

Supporting Information

Alicyclic annulated triazoles versus triazinediones by the reaction of cyclic imidates with methyl 2-hydrazinyl-2-oxoacetate

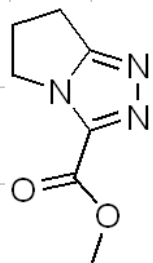
Viacheslav Lysenko ^a, Anton Portiankin ^a, Kostiantyn Nazarenko ^{a,b}, Kostiantyn Shvydenko ^a, Tetiana Shvydenko ^a, and Aleksandr Kostyuk ^{a,*}

Content

Copies of NMR spectra

Compound #	Page	Spectra NMR	Compound #	Page	Spectra NMR	Compound d #		NMR
3a	2	¹ H	3j	18	¹³ C	6g	34	¹³ C
3a	3	¹³ C	5a	19	¹ H	7d	35	¹ H
3d	4	¹ H	5a	20	¹³ C	7d	36	¹³ C
3d	5	¹³ C	5b	21	¹ H	7f	37	¹ H
3e	6	¹ H	5b	22	¹³ C	7f	38	¹³ C
3e	7	¹³ C	5c	23	¹ H	7g	39	¹ H
3e	8	¹⁹ F	5c	24	¹³ C	7g	40	¹³ C
3f	9	¹ H	5f	25	¹ H	7h	41	¹ H
3f	10	¹³ C	5f	26	APT	7h	42	¹³ C
3g	11	¹ H	5g	27	¹ H	8	43	¹ H
3g	12	¹³ C	5g	28	¹³ C	8	44	¹³ C
3h	13	¹ H	5g	29	APT ¹³ C	9	45	¹ H
3h	14	¹³ C	6a	30	¹ H	9	46	¹³ C
3i	15	¹ H	6a	31	¹³ C			
3i	16	¹³ C	6c	32	¹ H			
3j	17	¹ H	6g	33	¹ H			

PHLV1474



3a

CDCl₃

7.26

4.26

4.24

4.22

3.96

3.03

3.01

2.99

2.84

2.82

2.80

2.78

2.76

26

24

22

20

18

16

14

12

10

8

6

4

2

0

-2

11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

f1 (MД)

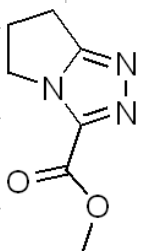
2.00

3.08

2.07

2.12

PHLV1474_C13
13C (1H-decoupled)



3a

CDCl₃

— 164.99

— 158.16

— 142.93

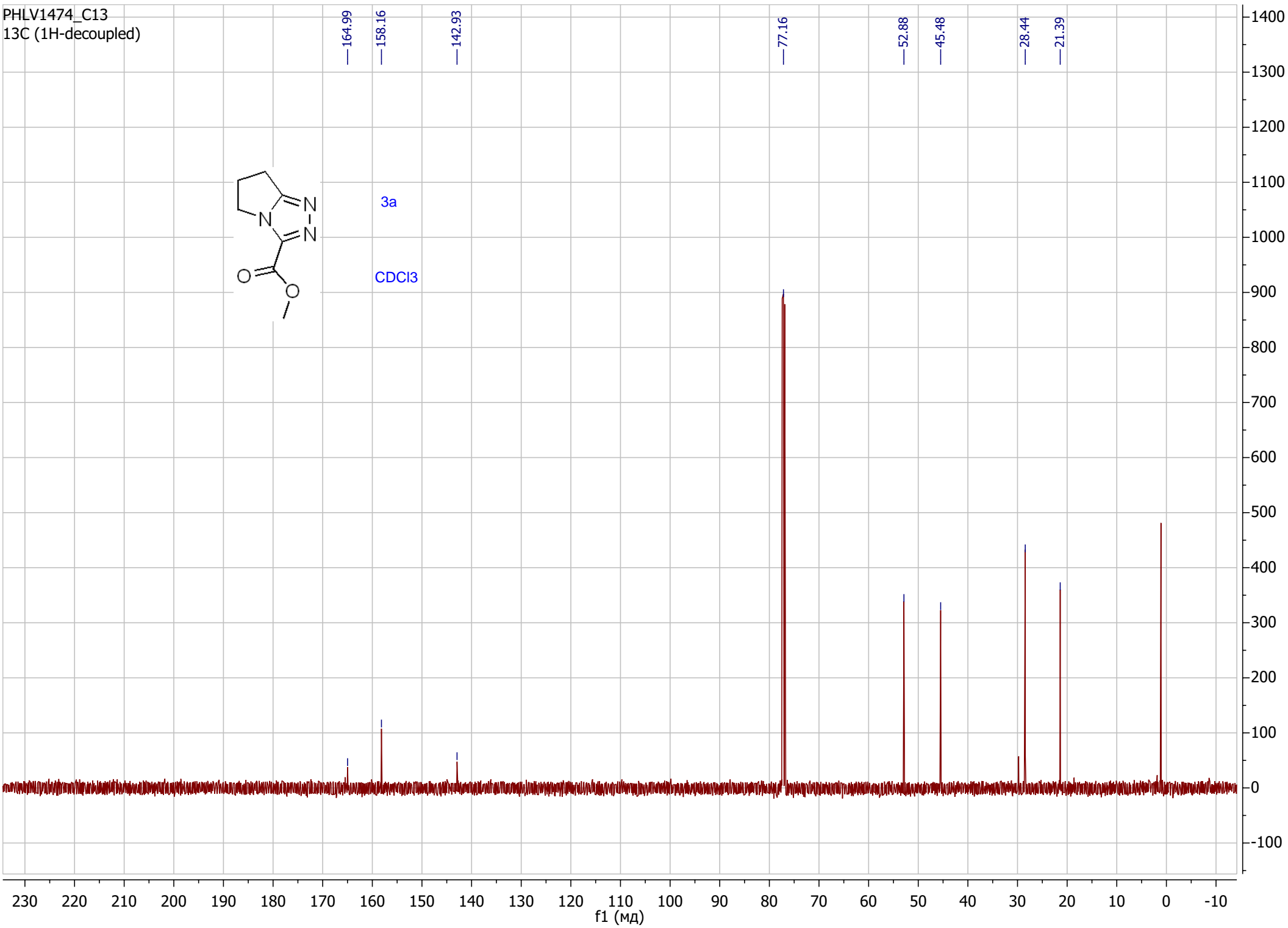
— 77.16

— 52.88

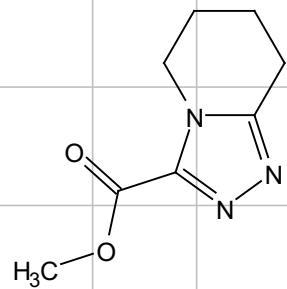
— 45.48

— 28.44

— 21.39



PHskv8-1



3d

CDCl₃

7.27

4.29

4.28

4.26

3.94

3.92

3.01

3.00

2.98

2.02

2.01

1.99

1.98

1.96

1.93

1.91

1.90

1.88

1.87

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (MД)

110

100

90

80

70

60

50

40

30

20

10

0

-10

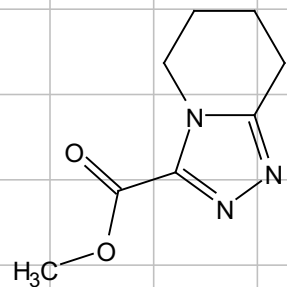
2.04

3.00

2.01

2.02

1.97



3d

DMSO-d6

158.57
154.40
144.52

52.77

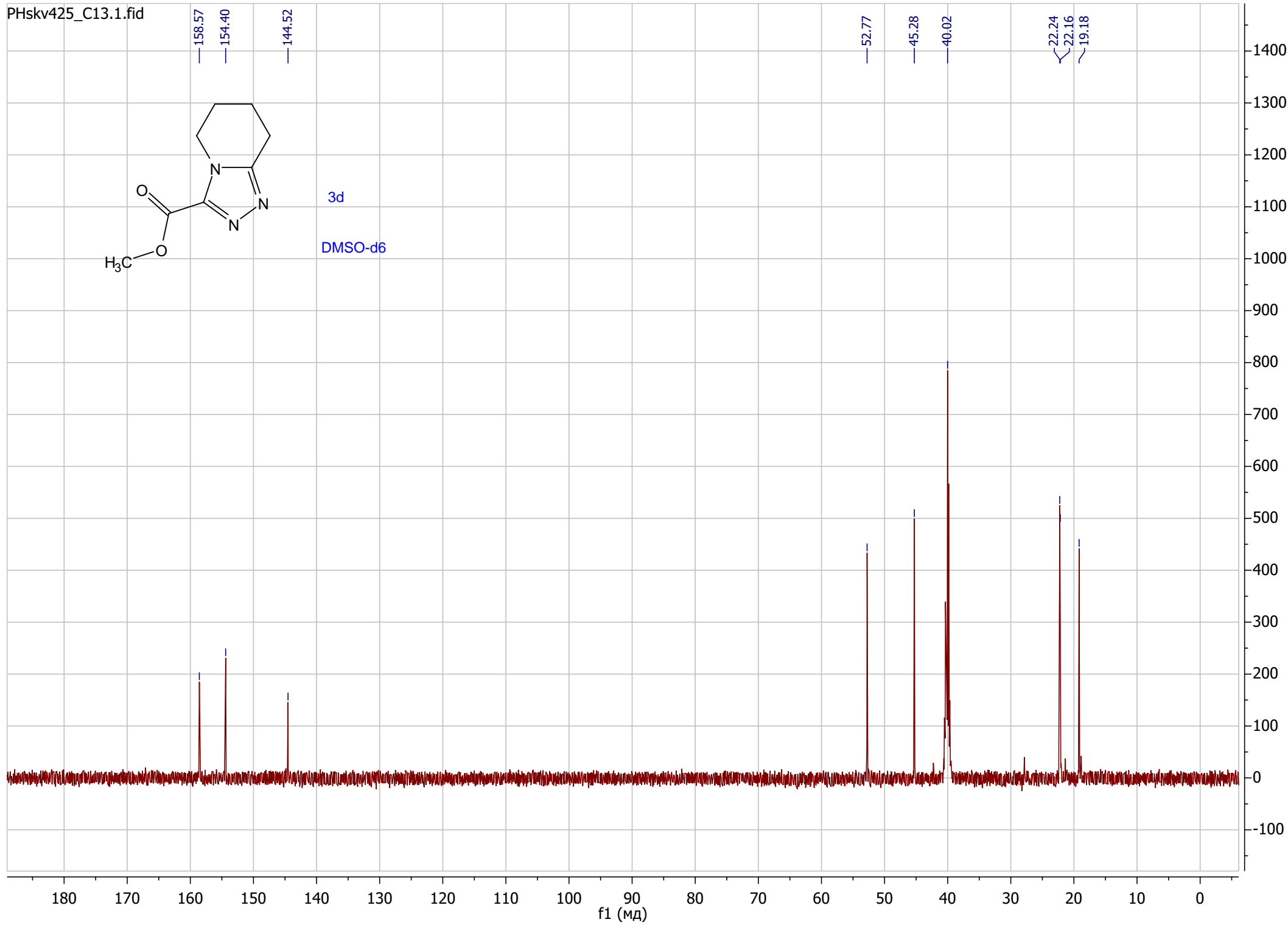
45.28

40.02

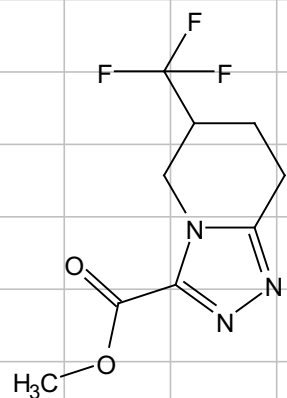
22.24

22.16

19.18



PHskv7-2

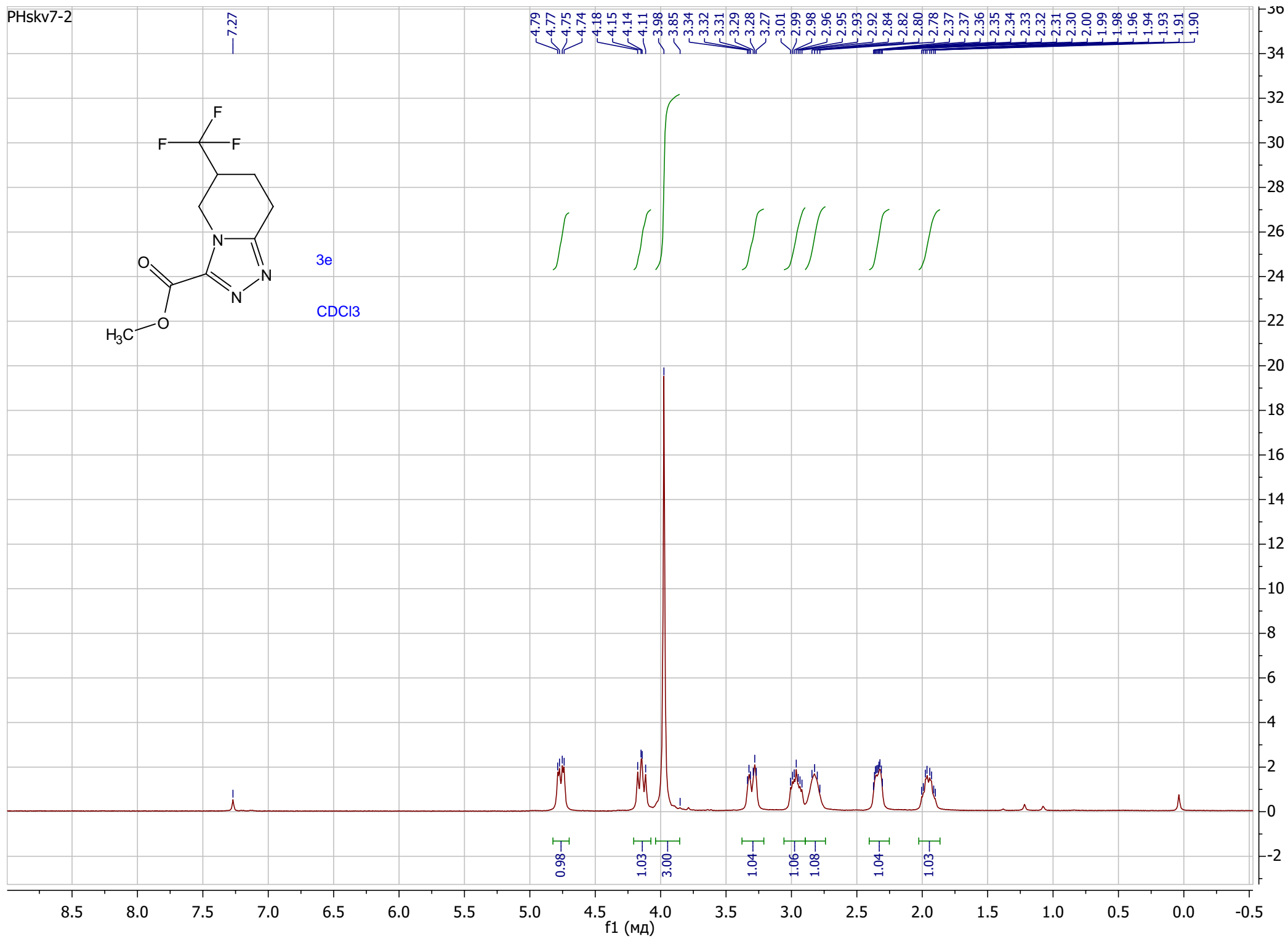


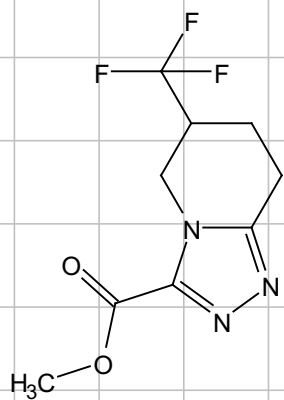
3e

CDCl₃

7.27

4.79
4.77
4.75
4.74
4.18
4.15
4.14
4.11
3.98
3.85
3.34
3.32
3.31
3.29
3.28
3.27
3.01
2.99
2.98
2.96
2.95
2.93
2.92
2.84
2.82
2.80
2.78
2.37
2.37
2.36
2.35
2.34
2.33
2.32
2.31
2.30
2.00
1.99
1.98
1.96
1.94
1.93
1.91
1.90





3e

CDCl₃

158.23

152.97

144.23

130.02

127.24

124.47

121.70

77.41

77.09

76.78

52.88

43.37

38.73

38.45

38.17

37.88

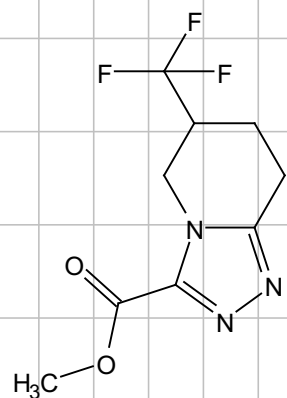
20.54

19.06

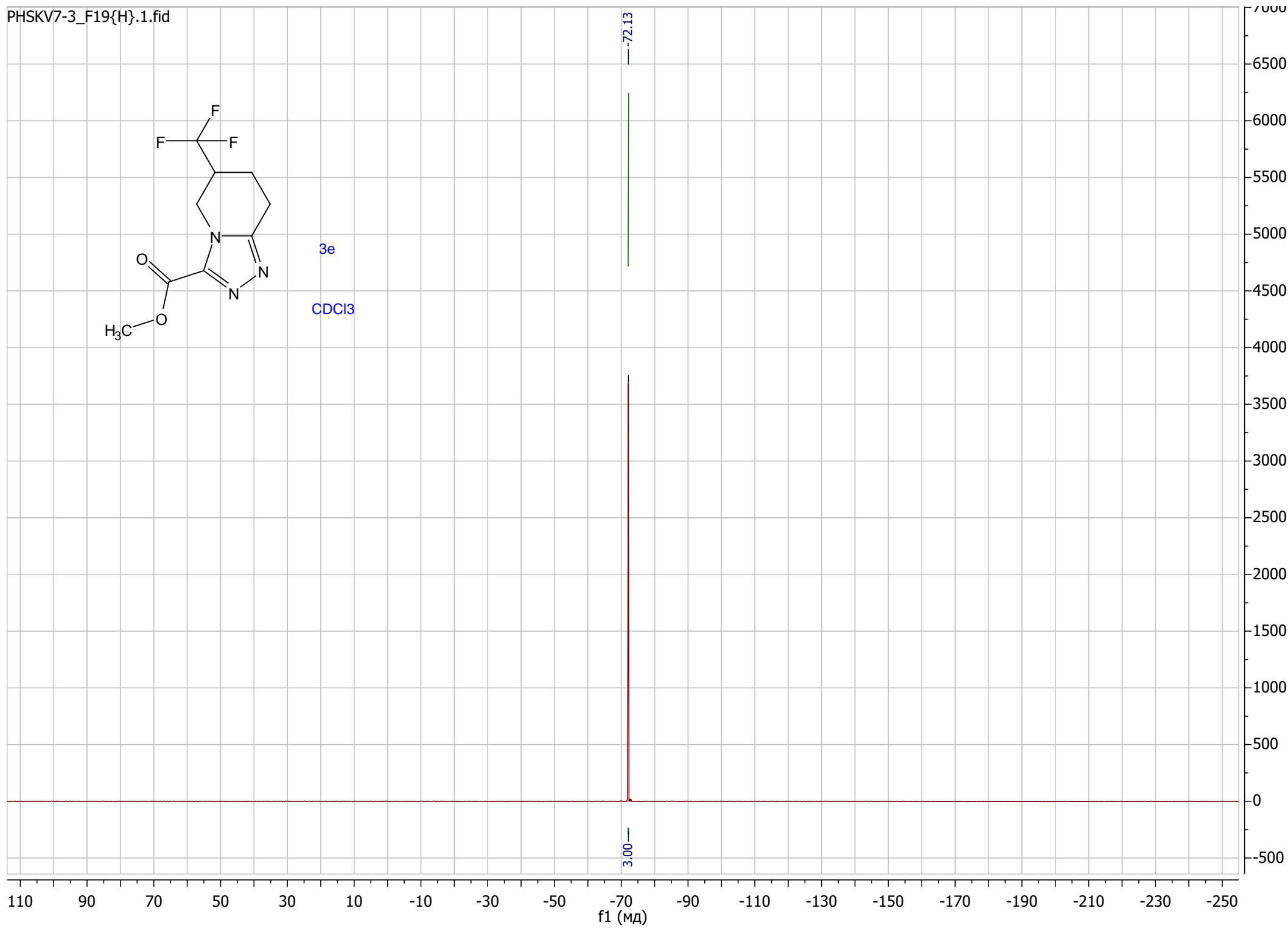
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f1 (MД)

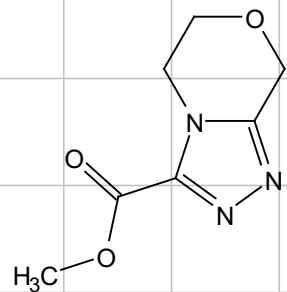
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000



3e
CDCl3

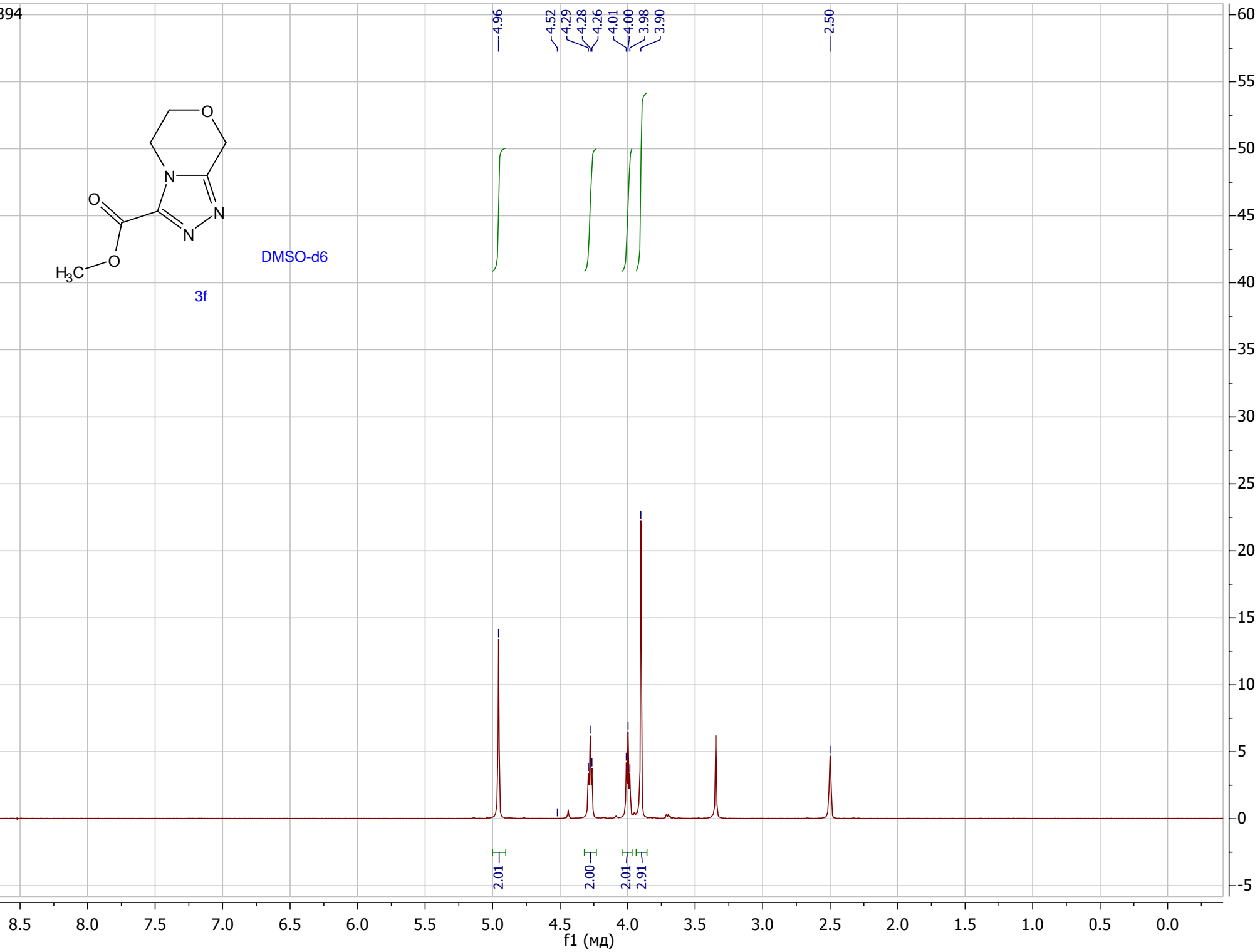


phskv394

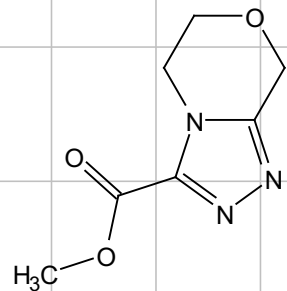


3f

DMSO-d6



phskv426_C13



3f

DMSO-d6

158.20

151.26

144.73

63.06

62.71

52.94

44.95

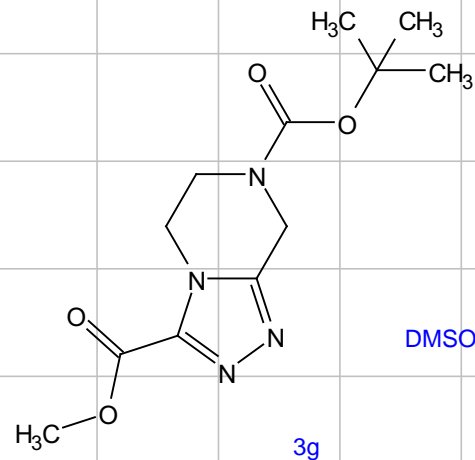
39.95

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

f1 (MД)

9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000

phskv6



4.75
4.28
4.27
4.26
3.90
3.78
3.76
3.75
3.33
2.50
1.43



1.99
2.00
3.03
2.02

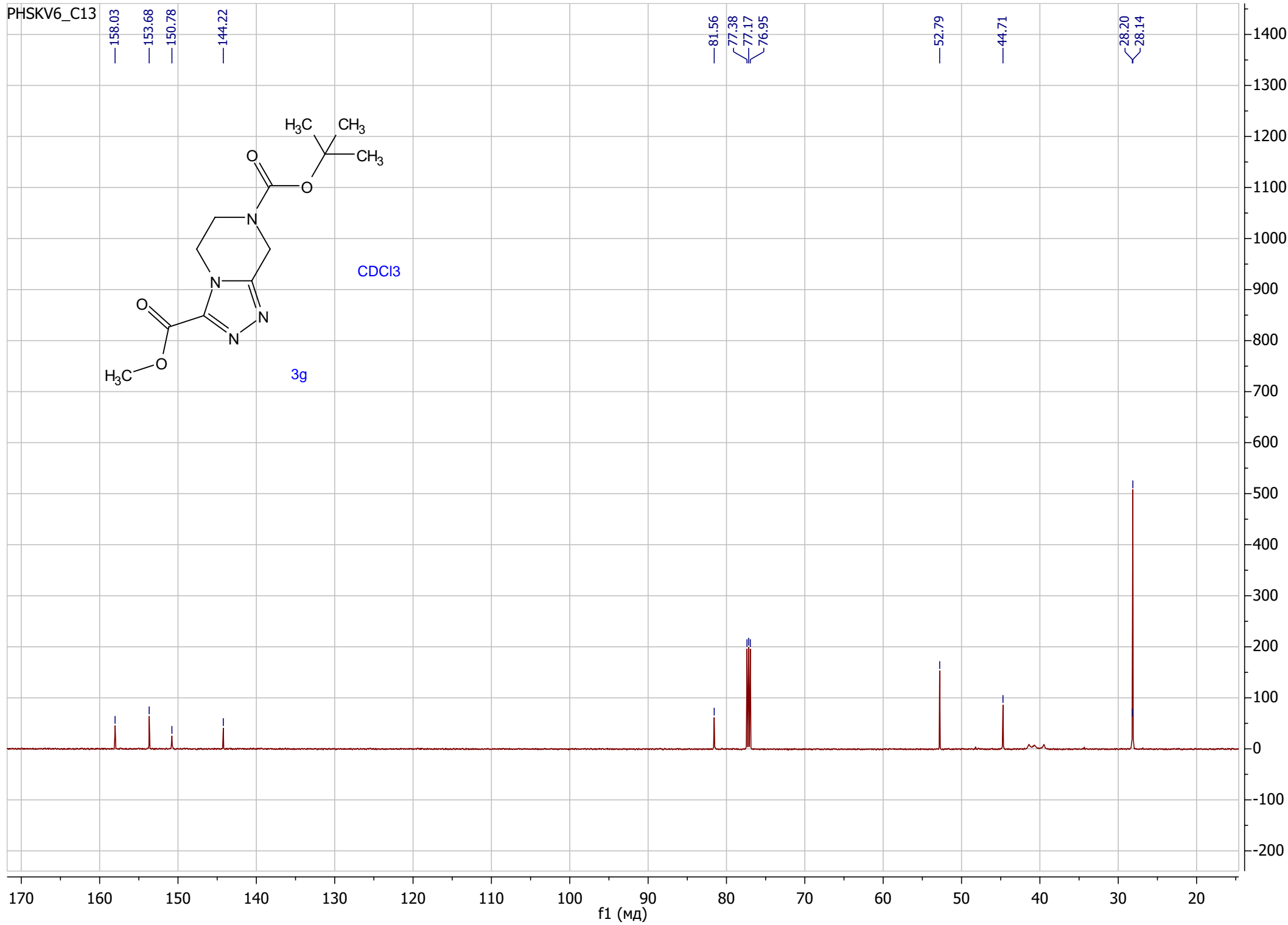
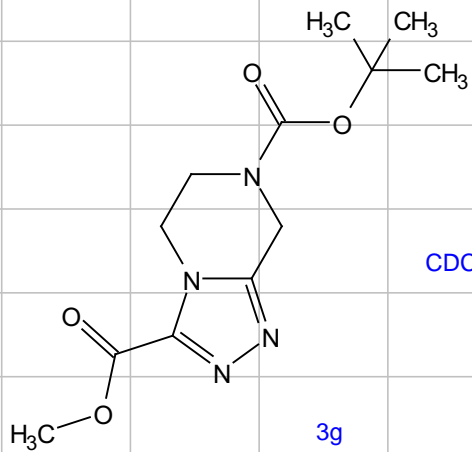
8.72

7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

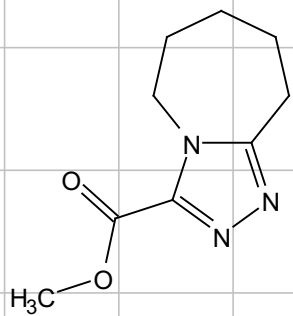
f1 (MД)

60
55
50
45
40
35
30
25
20
15
10
5
0
-5

PHSKV6_C13

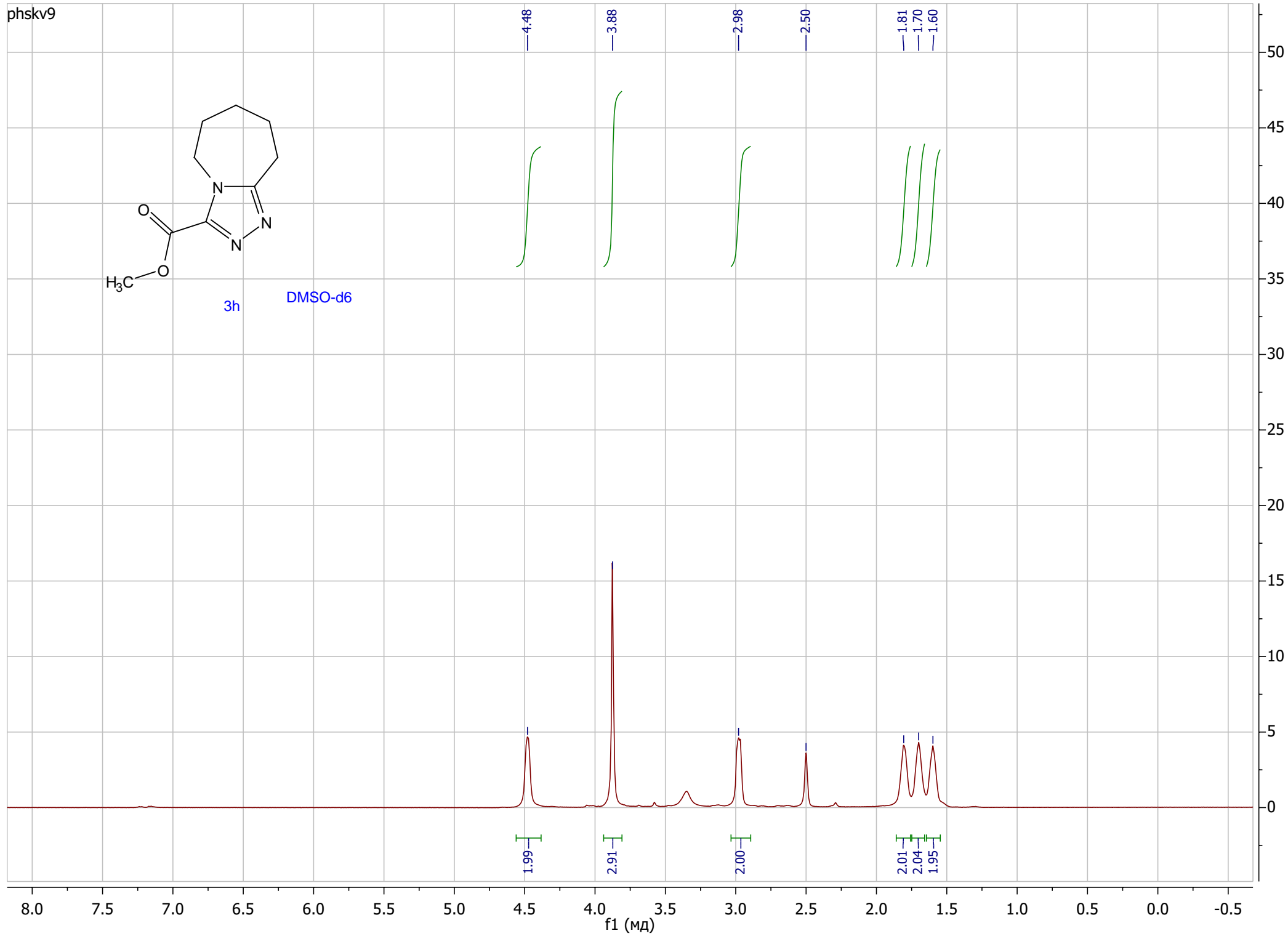


phskv9

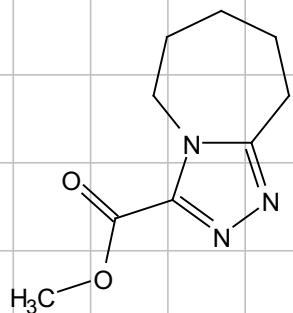


3h

DMSO-d6

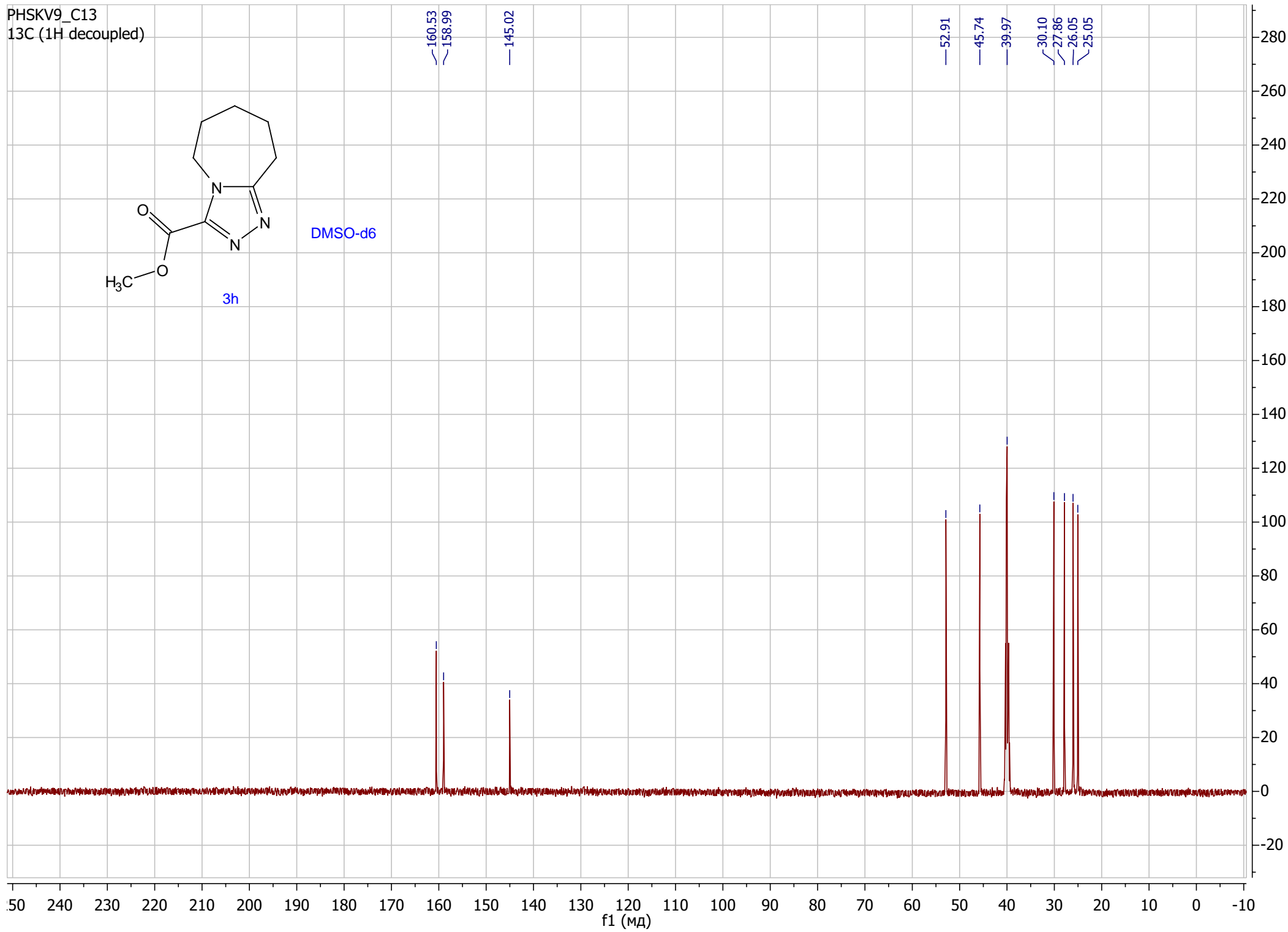


PHSKV9_C13
13C (1H decoupled)

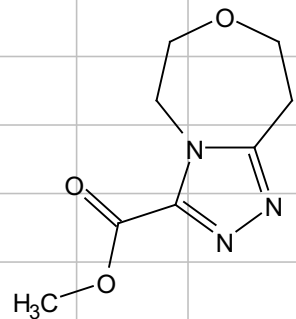


DMSO-d6

3h

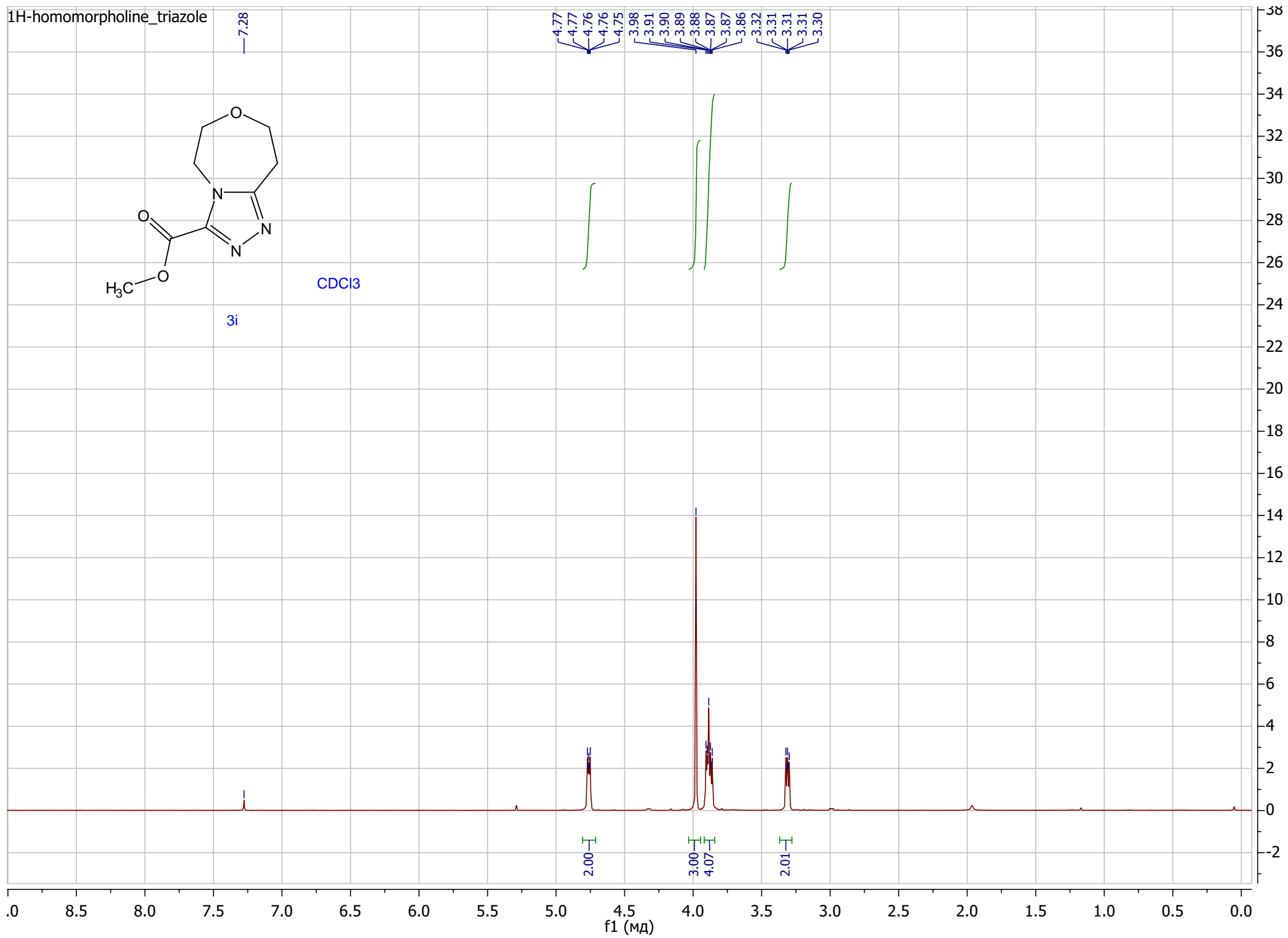


1H-homomorpholine_triazole

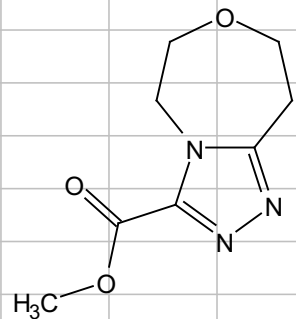


3i

CDCl3



PHSKV5_C13



3i

CDCl₃

158.96
158.64

144.84

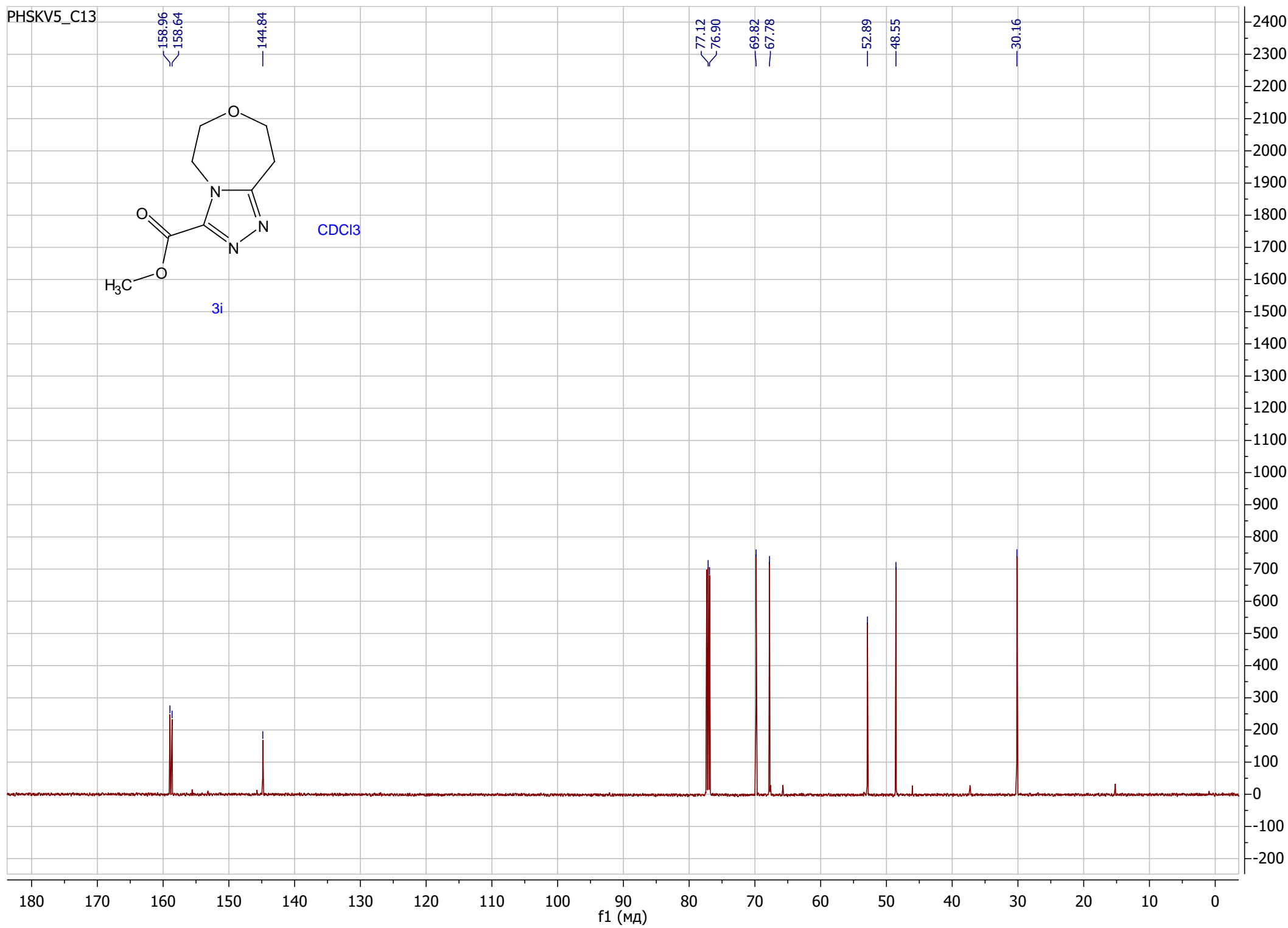
77.12
76.90

69.82
67.78

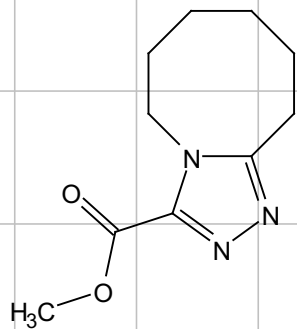
52.89

48.55

30.16



phskv427



3j

CDCl₃

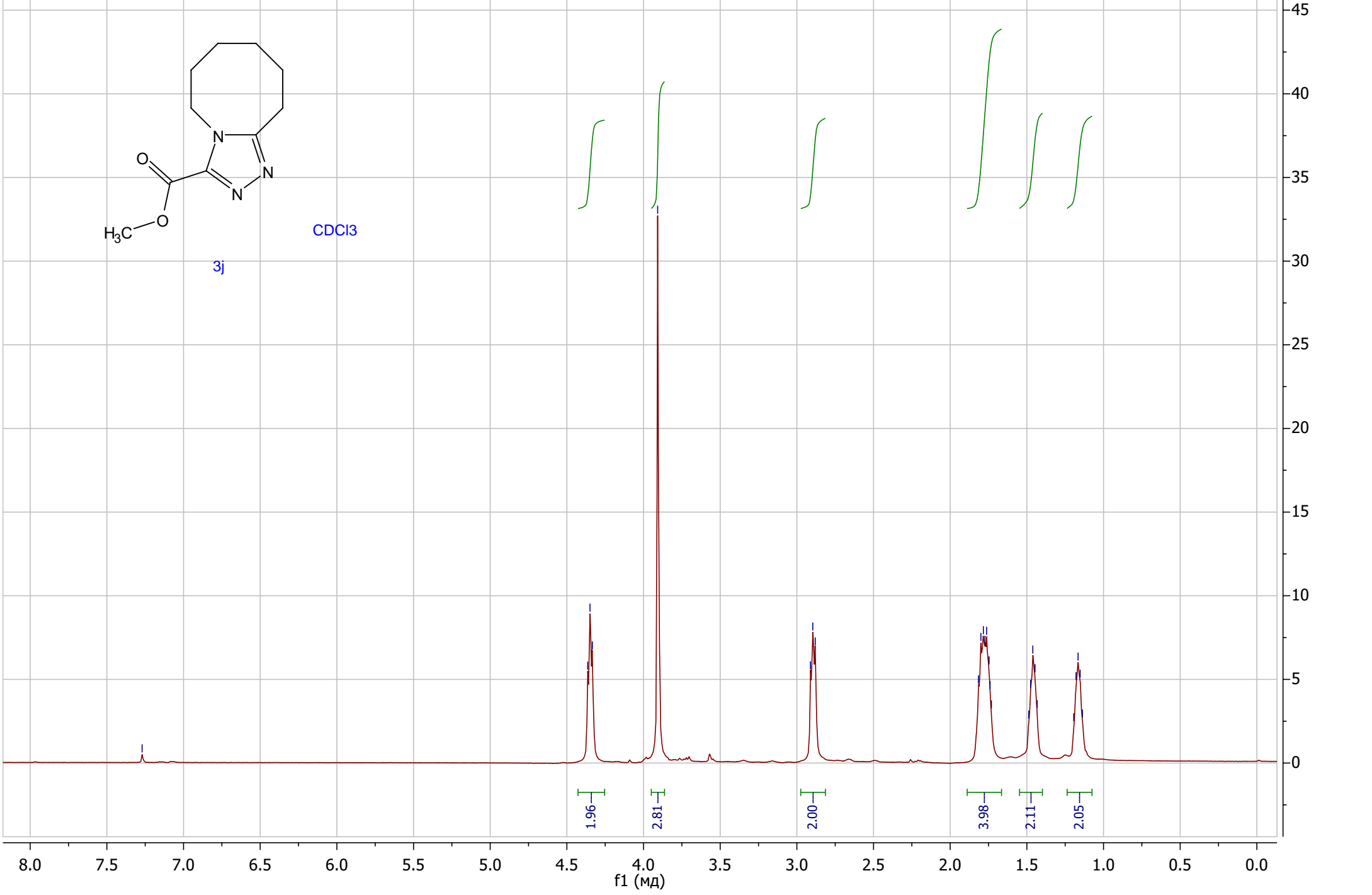
7.27

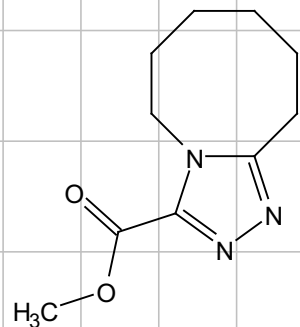
4.36
4.35
4.33

3.91

2.91
2.90
2.88

1.82
1.80
1.78
1.77
1.76
1.75
1.74
1.73
1.49
1.48
1.46
1.45
1.43
1.19
1.18
1.17
1.15
1.14



CDCl₃**3j**

159.33

158.40

144.34

77.42

77.16

76.91

52.61

42.98

30.38

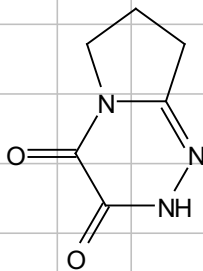
30.01

25.29

24.43

23.24

240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (MД)5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500



5a

DMSO-D6



12.11

3.86
3.85
3.83



2.83
2.81
2.79



2.50
2.14
2.12
2.11
2.09
2.07



0.97

2.06

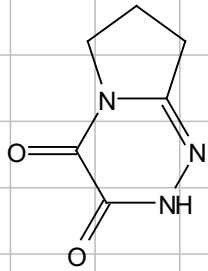
2.03

2.06

13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (M)

1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100



5a

DMSO-d6

154.90
154.85
148.52

46.61
40.55
40.34
40.13
39.92
39.71
39.50
39.29

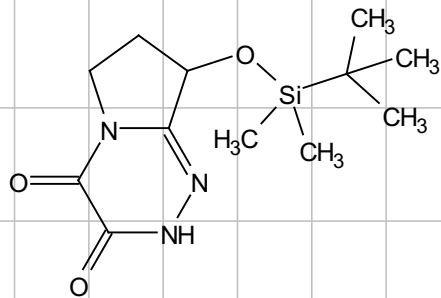
28.86
20.84

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

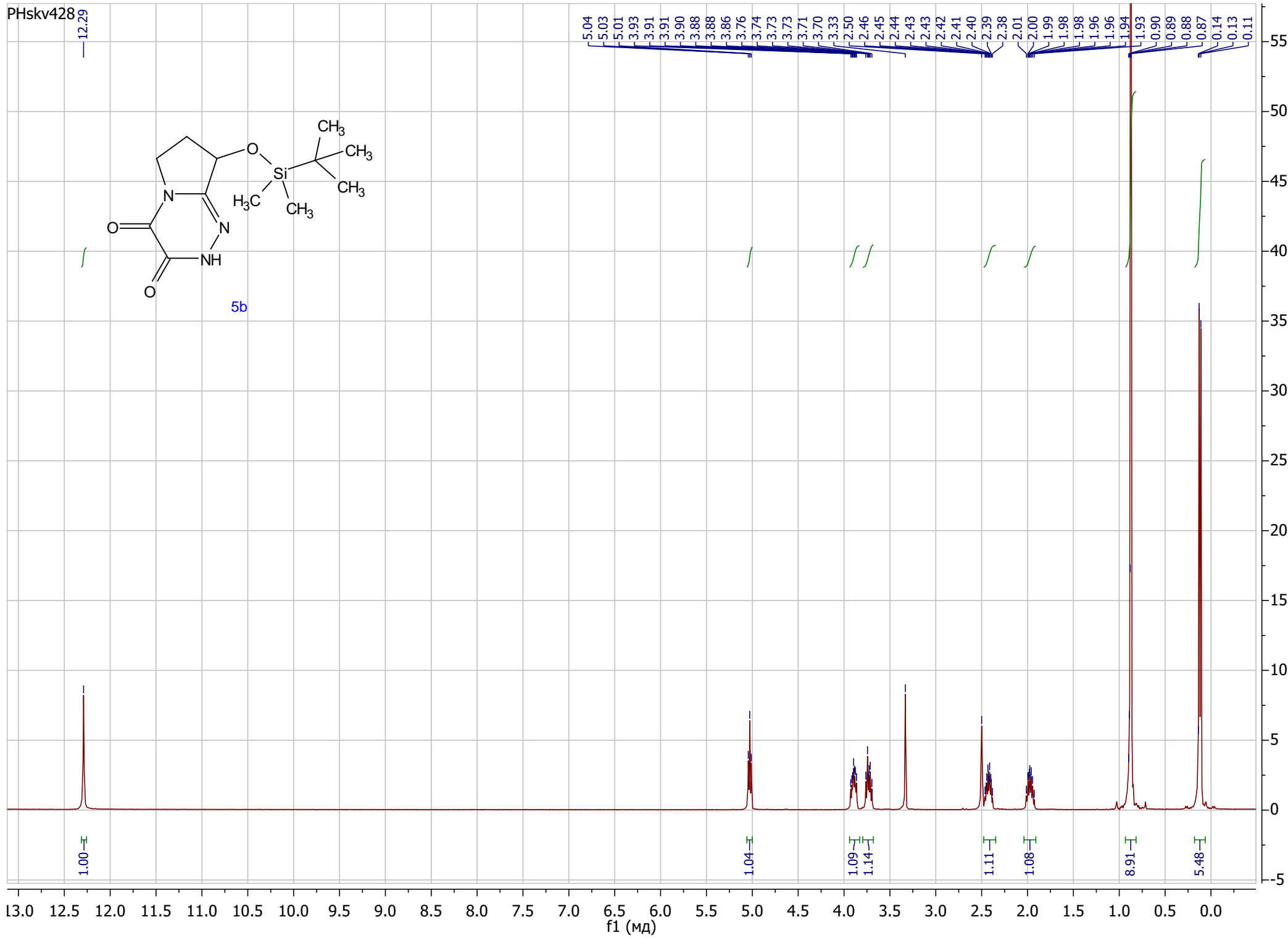
f1 (MД)

19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000

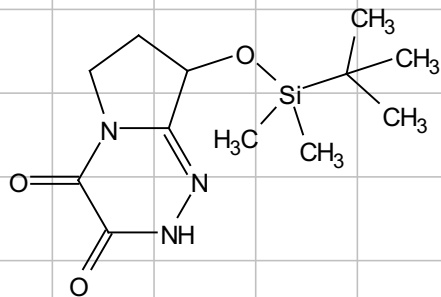
PHskv428



5b



PHSKV-428_C13
13C (1H decoupled)



5b

155.05
154.57

148.34

71.23

43.20

39.96

31.87

26.05

18.32

4.31
4.54

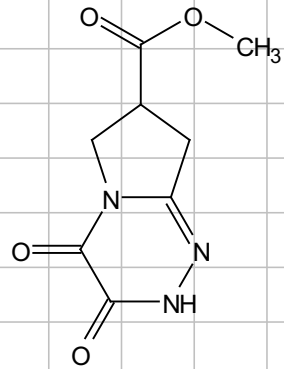
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (MД)

150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

PHSKV2

12.17



DMSO-d6

5c

4.12
4.11
4.10
4.08
4.04
4.03
4.01
4.00
3.70
3.67
3.63
3.60
3.58
3.57
3.54
3.17
3.17
3.15
3.13
3.12
3.09
3.07
3.05
3.04
2.50

0.96

2.12

3.00

1.13

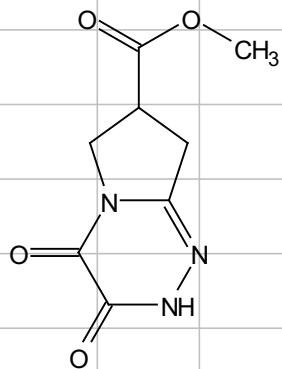
2.11

13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (MД)

23
22
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2

PHSKV2_C13
13C (1H decoupled)



5c

DMSO-d6

172.47

154.83

154.53

146.74

52.76

48.22

39.91

38.36

31.76

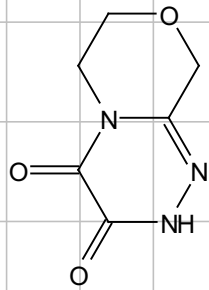
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (MД)

80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10

PHSKV3

12.29



5f

DMSO-d6

4.46
4.44
4.43
3.96
3.94
3.93
3.71
3.70
3.69

2.50

0.95

2.00

2.00

1.97

3.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (MД)

26
24
22
20
18
16
14
12
10
8
6
4
2
0
-2

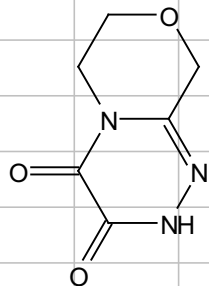
PHSKV3_C13
13C (1H decoupled)

156.18
154.52

138.97

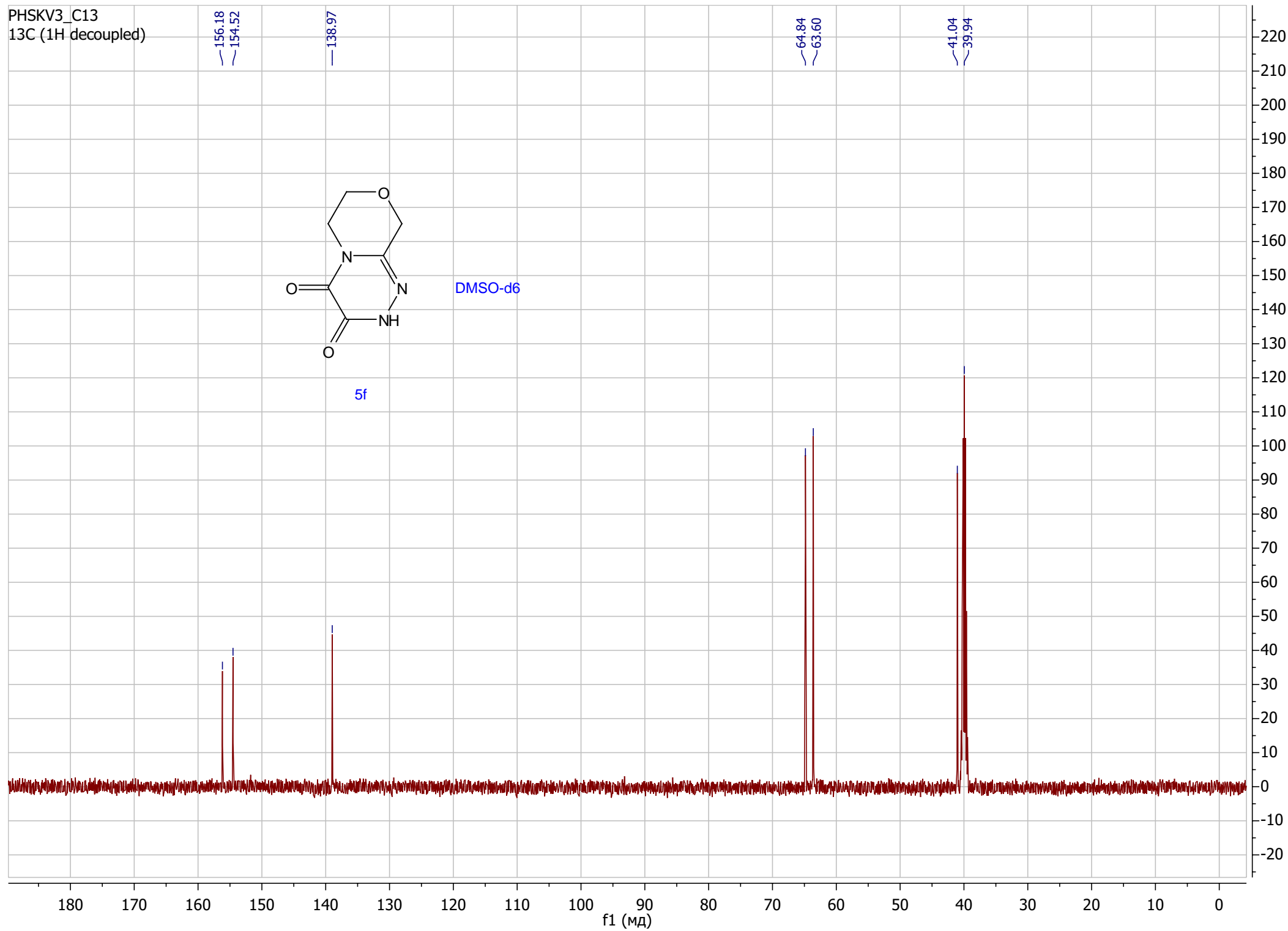
64.84
63.60

41.04
39.94

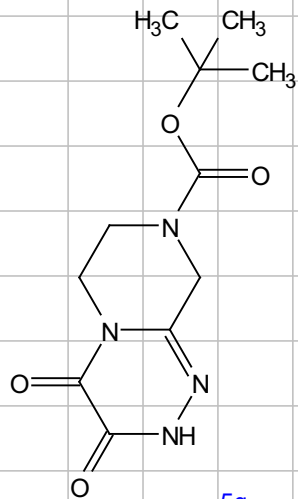


DMSO-d6

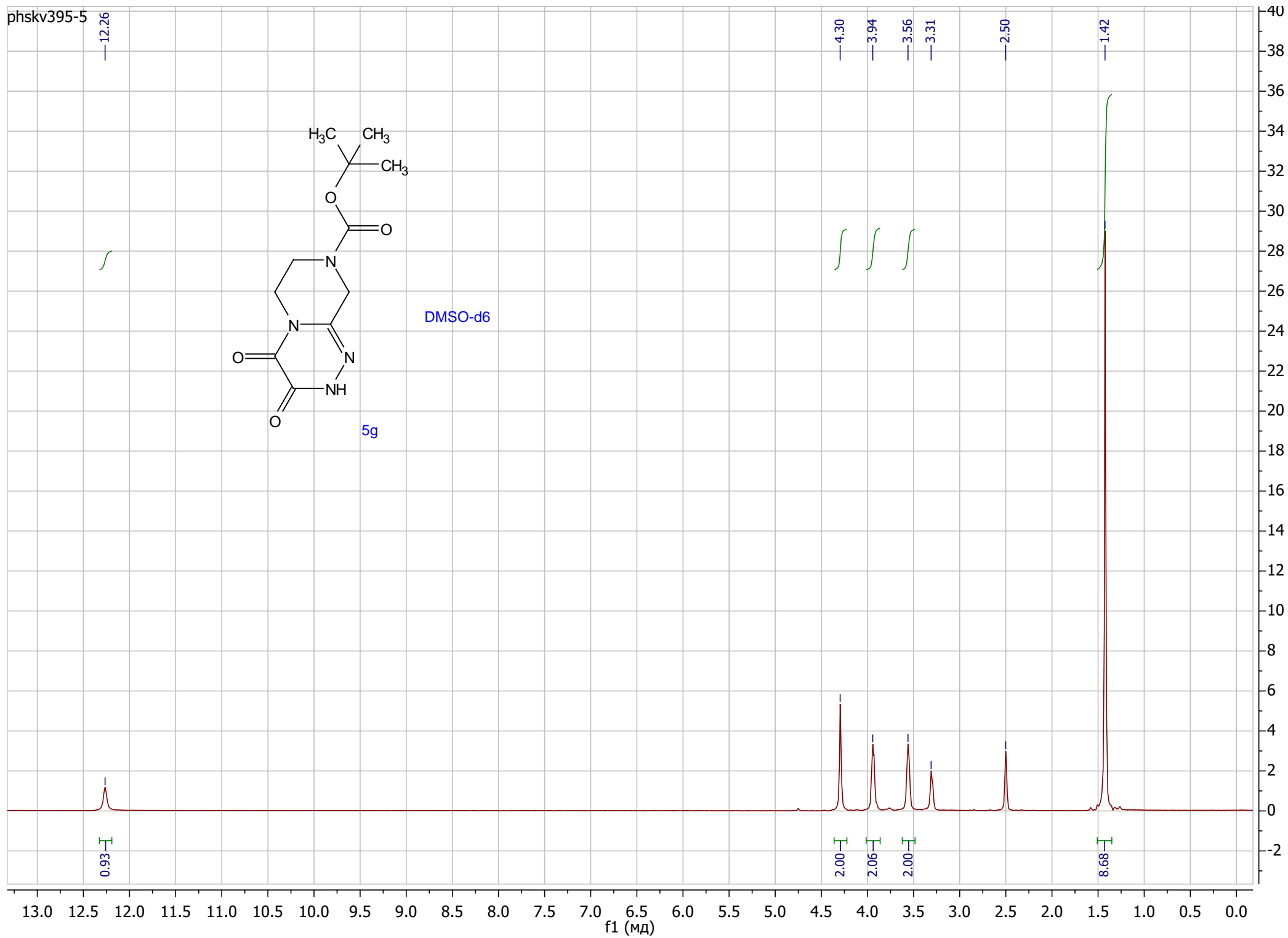
5f

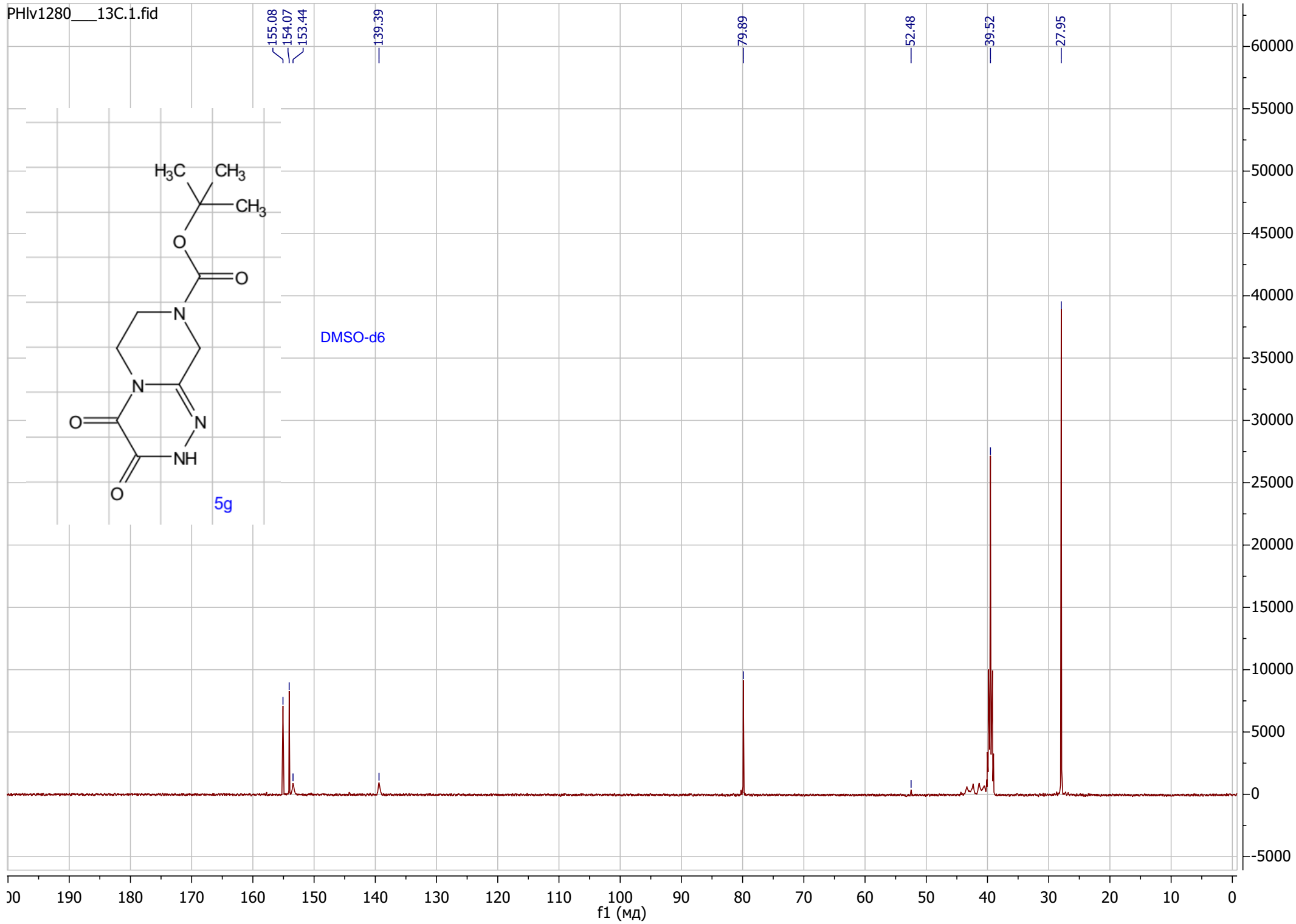


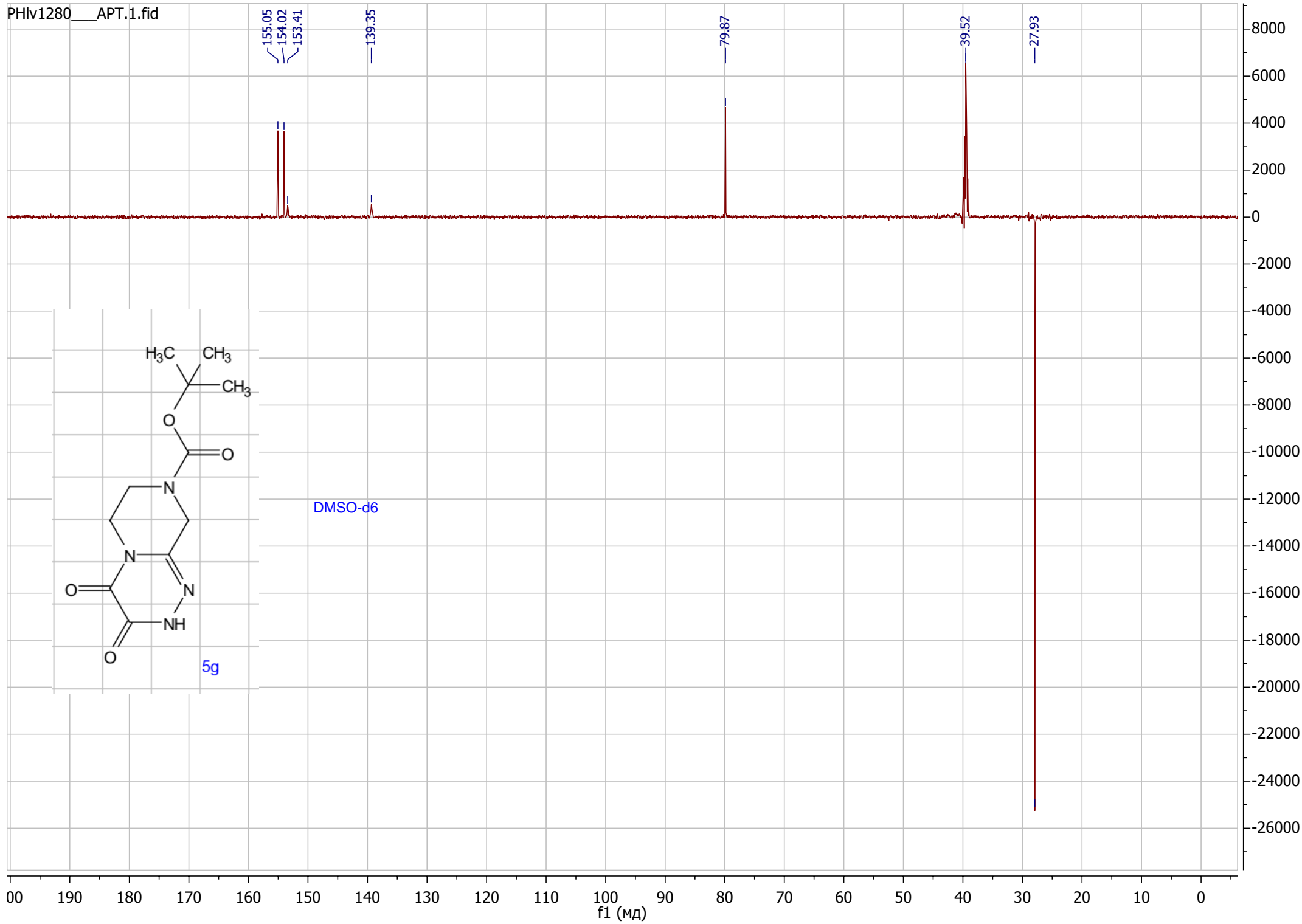
phskv395-5



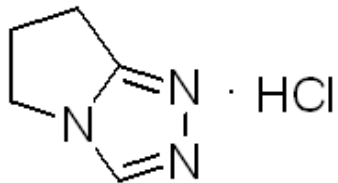
DMSO-d6







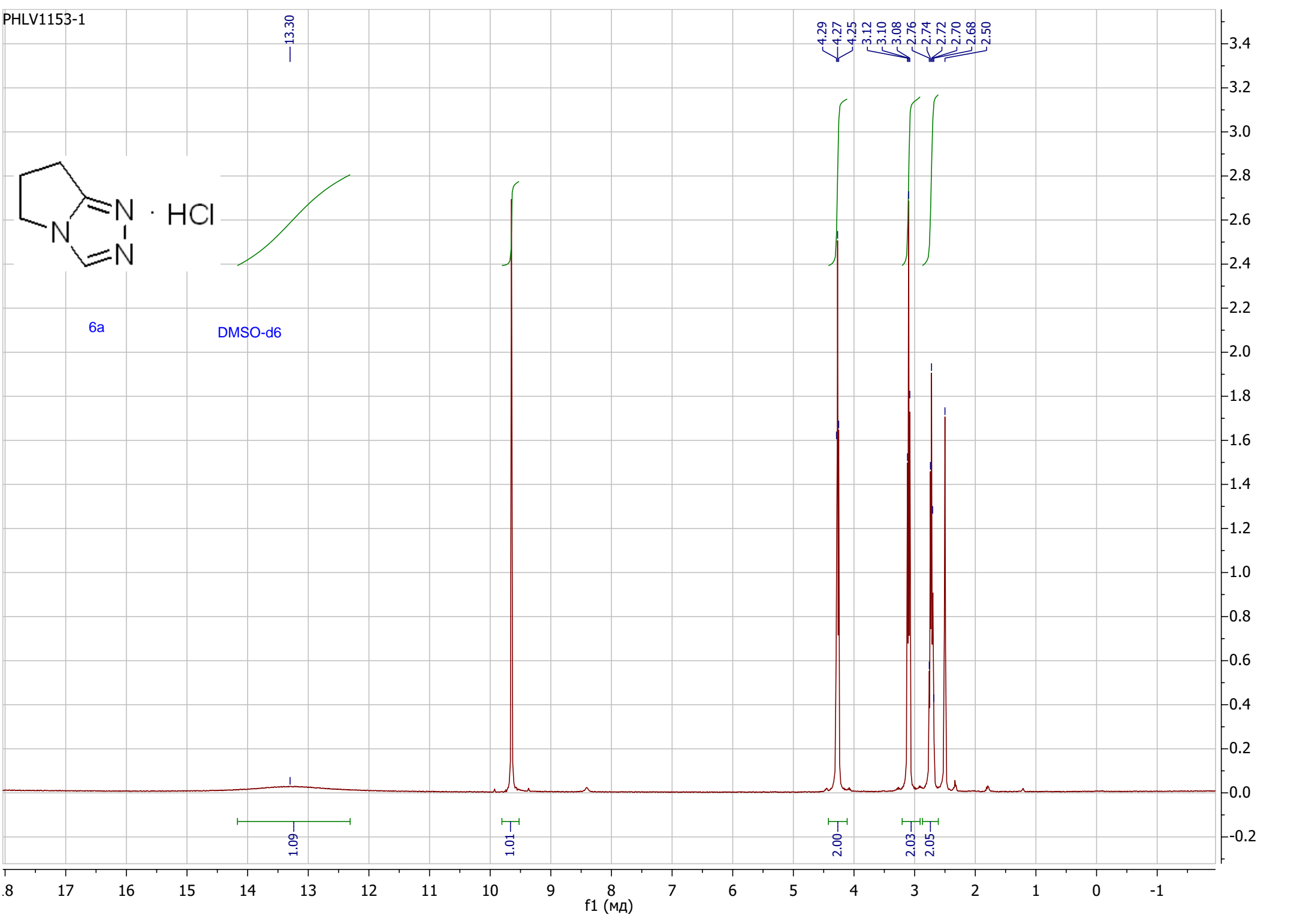
PHLV1153-1



6a

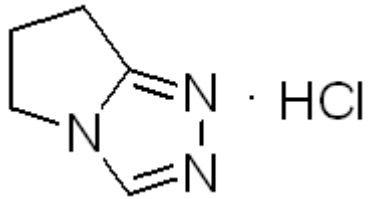
DMSO-d6

13.30



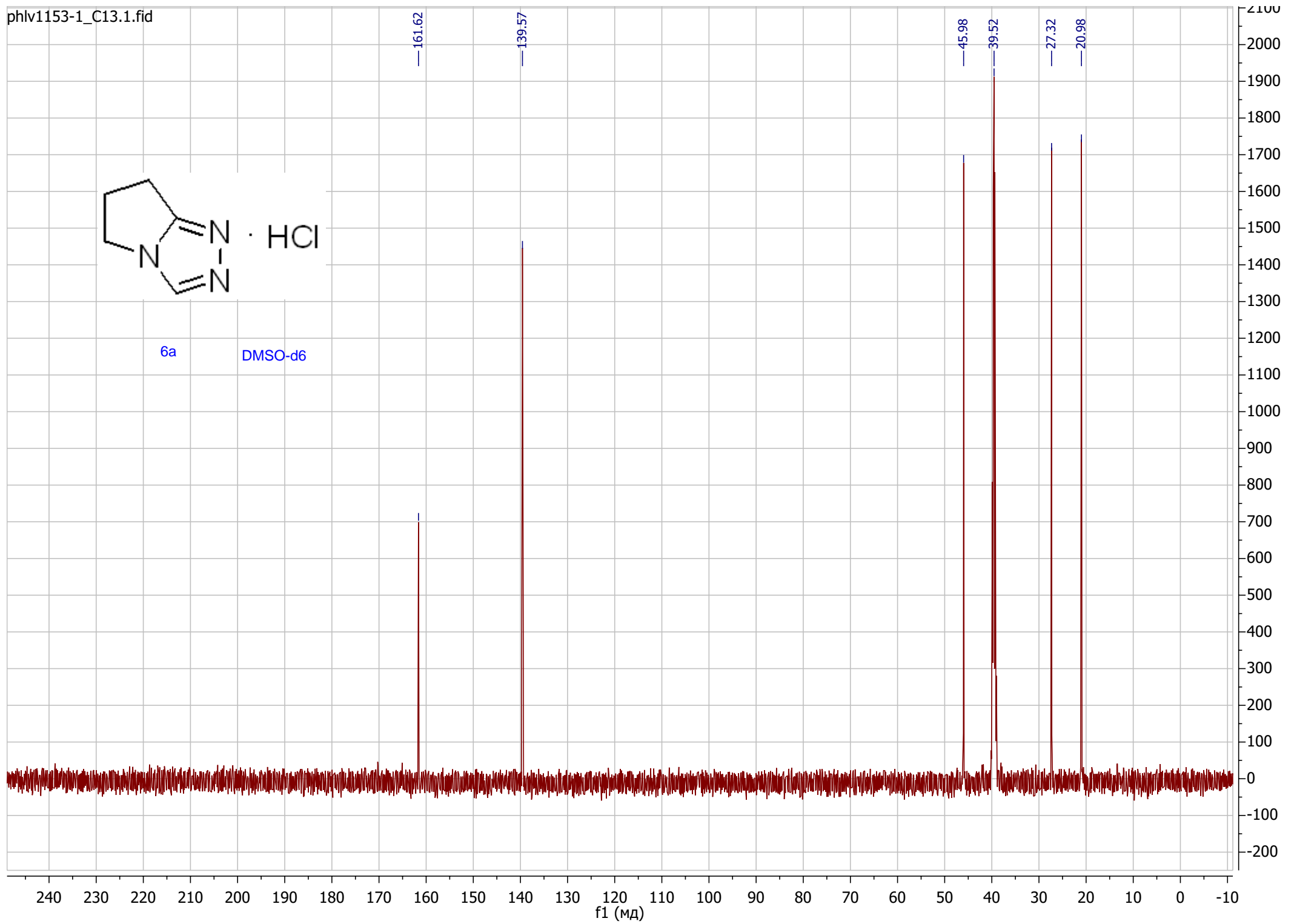
8 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1

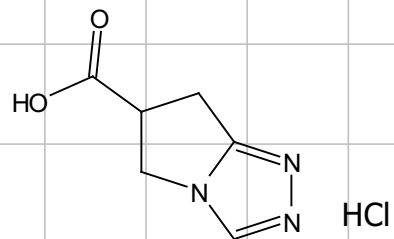
f1 (ppm)



6a

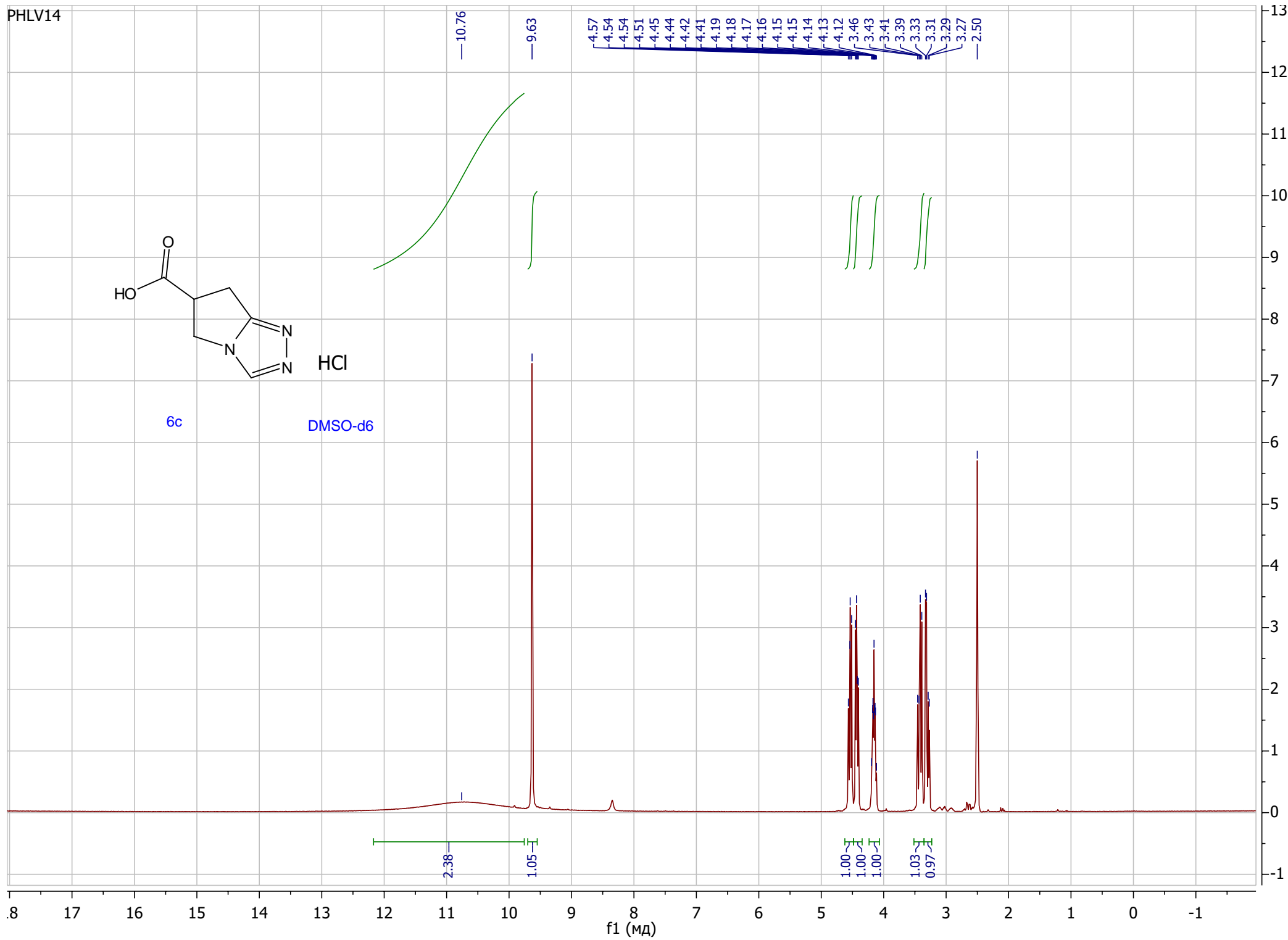
DMSO-d6



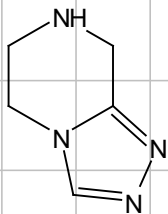


6c

DMSO-d6



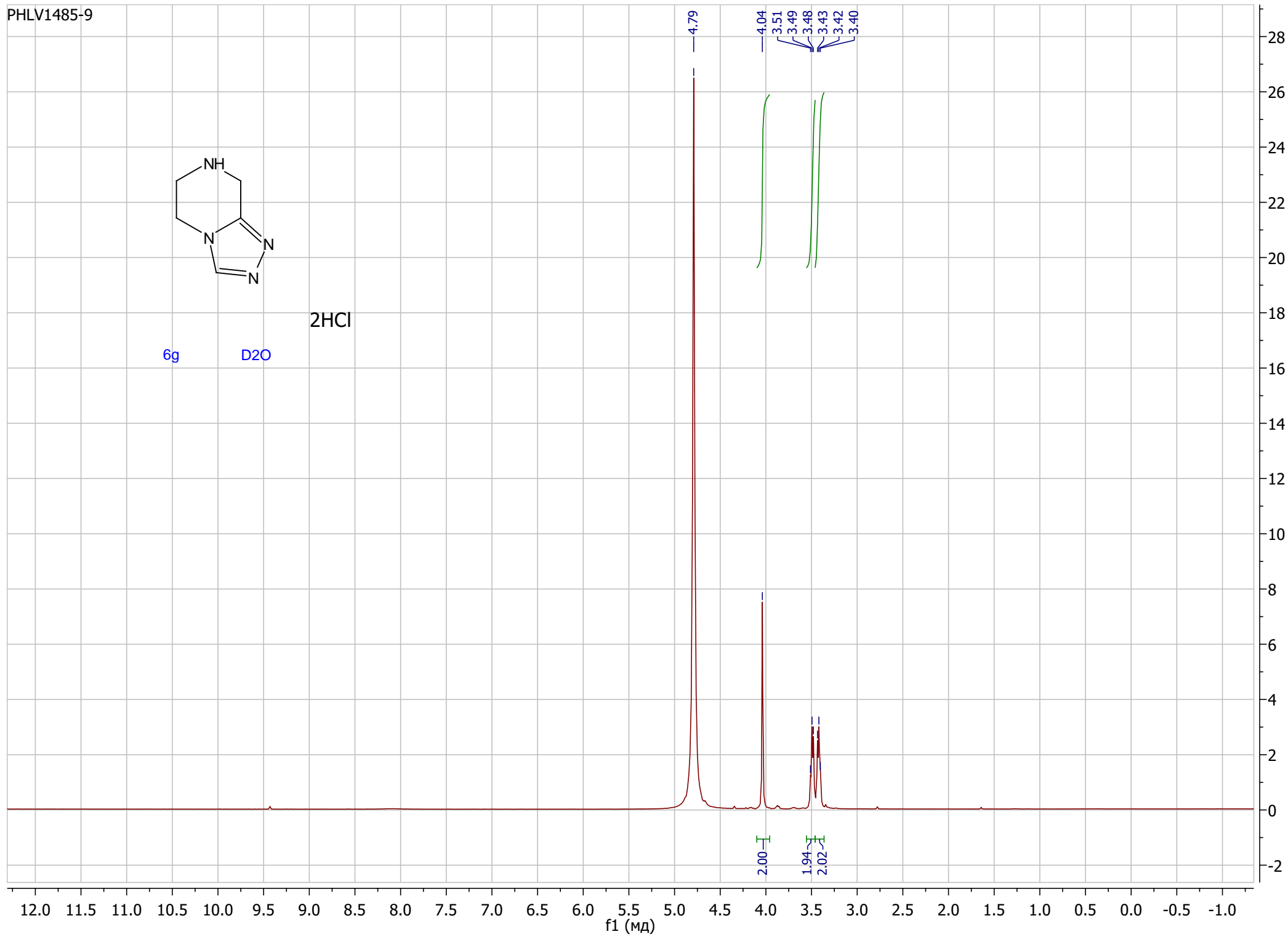
PHLV1485-9



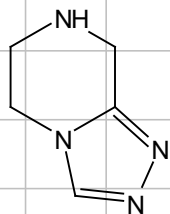
6g

D2O

2HCl



PHLV1485-9_C13



2HCl

6g

D2O

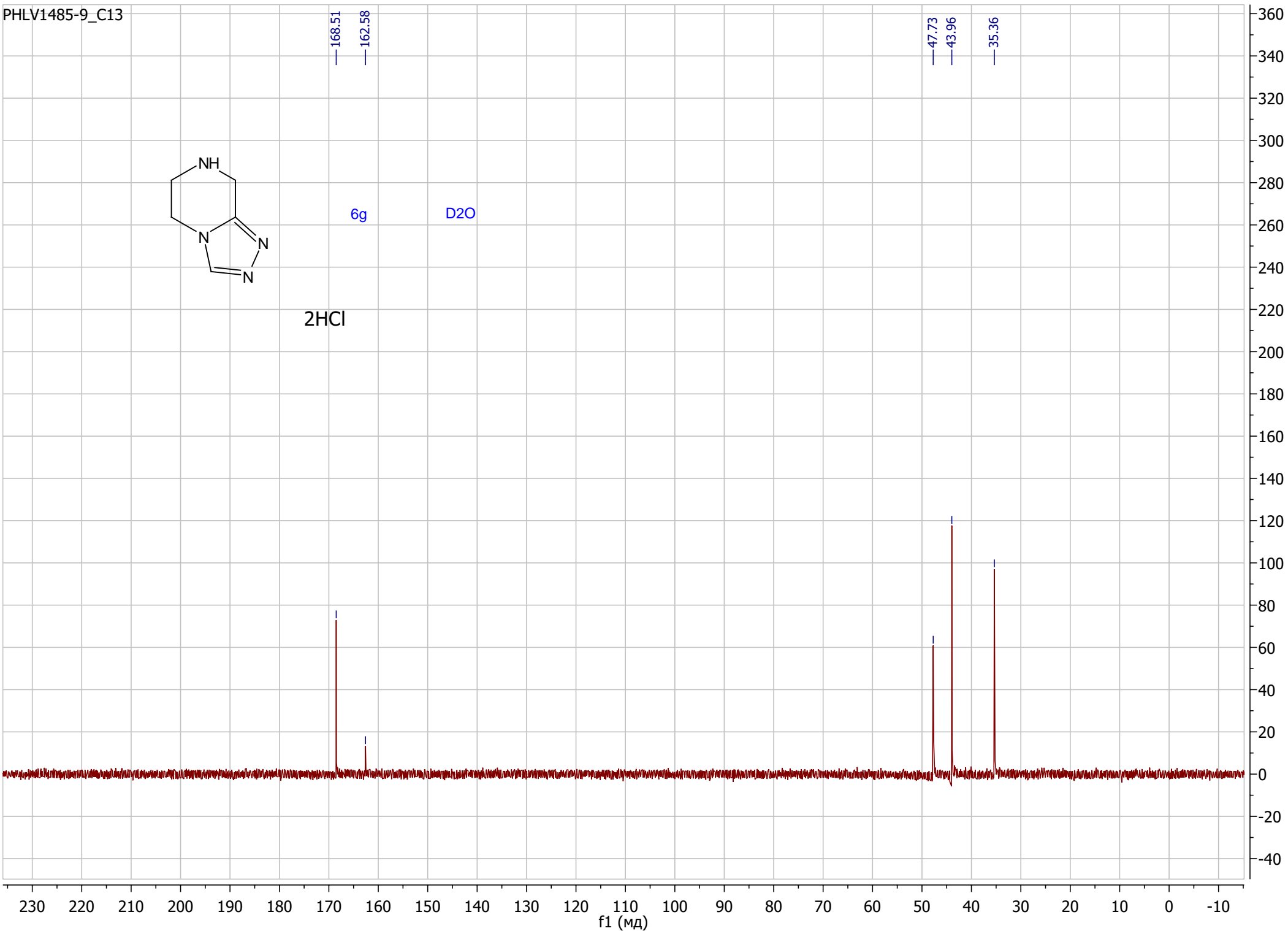
168.51

162.58

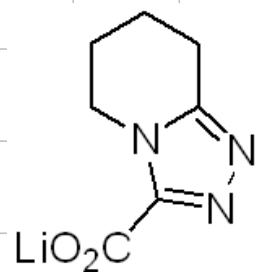
47.73

43.96

35.36

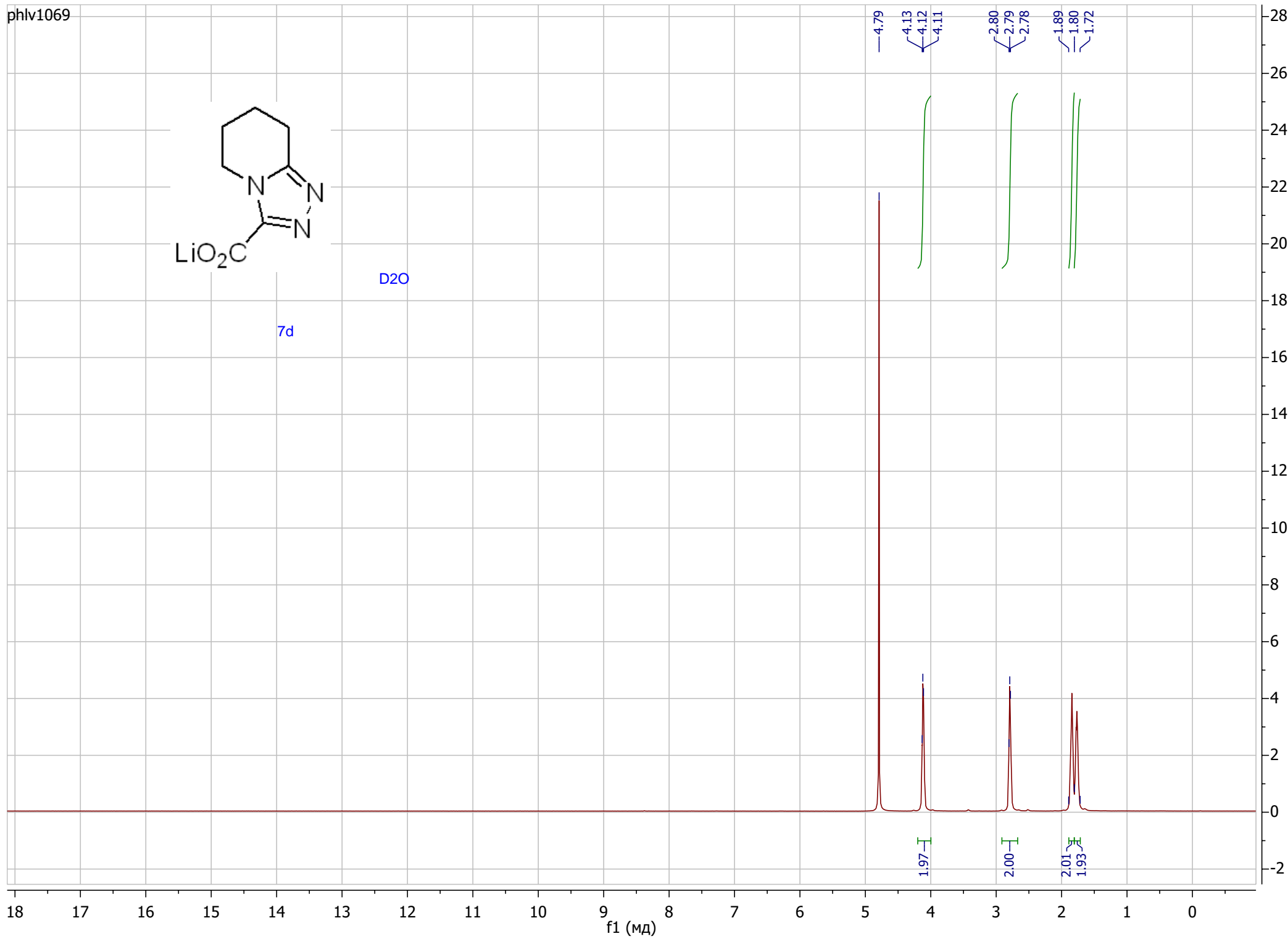


phlv1069

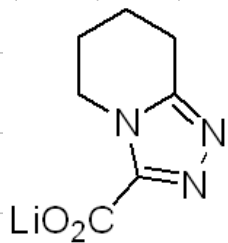


7d

D2O

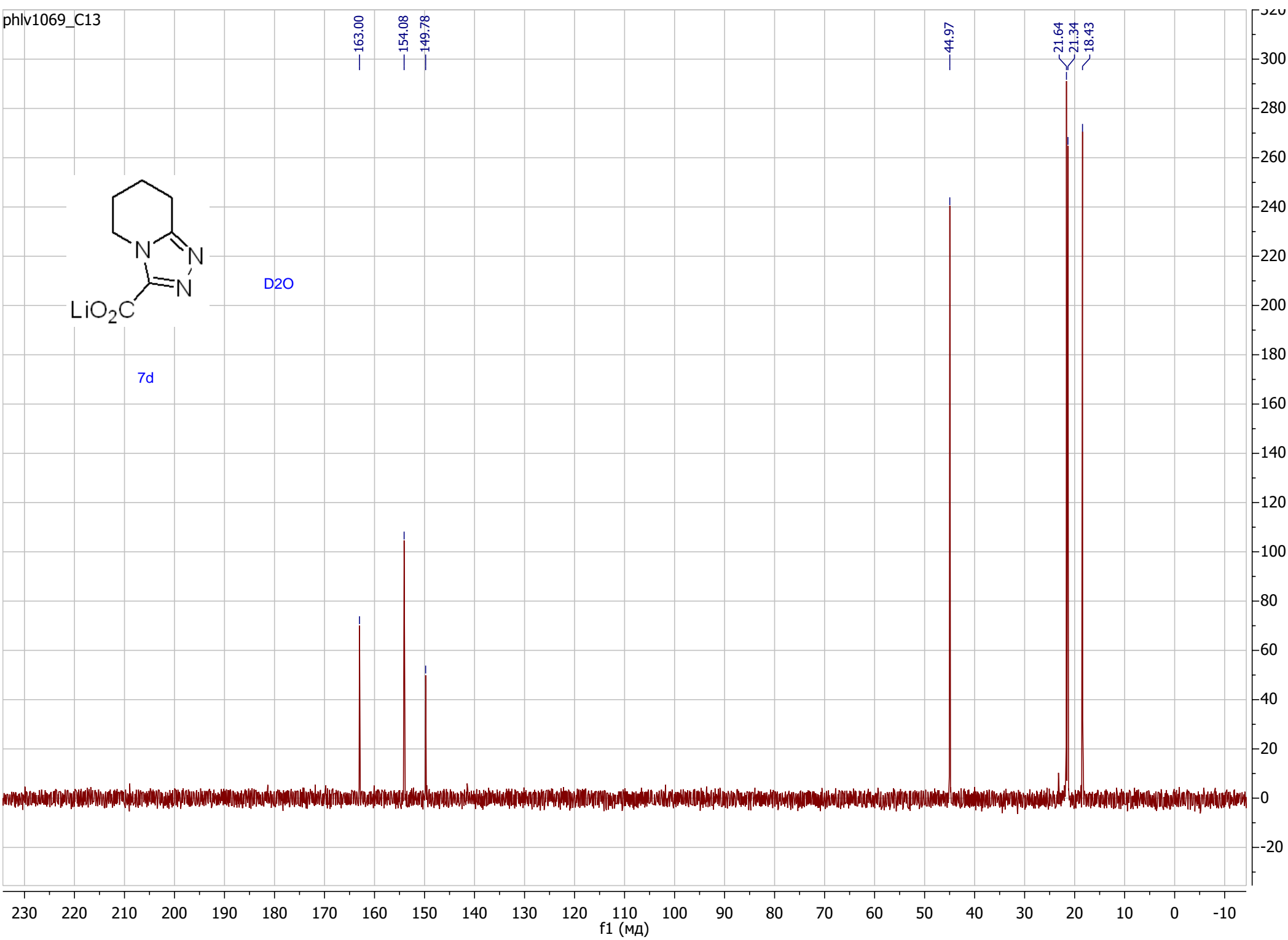


pflv1069_C13

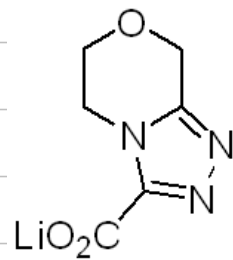


7d

D2O

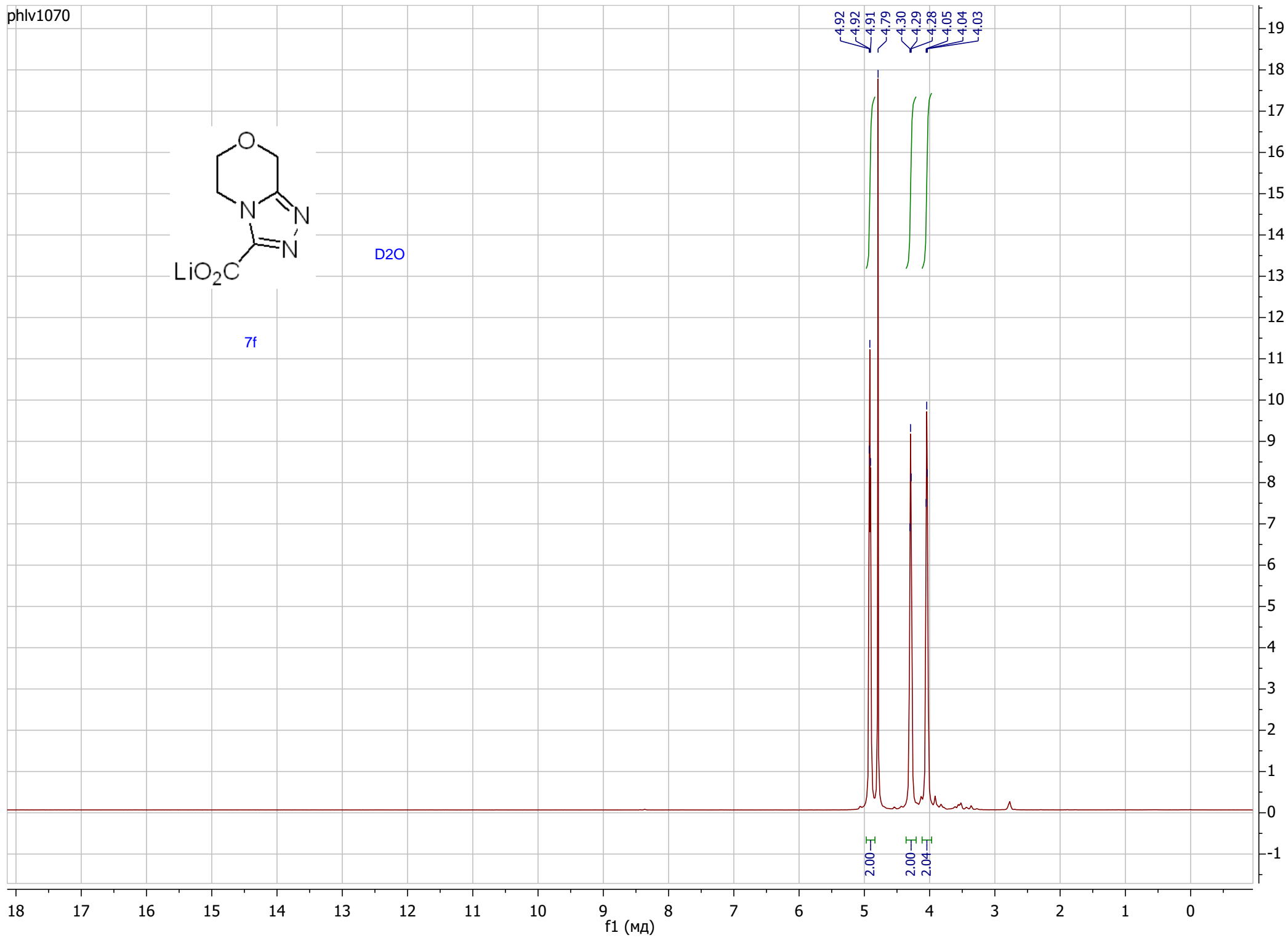


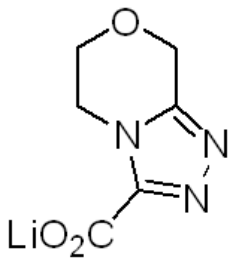
phlv1070



7f

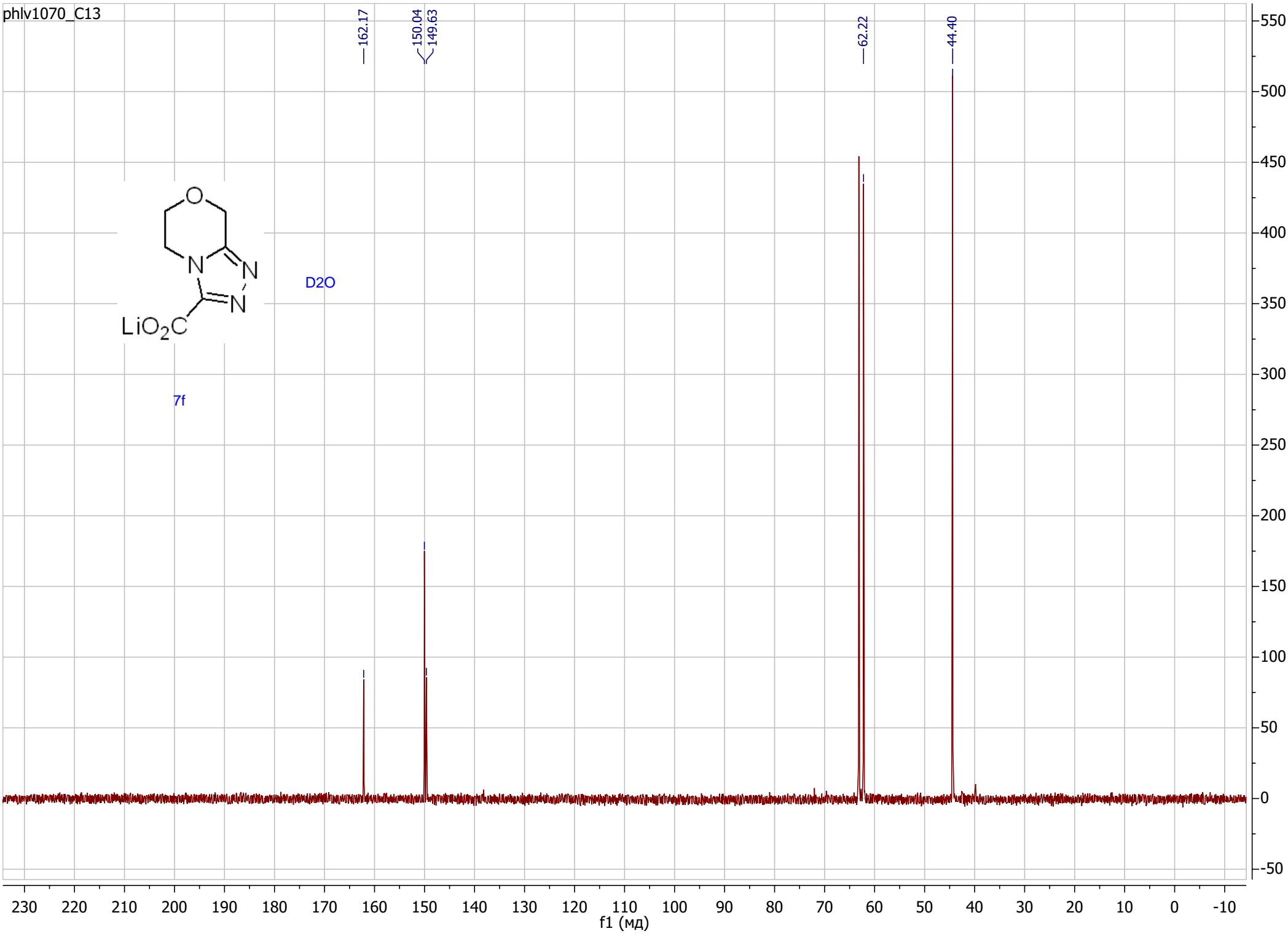
D2O



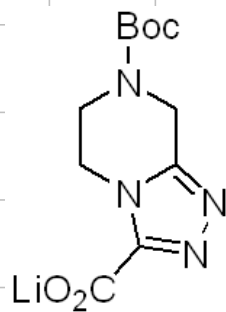


7f

D2O

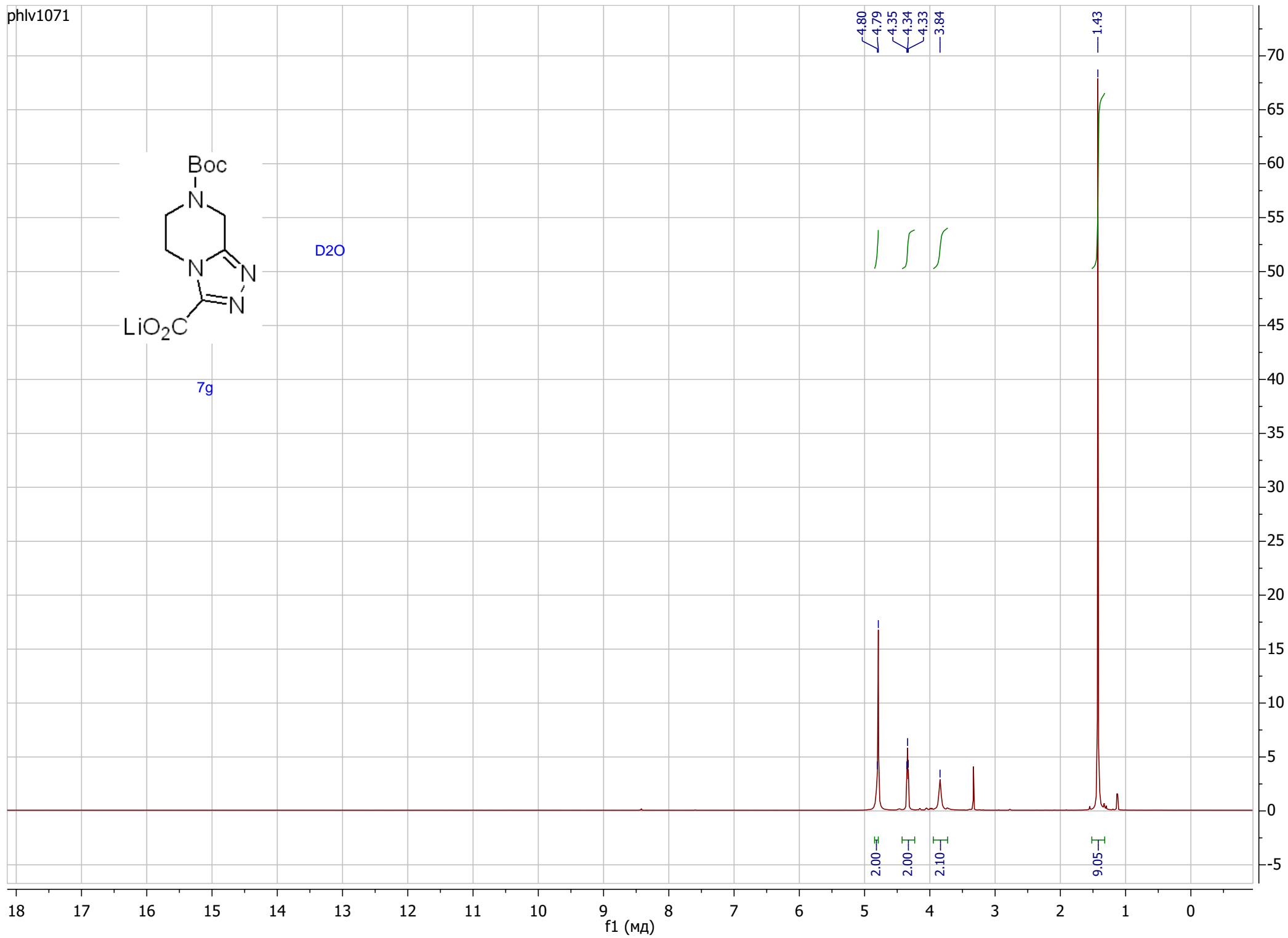


phlv1071

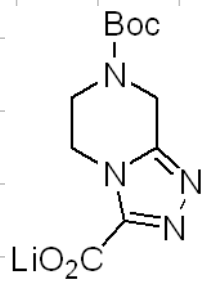


7g

D2O



phlv1071_C13



7g

D2O

162.32

155.65

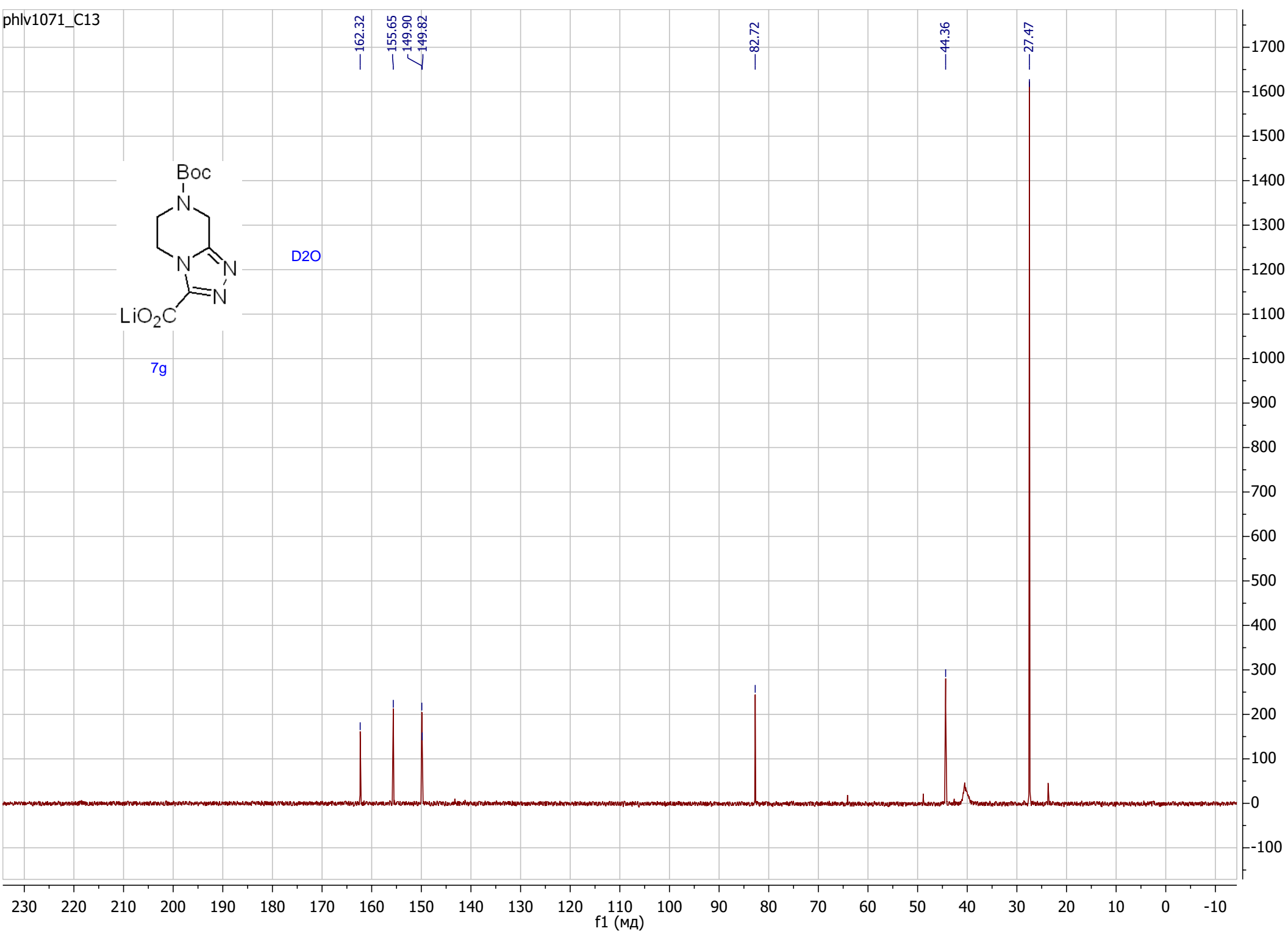
149.90

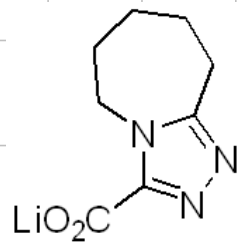
149.82

82.72

44.36

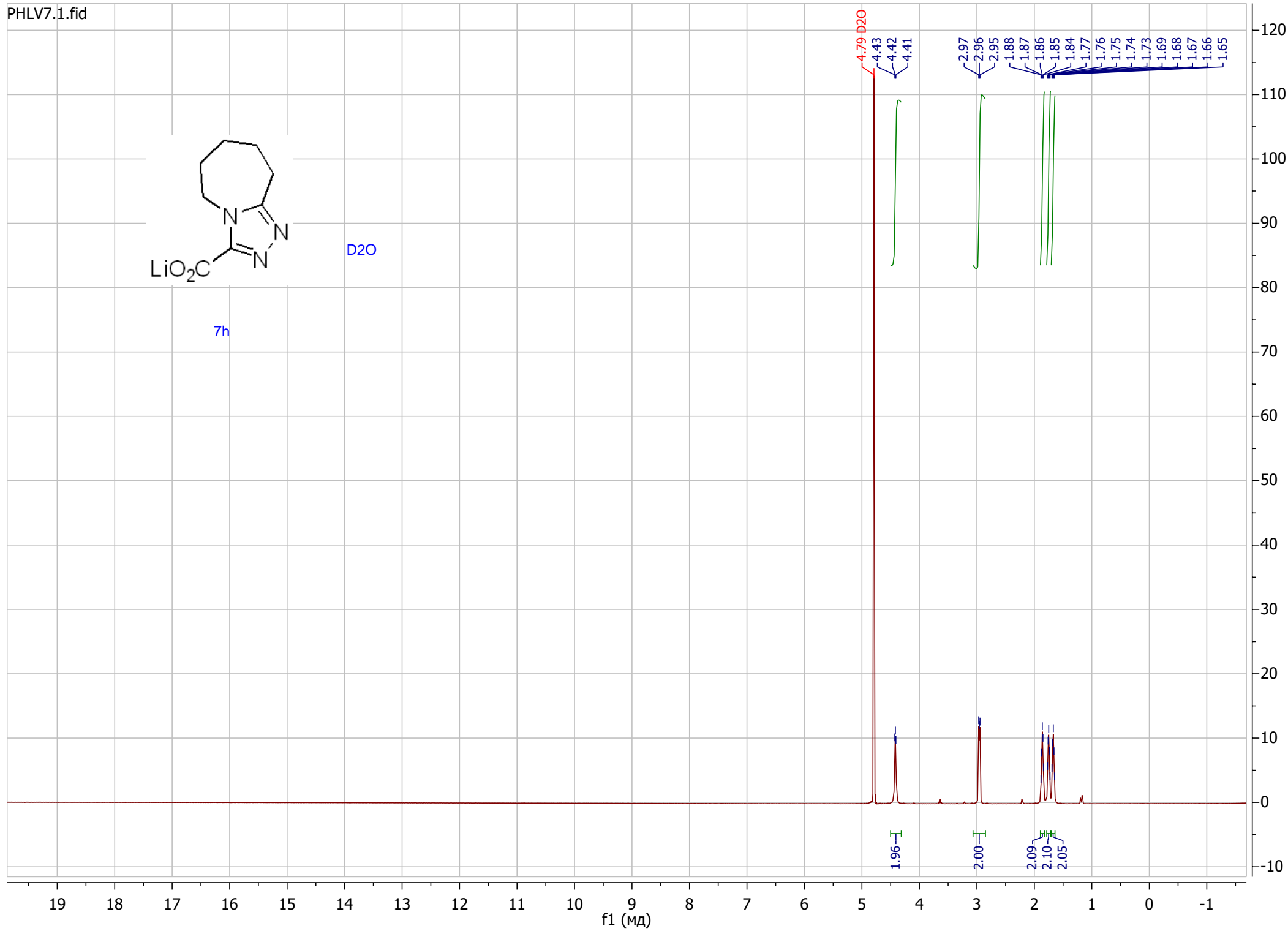
27.47

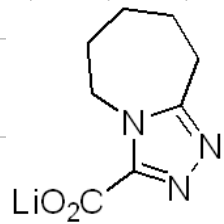




7h

D2O





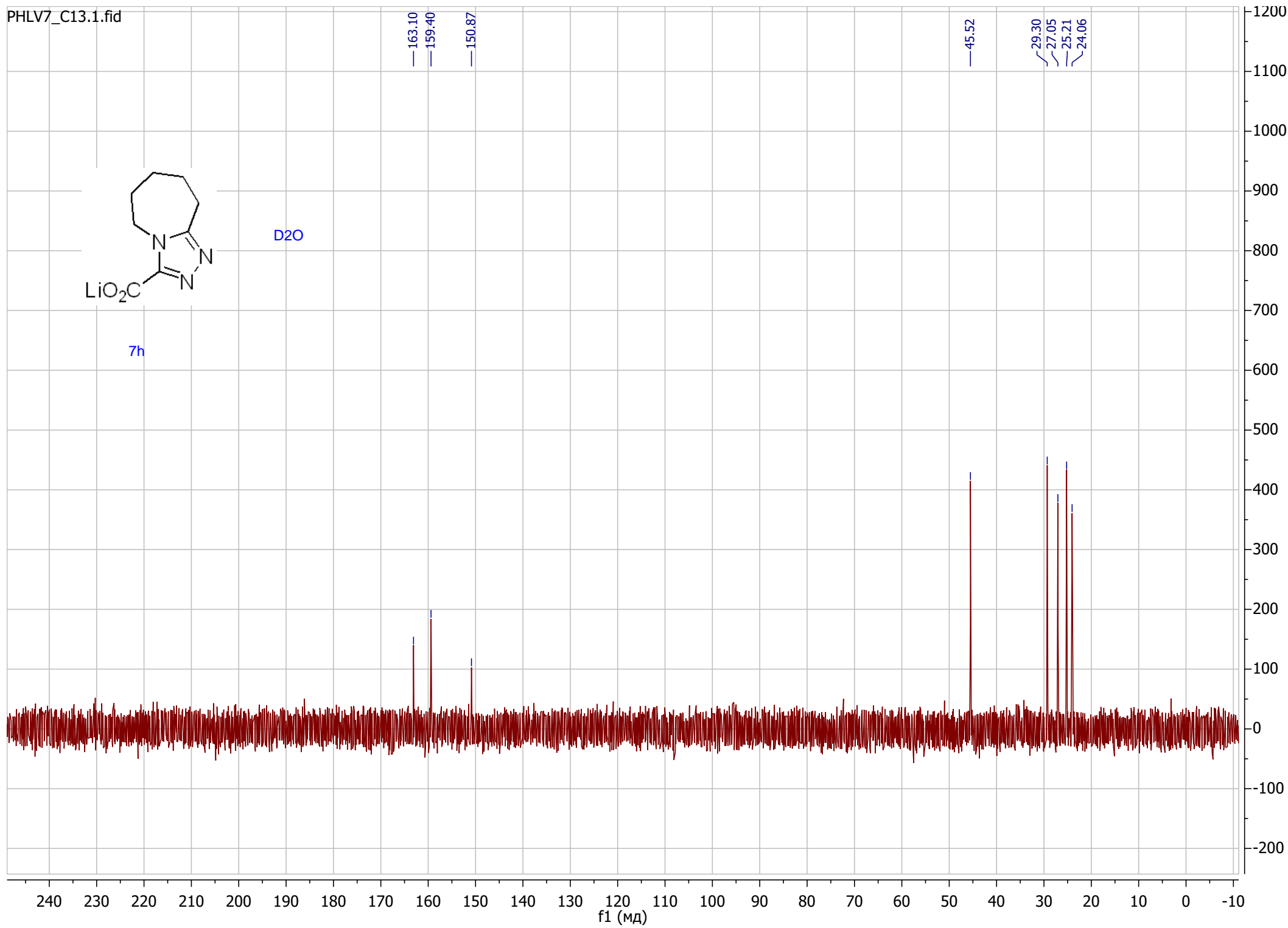
7h

D2O

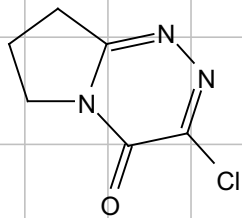
163.10
159.40
150.87

45.52

29.30
27.05
25.21
24.06

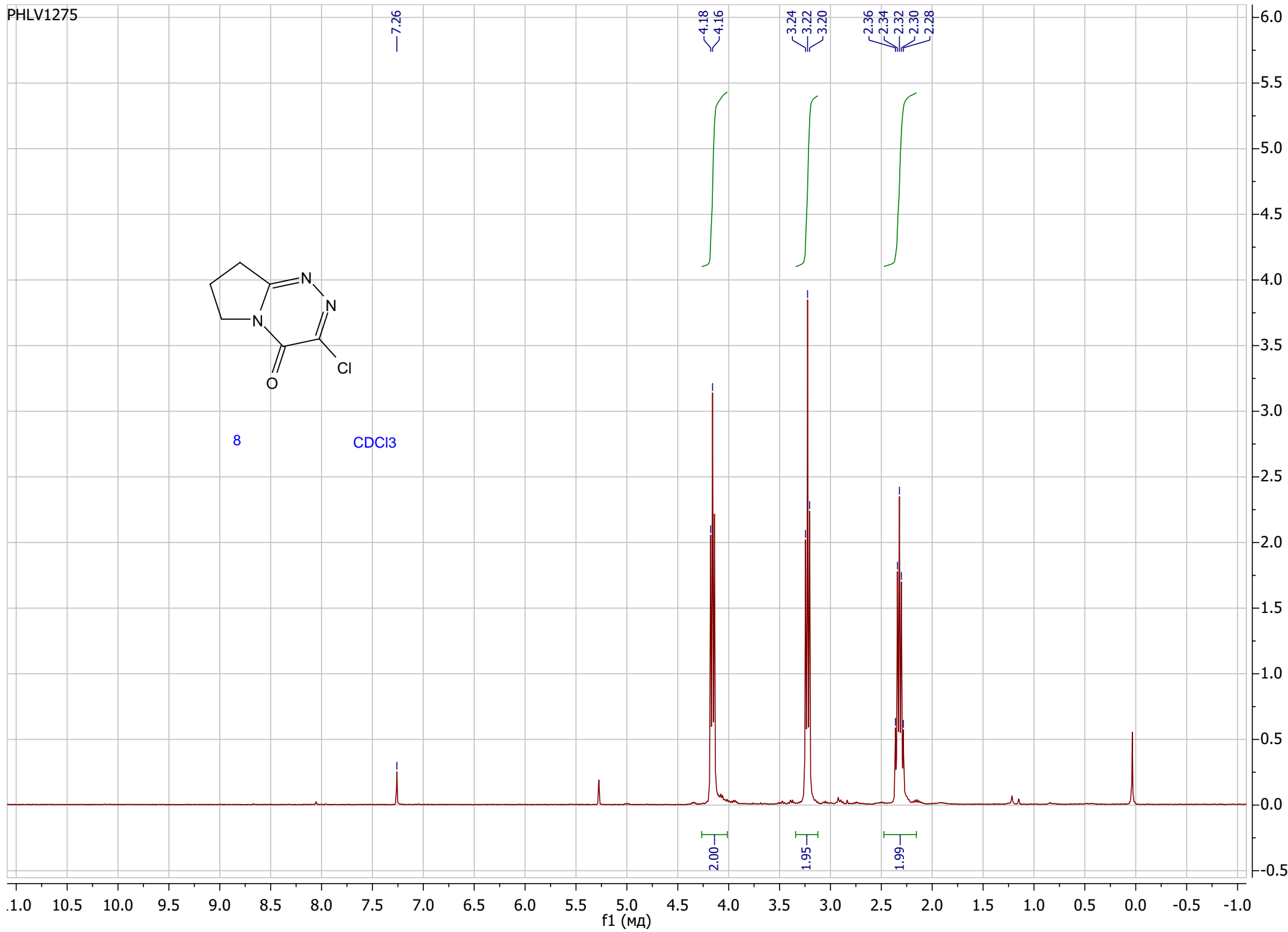


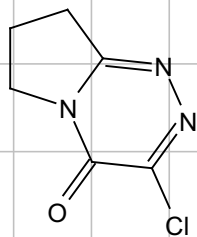
PHLV1275



8

CDCI3





8

CDCl3

161.00

152.08

149.11

77.41

77.16

76.91

48.13

30.68

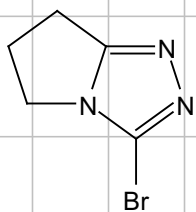
19.77

240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (MД)

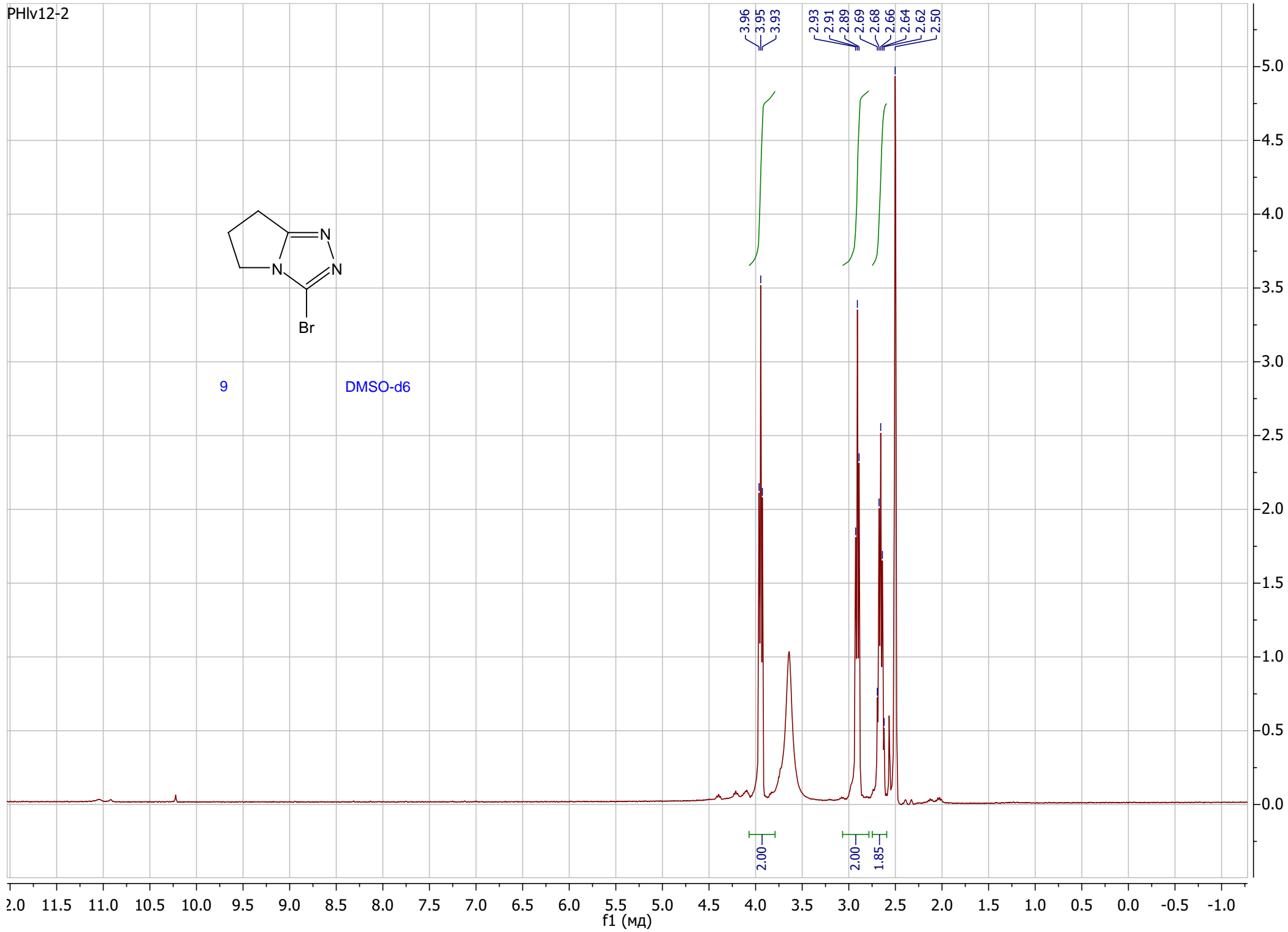
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000

PHlv12-2

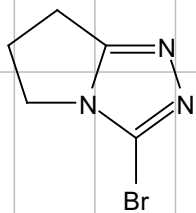


9

DMSO-d6



phlv12_C13



9

DMSO-d6

