	7e+005	

2: (Time: 1.22) Combine (486:494-(459:463+588:592))

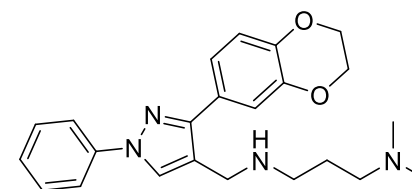
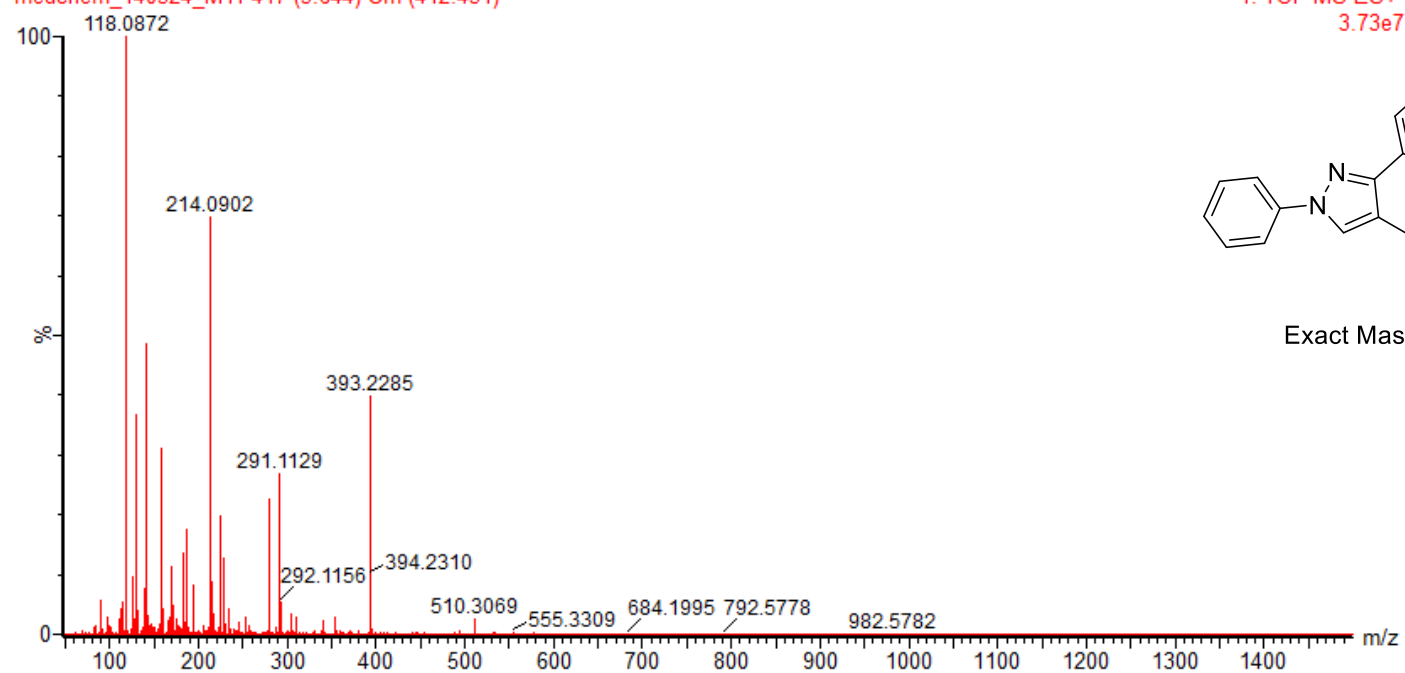
1: MS ES+
9.9e+006



29UAMC5296

medchem_140324_M11 417 (3.644) Cm (412:451)

1: TOF MS ES+
3.73e7



29

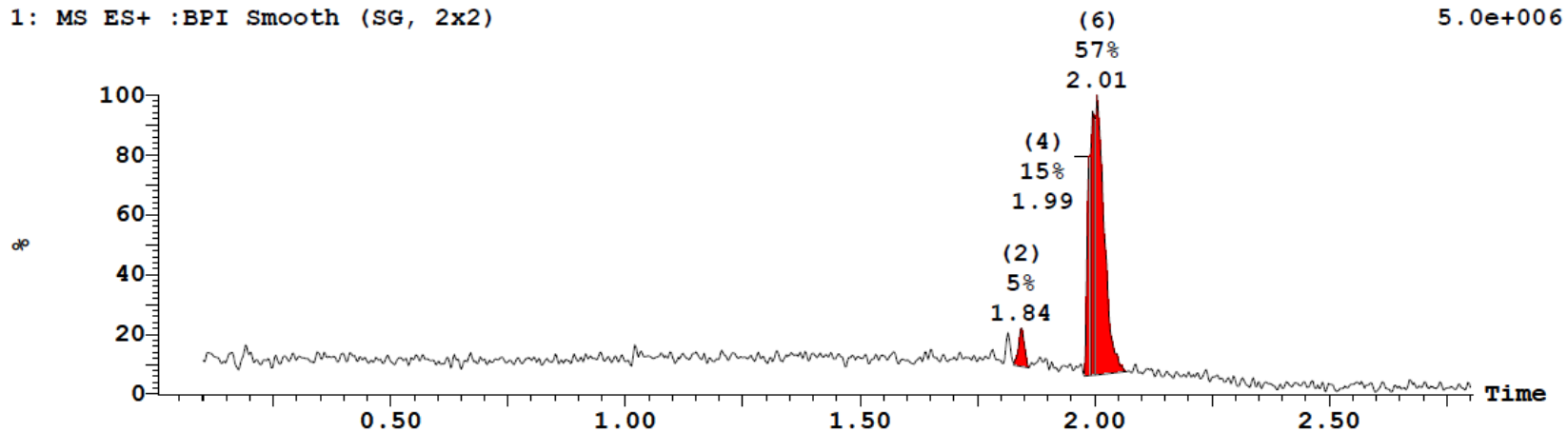
Exact Mass: 392,2212

2.7 3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-N-(4-fluorobenzyl)-1-phenyl-1H-pyrazole-4-carboxamide (33)

Sample 1 Vial 2:9 ID UAMC-5391 File UAMC-5391 Date 12-Apr-2023 Time 10:47:22 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

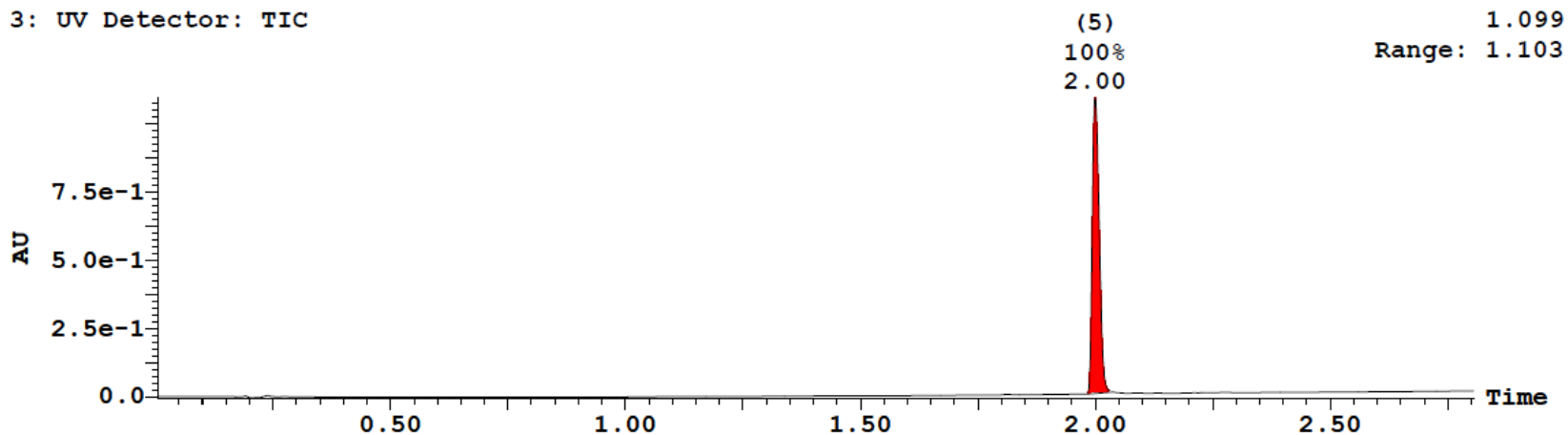
5.0e+006



3: UV Detector: TIC

1.099

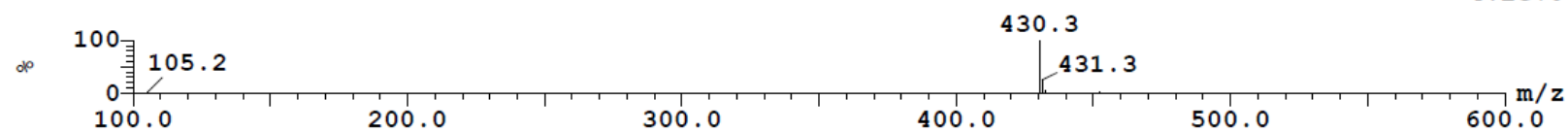
Range: 1.103



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
5		2.00	2e+004	100.00	0	1e+006	

5: (Time: 2.00) Combine (797:805-(785:789+820:824))

1:MS ES+
4.2e+006

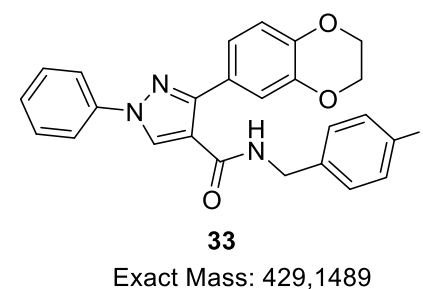
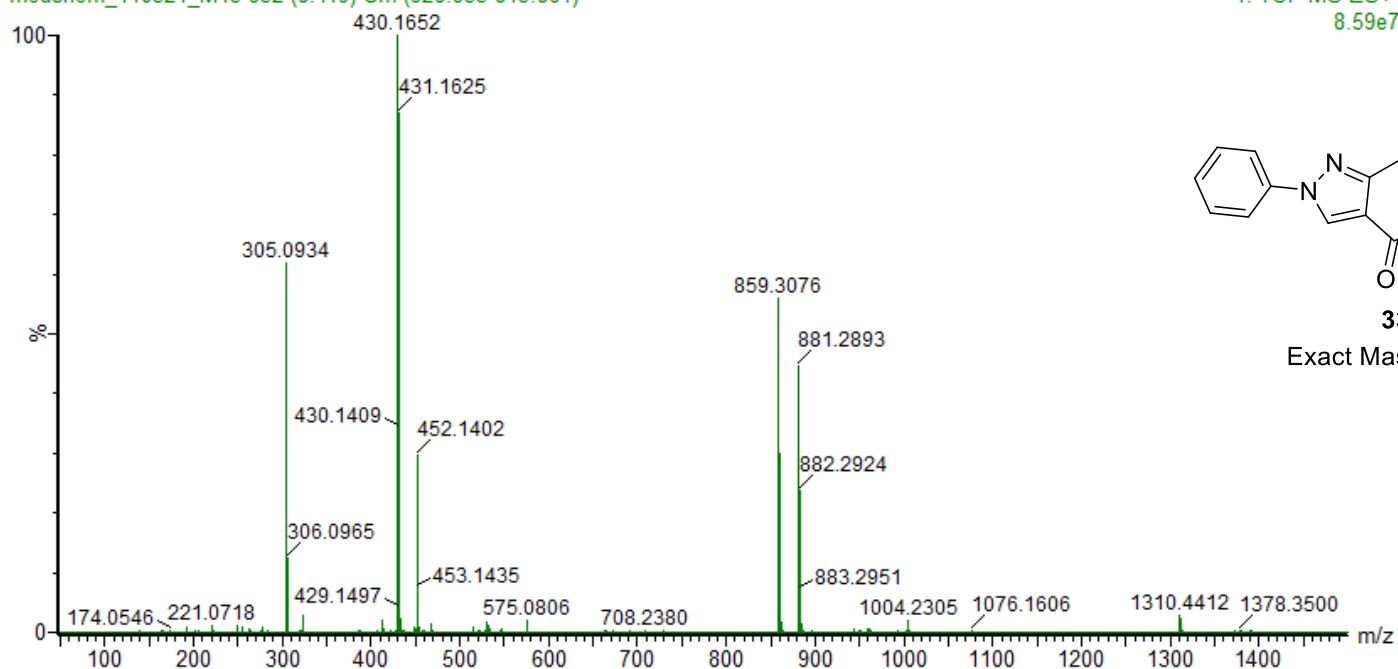


Peak ID	Compound	Time	Mass Found
6		2.01	

33UAMC5391

medchem_140324_M13 932 (8.119) Cm (928:935-845:861)

1: TOF MS ES+
8.59e7

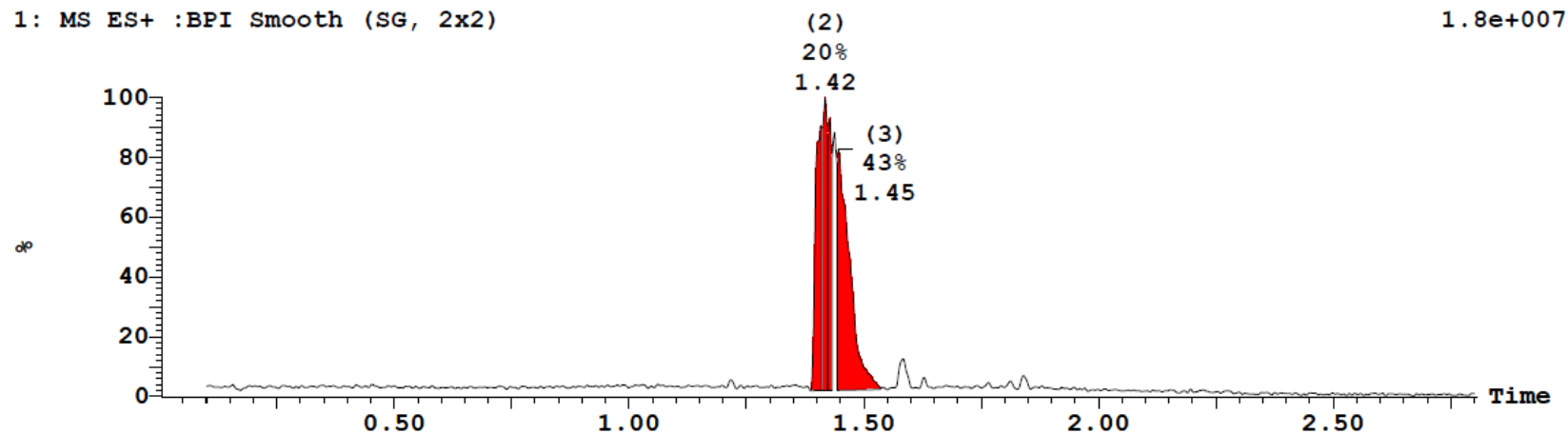


2.8 3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-1-phenyl-N-(2-(pyridin-4-yl)ethyl)-1H-pyrazole-4-carboxamide (35)

Sample 1 Vial 2:13 ID UAMC-5395 File UAMC-5395 Date 12-Apr-2023 Time 11:04:05 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

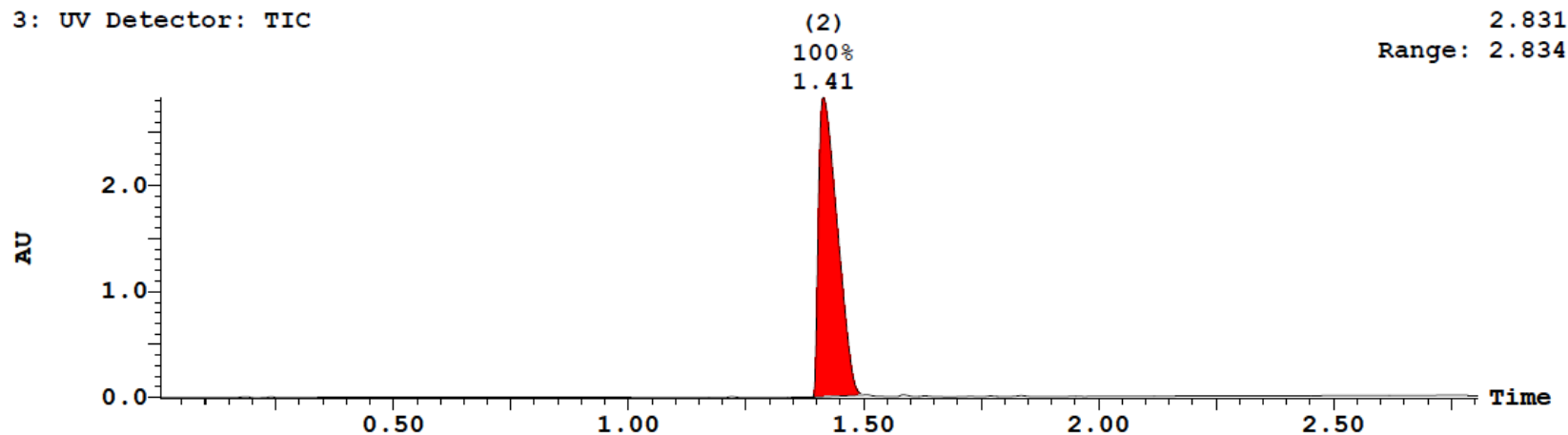
1.8e+007



3: UV Detector: TIC

2.831

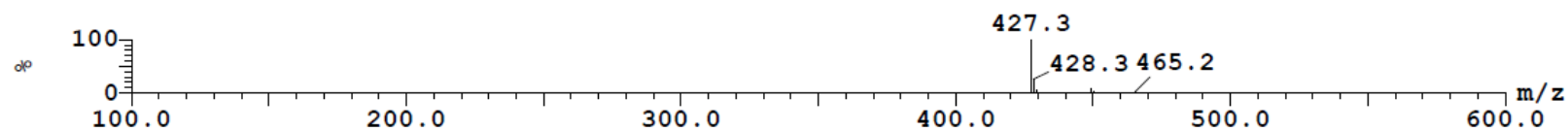
Range: 2.834



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
2		1.41	1e+005	100.00	0	3e+006	

2: (Time: 1.41) Combine (563:571- (548:552+606:610))

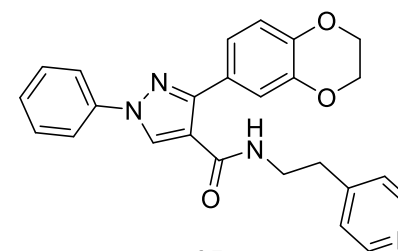
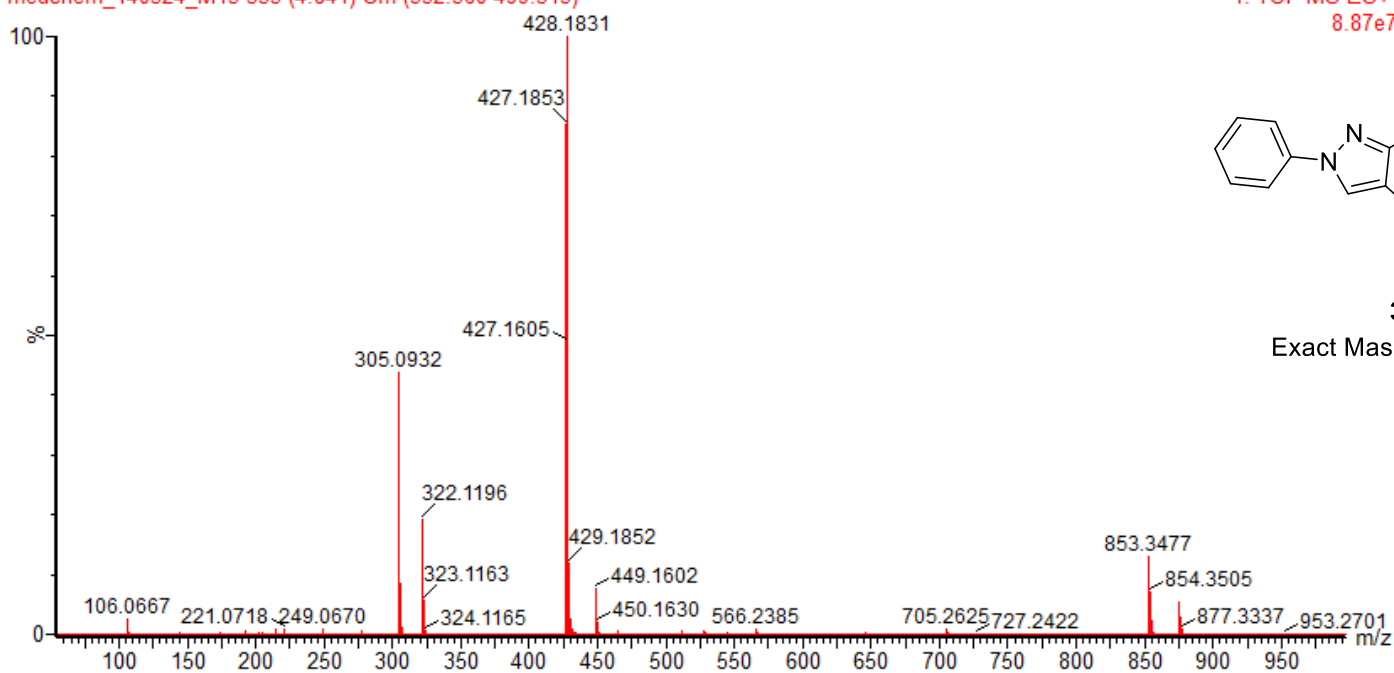
1: MS ES+
1.6e+007



35UAMC5395

medchem_140324_M15 555 (4.841) Cm (552:560-499:513)

1: TOF MS ES+
8.87e7



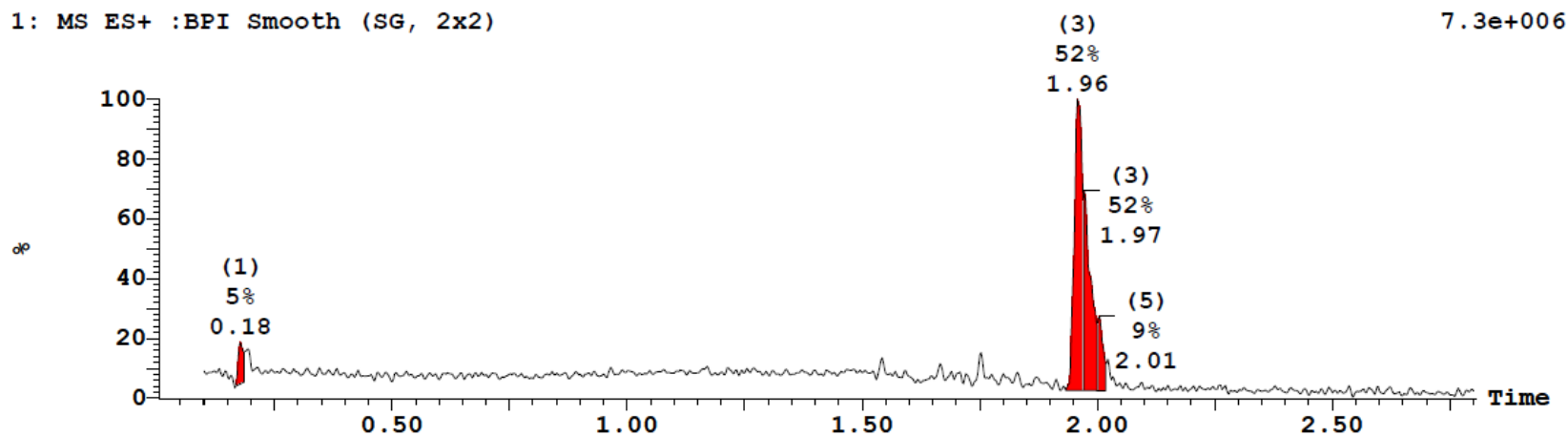
35

Exact Mass: 426,1692

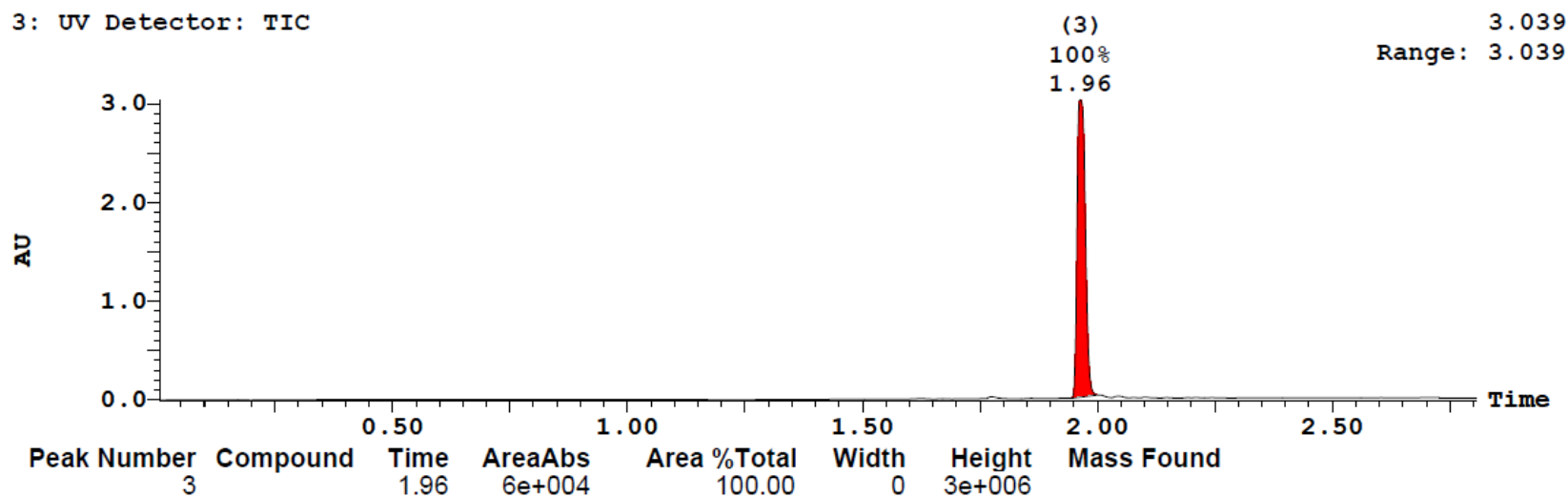
2.9 4-(4-(3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-1-phenyl-1H-pyrazole-4-carboxamido)phenoxy)-N-methylpicolinamide (38)

Sample 1 Vial 1:50 ID UAMC-5393-2 File UAMC-5393-2 Date 13-Apr-2023 Time 16:59:32 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

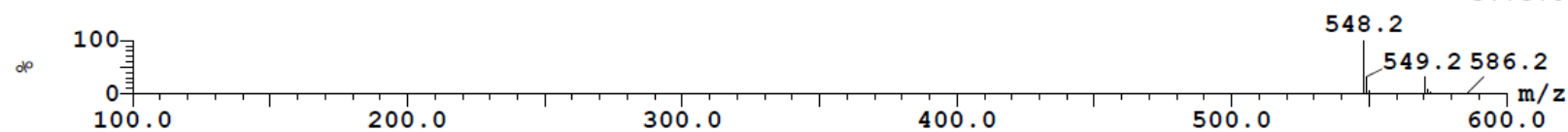


3: UV Detector: TIC



3: (Time: 1.96) Combine (782:790-(771:775+805:809))

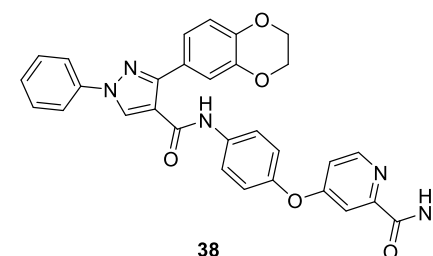
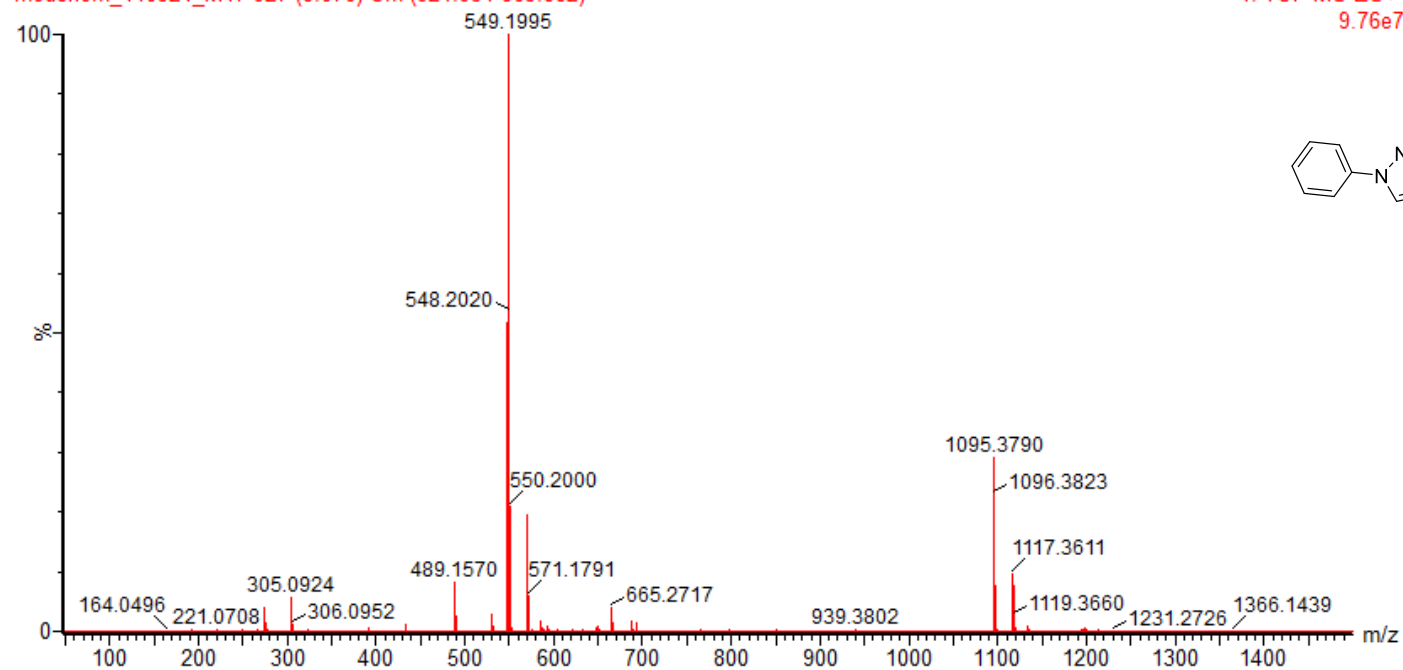
1: MS ES+
5.7e+006



38UAMC5393

medchem_140324_M17 927 (8.076) Cm (924:931-865:882)

1: TOF MS ES+
9.76e7

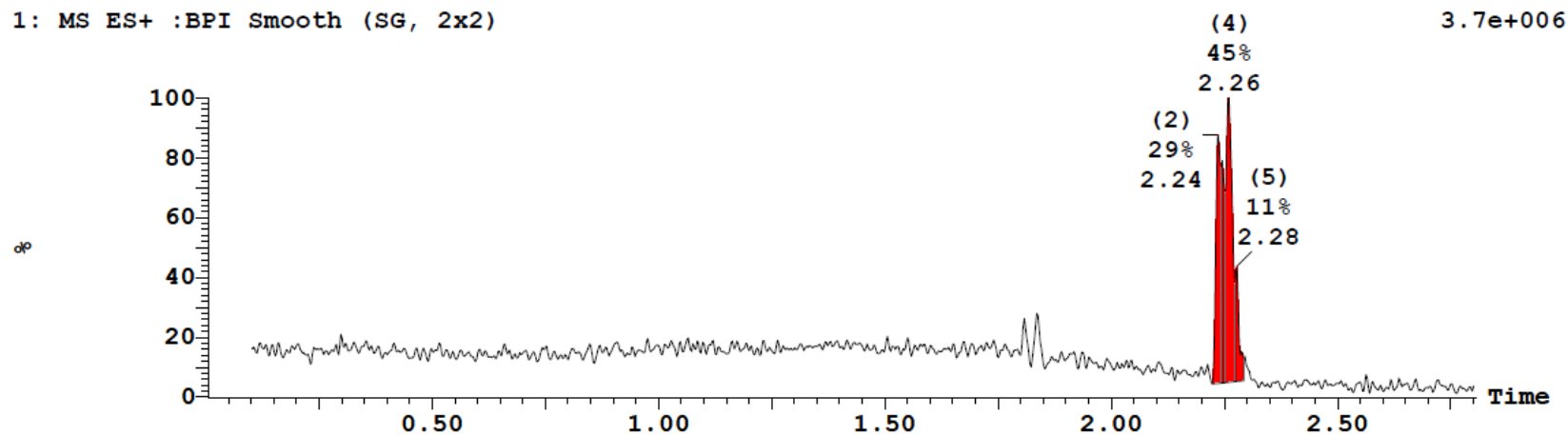


38
Exact Mass: 547,1856

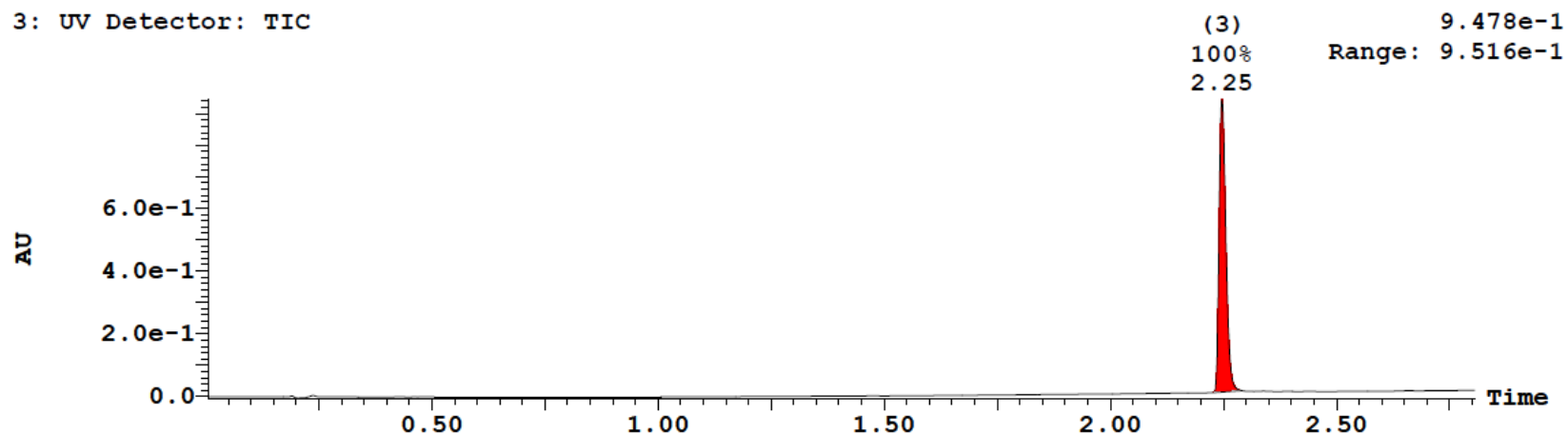
2.10 *N*-((1*r*,3*r*,5*r*,7*r*)-adamantan-2-yl)-3-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-1-phenyl-1*H*-pyrazole-4-carboxamide (41)

Sample 1 Vial 2:19 ID UAMC-5398 File UAMC-5398 Date 12-Apr-2023 Time 11:38:24 Description

1: MS ES+ :BPI Smooth (SG, 2x2)



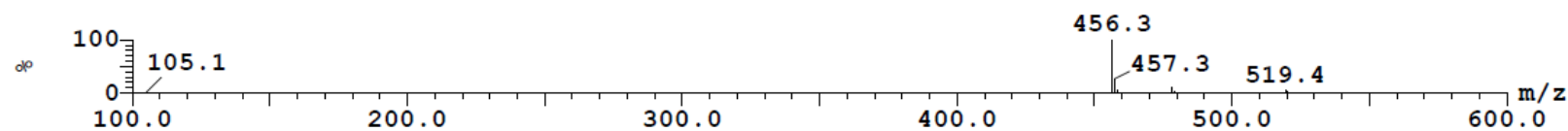
3: UV Detector: TIC



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
3		2.25	2e+004	100.00	0	9e+005	

3: (Time: 2.25) Combine (896:904-(883:887+921:925))

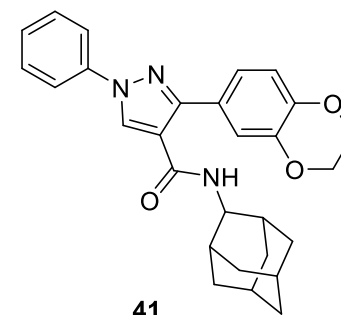
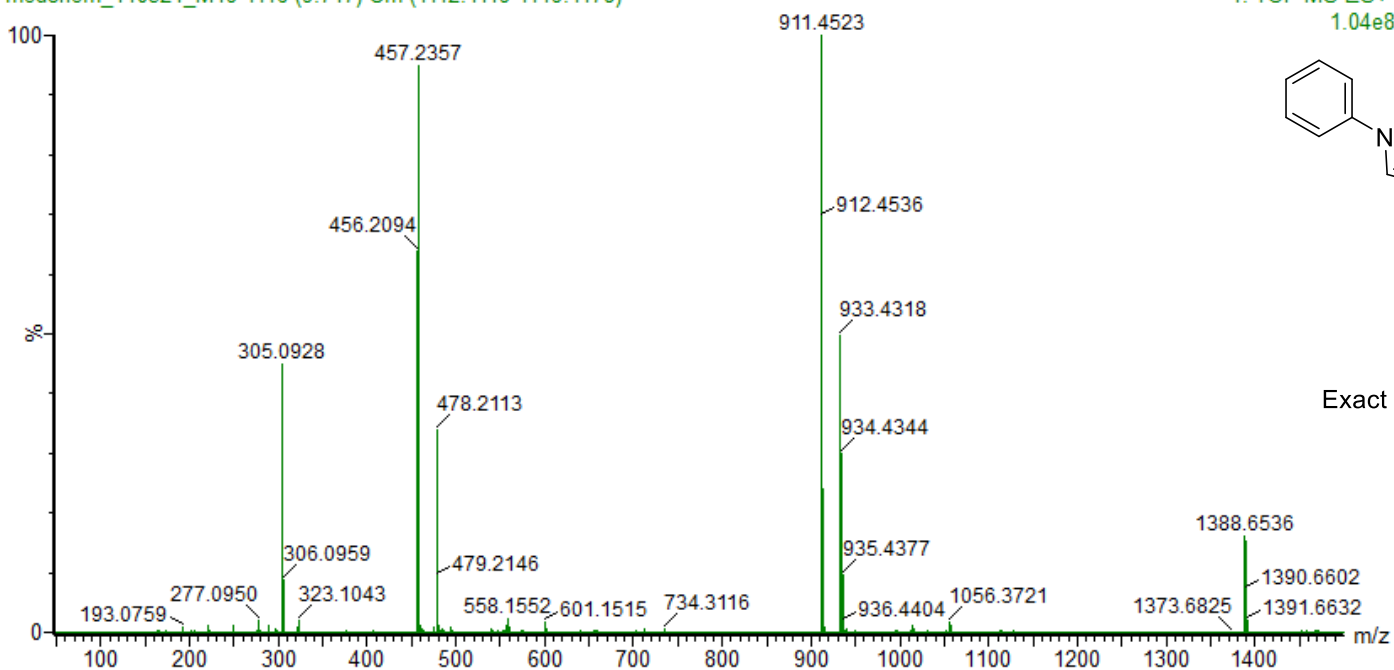
1: MS ES+
2.8e+006



41UAMC5398

medchem_140324_M19 1116 (9.717) Cm (1112:1119-1149:1178)

1: TOF MS ES+
1.04e8



41

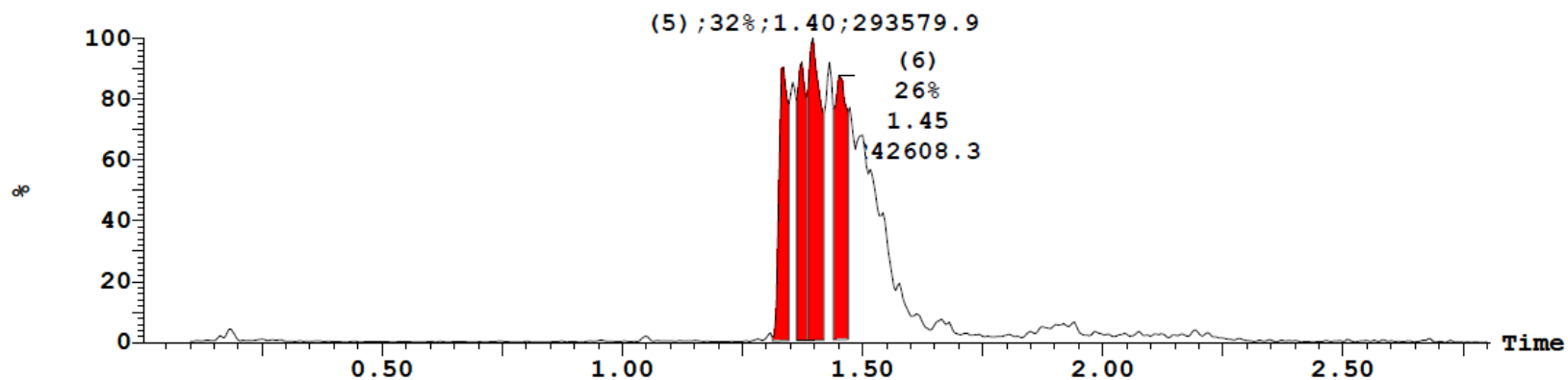
Exact Mass: 455,2209

2.11 3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-N-(2-morpholinoethyl)-1-phenyl-1H-pyrazole-4-carboxamide hydrochloride (44)

Sample 1 Vial 2:9 ID UAMC-5384 ACID FREE File UAMC-5384 ACID FREE Date 04-Nov-2023 Time 17:18:47 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

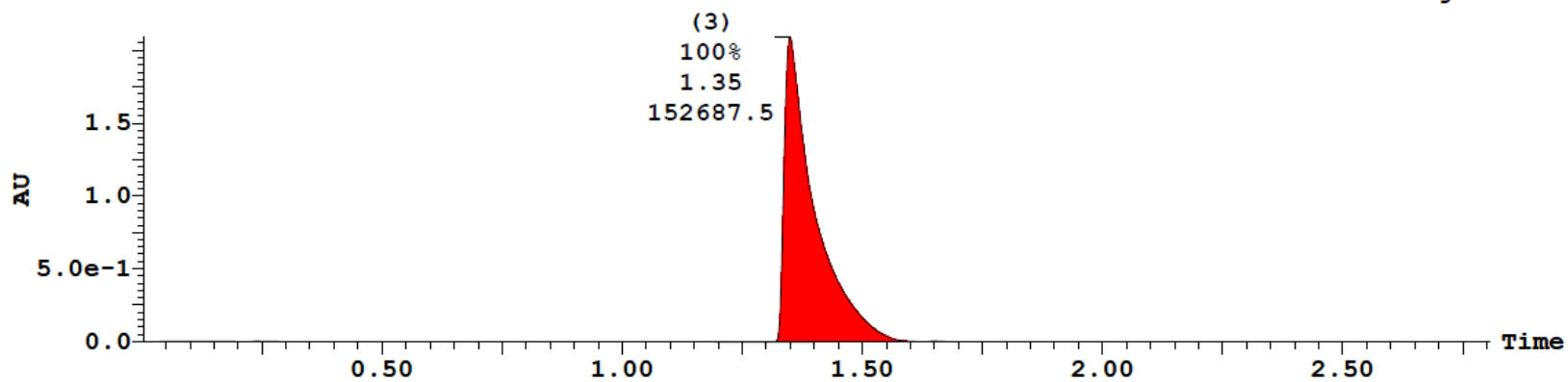
9.8e+006



3: UV Detector: TIC

2.09

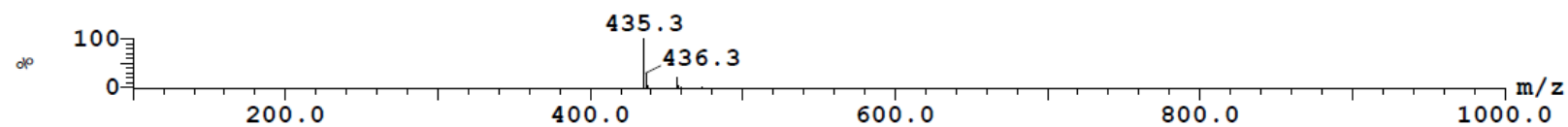
Range: 2.094



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
3		1.35	2e+005	100.00	0	2e+006	

3: (Time: 1.35) Combine (350:355- (333:336+425:428))

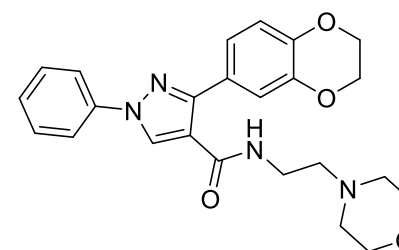
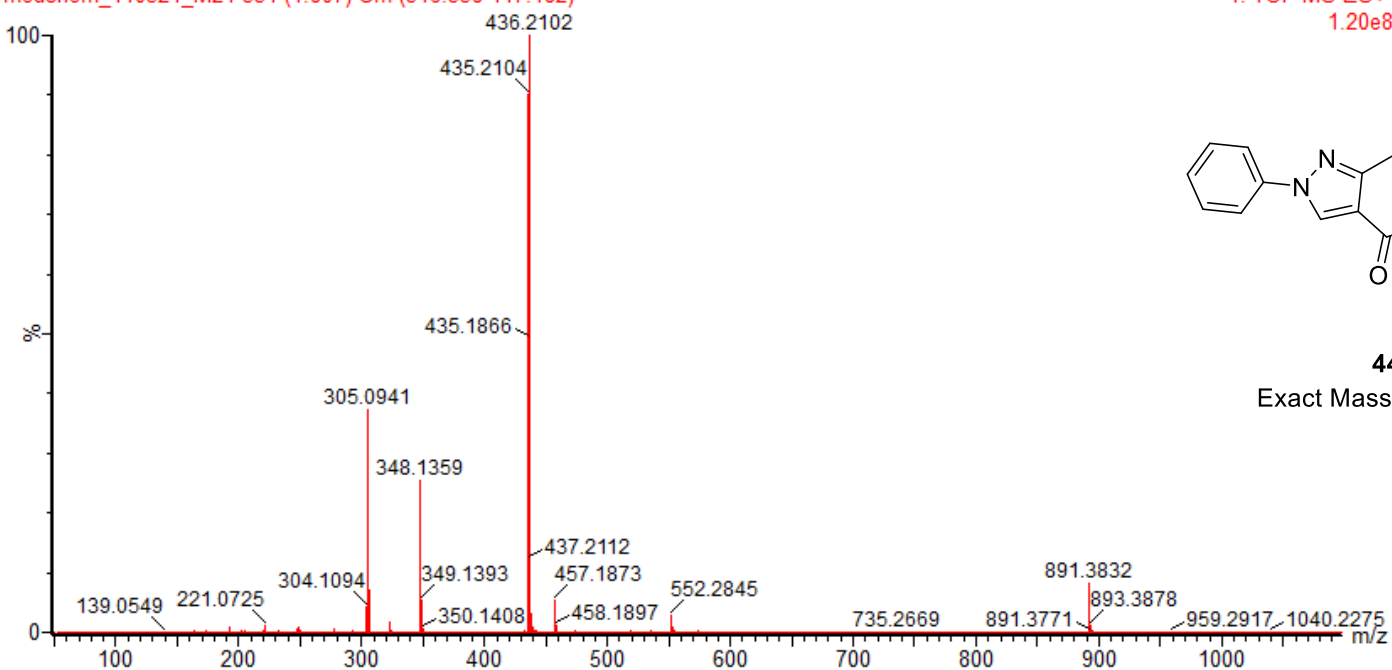
1: MS ES+
7.9e+006



44UAMC5384

medchem_140324_M21 551 (4.807) Cm (546:558-447:482)

1: TOF MS ES+
1.20e8



44

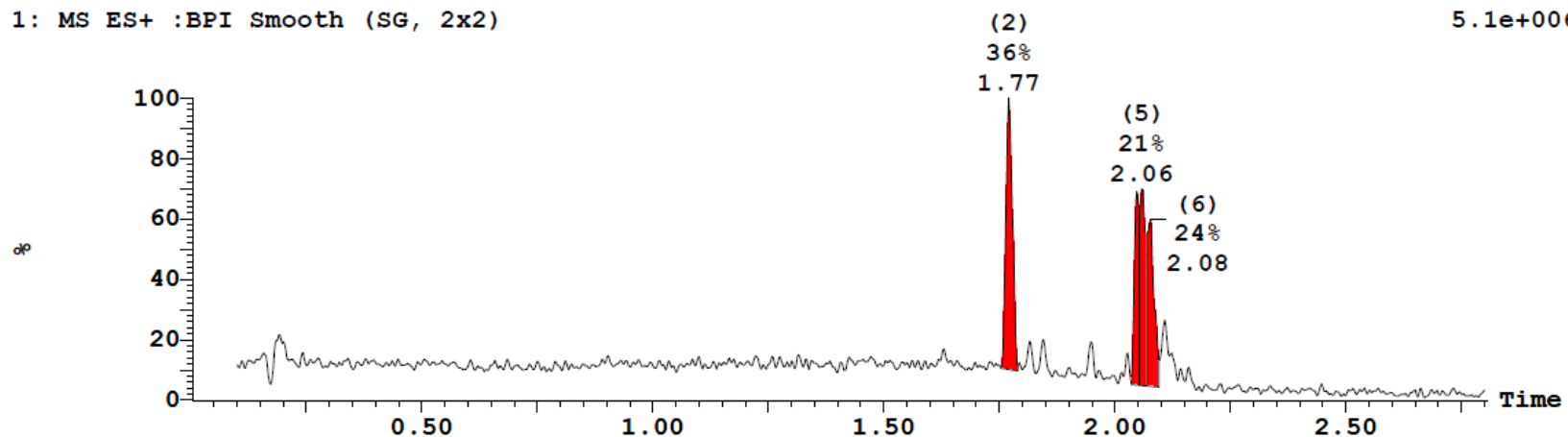
Exact Mass: 434,1954

2.12 1-benzyl-4-(((3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-1-phenyl-1H-pyrazol-4-yl)methoxy)methyl)-1H-1,2,3-triazole (48)

Sample 1 Vial 2:5 ID UAMC-5387 File UAMC-5387 Date 12-Apr-2023 Time 10:30:38 Description

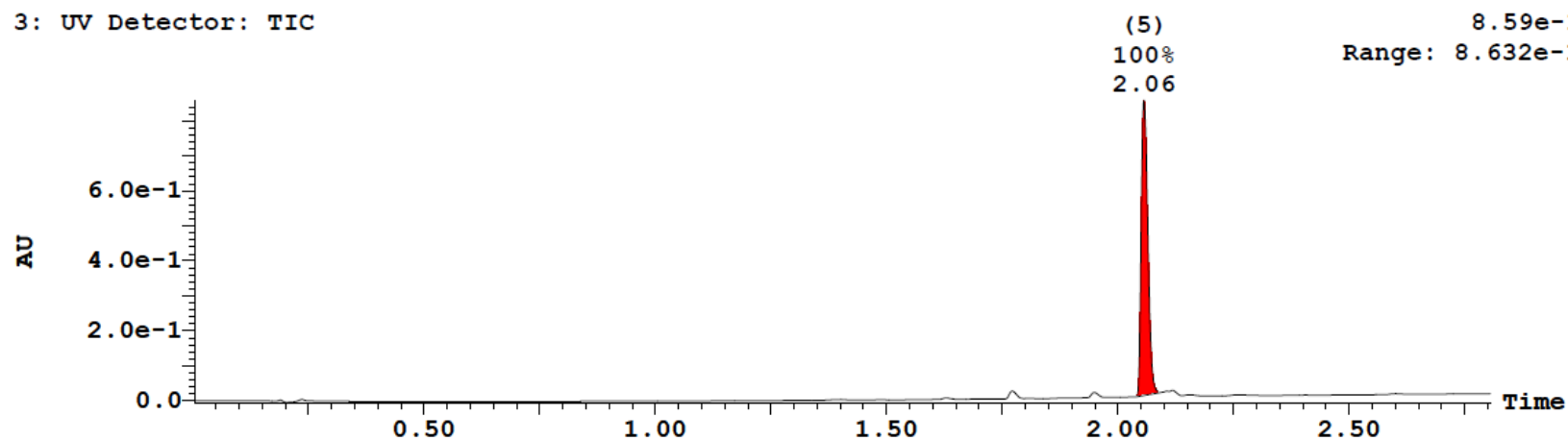
1: MS ES+ :BPI Smooth (SG, 2x2)

5.1e+006



3: UV Detector: TIC

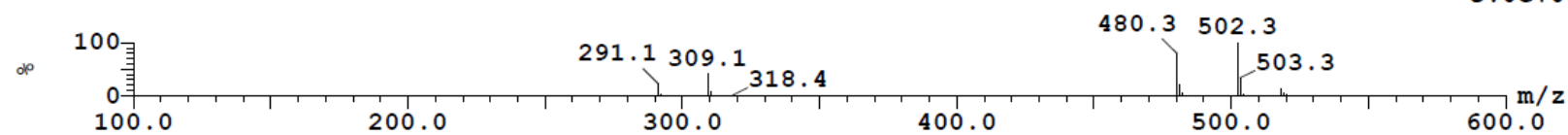
8.59e-1
Range: 8.632e-1



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
5		2.06	1e+004	100.00	0	8e+005	

5: (Time: 2.06) Combine (820:828-(809:813+842:846))

1: MS ES+
3.0e+006

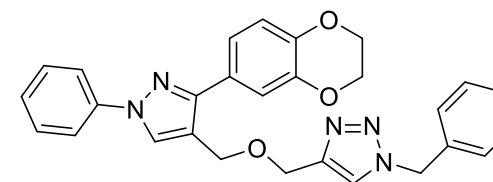
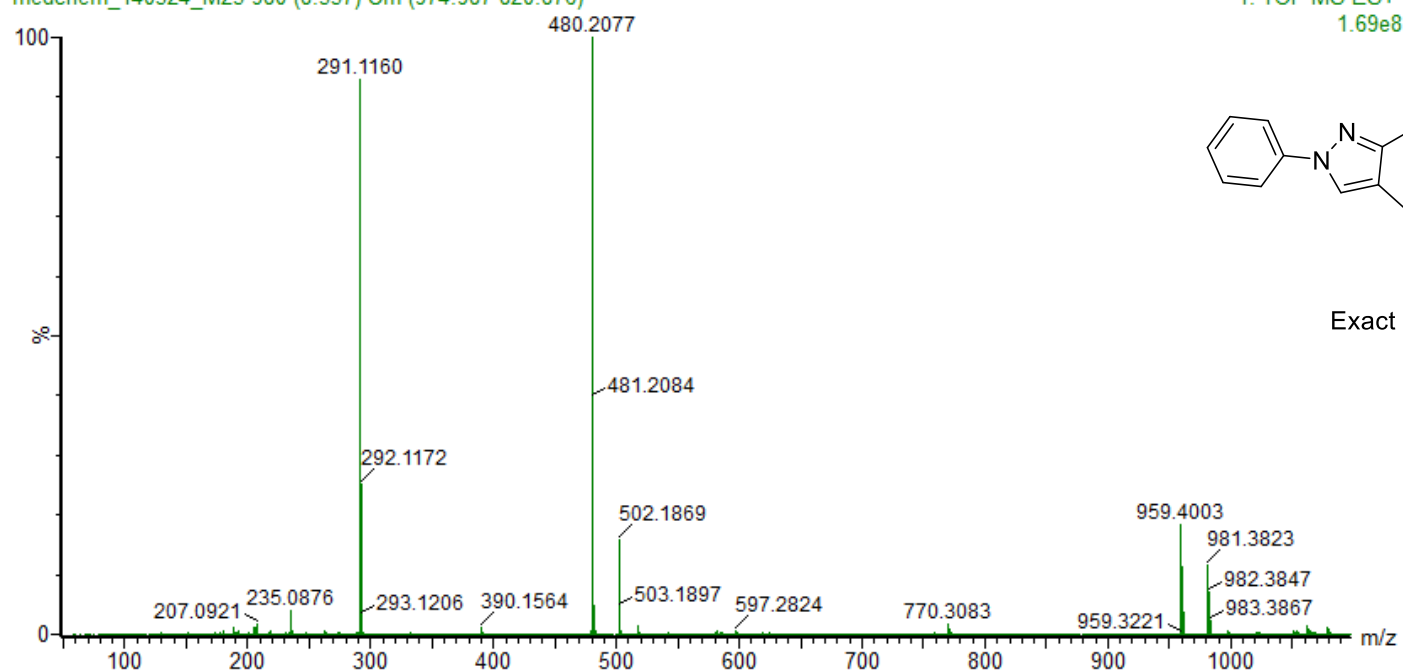


Peak ID	Compound	Time	Mass Found
6		2.08	

48UAMC5387

medchem_140324_M23 980 (8.537) Cm (974:987-820:876)

1: TOF MS ES+
1.69e8



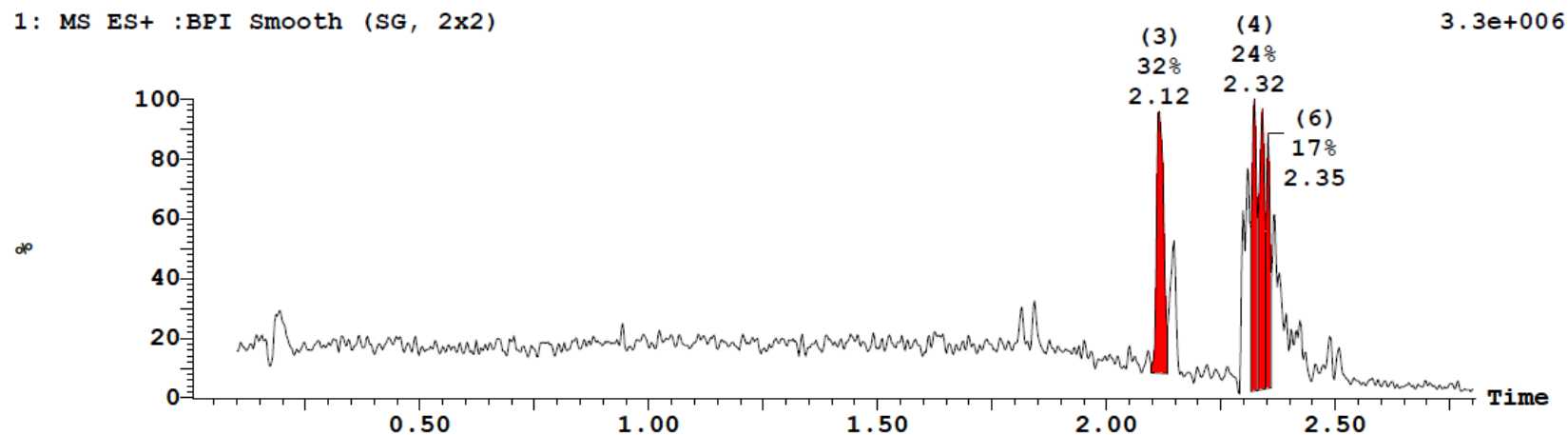
48

Exact Mass: 479,1957

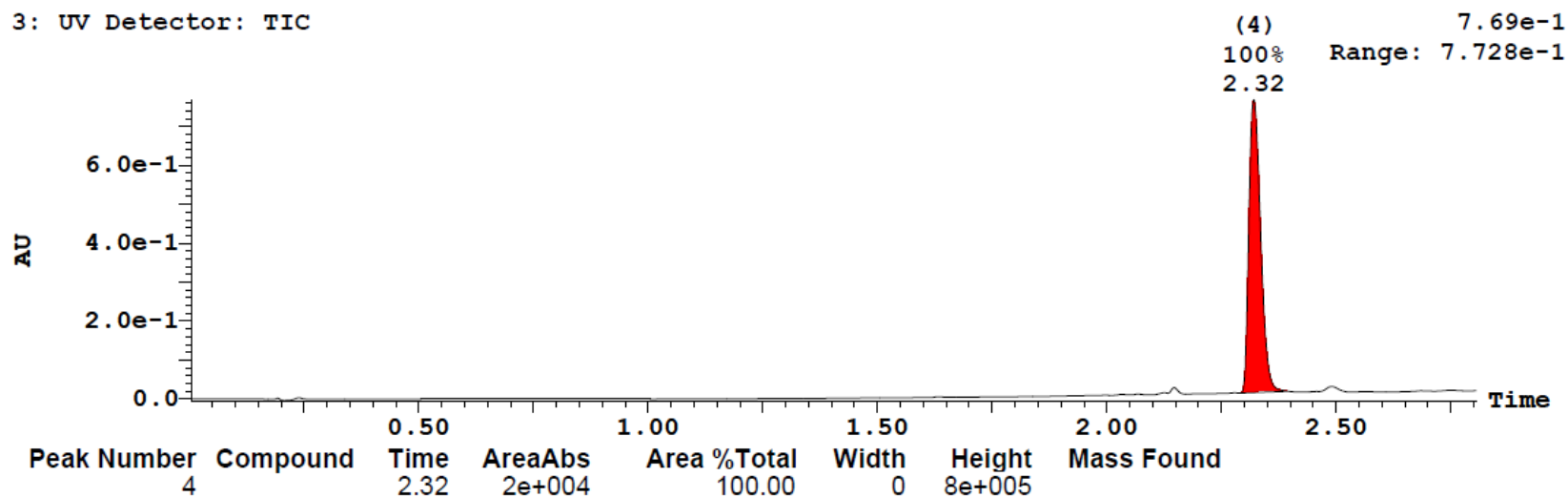
2.13 4-benzyl-3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-1-phenyl-1H-pyrazole (49)

Sample 1 Vial 2:12 ID UAMC-5394 File UAMC-5394 Date 12-Apr-2023 Time 10:59:54 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

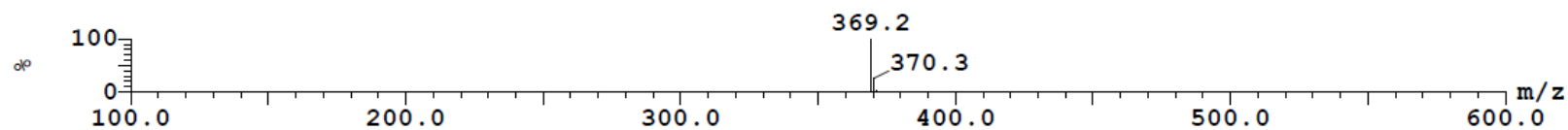


3: UV Detector: TIC



4: (Time: 2.32) Combine (925:933-(909:913+963:967))

1:MS ES+
2.1e+006

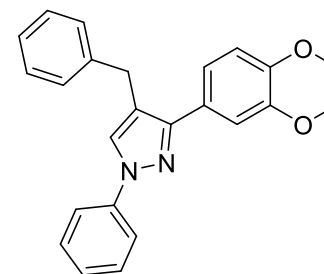
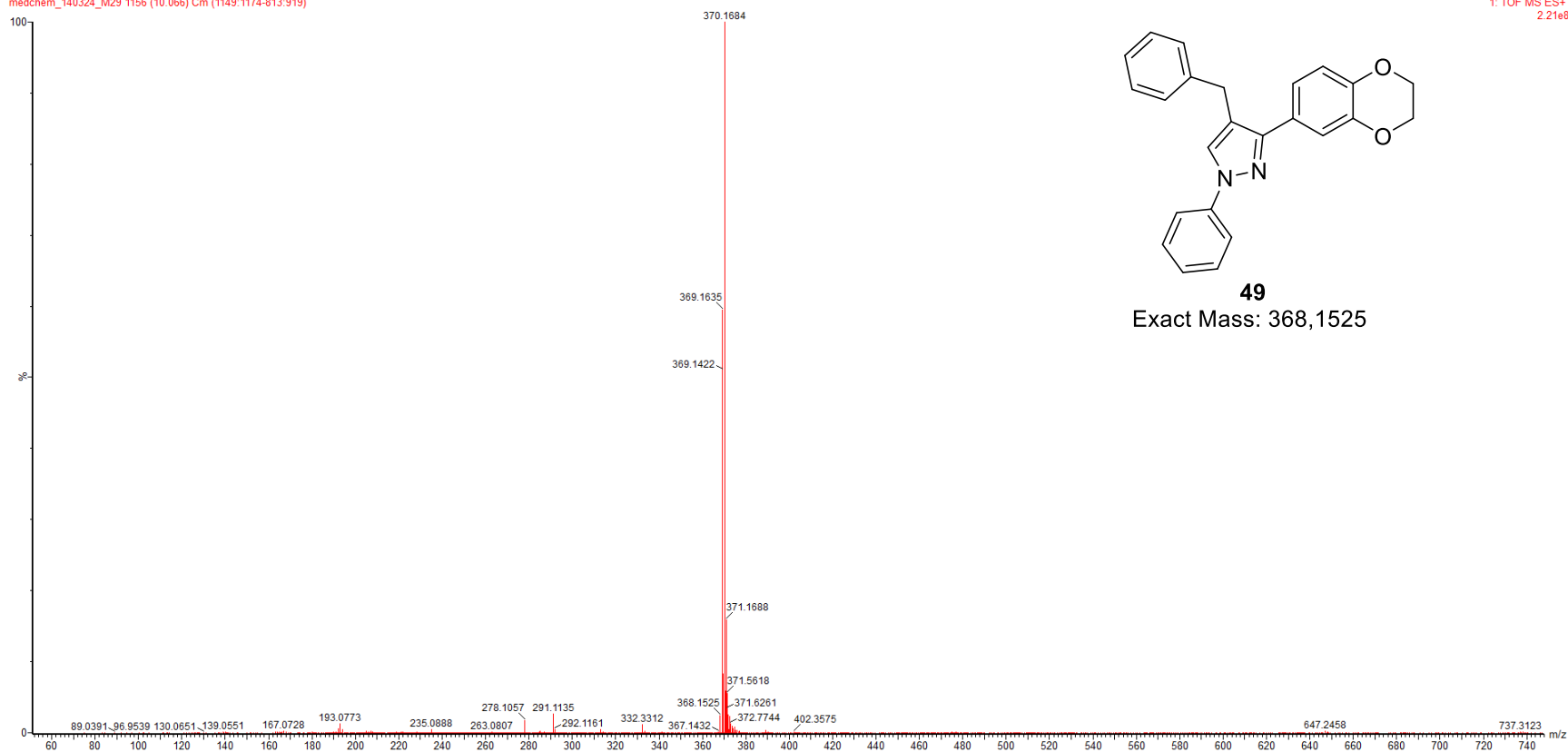


Peak ID	Compound	Time	Mass Found
5		2.34	

49UAMC5394

medchem_140324_M29 1156 (10.066) Cm (1149:1174-813:919)

1: TOF MS ES+
2.21e8



49

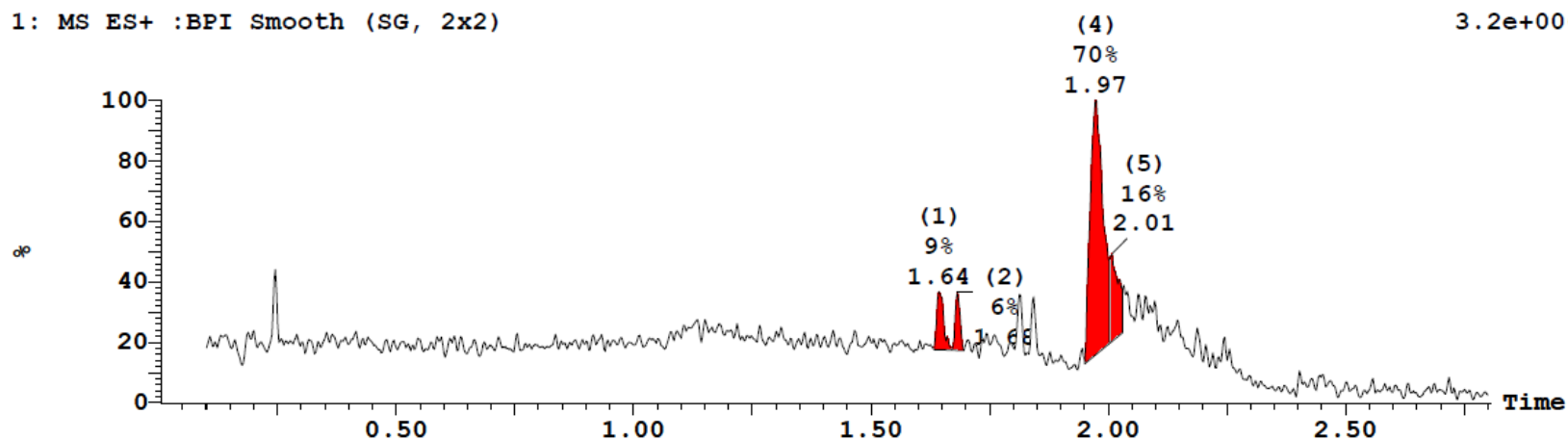
Exact Mass: 368,1525

2.14 1-((3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-1-phenyl-1H-pyrazol-4-yl)methyl)-3-(4-fluorophenyl)urea (54)

Sample 1 Vial 1:56 ID UAMC-5434 File UAMC-5434 Date 13-Apr-2023 Time 17:45:39 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

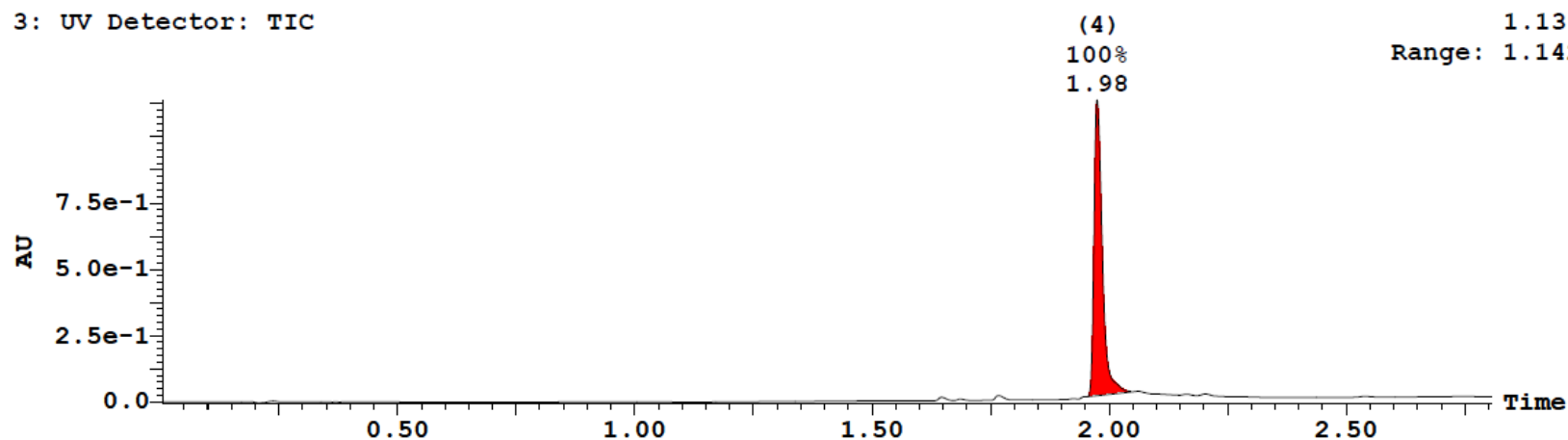
3.2e+006



3: UV Detector: TIC

1.139

Range: 1.142



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
4		1.98	2e+004	100.00	0	1e+006	

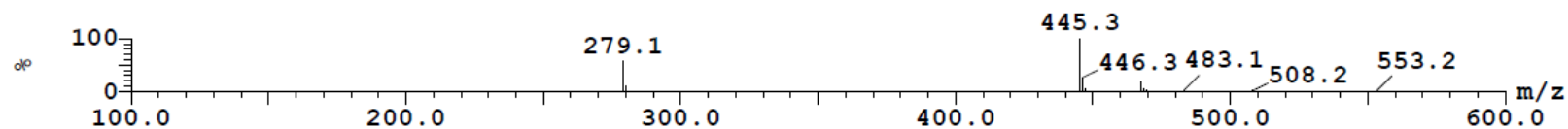
Peak ID Compound Time Mass Found

4 1.97

4: (Time: 1.98) Combine (787:795-(774:778+826:830))

1:MS ES+

2.4e+006

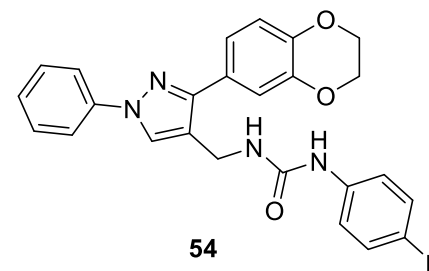
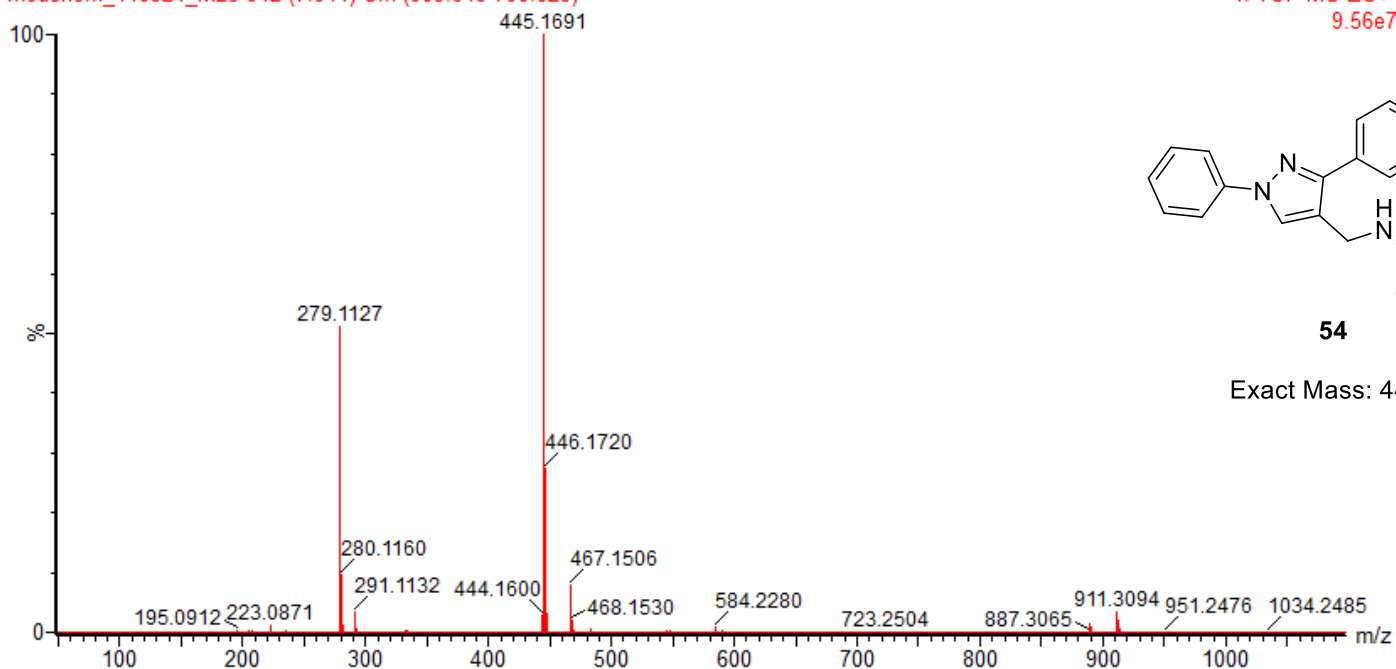


54UAMC5434

medchem_140324_M25 912 (7.941) Cm (905:919-790:823)

1: TOF MS ES+

9.56e7



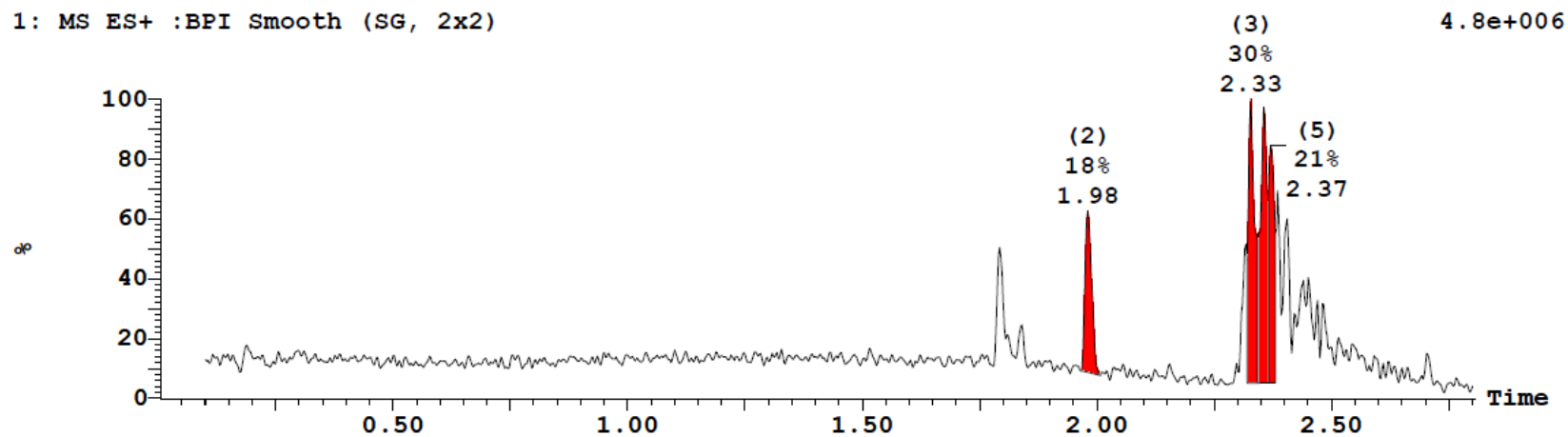
54

Exact Mass: 444,1598

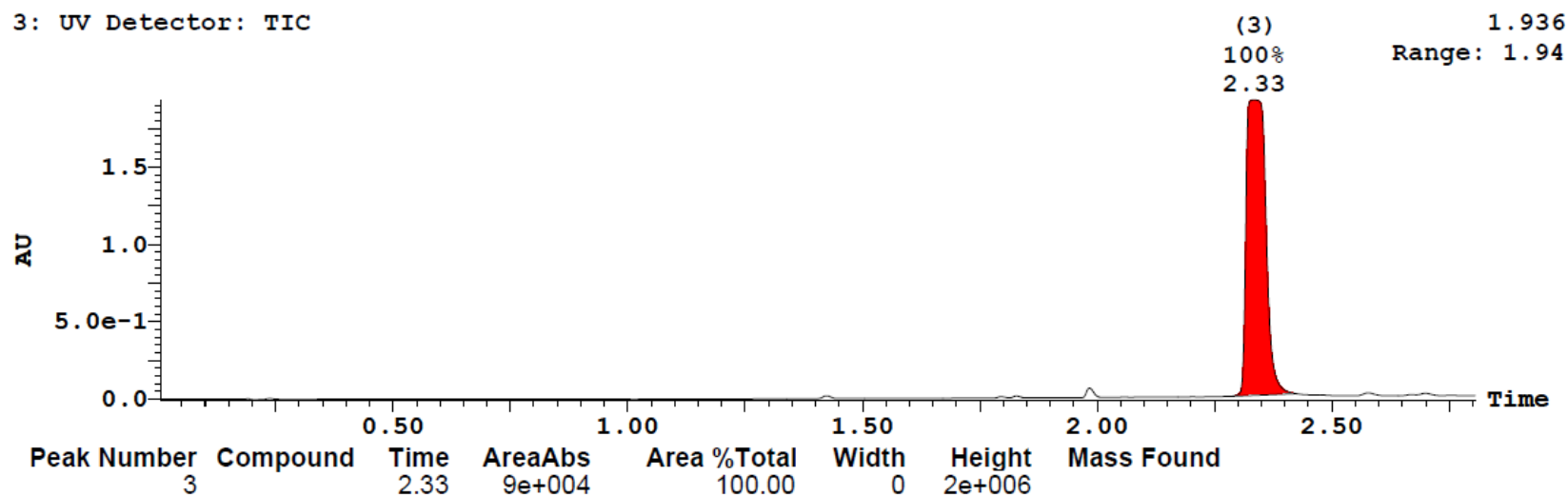
2.15 4-(((4-fluorobenzyl)oxy)methyl)-3-(4-methoxyphenyl)-1-phenyl-1H-pyrazole (68)

Sample 1 Vial 2:46 ID UAMC-5419 File UAMC-5419 Date 12-Apr-2023 Time 13:59:34 Description

1: MS ES+ :BPI Smooth (SG, 2x2)



3: UV Detector: TIC



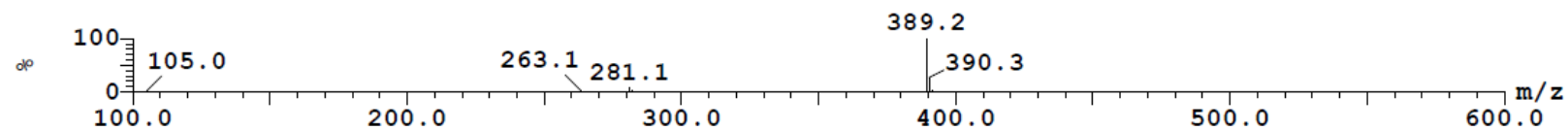
Peak ID Compound Time Mass Found

3 2.33

3: (Time: 2.33) Combine (931:939- (908:912+975:979))

1:MS ES+

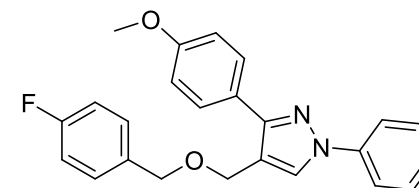
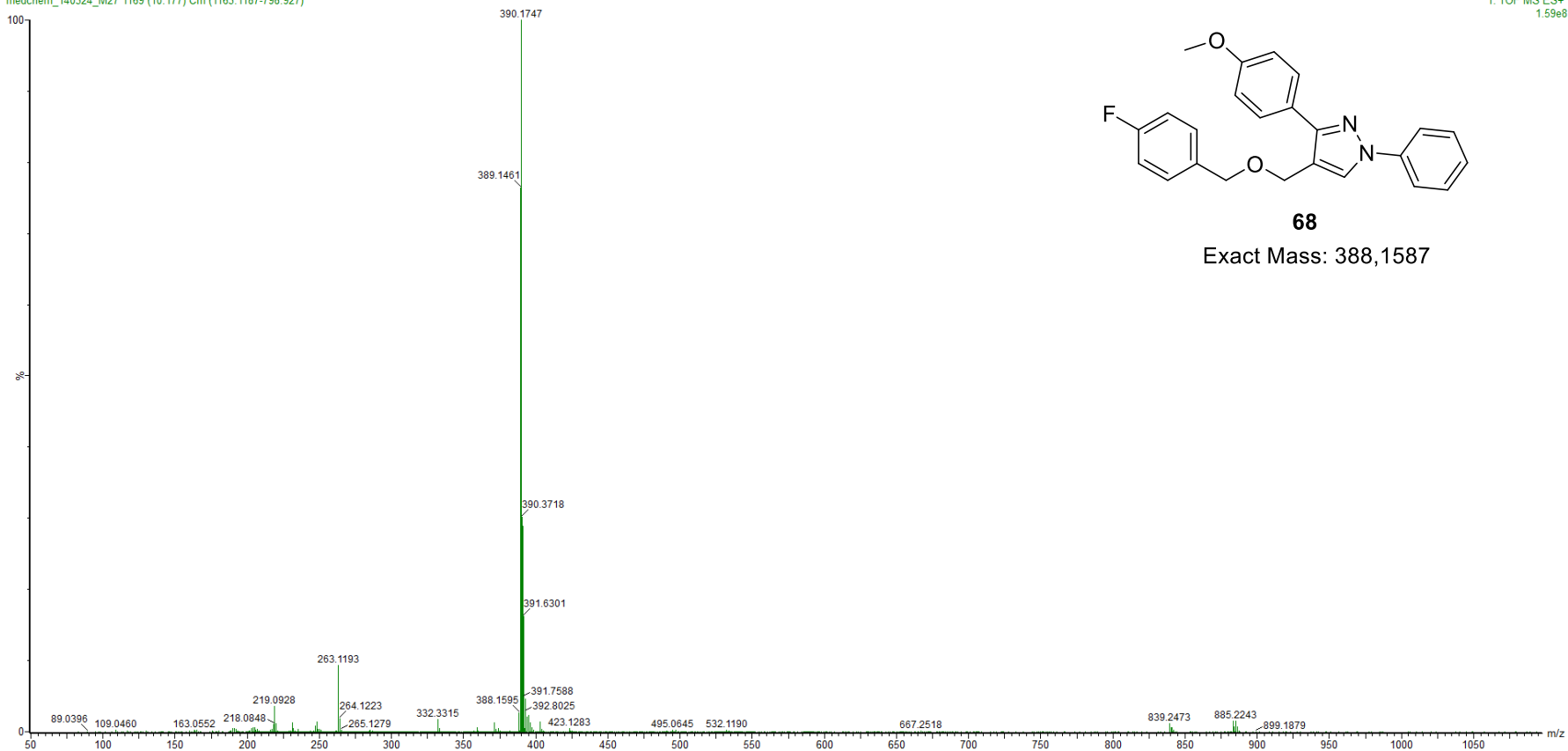
2.6e+006



68UAMC5419

medchem_140324_M27 1169 (10.177) Cm (1163:1187-798:927)

1: TOF MS ES+
1.59e8



68

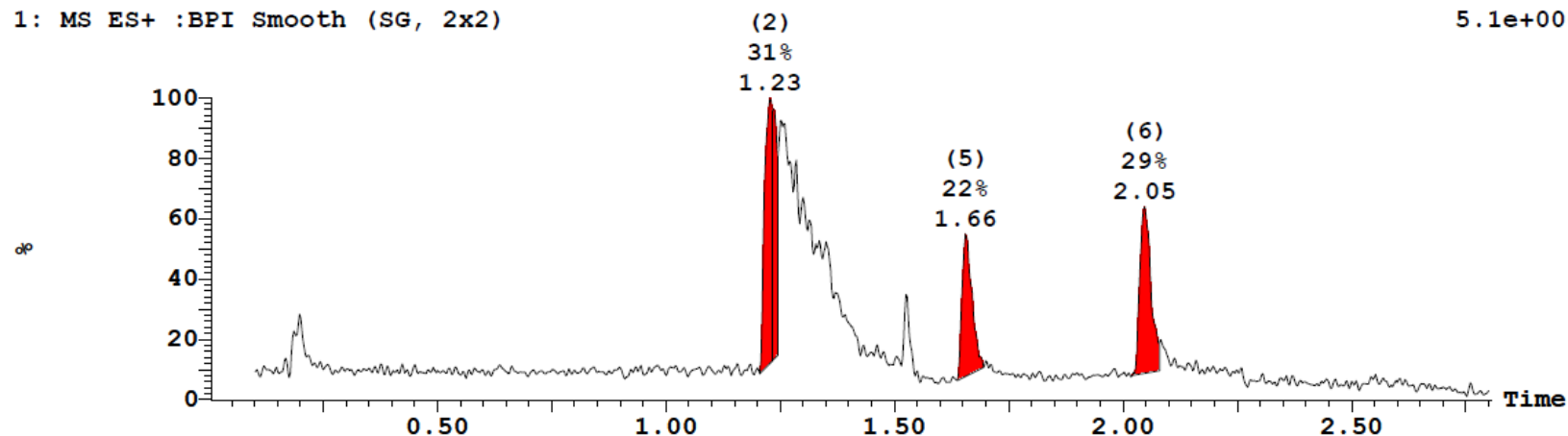
Exact Mass: 388,1587

2.16 *N*-((3-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-1-(pyridin-2-yl)-1*H*-pyrazol-4-yl)methyl)-2-(pyrrolidin-1-yl)ethan-1-amine dihydrochloride (69)

Sample 1 Vial 1:53 ID MB-2021-060E File MB-2021-060E Date 05-Jul-2023 Time 15:25:04 Description

1: MS ES+ :BPI Smooth (SG, 2x2)

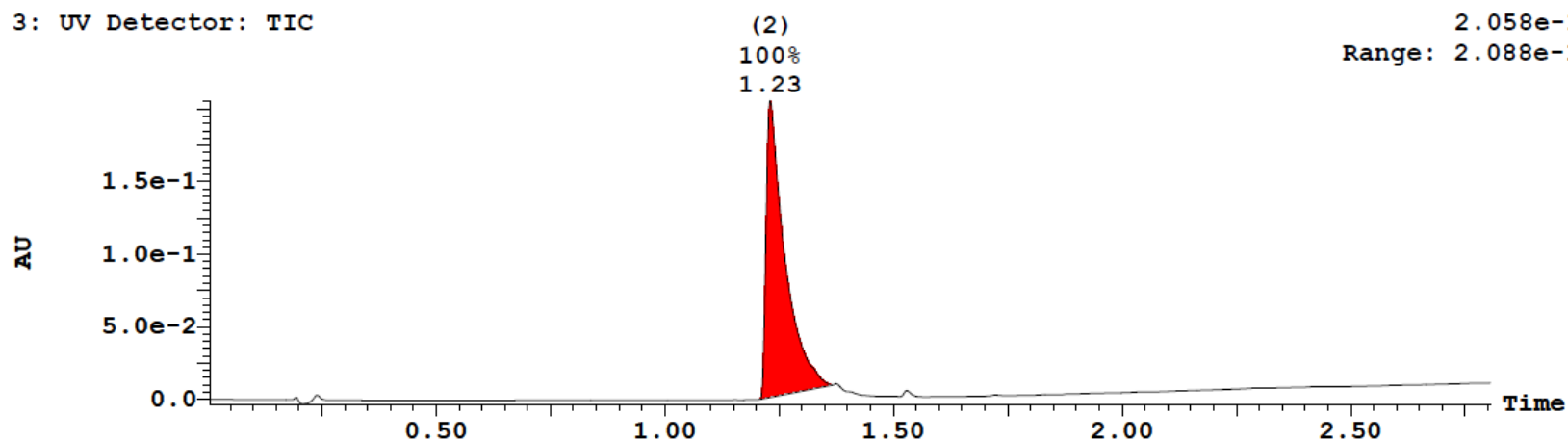
5.1e+006



3: UV Detector: TIC

2.058e-1

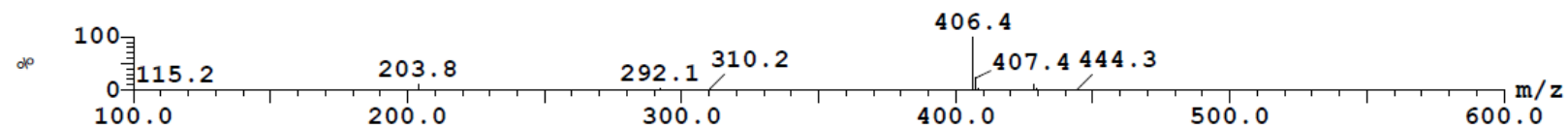
Range: 2.088e-1



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
2		1.23	1e+004	100.00	0	2e+005	

Peak ID Compound Time Mass Found
 2 1.23
 2: (Time: 1.23) Combine (489:497- (475:479+552:556))

1:MS ES+
 4.1e+006



69UAMC5462
 medchem_140324_M31 365 (3.192) Cm (365:378)

1: TOF MS ES+
 2.53e7

