Electronic Supplementary Information (ESI)

Versatile Synthesis of Pathogen Specific Bacterial Cell Wall Building Blocks †

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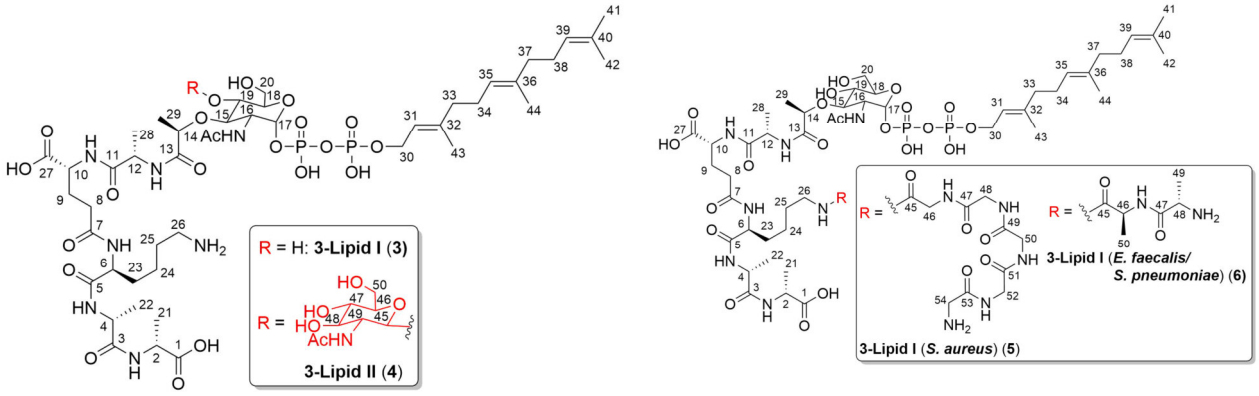


Table S1. NMR data for 3-lipid I (**3**), 3-lipid II (**4**), 3-lipid I (*S. aureus*, **5**) and 3-lipid I (*E. faecalis*, *S. pneumoniae*, **6**) in D_2O.[a]

	3-lipid I [**3**]		3-lipid II [**4**]		3-lipid I (*S. aureus*) [**5**]		3-lipid I (*S. pneumoniae, E. faecalis*) [**6**]	
position	δ_C	δ_H mult. (*J* in Hz)	δ_C	δ_H mult. (*J* in Hz)	δ_C	δ_H mult. (*J* in Hz)	δ_C	δ_H mult. (*J* in Hz)
1	179.8	-	179.8	-	179.9	-	181.4	-
2	51.0	4.20 – 4.10 m	51.0	4.15 – 4.12 m	51.0	4.16 – 4.10 m	51.1	4.19 – 4.14 m
3	174.0	-	174.0	-	174.0	-	174.1	-
4	78.0	4.35 q (7.2)	49.6	4.35 q (7.1)	49.8	4.30 q (7.2)	50.2	4.31 – 4.29 m
5	174.1	-	174.1	-	174.2	-	174.8	-
6	54.2	4.25 – 4.22 m	54.3	4.24 – 4.20 m/	54.3	4.26 – 4.17 m	54.3	4.29 – 4.24 m
7	175.7	-	175.7	-	175.6	-	175.8	-
8	31.7	2.32 t (7.8)	31.8	2.34 – 2.33 m	31.8	2.37 – 2.28 m	31.9	2.33 – 2.28 m
9	28.1	2.20 – 2.15 m/ 1.93 – 1.89 m	28.2	2.19 – 2.17 m/ 1.93 – 1.89 m	28.1	2.20 – 2.16 m/ 1.93 – 1.88 m	28.2	2.20 – 2.14 m/ 1.93 – 1.88 m
10	54.2	4.20 – 4.10 m	53.7	4.24 – 4.20 m/	54.3	4.26 – 4.17 m	54.3	4.29 – 4.24 m
11	175.8	-	175.7	-	175.5	-	175.9	-
12	49.9	4.29 q (7.2)	50.0	4.32 – 4.27 m	78.0	4.26 – 4.17 m	78.2	4.29 – 4.24 m
13	173.6	-	173.6	-	173.6	-	173.7	-
14	49.6	4.25 – 4.22 m	78.4	4.32 – 4.27 m	49.5	4.37 q (7.2)	49.5	4.36 q (7.2)
15	79.9	3.80 dd (9.6, 9.6)	77.9	3.86 – 3.81 m	79.9	3.80 dd (9.6, 9.6)	79.9	3.80 dd (9.7, 9.7)
16	53.4	4.20 – 4.10 m	53.5	4.15 – 4.12 m	53.4	4.16 – 4.10 m	53.3	4.19 – 4.14 m
NHAc-C=O	174.1	-	174.4	-	174.1	-	174.1	-
NHAc-C=O	-	-	174.2	-	-	-	-	-
NHAc-CH_3	22.2	2.02 s	22.2	2.01 s	22.4	2.02 s	22.3	2.00 s
NHAc-CH_3	-	-	22.1	2.07 s	-	-	-	-
17	94.7	5.50 – 5.47 m	94.2	5.50 – 5.47 m	94.7	5.50 – 5.48 m	94.8	5.50 – 5.46 m
18	73.0	3.98 – 3.96 m	73.8	3.98 – 3.89 m	73.0	3.98 – 3.96 m	73.1	3.99 – 3.94 m
19	68.0	3.66 dd (9.6, 9.6)	72.4	3.98 – 3.89 m	68.0	3.66 dd (9.6, 9.6)	68.2	3.64 pt (9.7)
20	60.3	3.92 – 3.84 m	61.1/ 59.7	3.98 – 3.89 m/ 3.79 – 3.74 m	60.3	3.90 – 3.83 m	58.2	3.91 – 3.85 m
21	17.4	1.35 d (7.2)	17.4	1.35 d (7.2)	17.4	1.35 d (7.2)	17.5	1.34 d (7.1)
22	18.6	1.39 d (7.2)	18.7	1.40 d (7.2)	16.9	1.46 d (7.2)	17.0	1.45 d (7.2)
23	30.5	1.87 – 1.77 m	30.5	1.86 – 1.82 m/ 1.81 – 1.79 m	30.7	1.83 – 1.73 m	30.7	1.83 – 1.76 m
24	22.0	1.52 – 1.47 m	22.2	1.45 – 1.39 m	22.2	1.56 – 1.51 m	22.2	1.53 – 1.50 m
25	26.3	1.72 – 1.70 m	26.5	1.69 – 1.66 m	27.8	1.72 – 1.70 m	27.7	1.72 – 1.70 m
26	39.1	3.02 t (7.5)	39.2	2.97 t (7.0)	39.0	3.23 t (6.7)	38.9	3.26 – 3.23 m
27	177.6	-	177.6	-	177.7	-	177.9	-
28	16.8	1.46 d (7.3)	16.9	1.47 d (6.9)	18.7	1.43 d (6.8)	18.7	1.42 d (6.9)
29	16.5	1.43 d (6.8)	16.5	1.46 d (6.8)	16.6	1.38 d (7.2)	16.7	1.38 d (7.1)
30	63.1	4.54 – 4.49 m	63.1	4.51 – 4.49 m	63.2	4.54 – 4.49 m	63.2	4.52 – 4.47 m
31	119.3	5.46 t (7.1)	119.3	5.46 t (6.9)	119.3	5.46 t (6.7)	119.3	5.46 t (6.8)
32	143.2	-	143.2	-	143.2	-	143.2	-
33	38.8	2.15 – 2.11 m	38.8	2.14 – 2.11 m	38.8	2.15 – 2.11 m	38.9	2.15 – 2.11 m
34	25.5	2.20 – 2.15 m	25.6	2.19 – 2.17 m	25.5	2.20 – 2.16 m	25.5	2.20 – 2.14 m

	3-lipid I [**3**]		3-lipid II [**4**]		3-lipid I (*S. aureus*) [**5**]		3-lipid I (*S. pneumoniae, E. faecalis*) [**6**]	
position	δ_C	δ_H mult. (*J* in Hz)	δ_C	δ_H mult. (*J* in Hz)	δ_C	δ_H mult. (*J* in Hz)	δ_C	δ_H mult. (*J* in Hz)
35	124.2	5.22 t (6.5)	124.2	5.23 t (6.4)	124.2	5.22 t (6.7)	124.4	5.23 t (6.8)
36	136.7	-	136.7	-	136.7	-	136.8	-
37	38.8	2.04 t (7.1)	38.8	2.05 t (7.7)	38.8	2.04 t (7.1)	38.9	2.02 t (7.5)
38	25.8	2.15 – 2.11 m	25.8	2.14 – 2.11 m	25.8	2.15 – 2.11 m	25.9	2.15 – 2.11 m
39	124.4	5.20 t (7.8)	124.4	5.20 t (6.4)	124.4	5.20 t (6.7)	124.5	5.21 – 5.16 m
40	133.4	-	133.5	-	133.4	-	133.4	-
41	-	1.64 s	17.0	1.64 s	17.0	1.64 s	17.0	1.64 s
42	24.9	1.70 s	24.9	1.71 s	24.9	1.71 s	25.0	1.70 s
43	15.7	1.74 s	15.7	1.74 s	15.7	1.74 s	15.7	1.73 s
44	15.3	1.64 s	15.3	1.64 s	15.3	1.64 s	15.3	1.63 s
45	-	-	100.1	4.63 d (8.3)	171.0	3.82 s	172.1	-
46	-	-	75.9	3.46 – 3.41 m	42.5	3.91 s	52.2	4.23 – 4.21 m
47	-	-	70.3	3.46 – 3.41 m	172.2/172.1/ 172.0	-	172.0	-
48	-	-	74.0	3.58 pt (8.6, 8.6)	42.6/42.5	4.03 s/ 4.01 s	49.9	4.21 – 4.19 m
49	-	-	56.1	3.79 – 3.74 m	172.2/172.1/ 172.0	-	16.6	1.37 d (7.2)
50	-	-	61.1/ 59.7	3.98 – 3.89 m/ 3.79 – 3.74 m	42.6/42.5	4.03 s/ 4.01 s	19.2	1.55 d (7.1)
51	-	-	-	-	172.2/172.1/ 172.0	-	-	-
52	-	-	-	-	42.4	4.08 s	-	-
53	-	-	-	-	169.9	-	-	-
54	-	-	-	-	41.2	-	-	-

[a] Recorded at 700 MHz and 500 MHz (^{1}H) and 150 MHz (^{13}C).

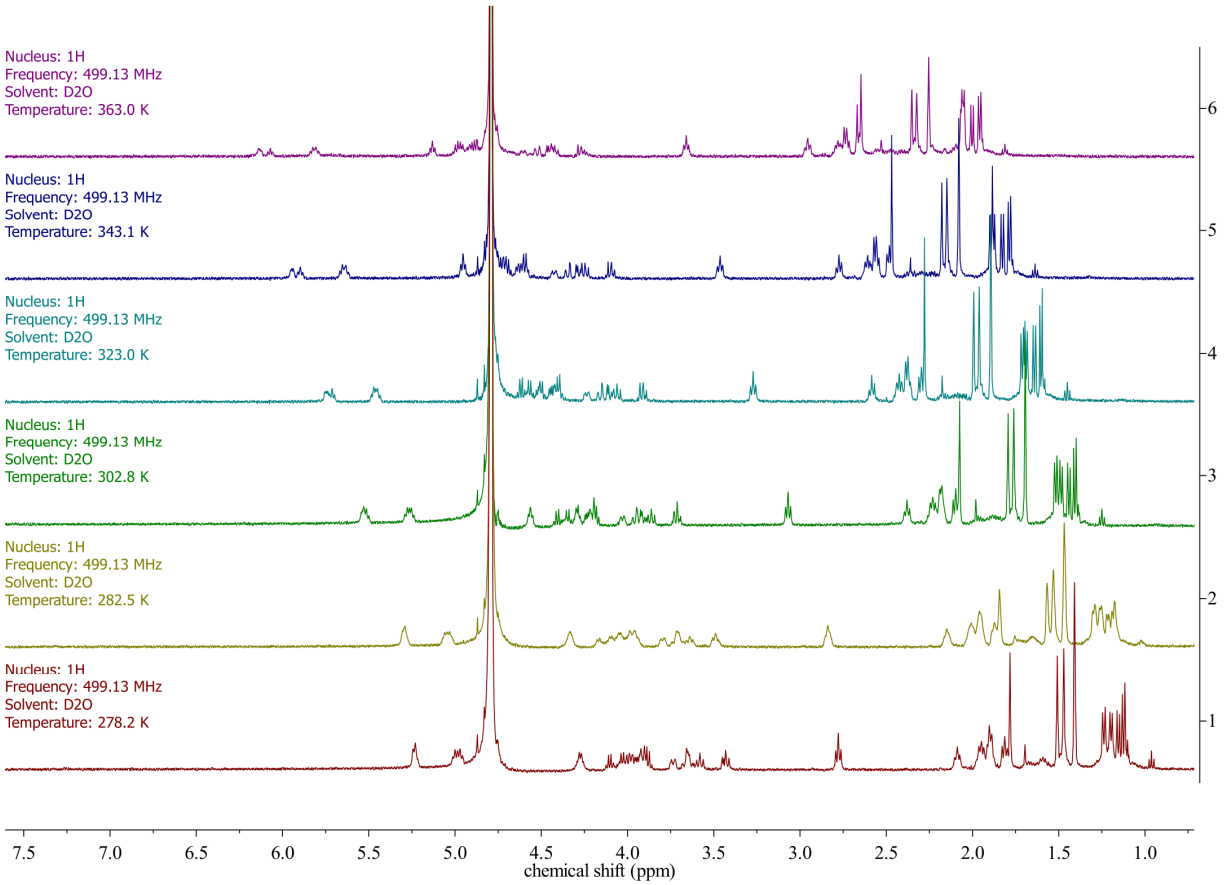


Figure S1: Temperature dependency of ^{1}H-NMR spectra of farnesyl lipid I analog **3**.

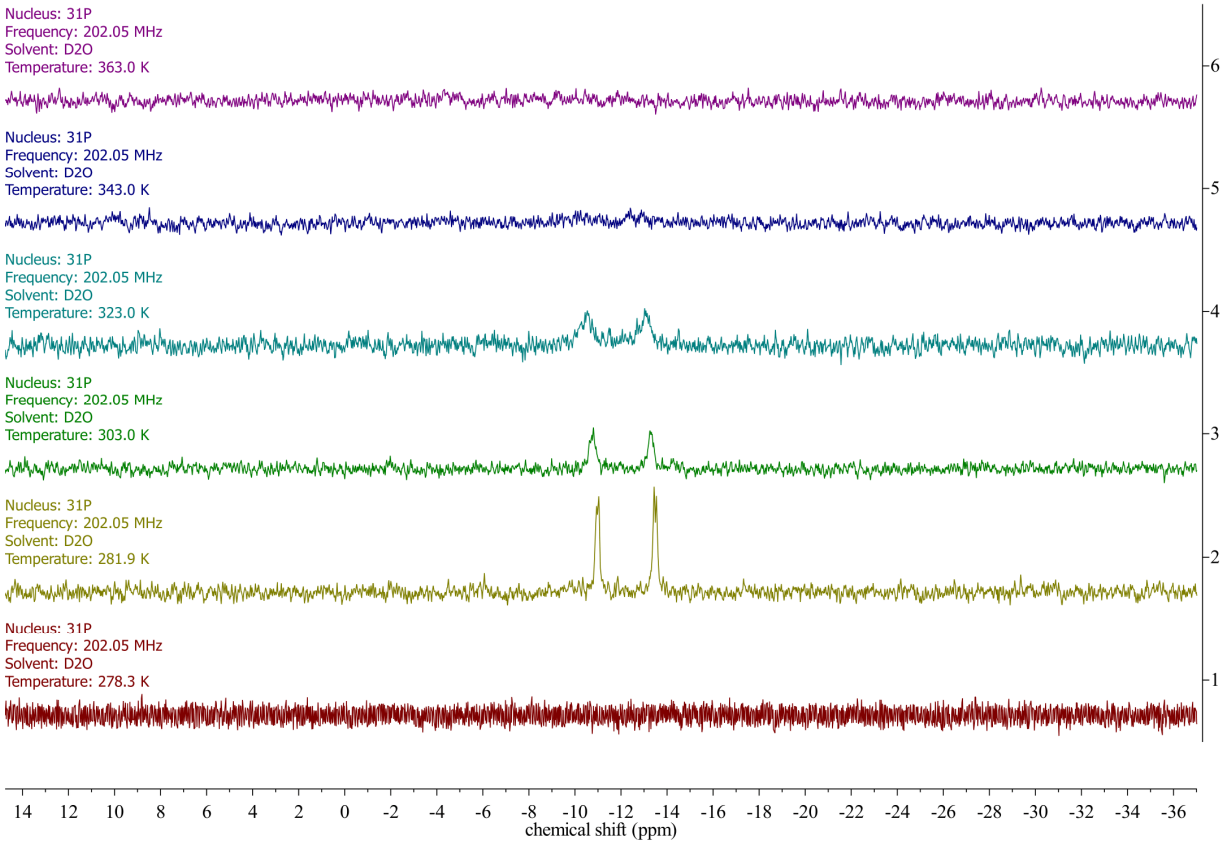
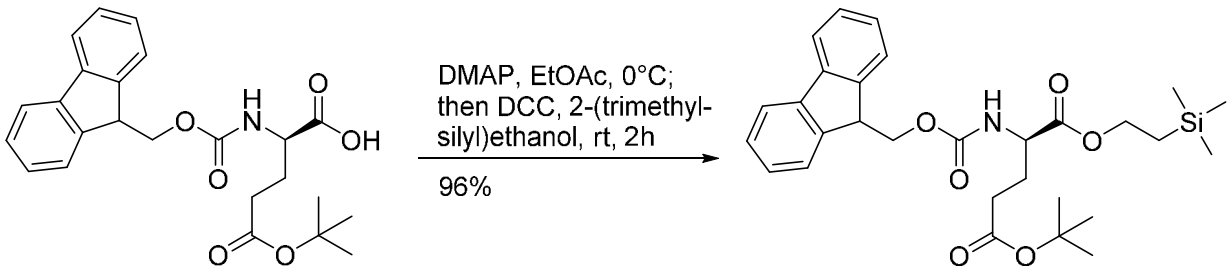
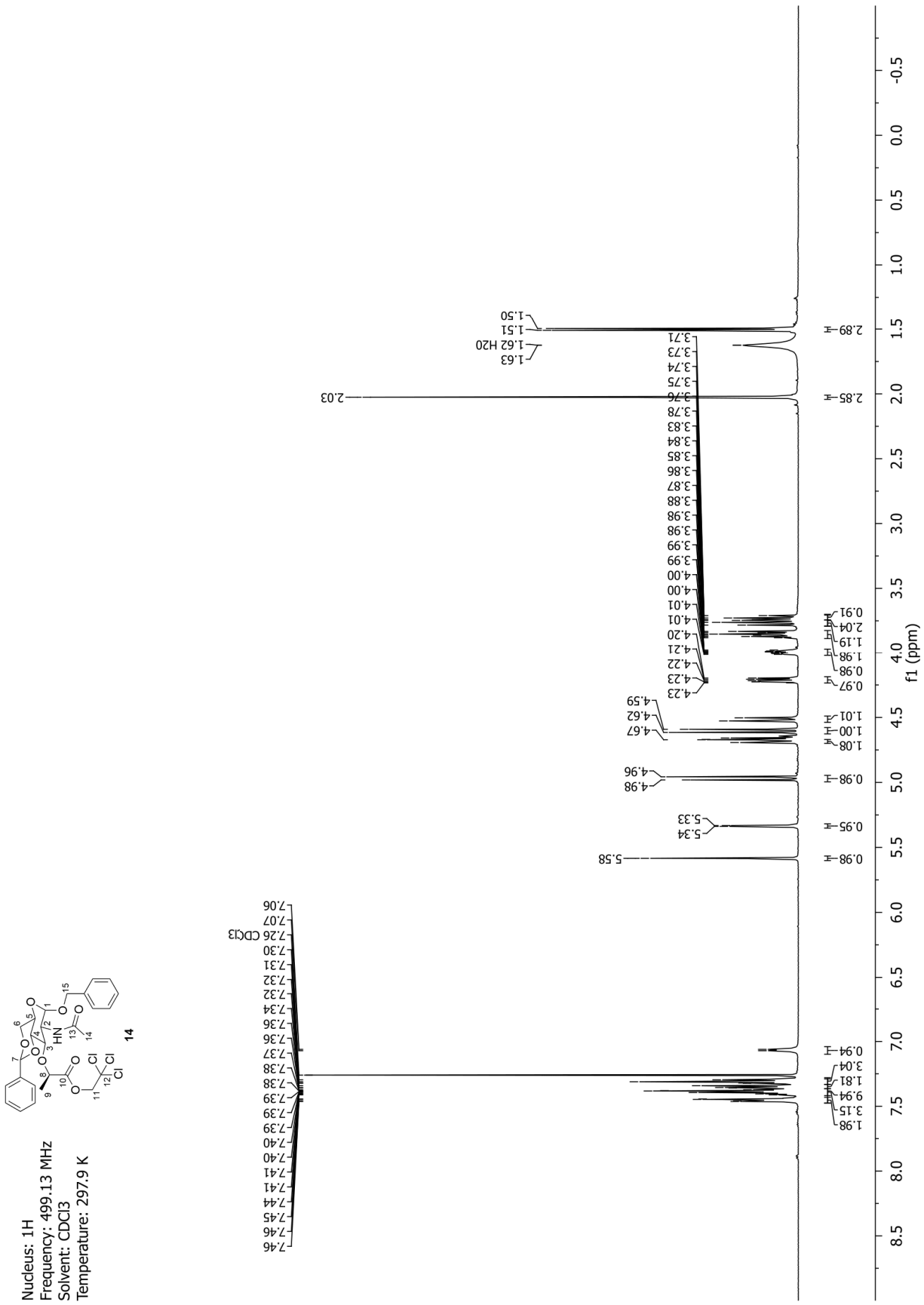


Figure S2: Temperature dependency of ^{31}P-NMR spectra of farnesyl lipid I analog **3**.



76 **19**

Fmoc-D-Glu(O-tBu)-OH (1.50 g, 3.53 mmol) and DMAP (86.1 mg, 705 µmol) were dissolved in 20 mL EtOAc and cooled to 0 °C. 2-(trimethylsilyl)ethanol (758 µL, 5.29 mmol) and DCC (1 M in CH_2Cl_2, 4.23 mL, 4.23 mmol) were added. After stirring for 2 h at rt, the reaction was filtered over celite and the residue was washed with EtOAc (2 x 20 mL). The solvent was removed under reduced pressure and the crude product was purified by flash chromatography (15% EtOAc/cyclohexane) to yield 1.77 g (3.37 mmol, 96%) of a white solid.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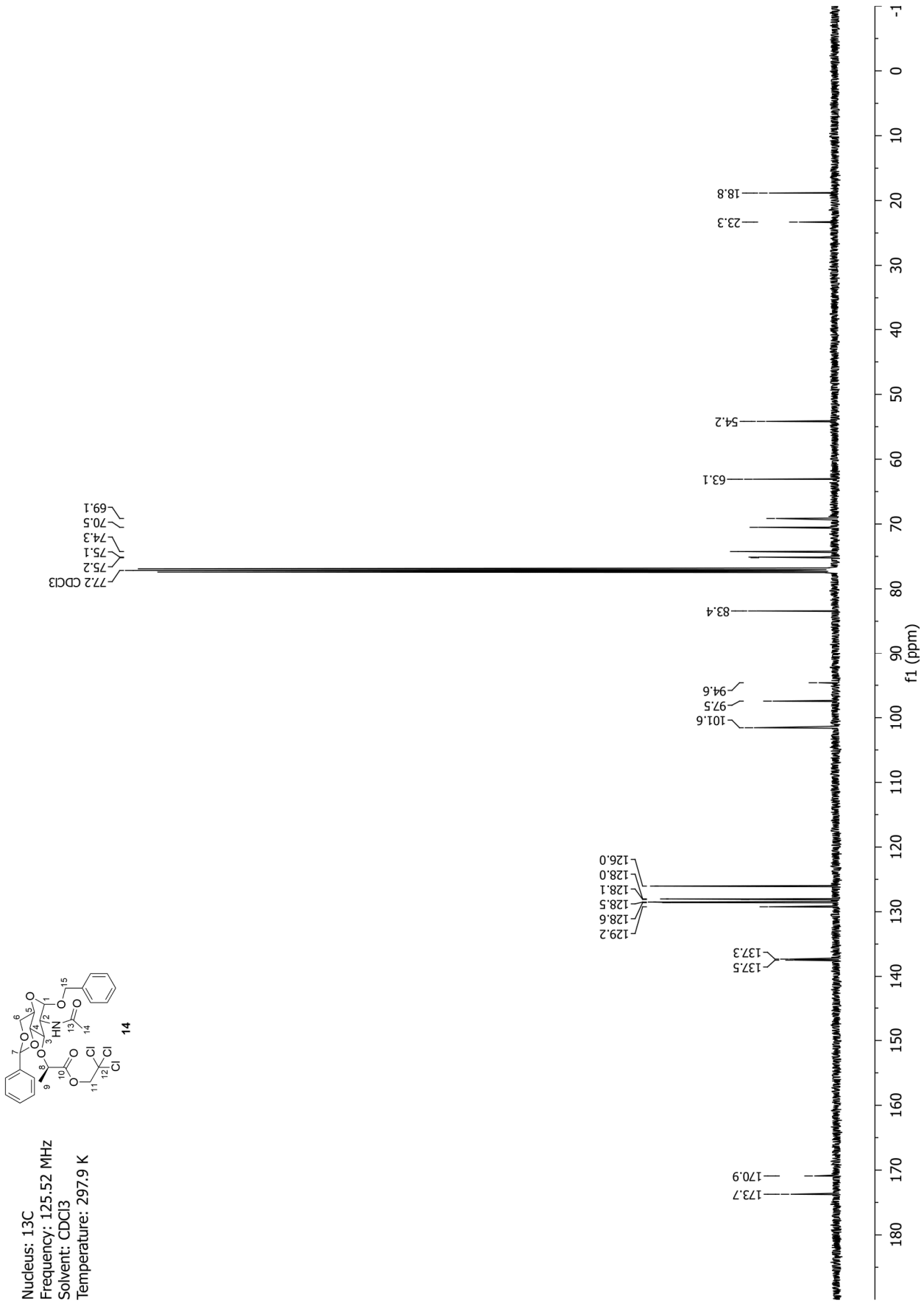
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75.1
75.2
77.2 CDCl3
83.4
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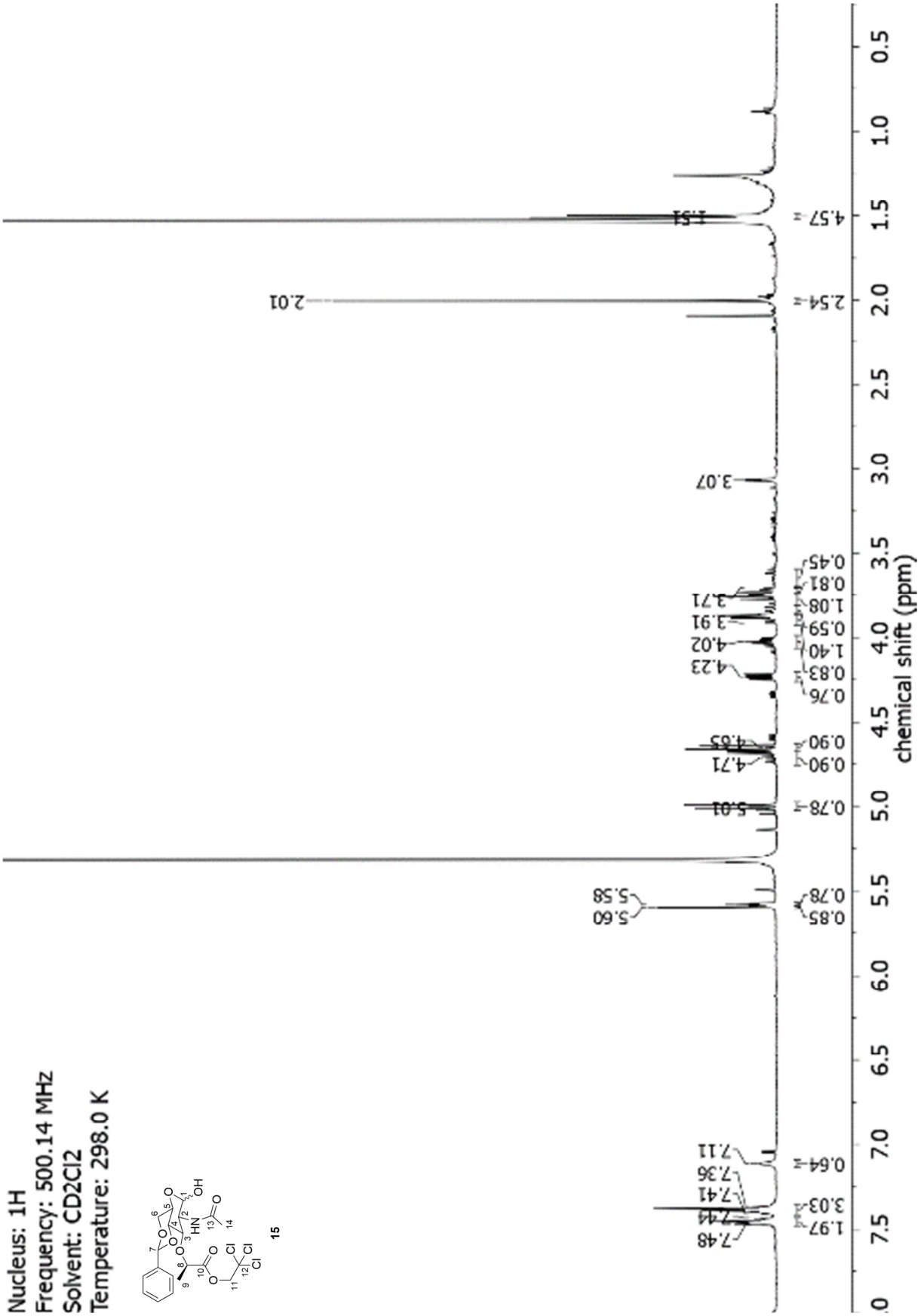
173.7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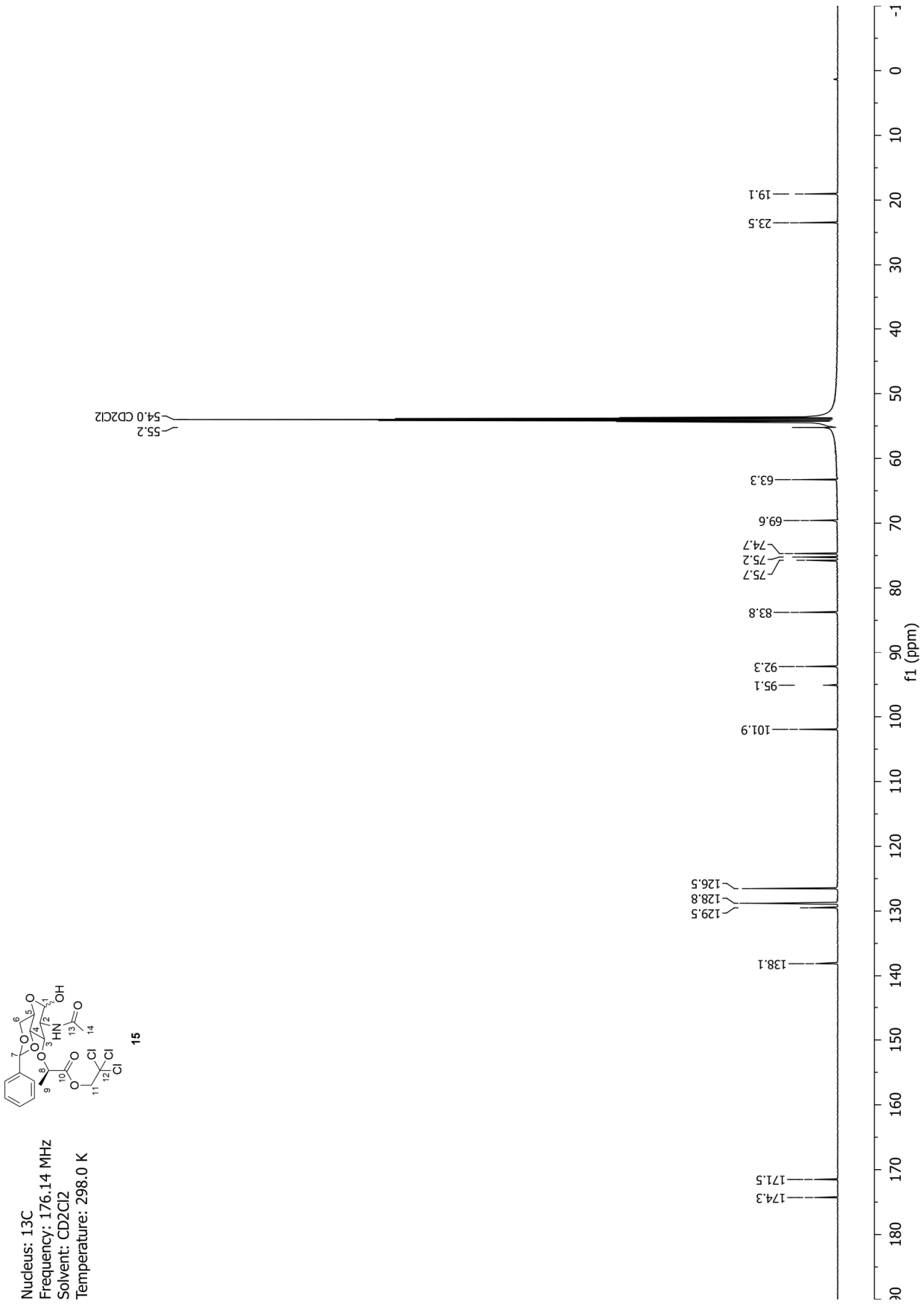
chemical shift (ppm)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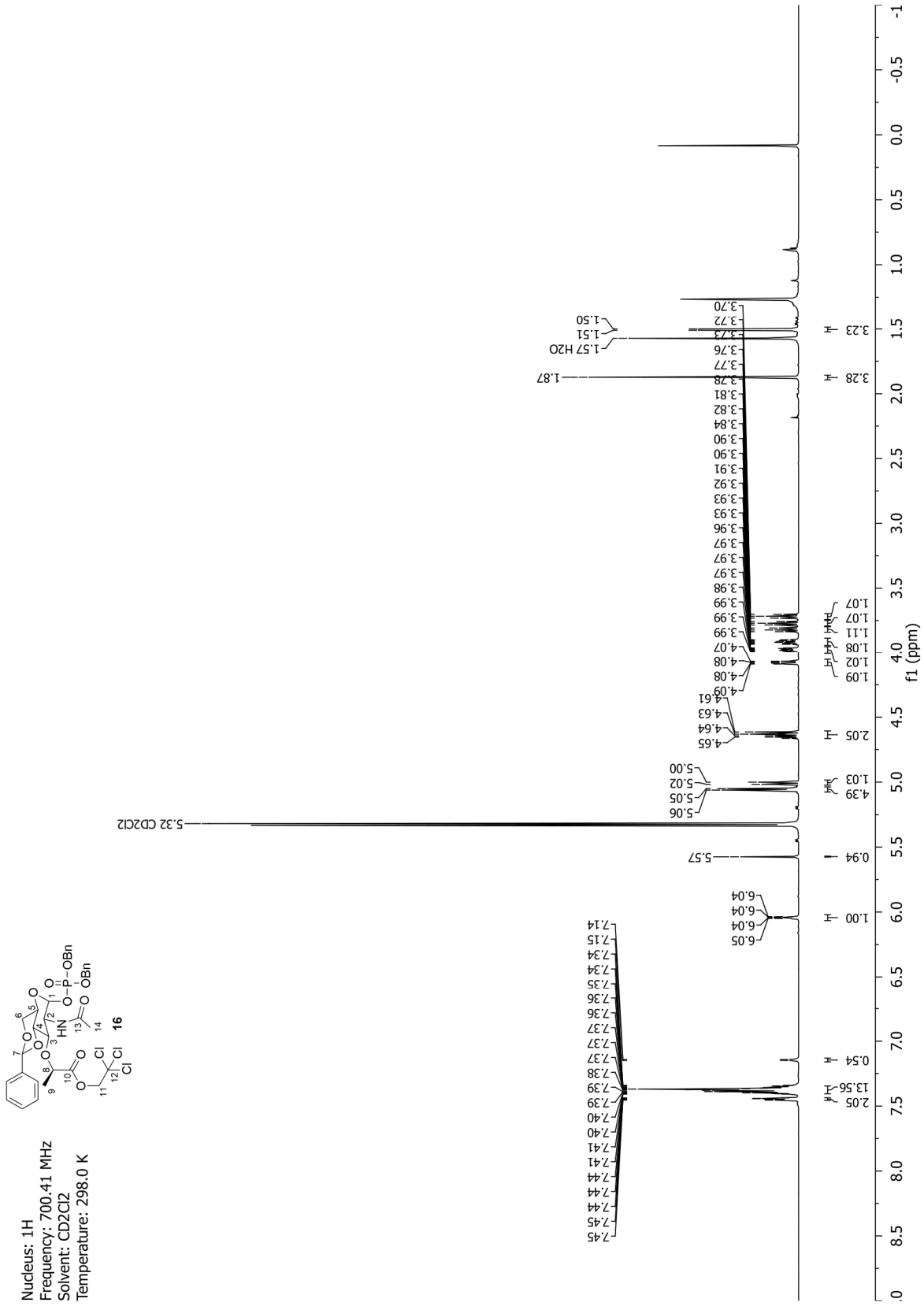
174.3
f1 (ppm)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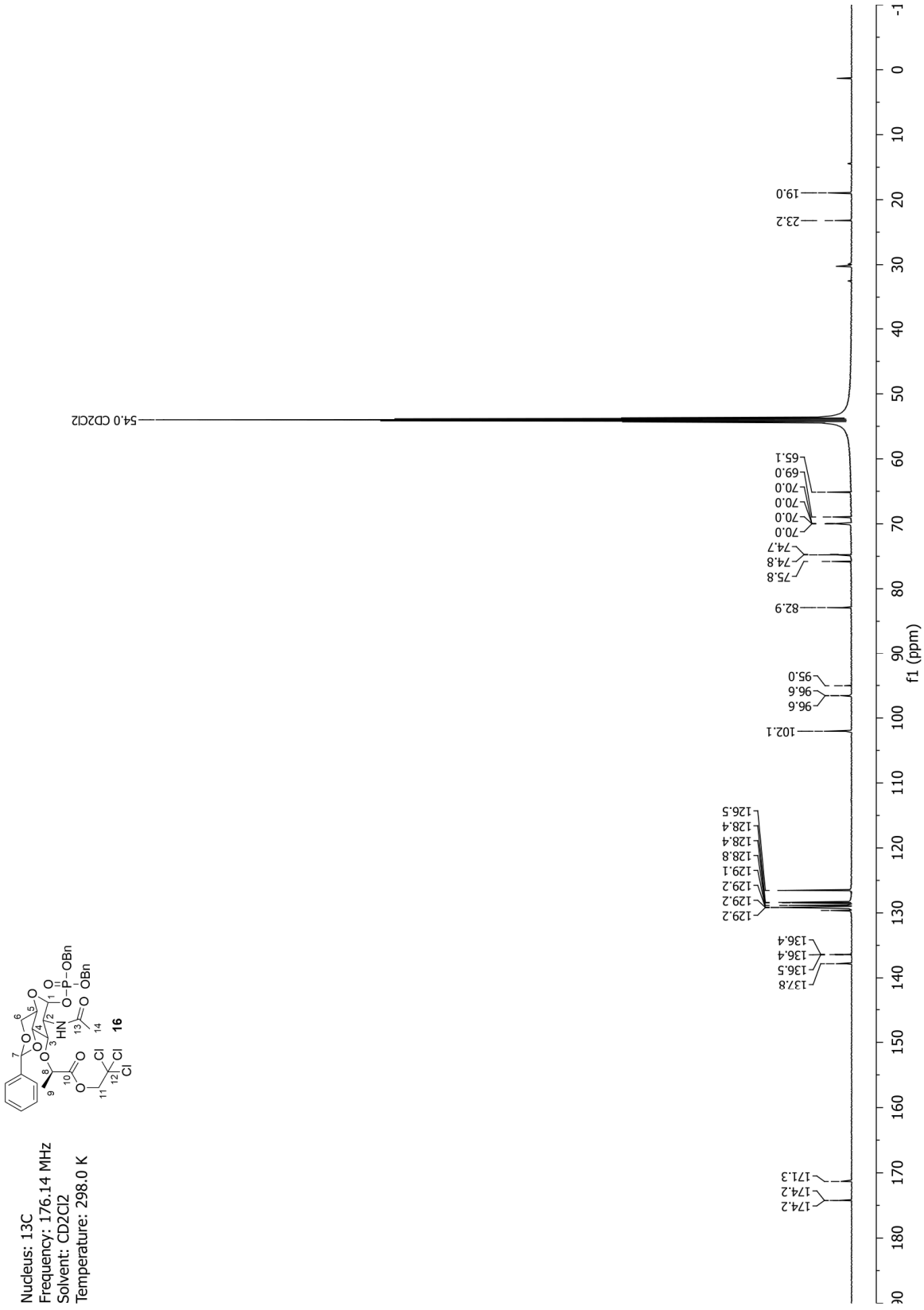
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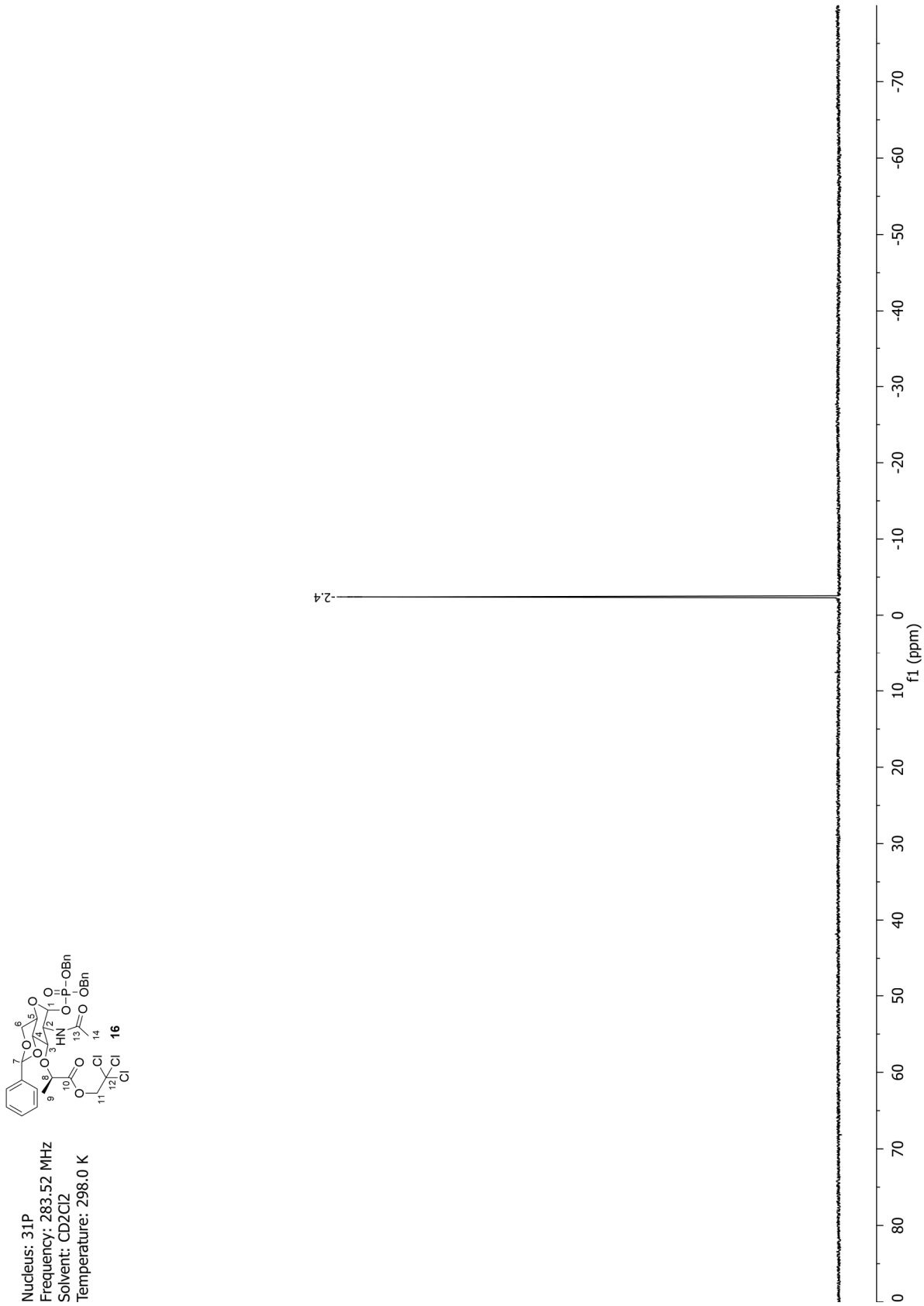
174.2
174.2
f1 (ppm)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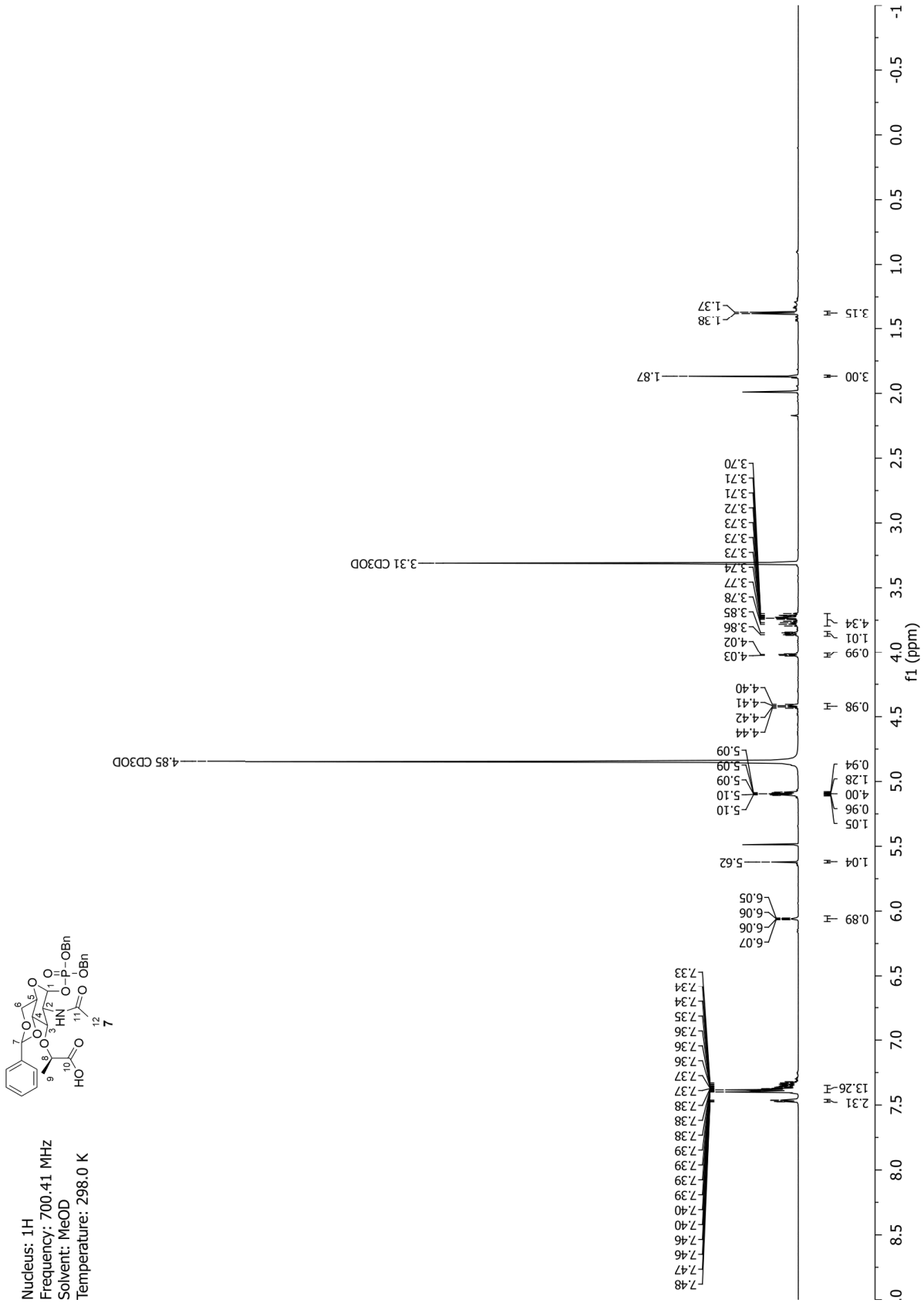
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0.98
0.99
1.01
4.34
4.03
4.02
3.86
3.85
3.78
3.77
3.74
3.73
3.73
3.72
3.71
3.71
3.70
1.38
1.37
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6.06
6.05
5.10
5.10
5.09
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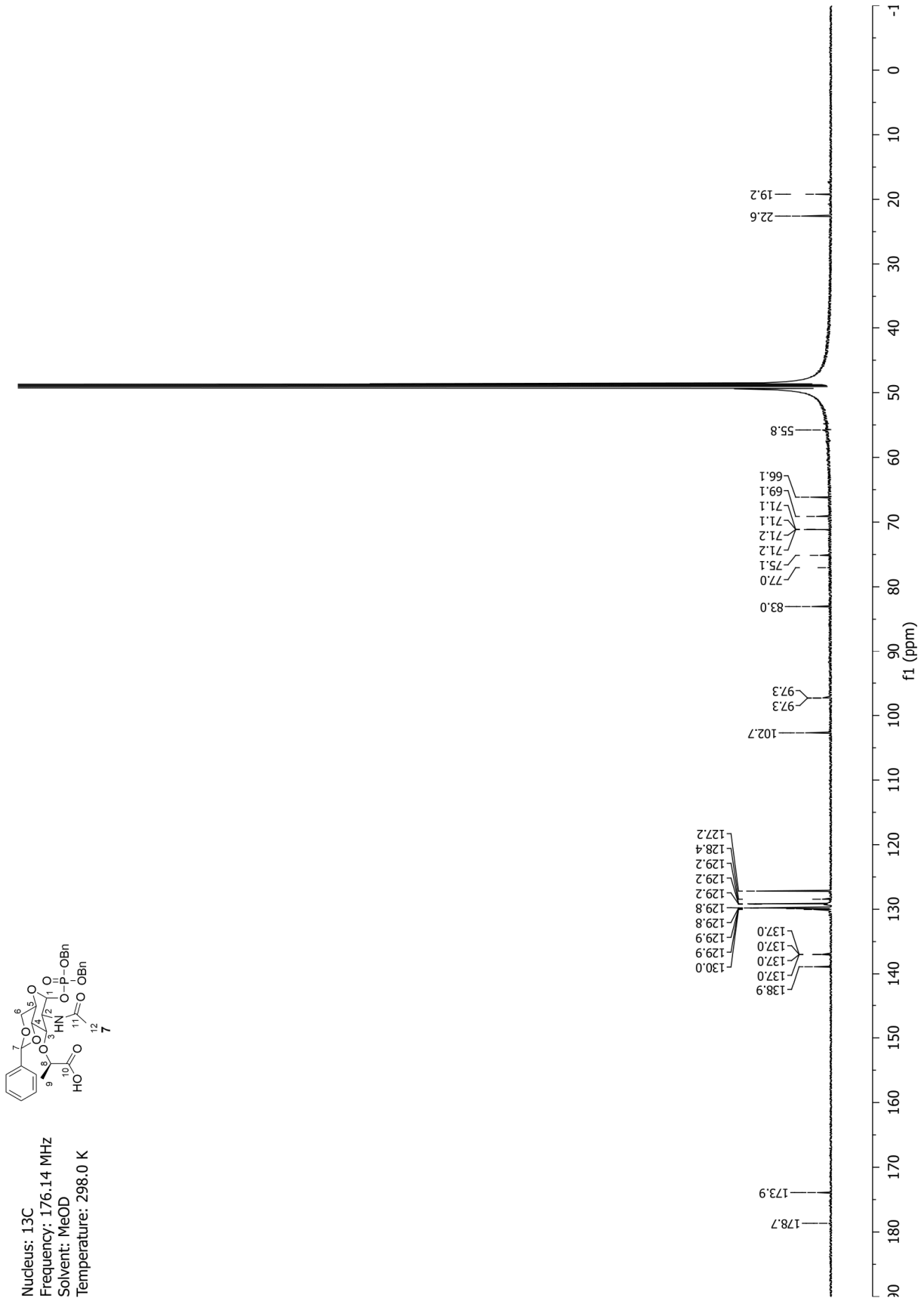
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71.1
71.2
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75.1
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83.0
97.3
97.3
102.7
127.2
128.4
129.2
129.2
129.2
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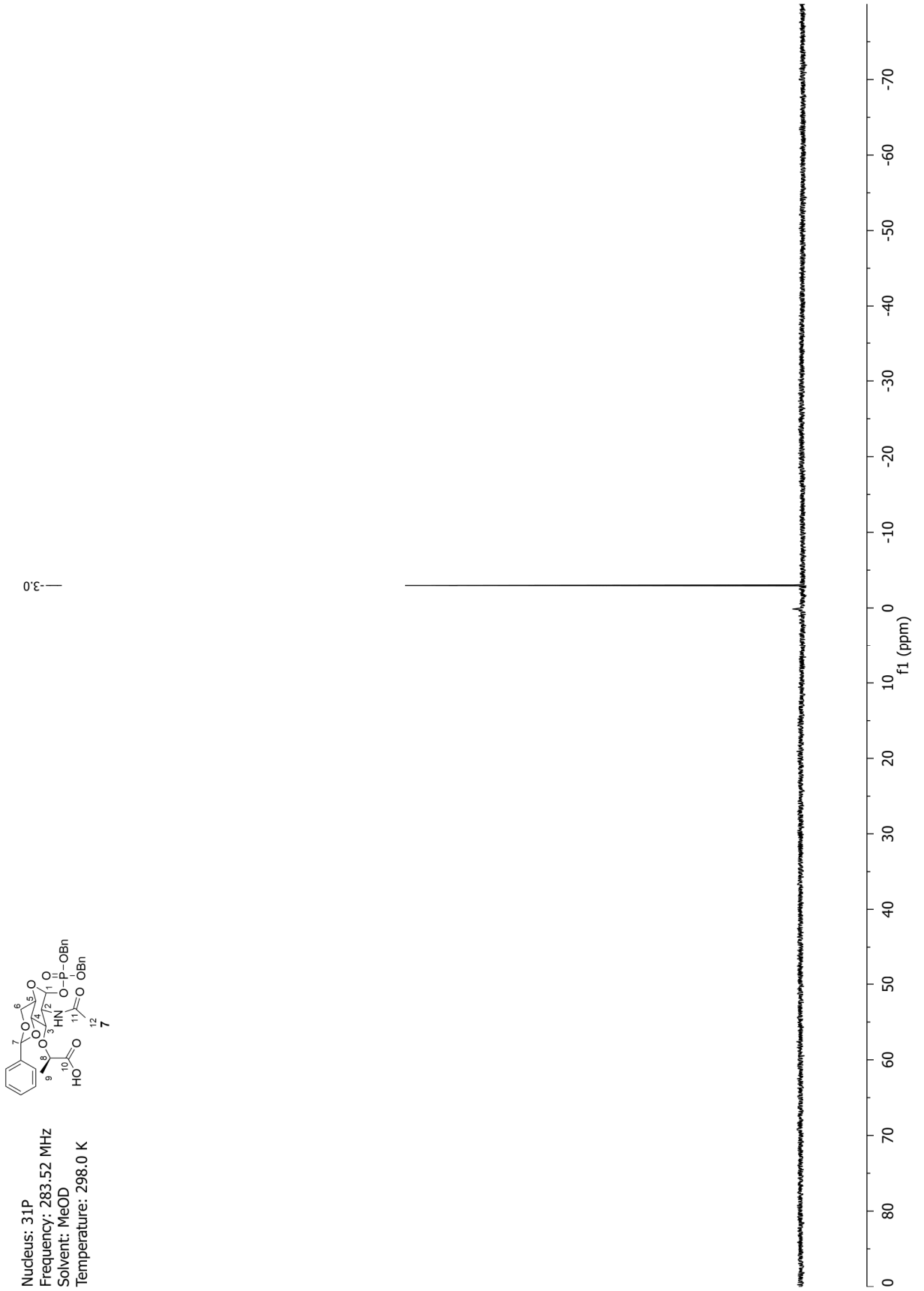
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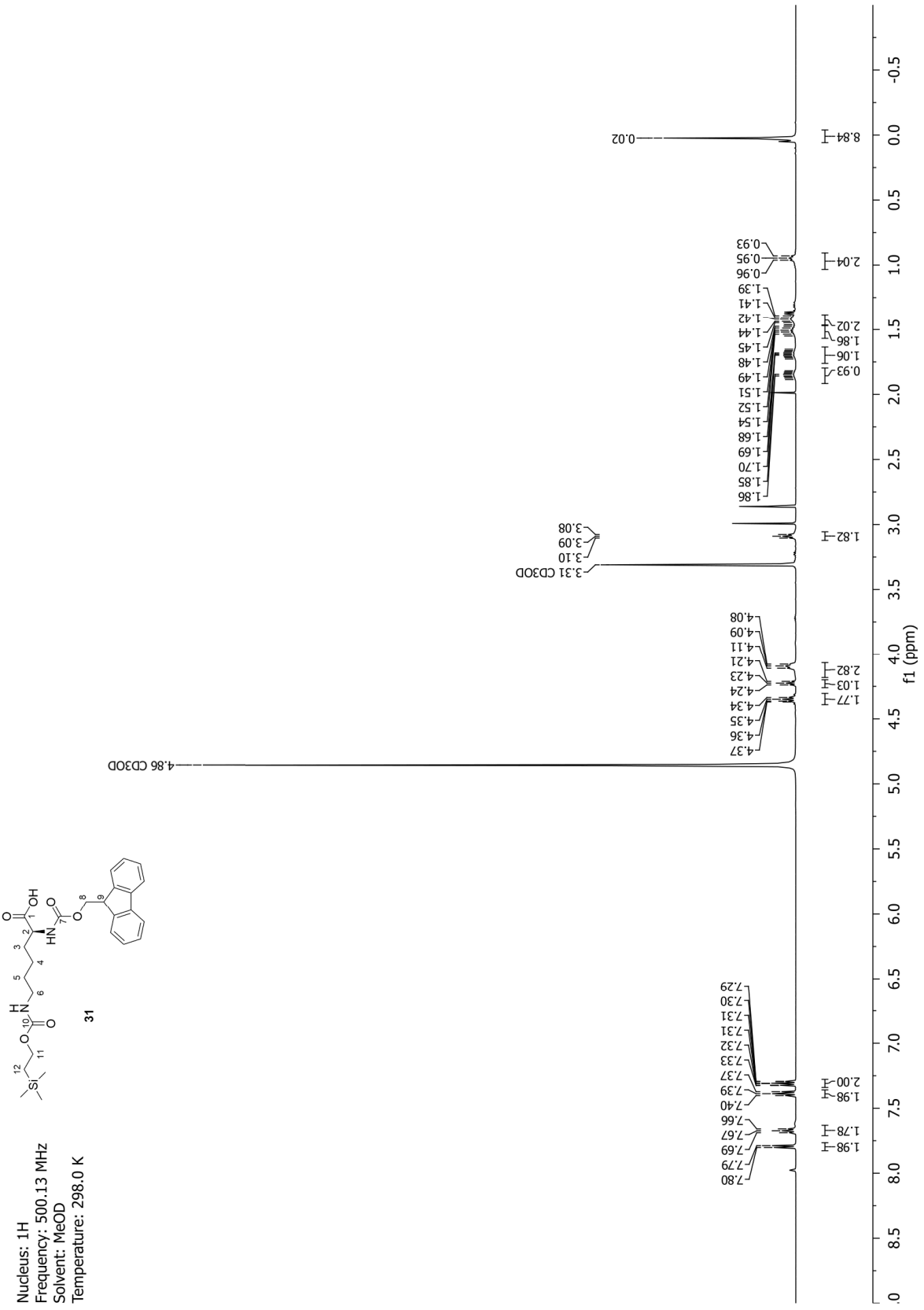
-3.0
f1 (ppm)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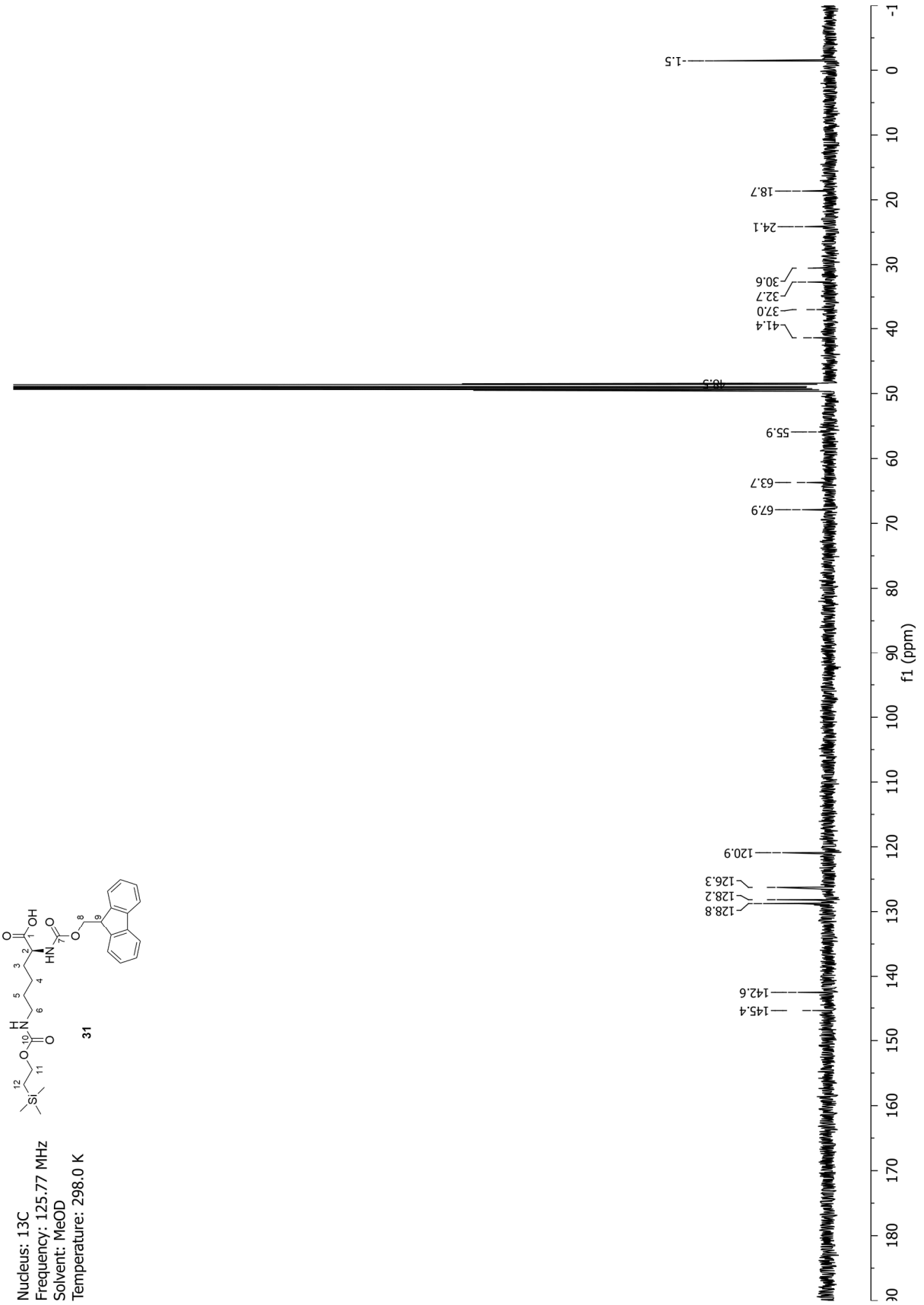
31
f1 (ppm)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37.0
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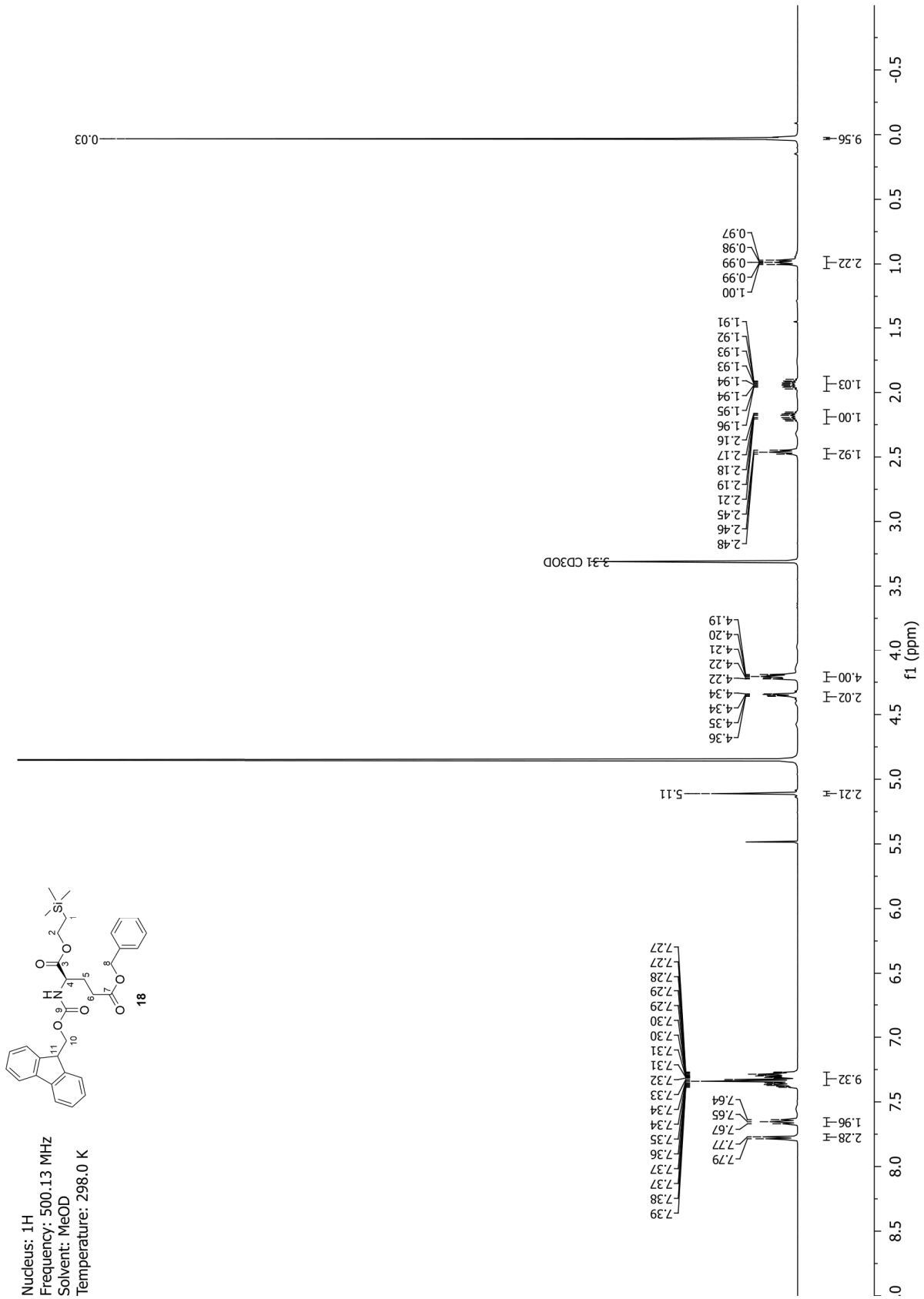
f1 (ppm)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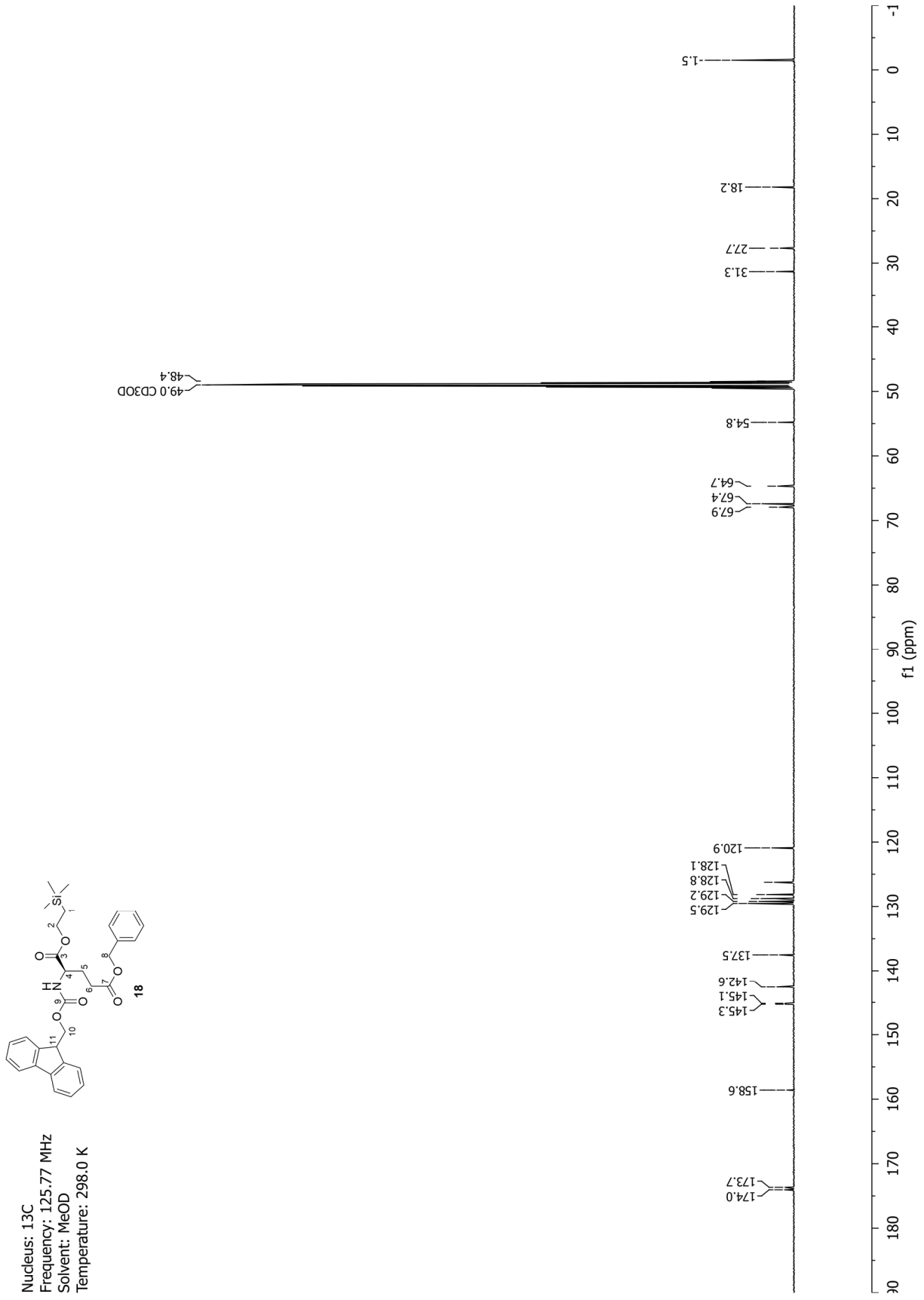
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145.1
145.3
158.6
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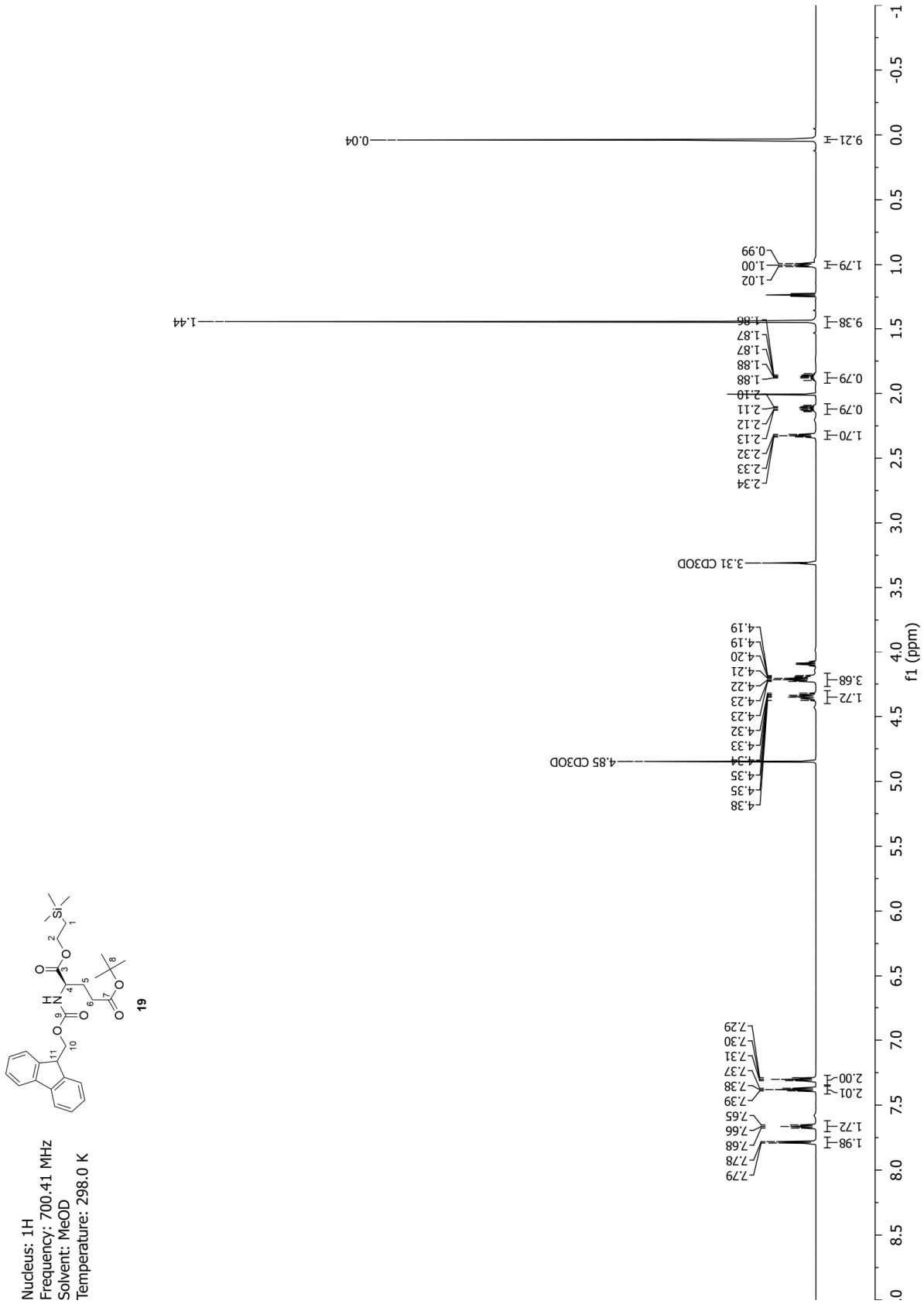
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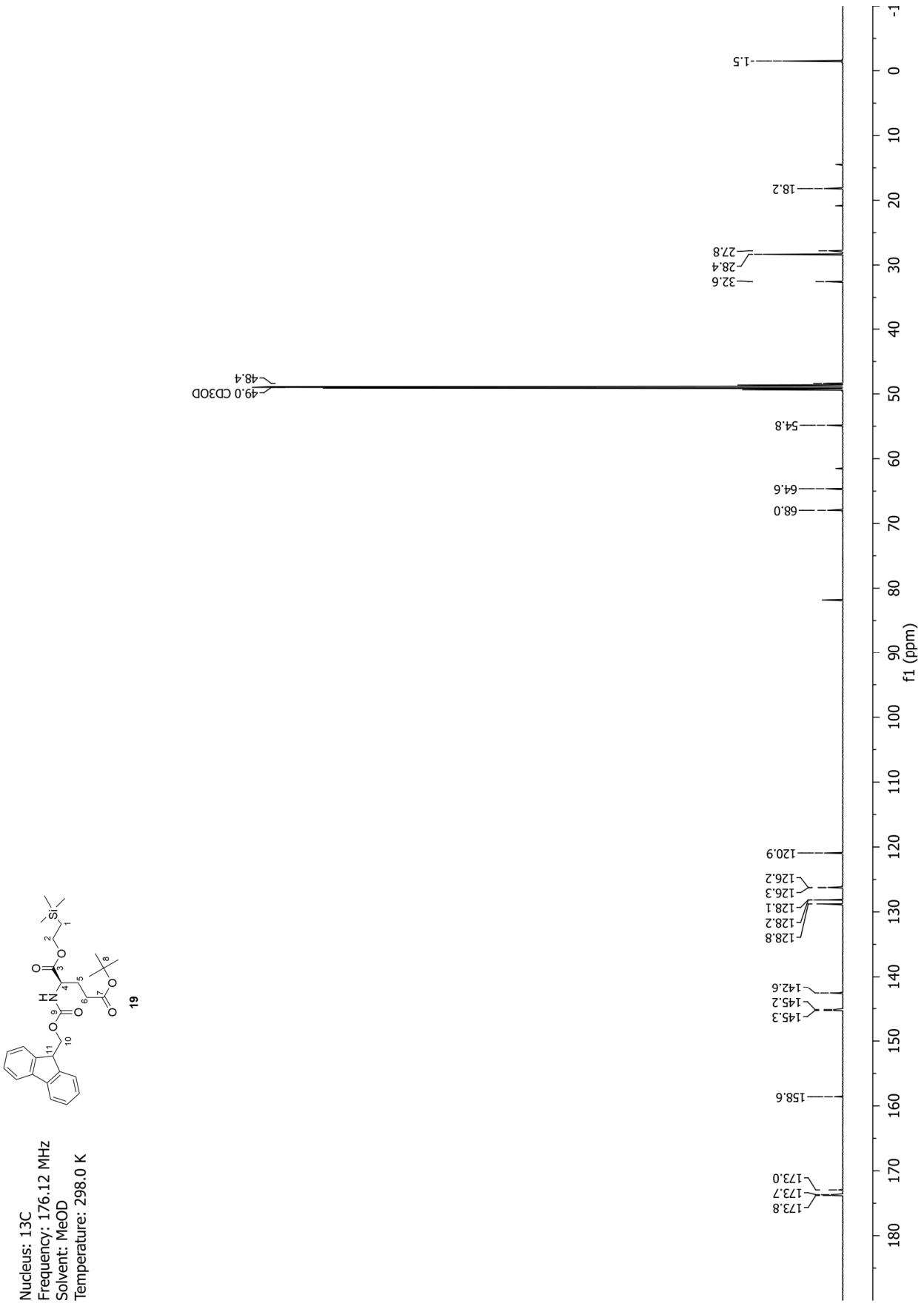
4.85 CD3OD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f1 (ppm)
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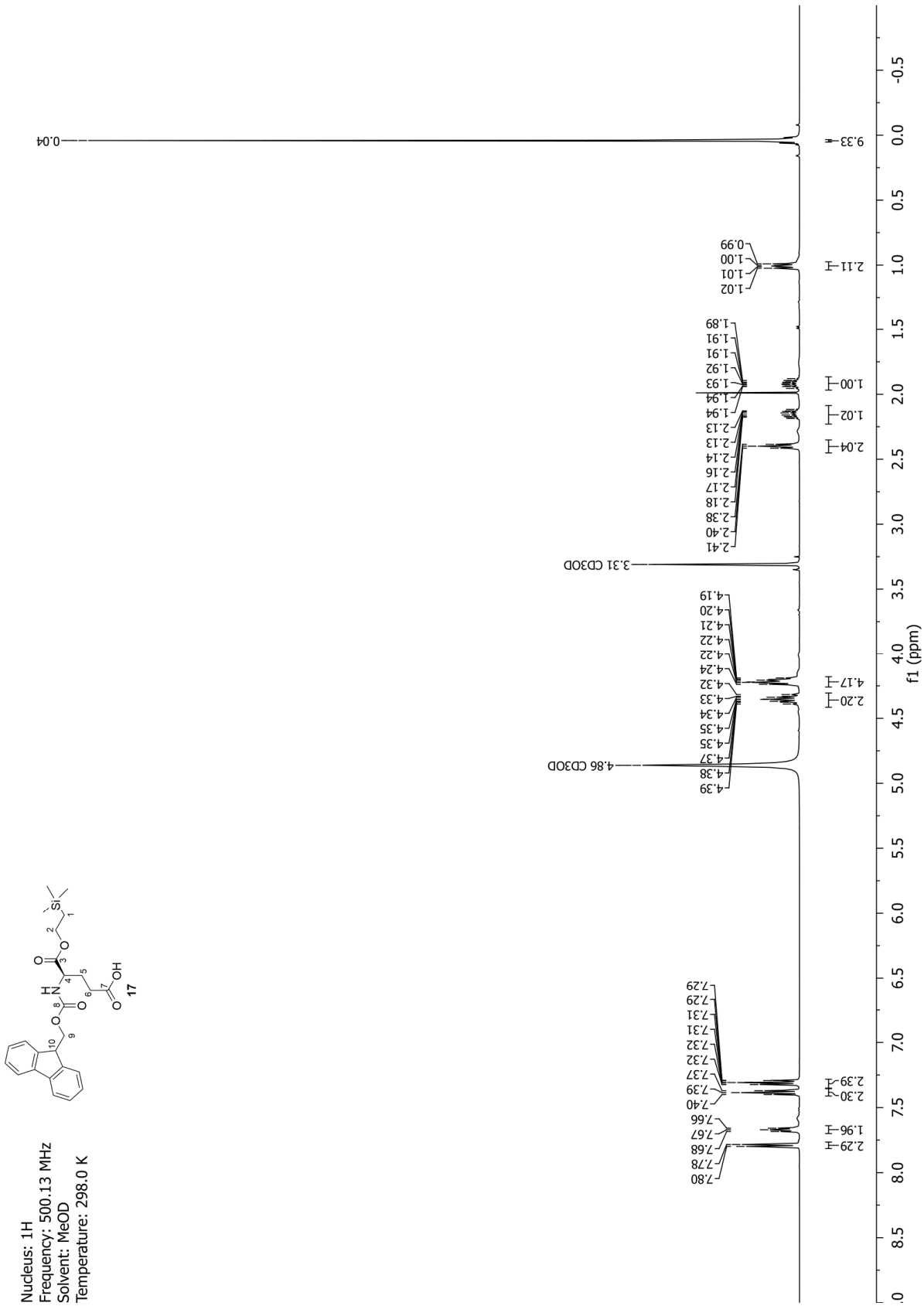
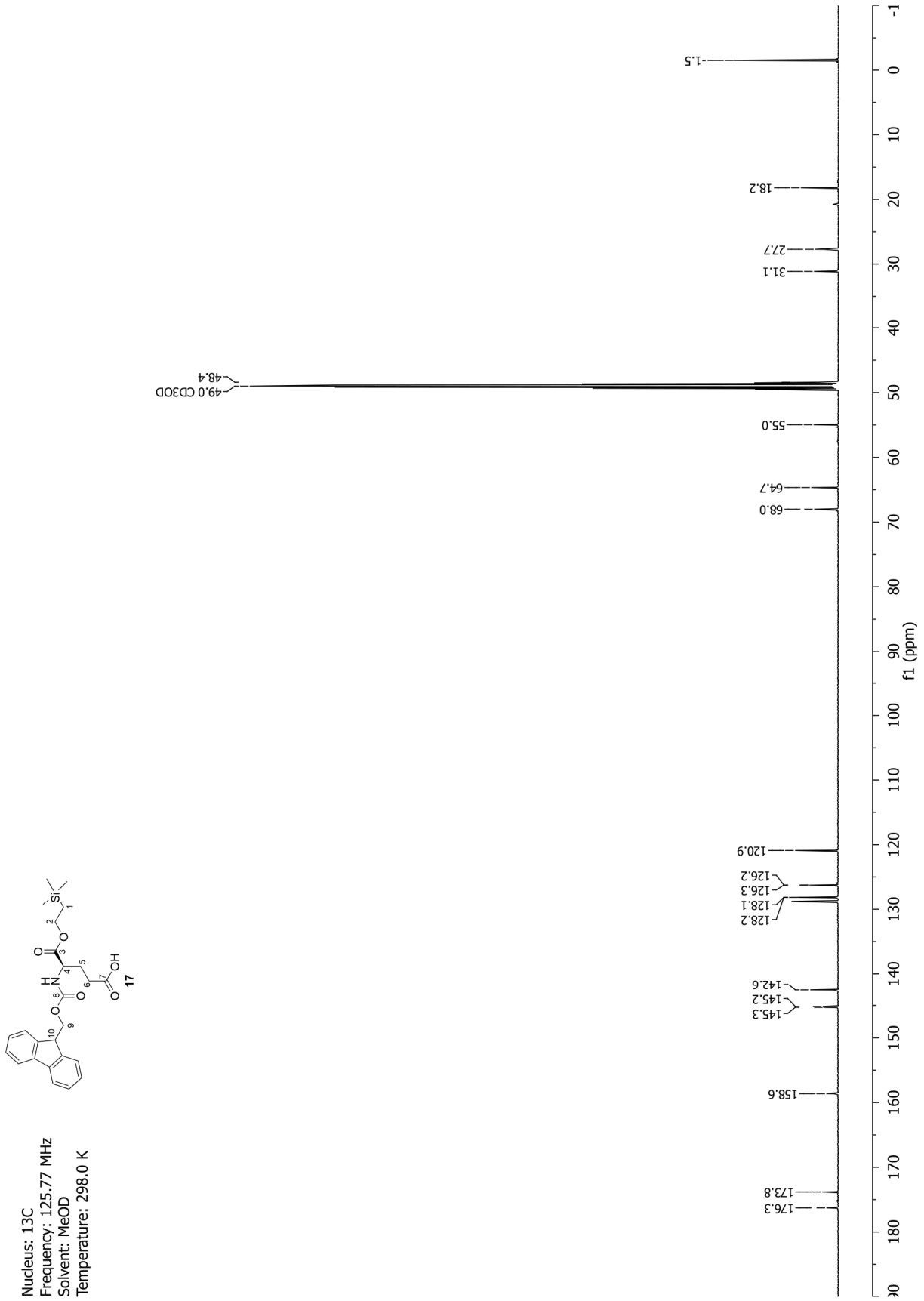
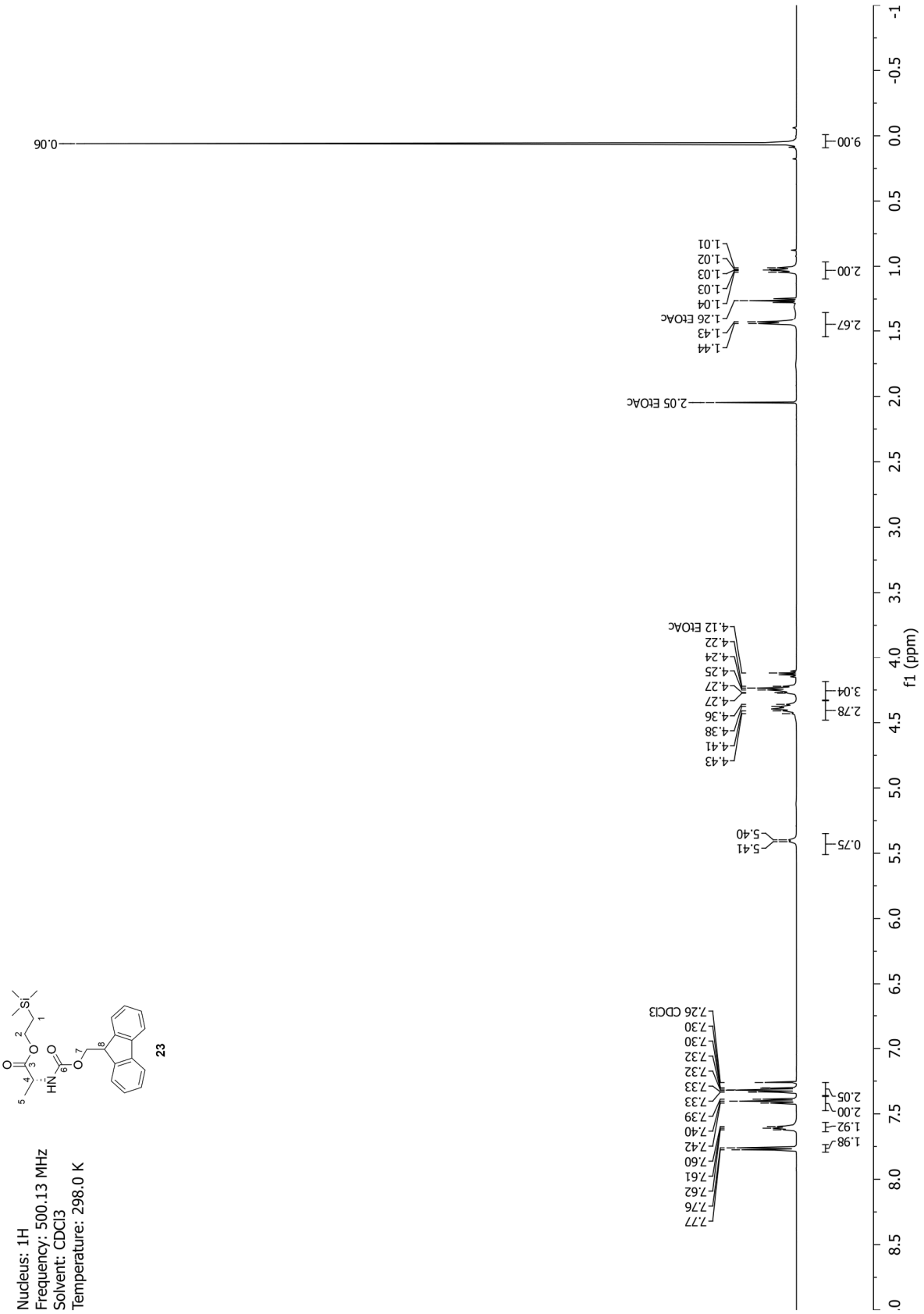
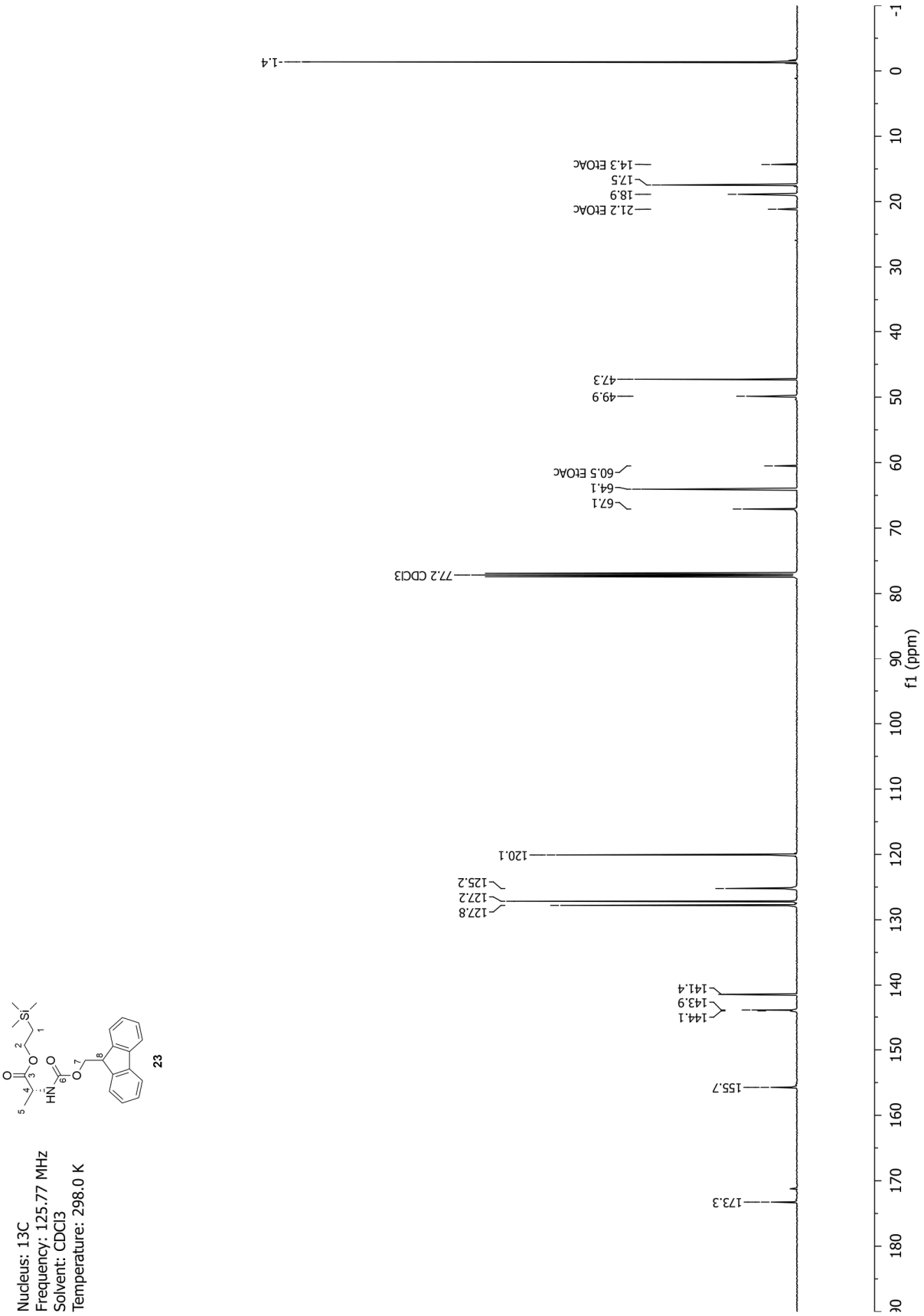
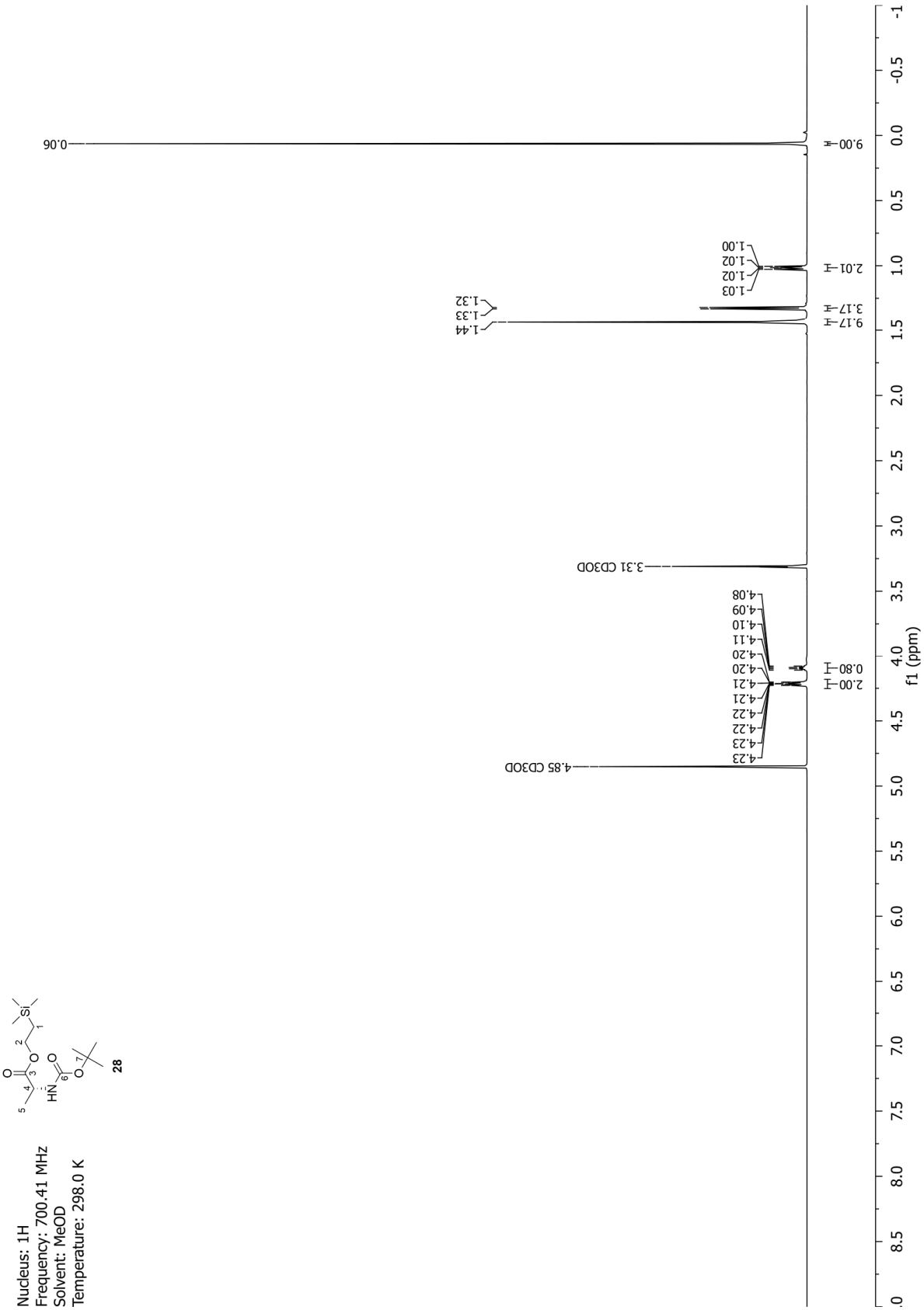
27.8
28.4
32.6
48.4
49.0 CD3OD
54.8
64.6
68.0
120.9
126.2
126.3
128.1
128.2
128.8
142.6
145.2
145.3
158.6
173.0
173.7
173.8

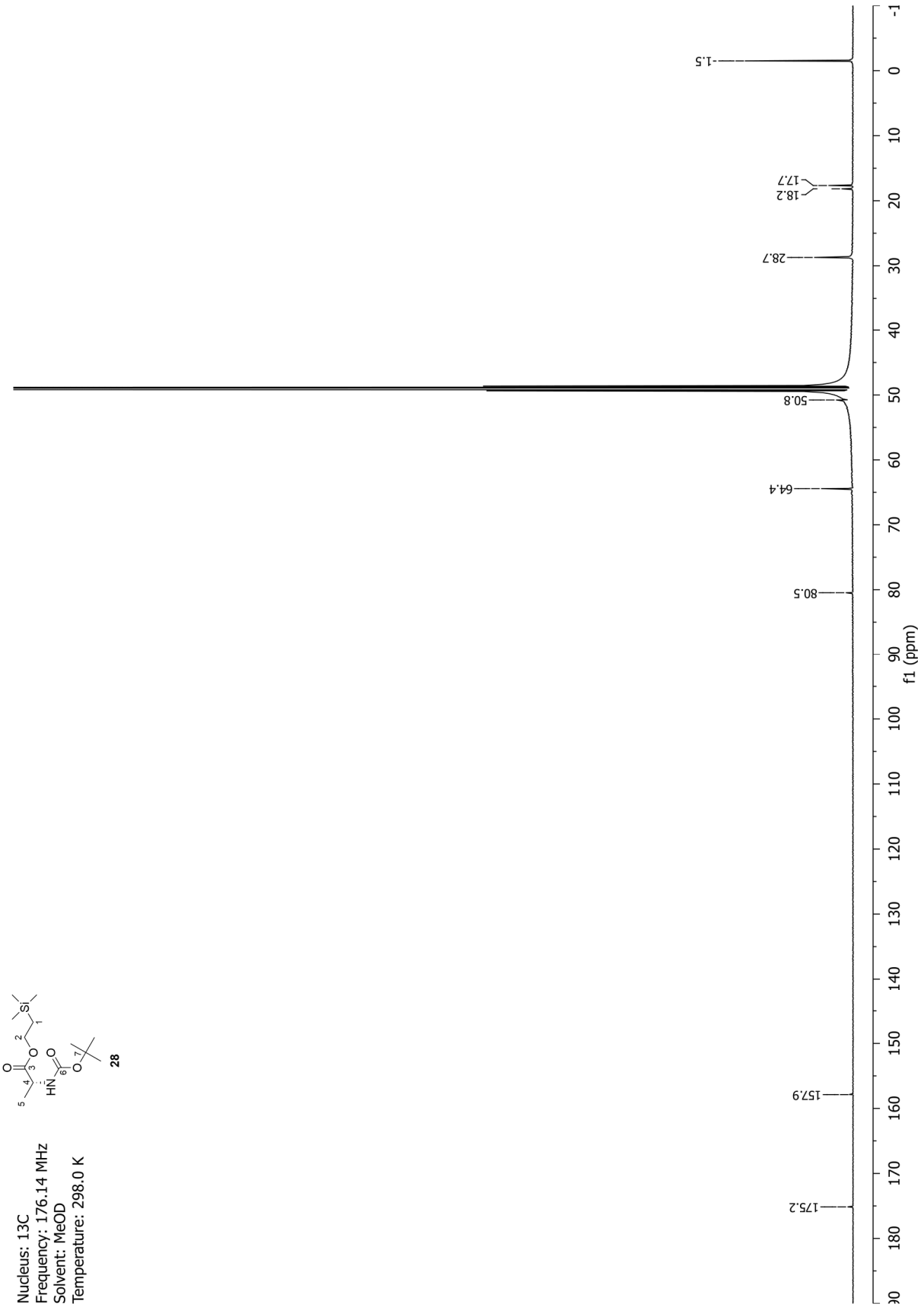

Nucleus: 1H
Frequency: 500.13 MHz
Solvent: MeOD
Temperature: 298.0 K
17
f1 (ppm)
0.04
3.31 CD3OD
4.86 CD3OD

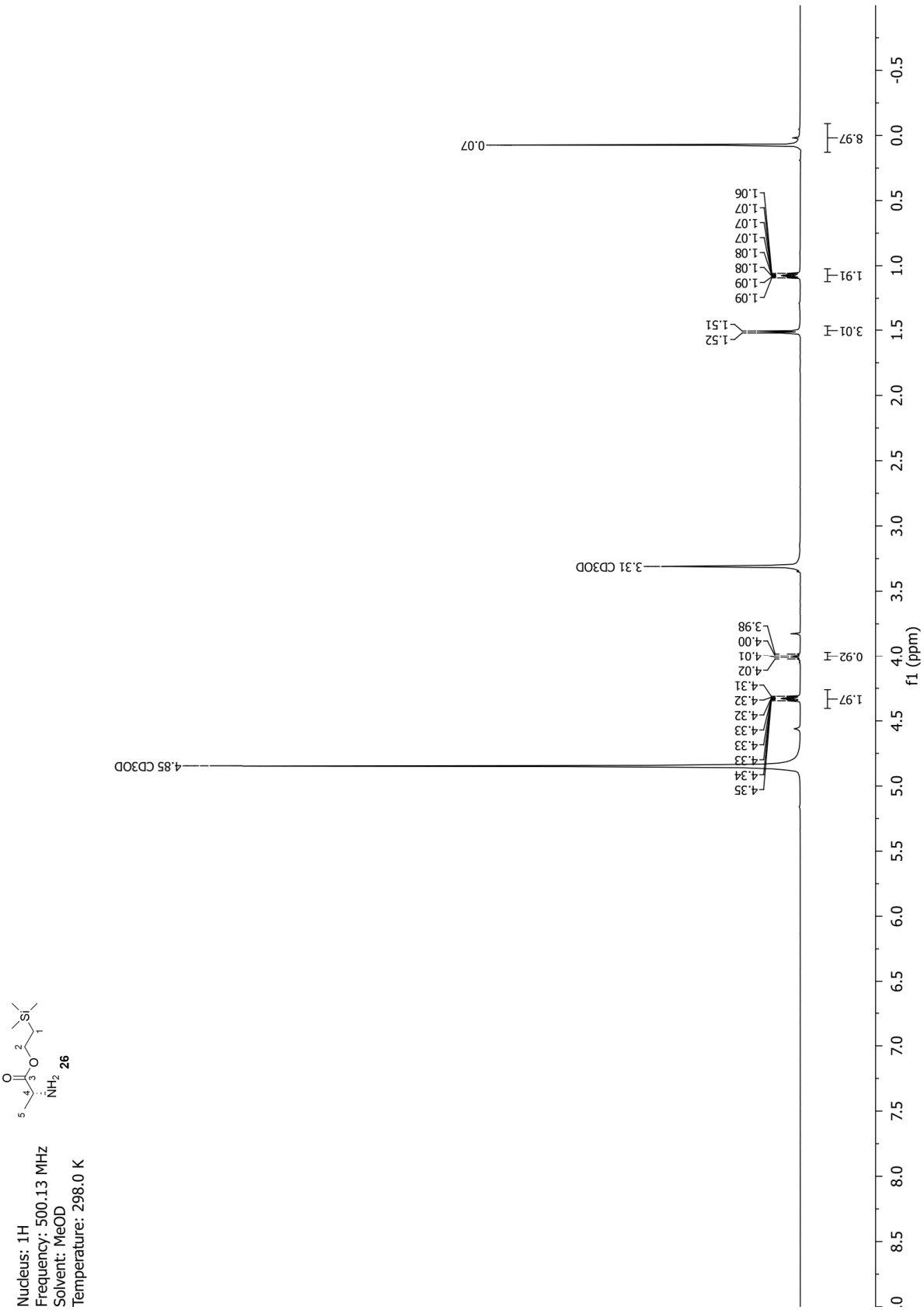

-1.5
18.2
27.7
31.1
48.4
49.0 CD3OD
55.0
64.7
68.0
120.9
126.2
126.3
128.1
128.2
142.6
145.2
145.3
158.6
173.8
176.3
f1 (ppm)
Nucleus: 13C
Frequency: 125.77 MHz
Solvent: MeOD
Temperature: 298.0 K
17

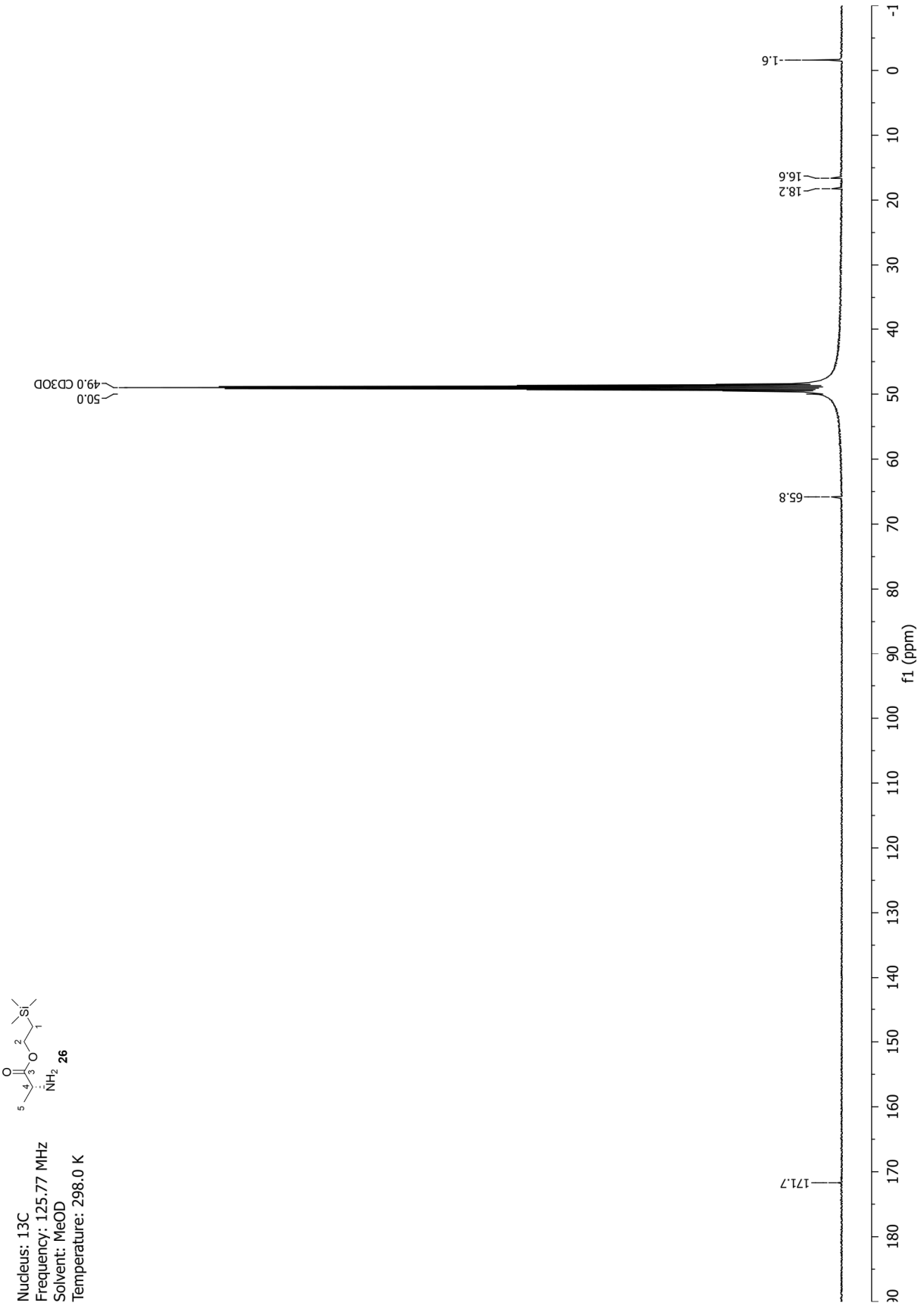

0.06
9.00
1.01
1.02
1.03
1.03
1.04
1.26 EtOAc
1.43
1.44
2.00
2.67
2.05 EtOAc
4.12 EtOAc
4.22
4.24
4.25
4.27
4.27
4.36
4.38
4.41
4.43
3.04
2.78
5.40
5.41
0.75
7.26 CDCl3
7.30
7.30
7.32
7.32
7.33
7.33
7.39
7.40
7.42
7.60
7.61
7.62
7.76
7.77
2.05
2.00
1.92
1.98
f1 (ppm)
Nucleus: 1H
Frequency: 500.13 MHz
Solvent: CDCl3
Temperature: 298.0 K
23

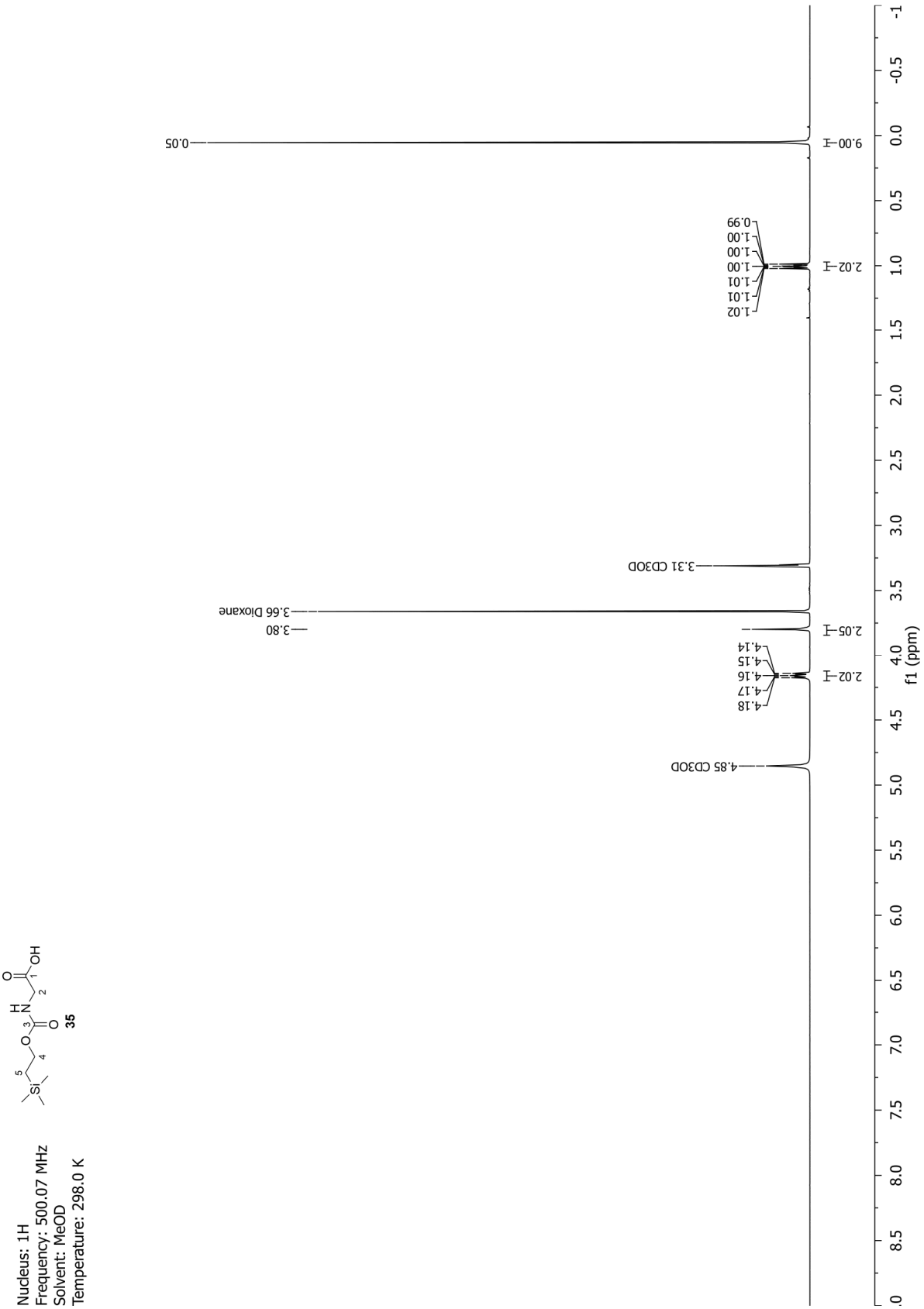

Nucleus: 13C
Frequency: 125.77 MHz
Solvent: CDCl3
Temperature: 298.0 K
23
-1.4
14.3 EtOAc
17.5
18.9
21.2 EtOAc
47.3
49.9
60.5 EtOAc
64.1
67.1
77.2 CDCl3
120.1
125.2
127.2
127.8
141.4
143.9
144.1
155.7
173.3
f1 (ppm)

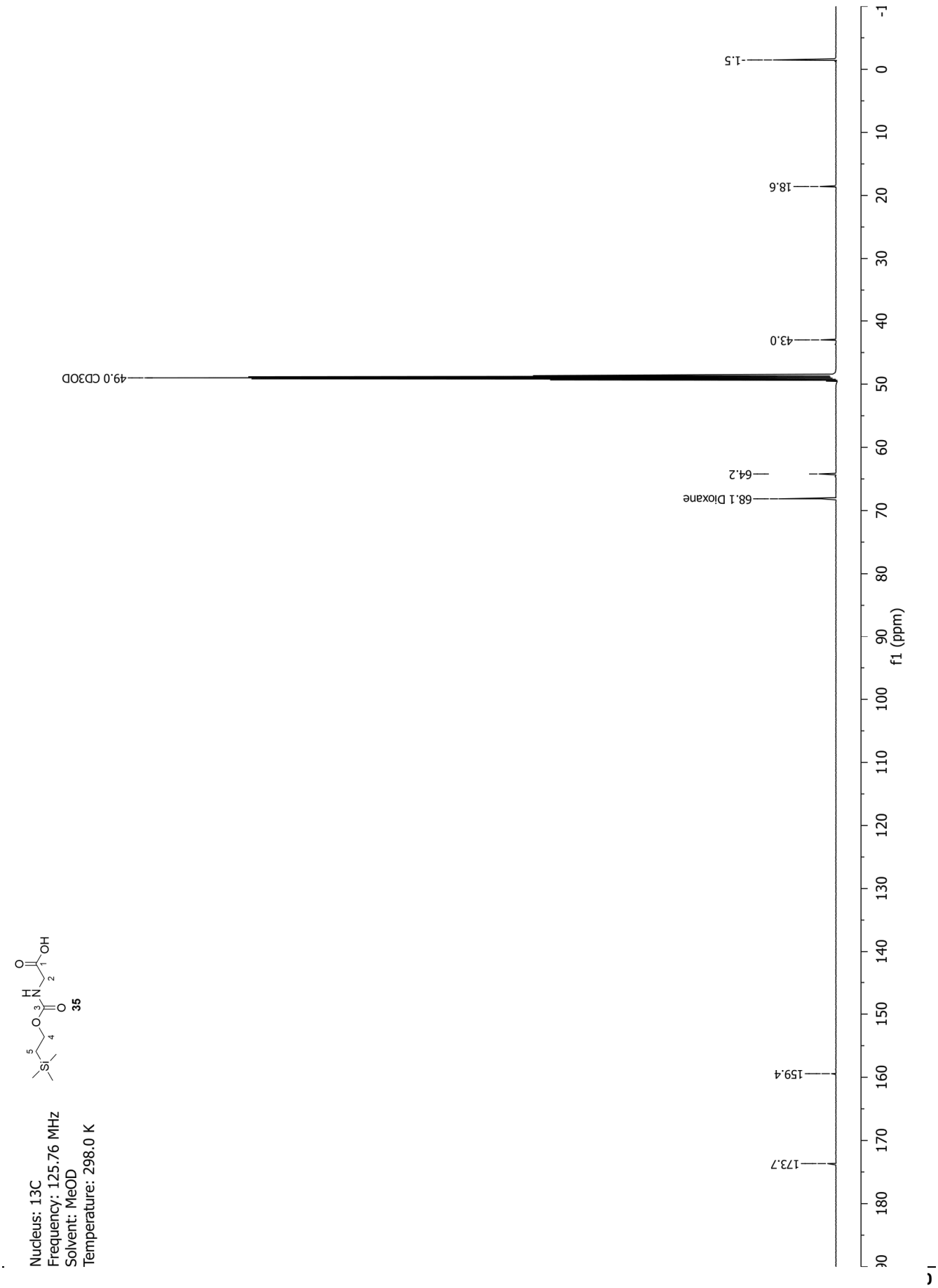

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: MeOD
Temperature: 298.0 K
28
f1 (ppm)
0.06
1.32
1.33
1.44
1.00
1.02
1.02
1.03
3.31 CD3OD
4.08
4.09
4.10
4.11
4.20
4.20
4.21
4.21
4.22
4.22
4.23
4.23
4.85 CD3OD
9.00
2.01
3.17
9.17
0.80
2.00

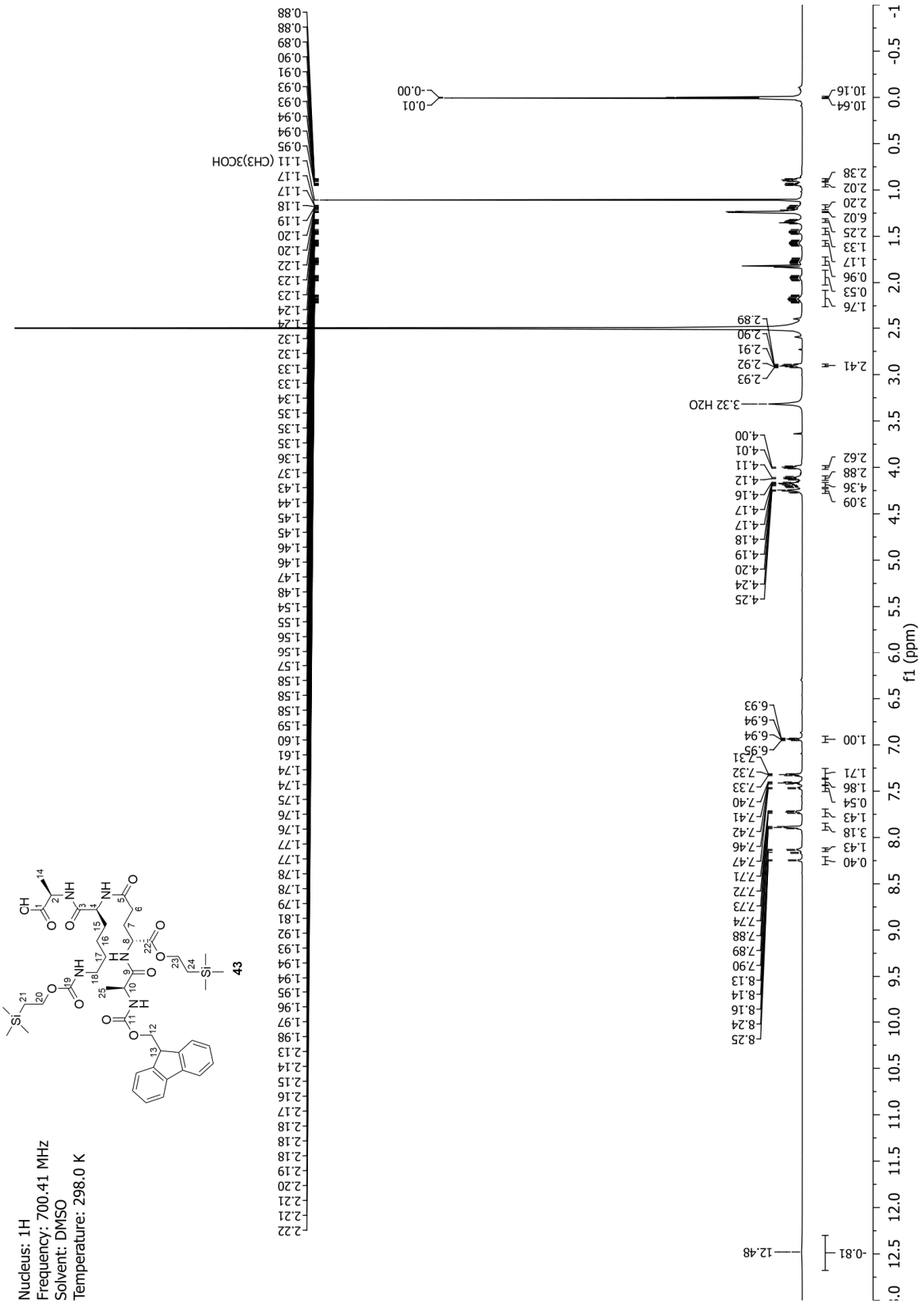

Nucleus: 13C
Frequency: 176.14 MHz
Solvent: MeOD
Temperature: 298.0 K
28
1.5
17.7
18.2
28.7
50.8
64.4
80.5
157.9
175.2
f1 (ppm)

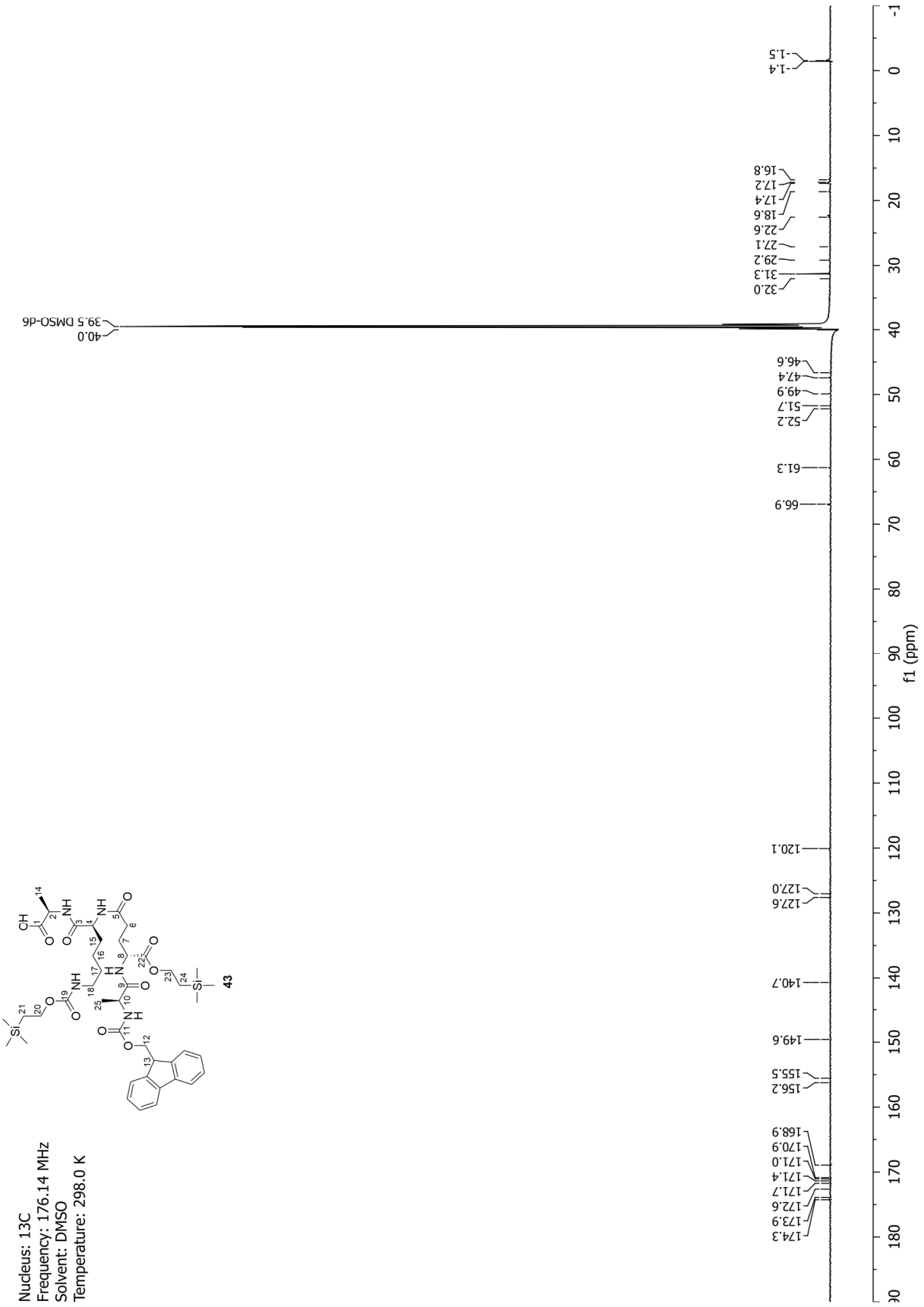

Nucleus: 1H
Frequency: 500.13 MHz
Solvent: MeOD
Temperature: 298.0 K
26
0.07
1.06
1.07
1.07
1.07
1.08
1.08
1.09
1.09
1.51
1.52
3.31 CD3OD
3.98
4.00
4.01
4.02
4.31
4.32
4.32
4.32
4.33
4.33
4.33
4.34
4.35
4.85 CD3OD
8.97
1.91
3.01
0.92
1.97
f1 (ppm)

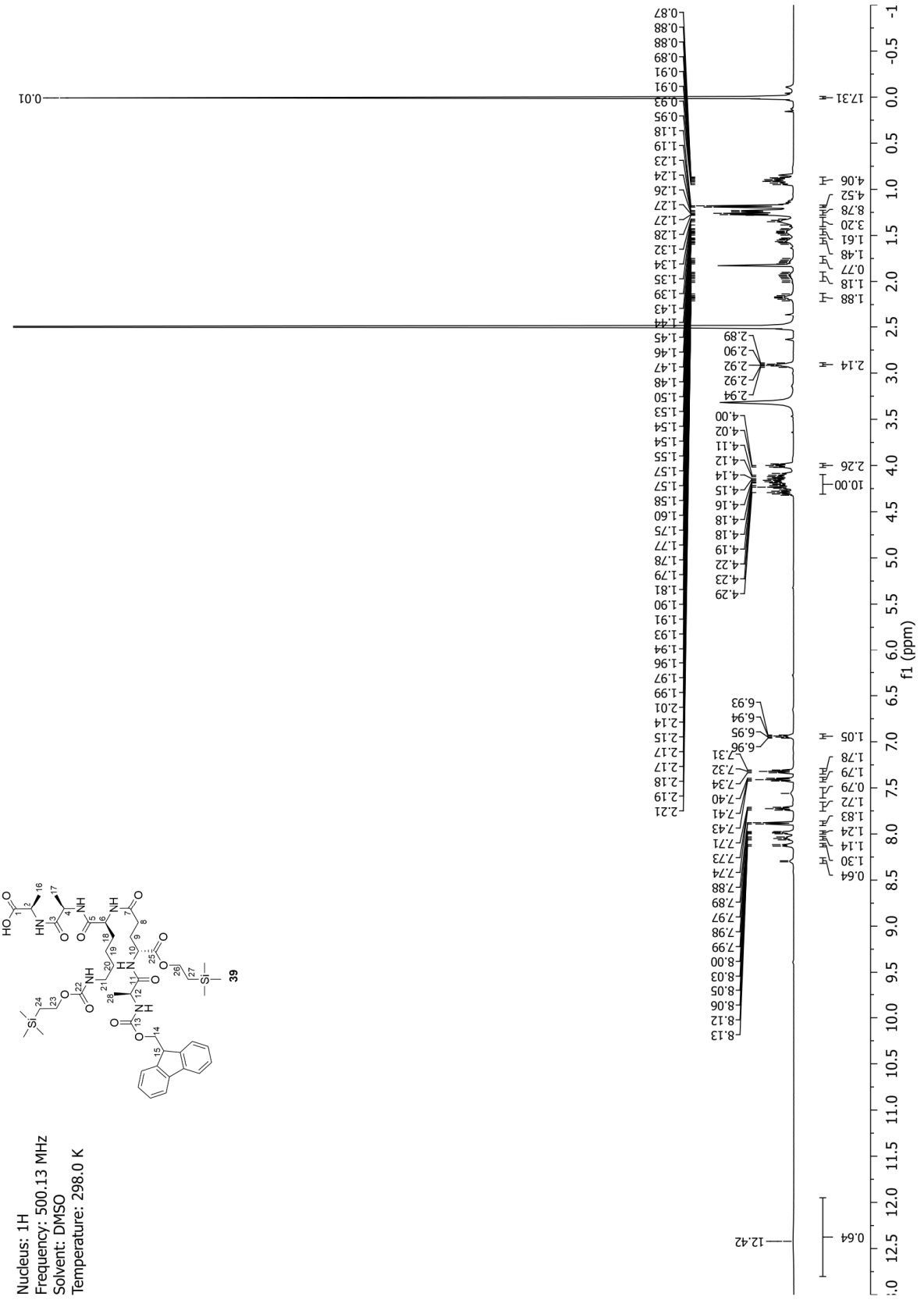

Nucleus: 13C
Frequency: 125.77 MHz
Solvent: MeOD
Temperature: 298.0 K
26
-1.6
16.6
18.2
49.0 CD3OD
50.0
65.8
171.7
f1 (ppm)

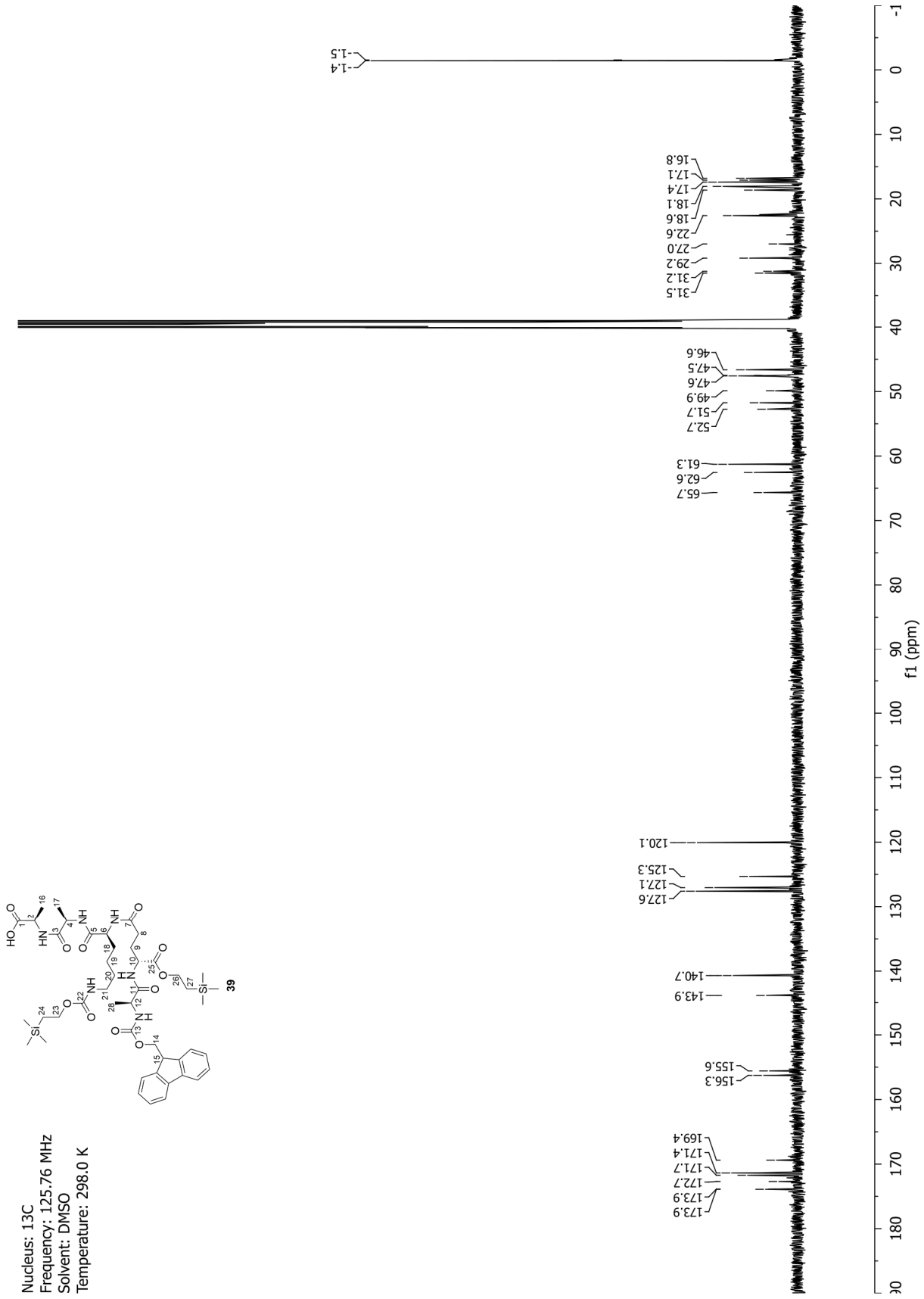

Nucleus: 1H
Frequency: 500.07 MHz
Solvent: MeOD
Temperature: 298.0 K
35
0.05
3.31 CD3OD
3.66 Dioxane
3.80
4.85 CD3OD
9.00
2.02
2.05
2.02
f1 (ppm)

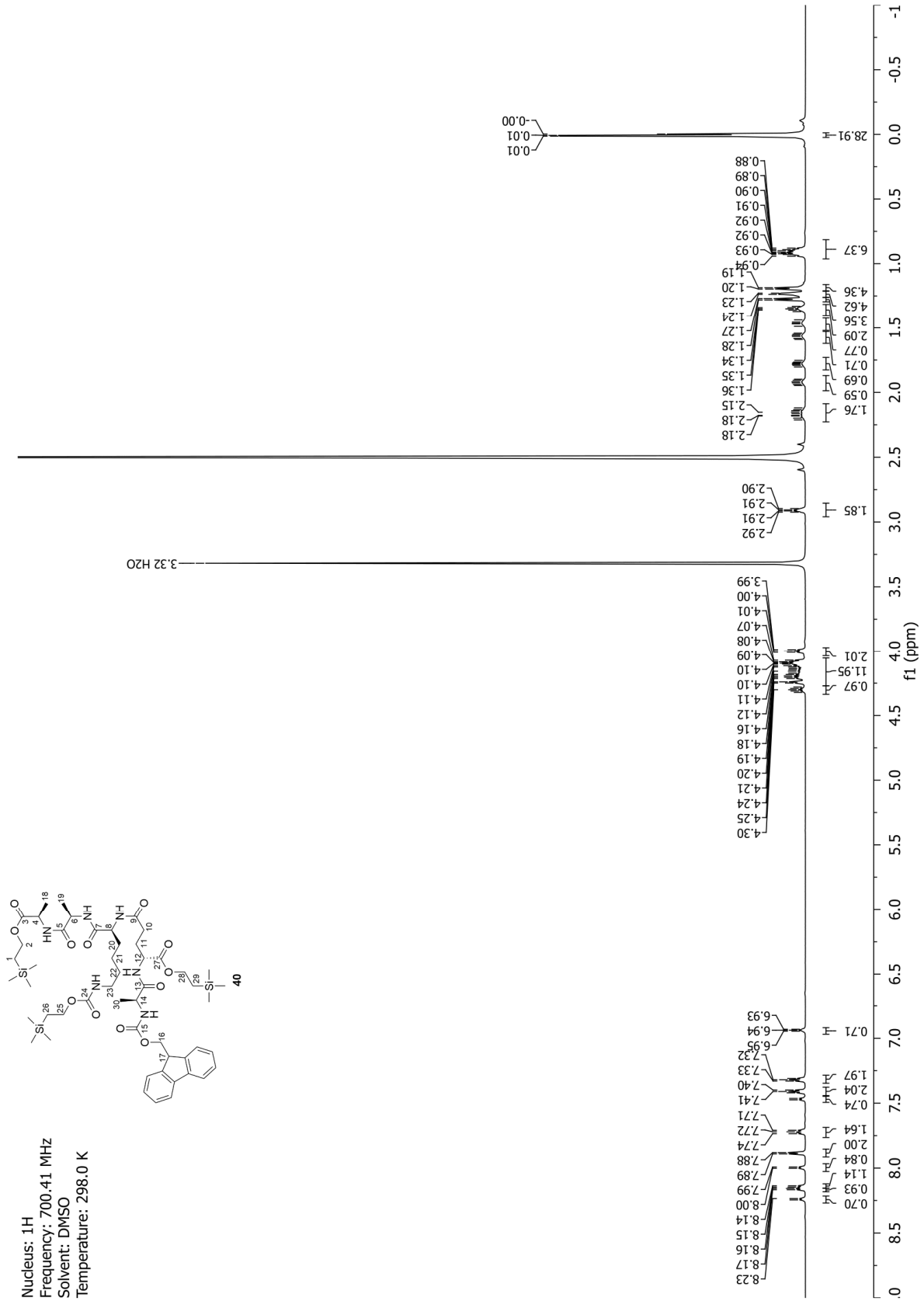

Nucleus: 13C
Frequency: 125.76 MHz
Solvent: MeOD
Temperature: 298.0 K
35
173.7
159.4
68.1 Dioxane
64.2
49.0 CD3OD
43.0
18.6
-1.5
f1 (ppm)

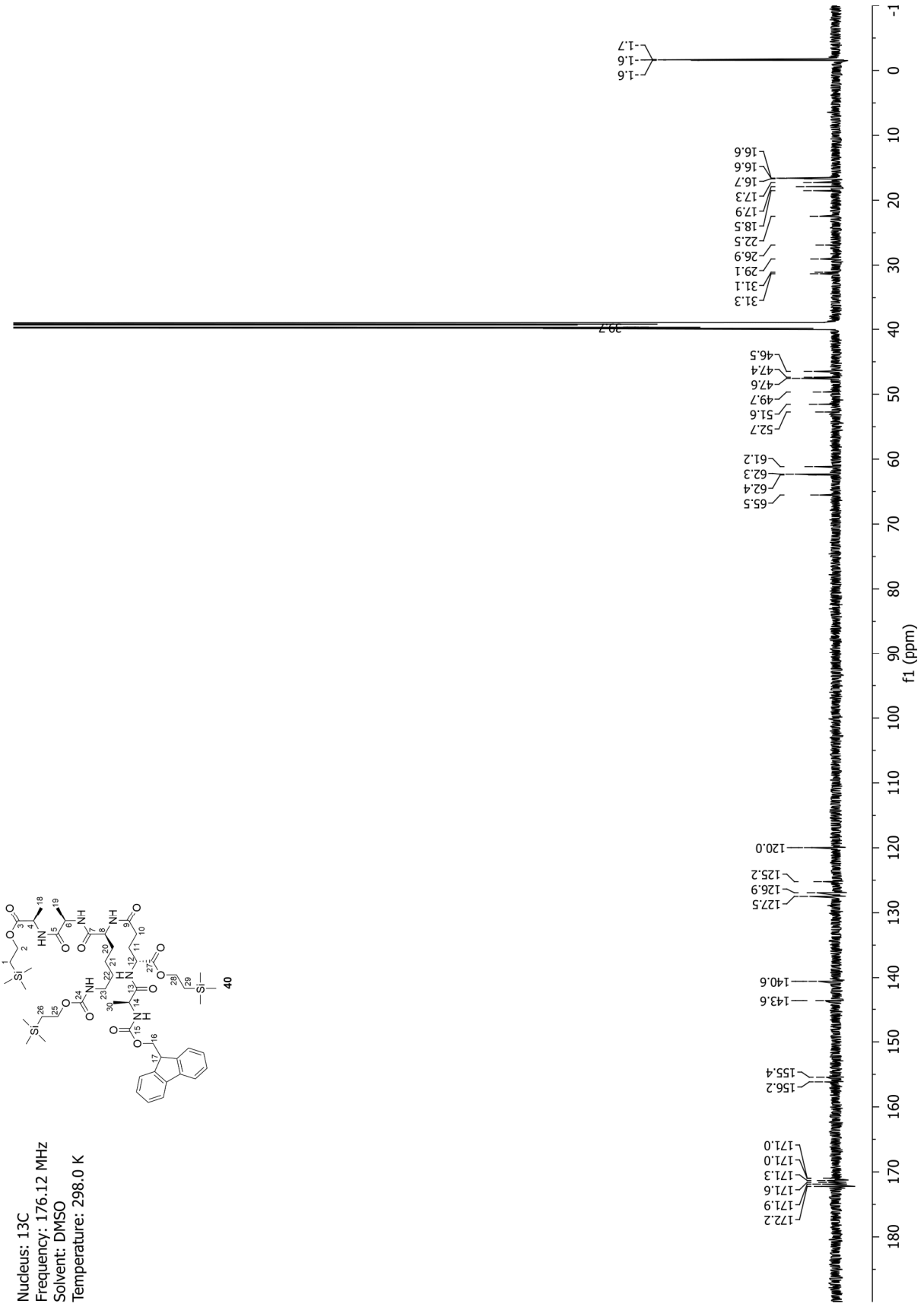

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: DMSO
Temperature: 298.0 K
43
f1 (ppm)

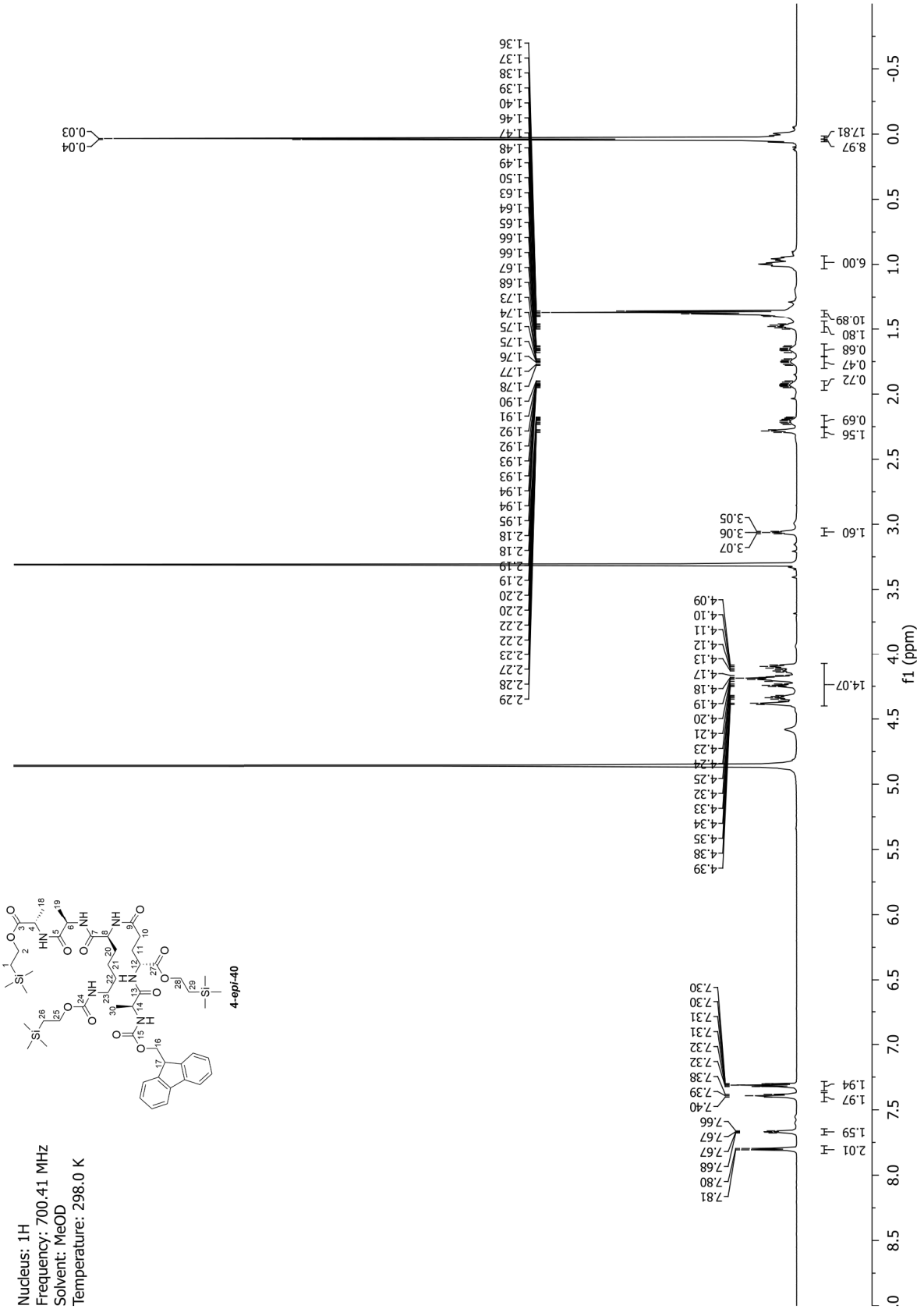

Nucleus: 13C
Frequency: 176.14 MHz
Solvent: DMSO
Temperature: 298.0 K
43
f1 (ppm)
39.5 DMSO-d6

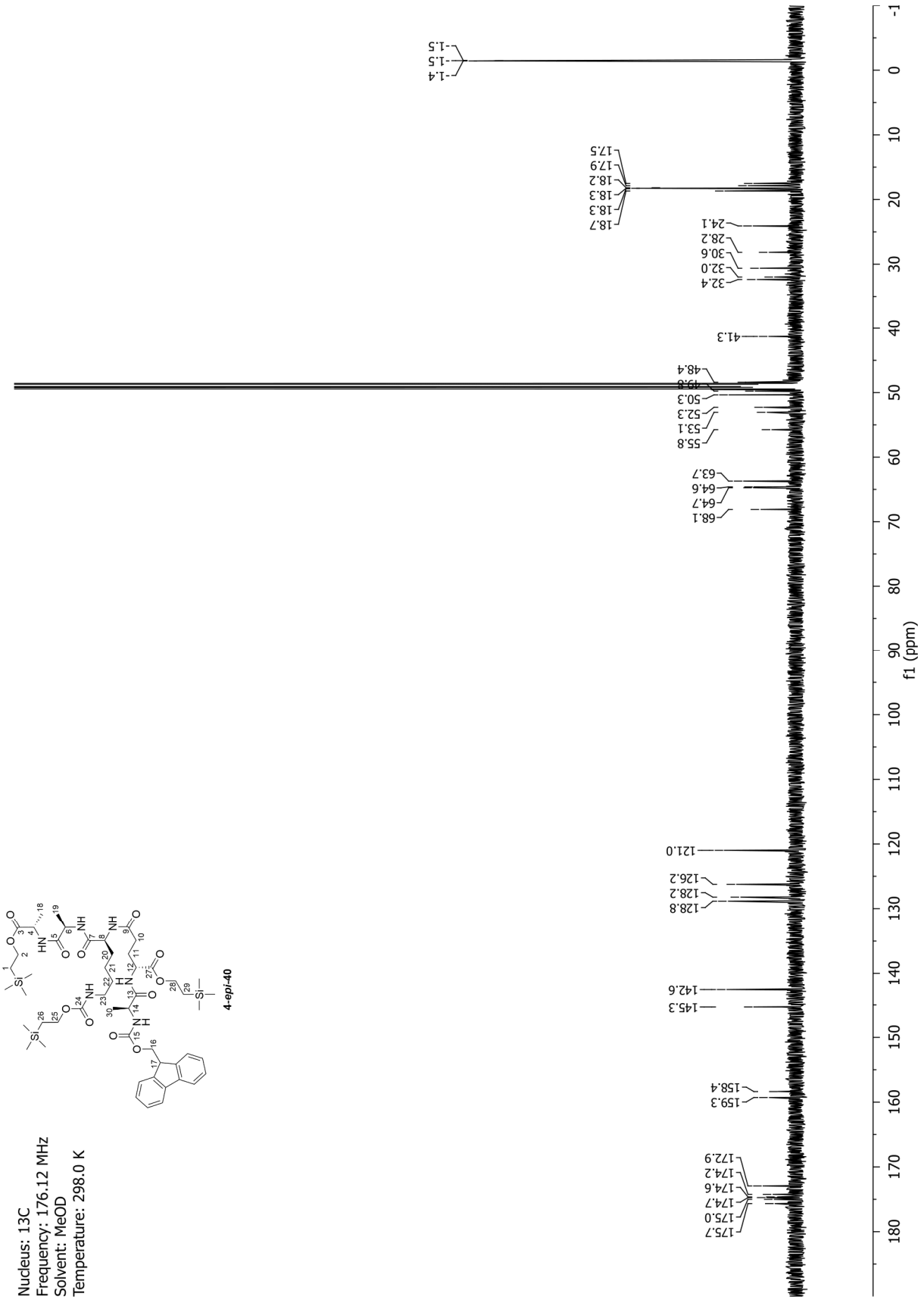

Nucleus: 1H
Frequency: 500.13 MHz
Solvent: DMSO
Temperature: 298.0 K
39
f1 (ppm)

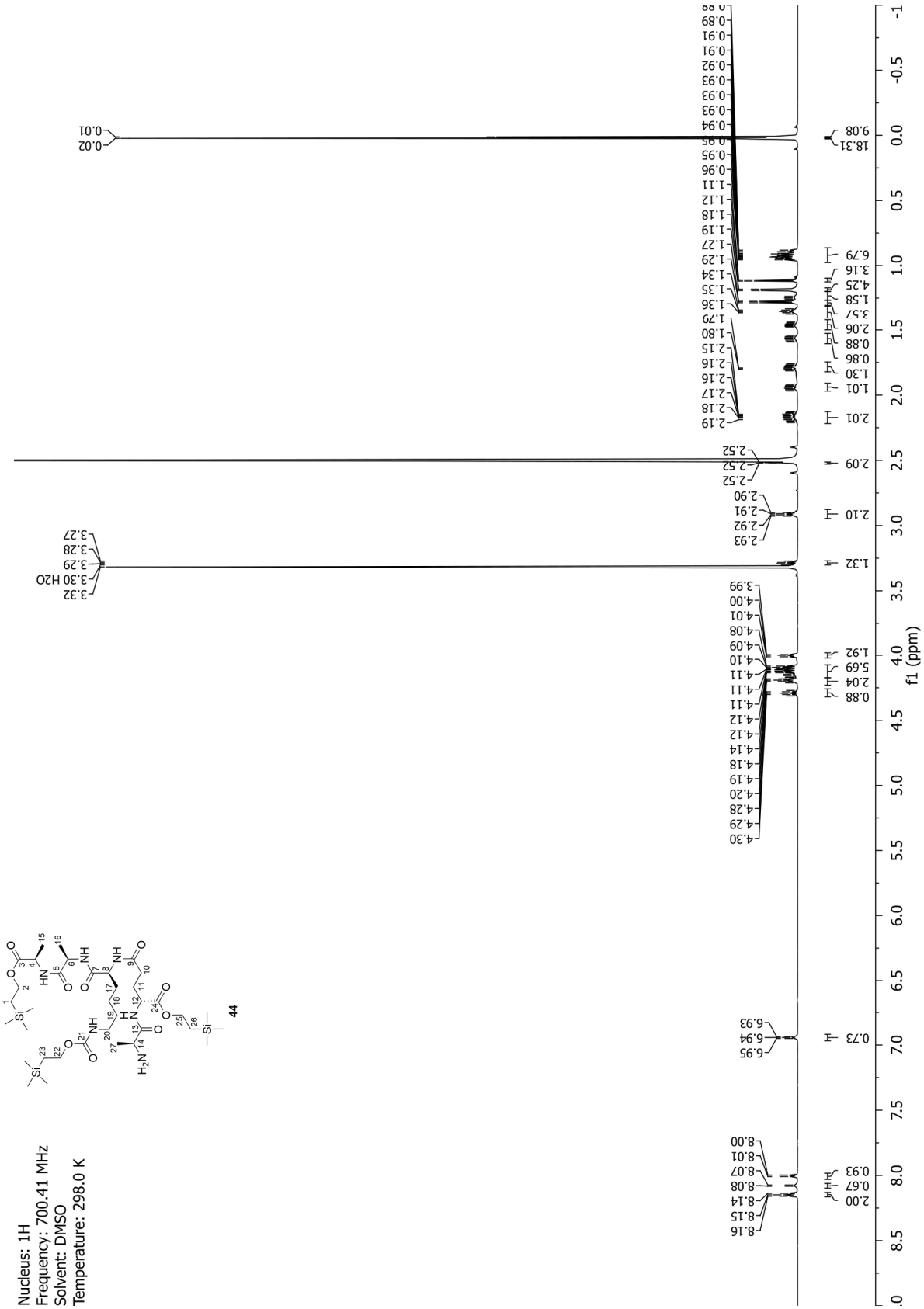

Nucleus: 13C
Frequency: 125.76 MHz
Solvent: DMSO
Temperature: 298.0 K
39
f1 (ppm)

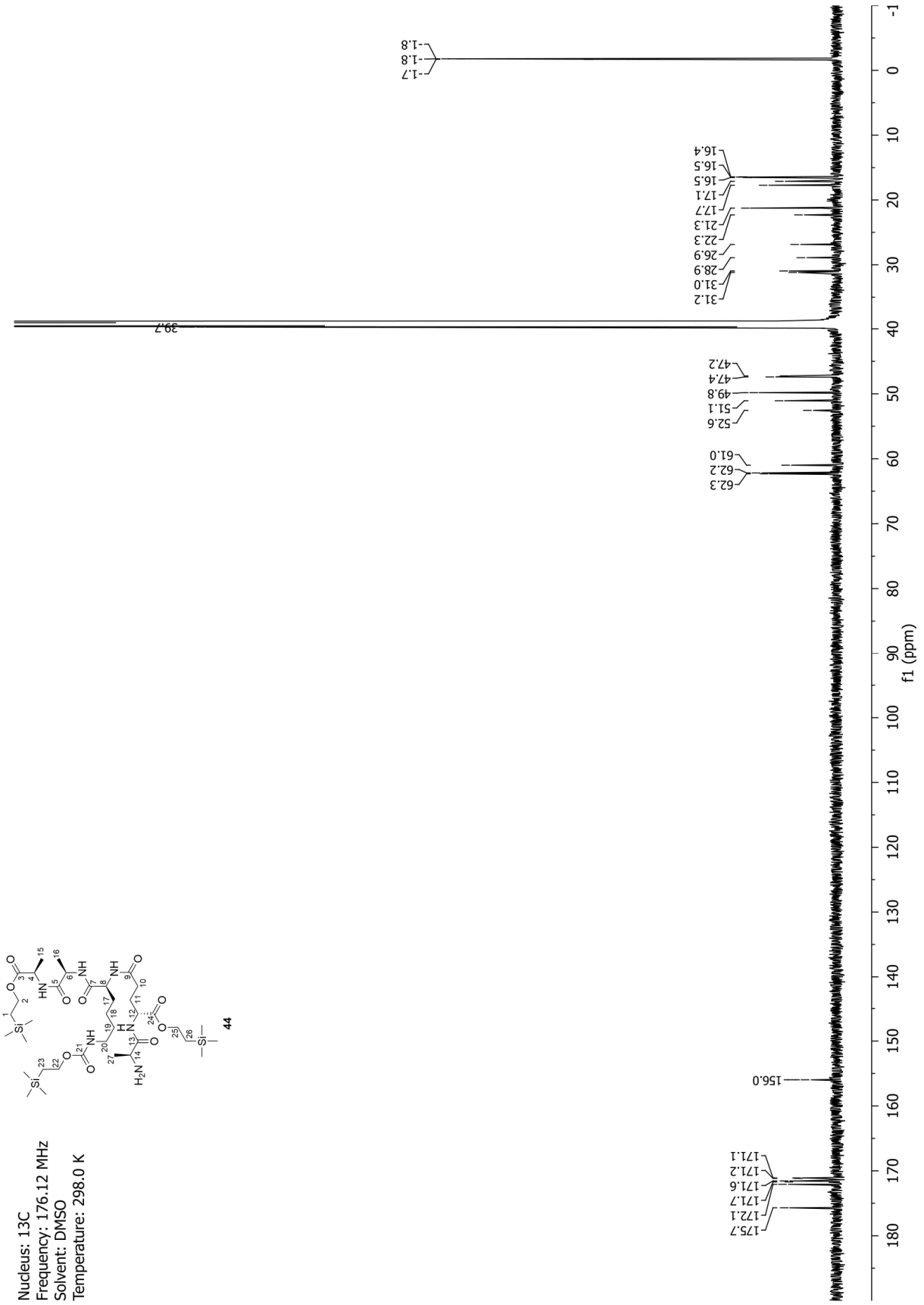

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: DMSO
Temperature: 298.0 K
40
3.32 H2O
f1 (ppm)

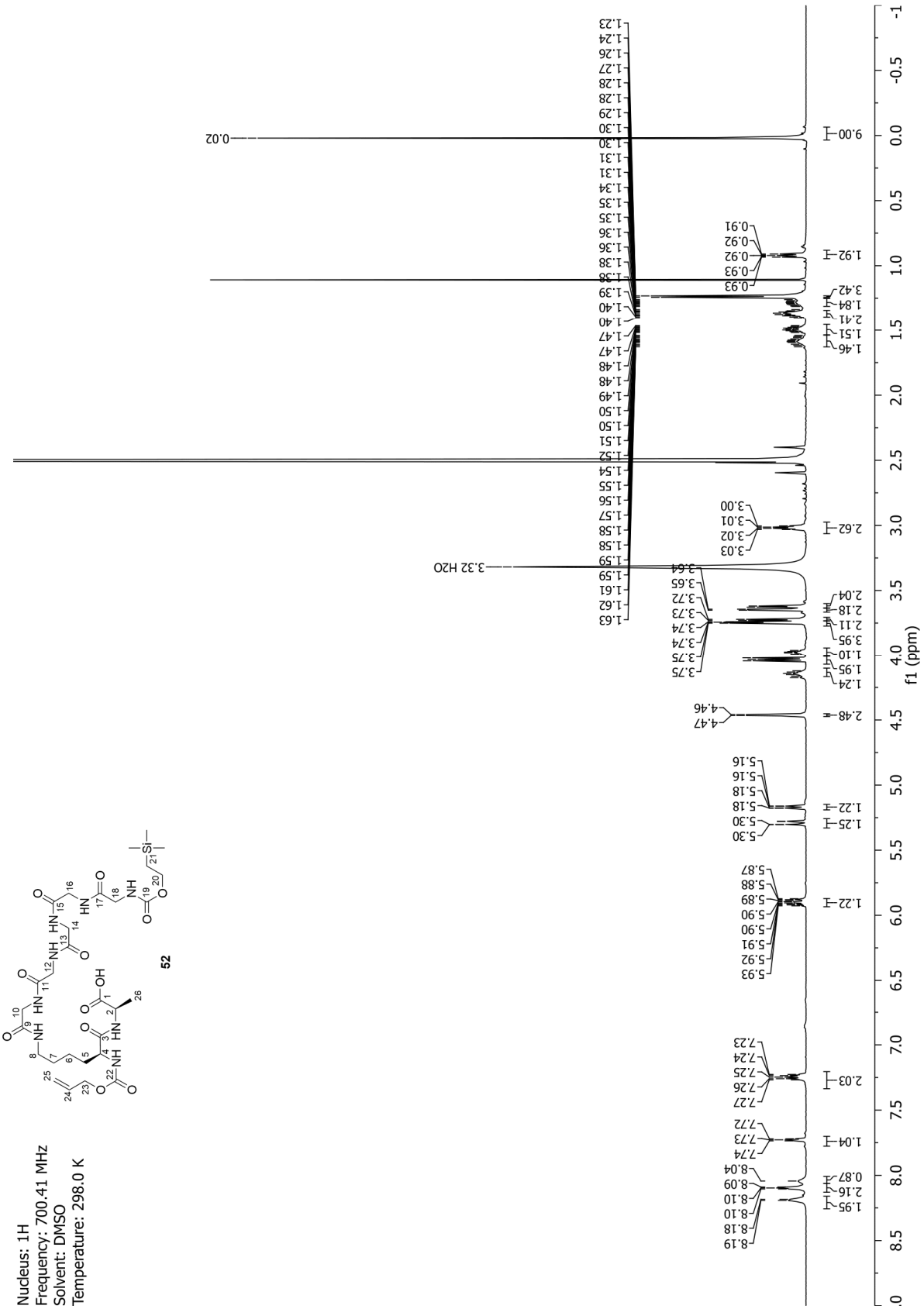

-1.7
-1.6
-1.6
16.6
16.6
16.7
17.3
17.9
18.5
22.5
26.9
29.1
31.1
31.3
39.7
46.5
47.4
47.6
49.7
51.6
52.7
61.2
62.3
62.4
65.5
120.0
125.2
126.9
127.5
140.6
143.6
155.4
156.2
171.0
171.0
171.3
171.6
171.9
172.2
f1 (ppm)
Nucleus: 13C
Frequency: 176.12 MHz
Solvent: DMSO
Temperature: 298.0 K
40

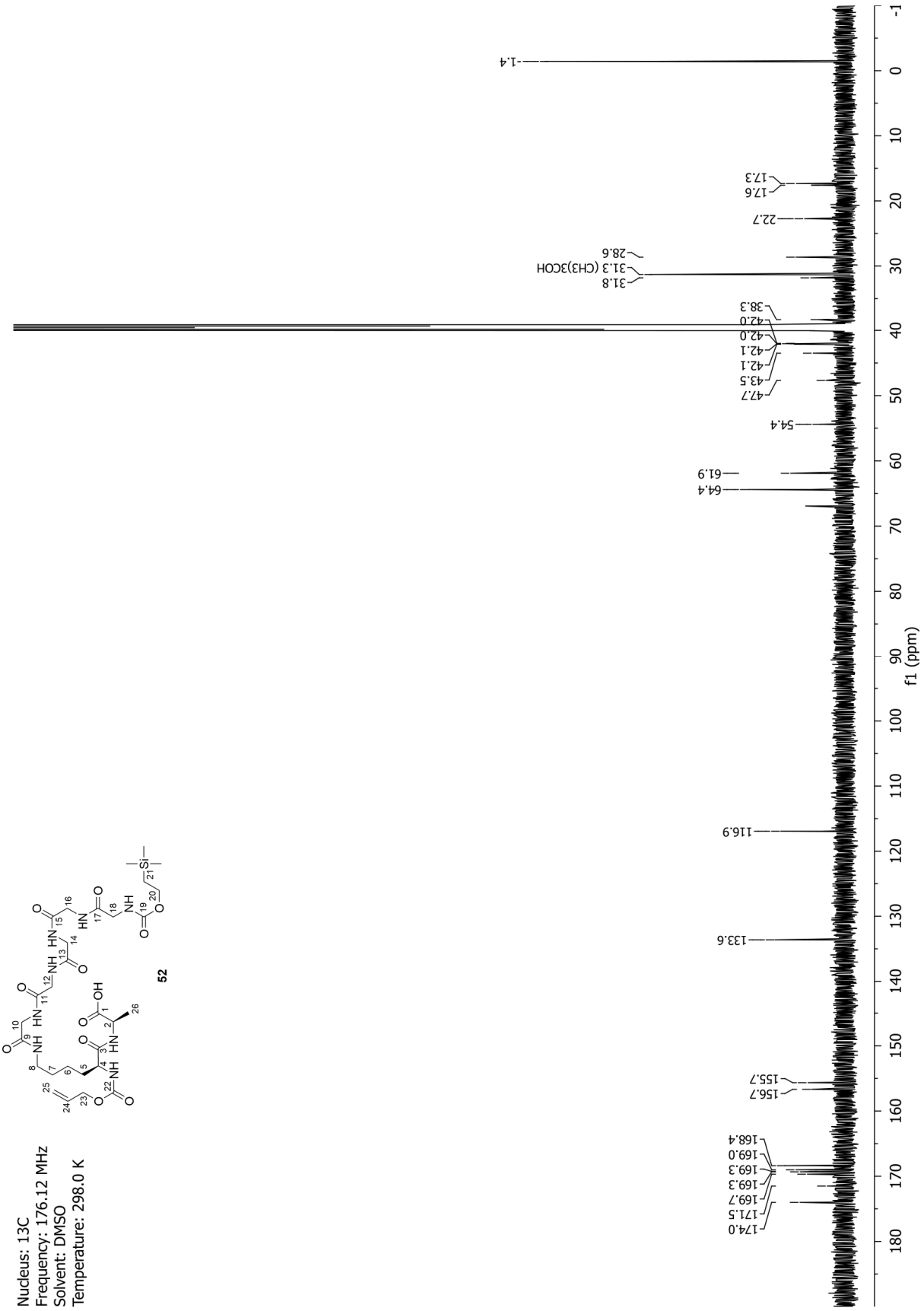

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: MeOD
Temperature: 298.0 K
4-epi-40
f1 (ppm)

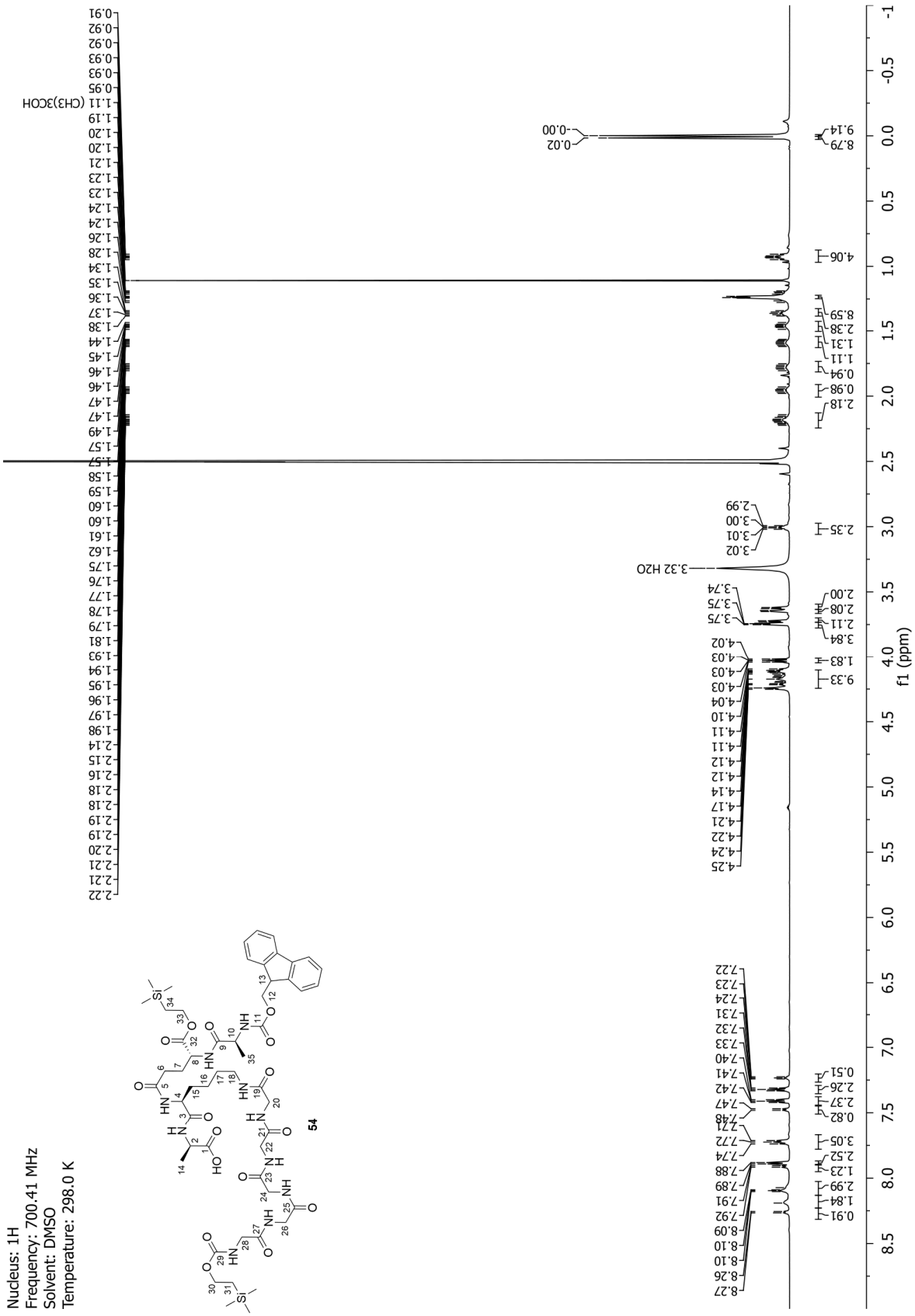

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: MeOD
Temperature: 298.0 K
4-epi-40
f1 (ppm)

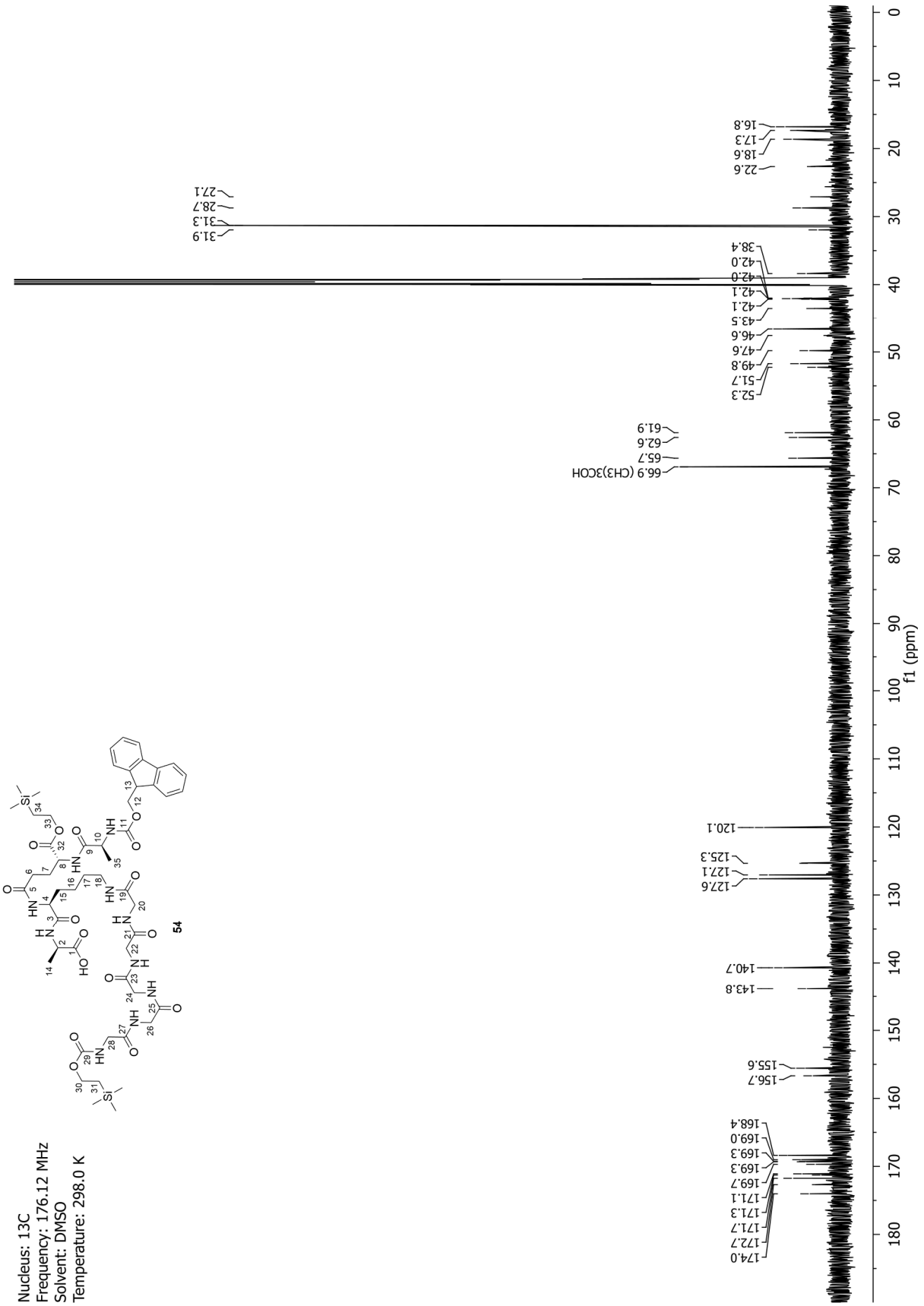

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: DMSO
Temperature: 298.0 K
44
f1 (ppm)

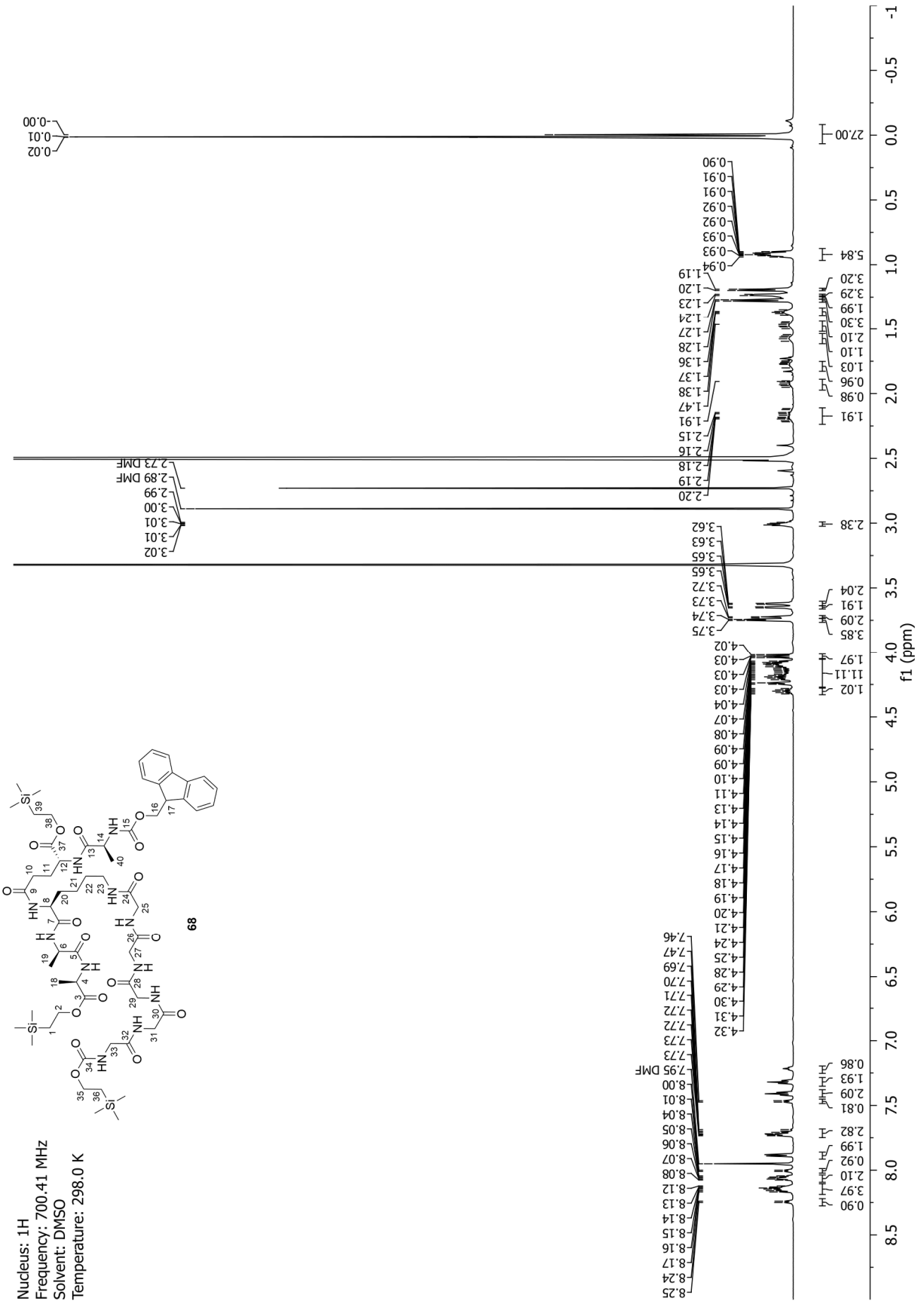

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: DMSO
Temperature: 298.0 K
f1 (ppm)
-1.7
-1.8
-1.8
16.4
16.5
16.5
17.1
17.7
21.3
22.3
26.9
28.9
31.0
31.2
39.7
47.2
47.4
49.8
51.1
52.6
61.0
62.2
62.3
156.0
171.1
171.2
171.6
171.7
172.1
175.7
44

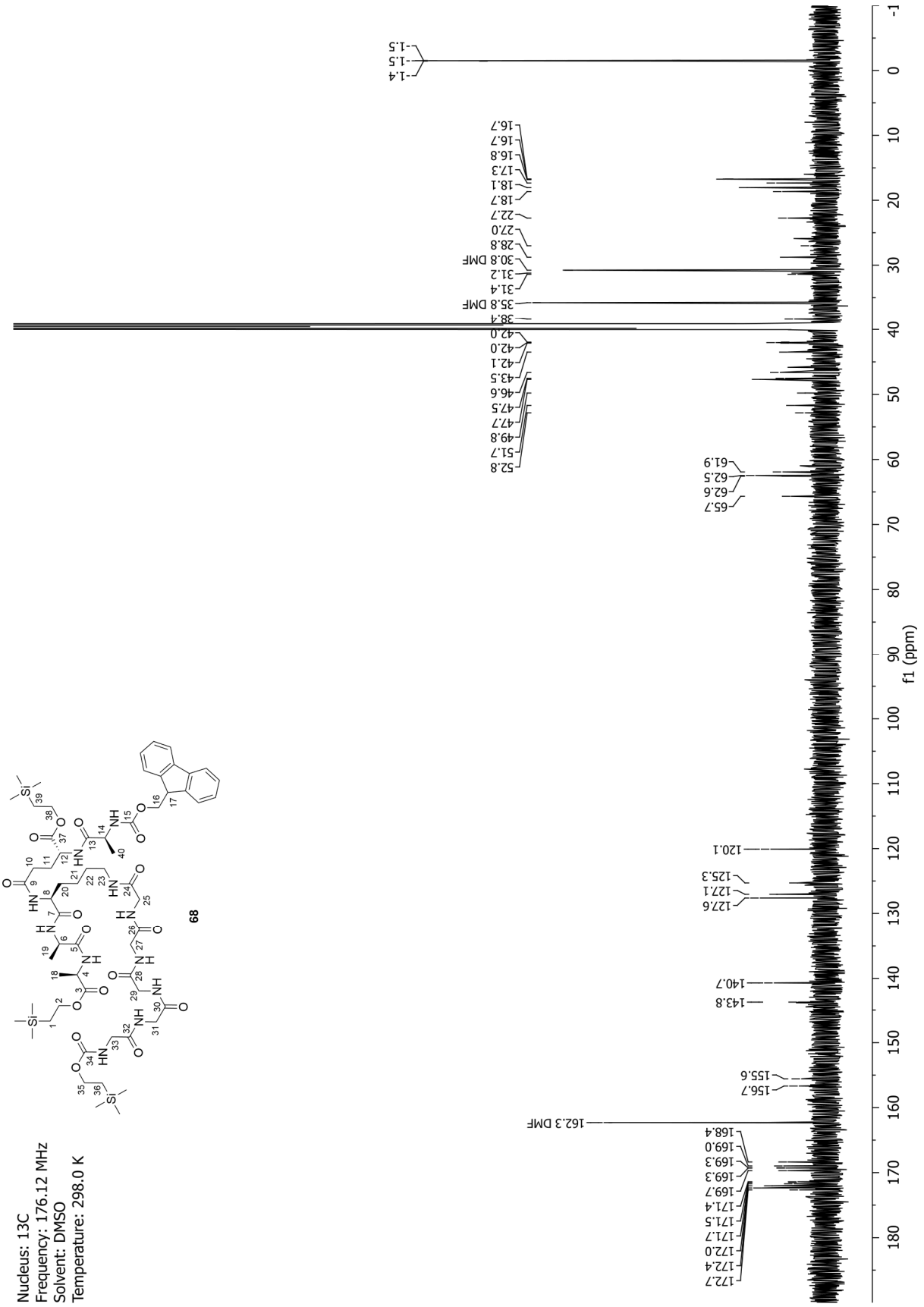

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: DMSO
Temperature: 298.0 K
52
f1 (ppm)
3.32 H2O
0.02

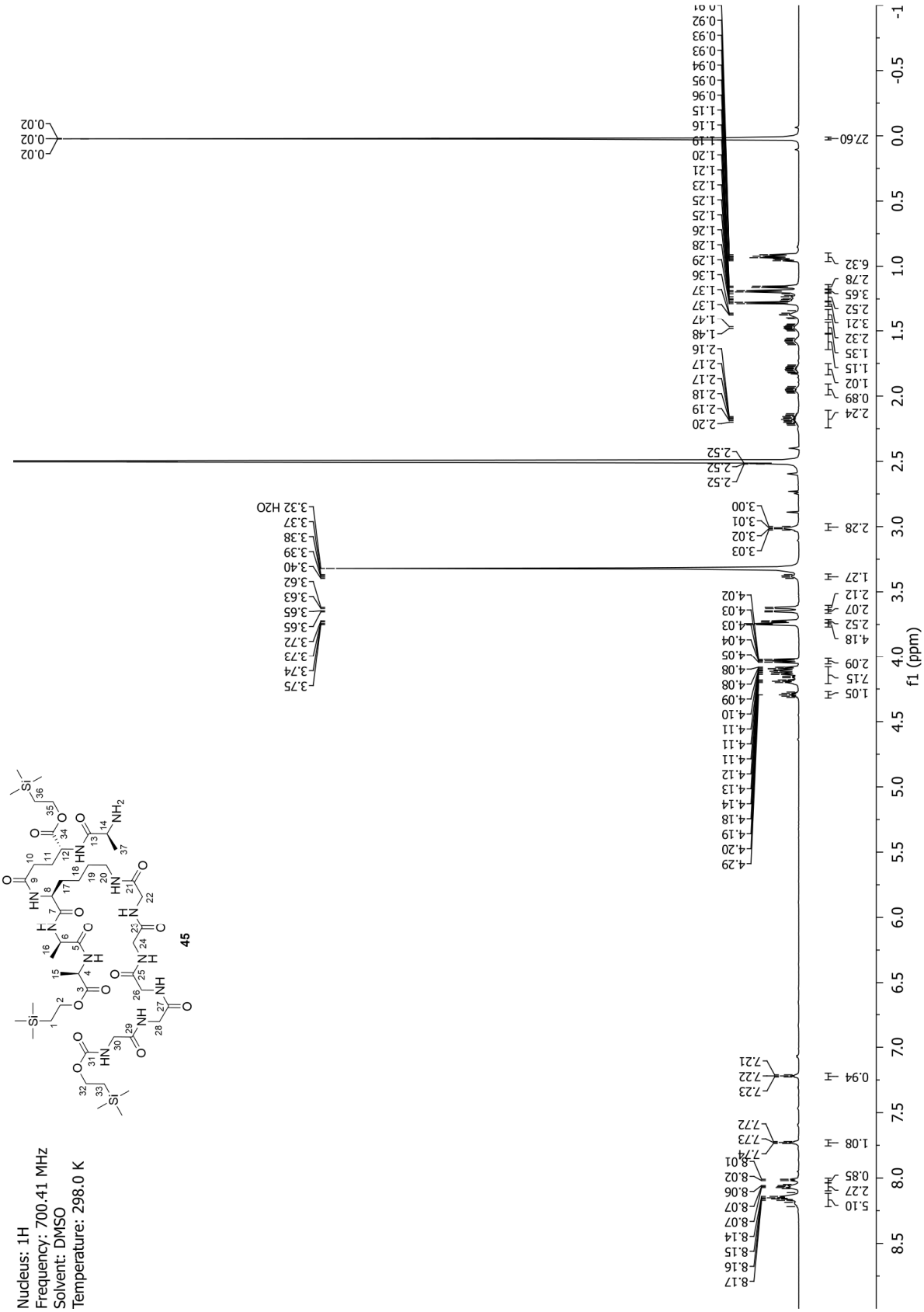

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: DMSO
Temperature: 298.0 K
52
f1 (ppm)
-1.4
17.3
17.6
22.7
28.6
31.3 (CH3)3COH
31.8
38.3
42.0
42.0
42.1
42.1
43.5
47.7
54.4
61.9
64.4
116.9
133.6
155.7
156.7
168.4
169.0
169.3
169.3
169.7
171.5
174.0

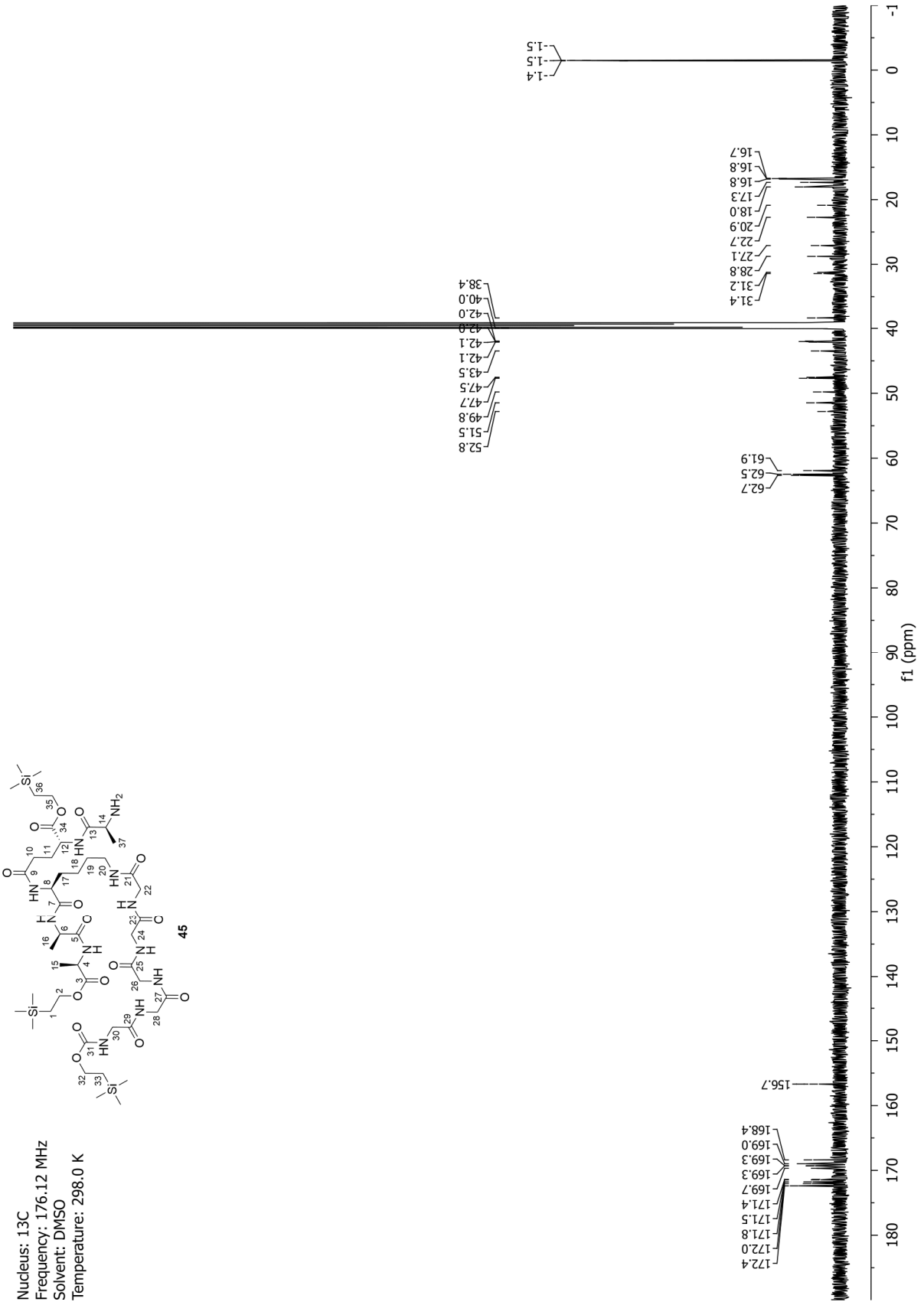

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: DMSO
Temperature: 298.0 K
f1 (ppm)
(CH3)3COH
3.32 H2O
54

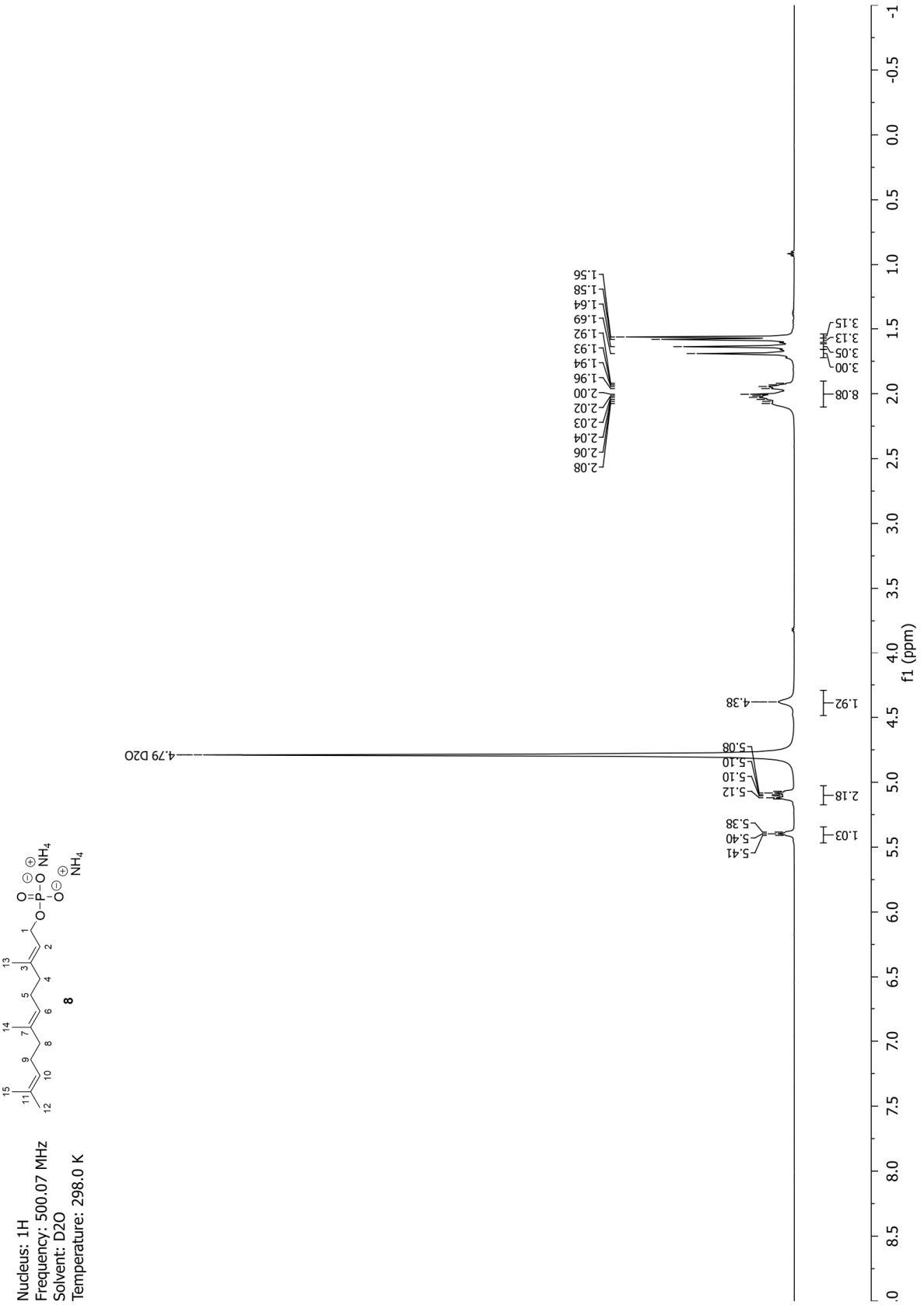

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: DMSO
Temperature: 298.0 K
f1 (ppm)
16.8
17.3
18.6
22.6
27.1
28.7
31.3
31.9
38.4
42.0
42.0
42.1
42.1
43.5
46.6
47.6
49.8
51.7
52.3
61.9
62.6
65.7
66.9 (CH3)3COH
120.1
125.3
127.1
127.6
140.7
143.8
155.6
156.7
168.4
169.0
169.3
169.3
169.7
171.1
171.3
171.7
172.7
174.0
54

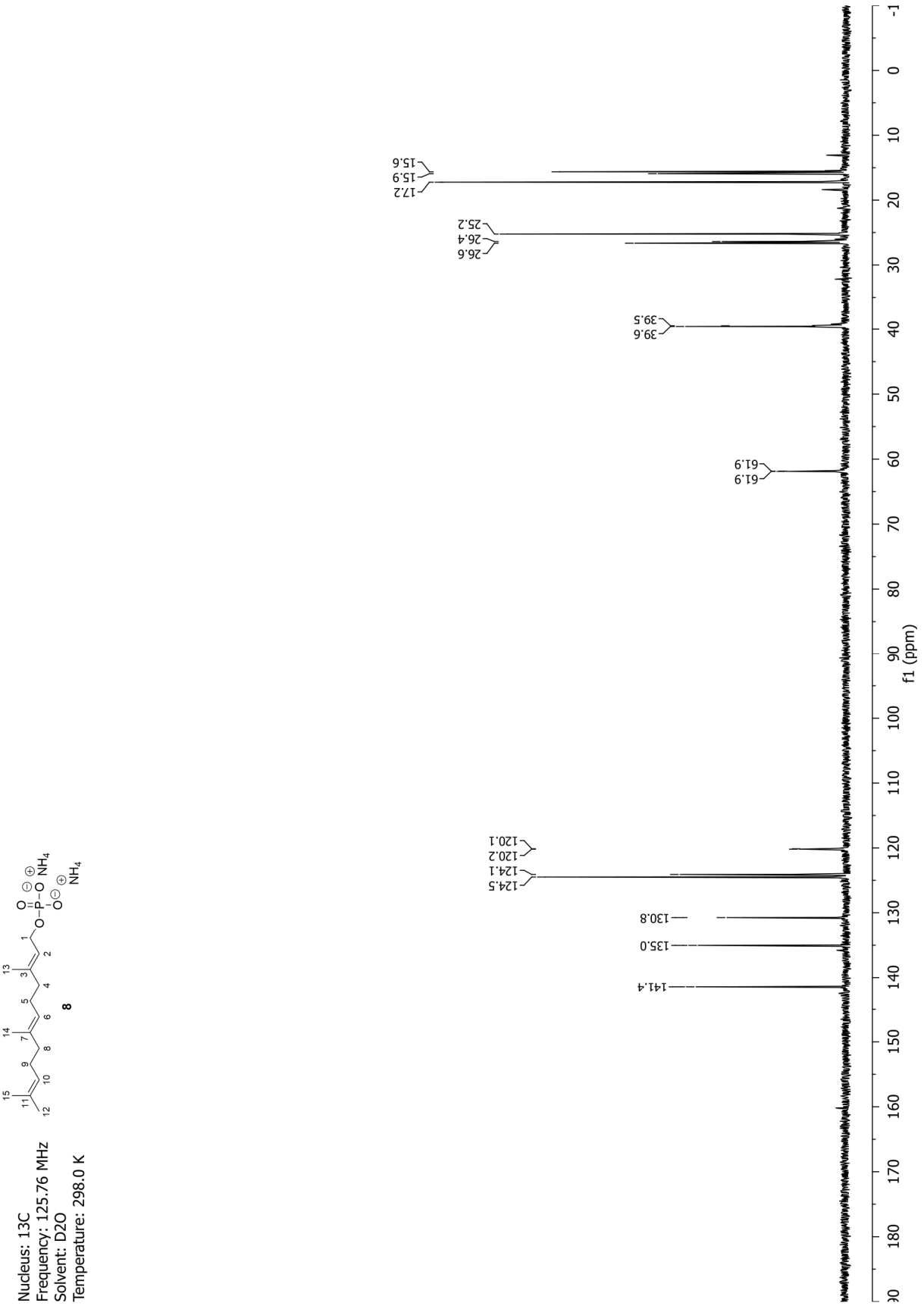

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: DMSO
Temperature: 298.0 K
68
f1 (ppm)

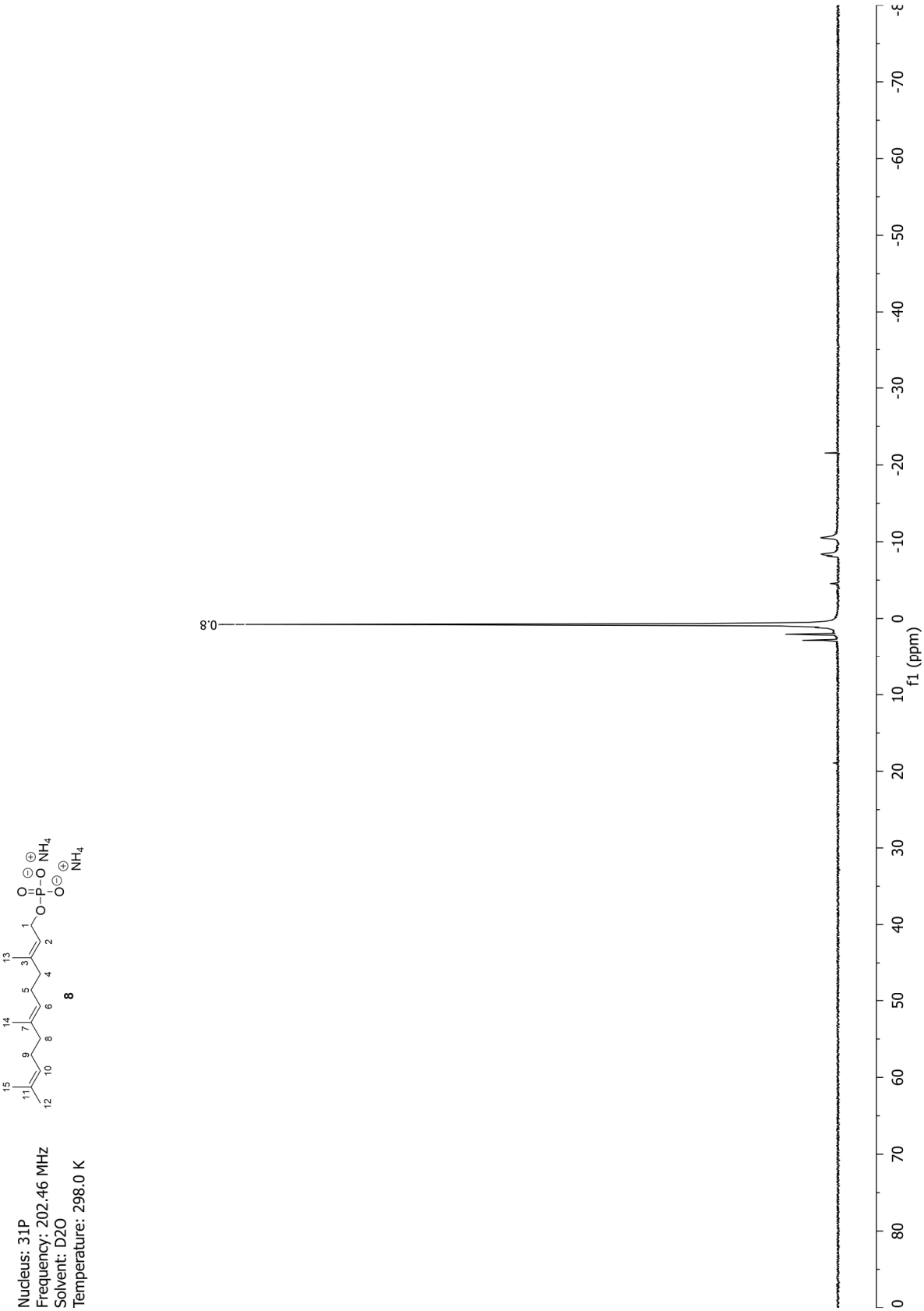

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: DMSO
Temperature: 298.0 K
68
f1 (ppm)
-1.4
-1.5
-1.5
16.7
16.7
16.8
17.3
18.1
18.7
22.7
27.0
28.8
30.8 DMF
31.2
31.4
35.8 DMF
38.4
42.0
42.0
42.1
43.5
46.6
47.5
47.7
49.8
51.7
52.8
61.9
62.5
62.6
65.7
120.1
125.3
127.1
127.6
140.7
143.8
155.6
156.7
162.3 DMF
168.4
169.0
169.3
169.3
169.7
171.4
171.5
171.7
172.0
172.4
172.7

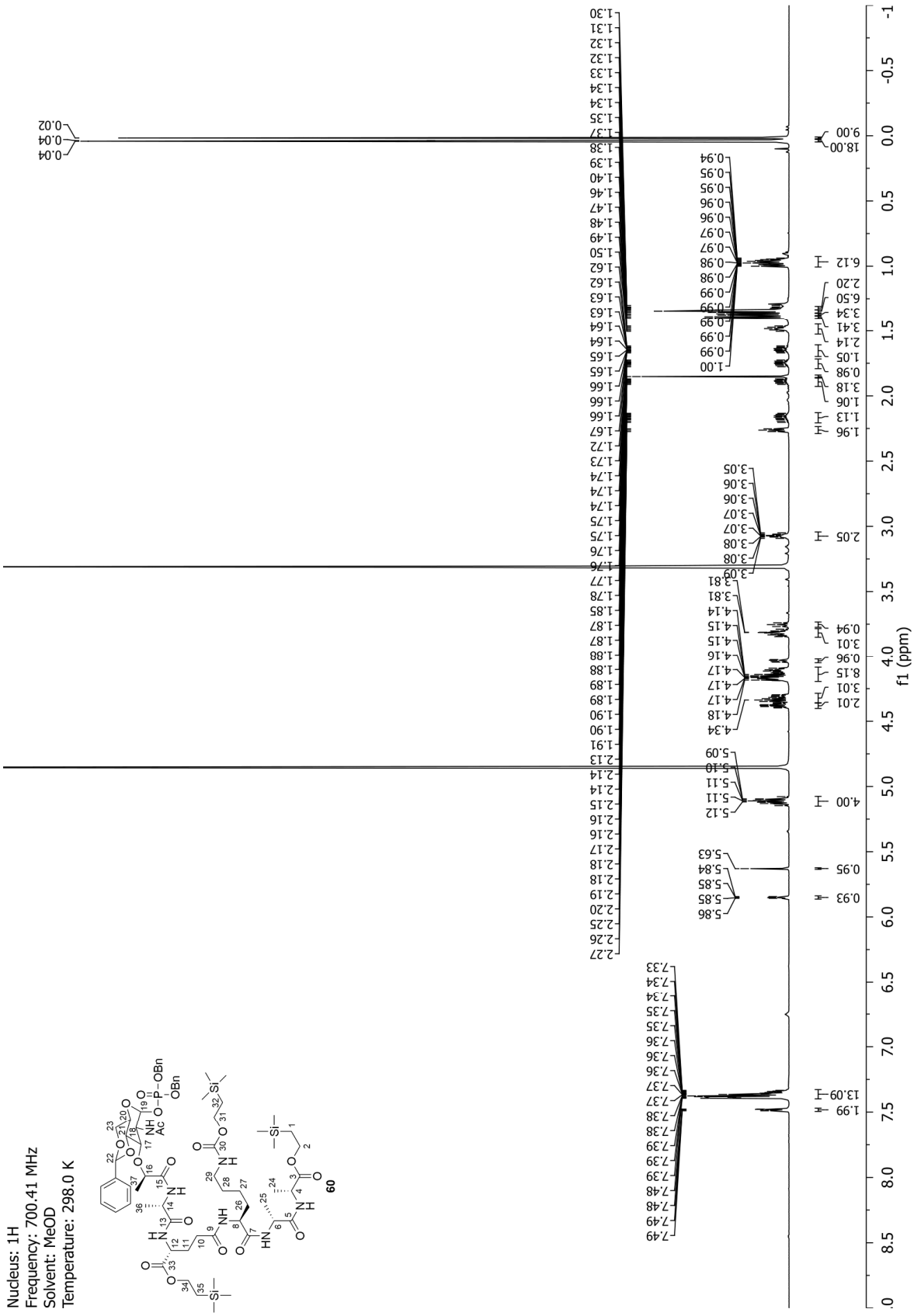

45
Nucleus: 1H
Frequency: 700.41 MHz
Solvent: DMSO
Temperature: 298.0 K
f1 (ppm)
3.32 H2O

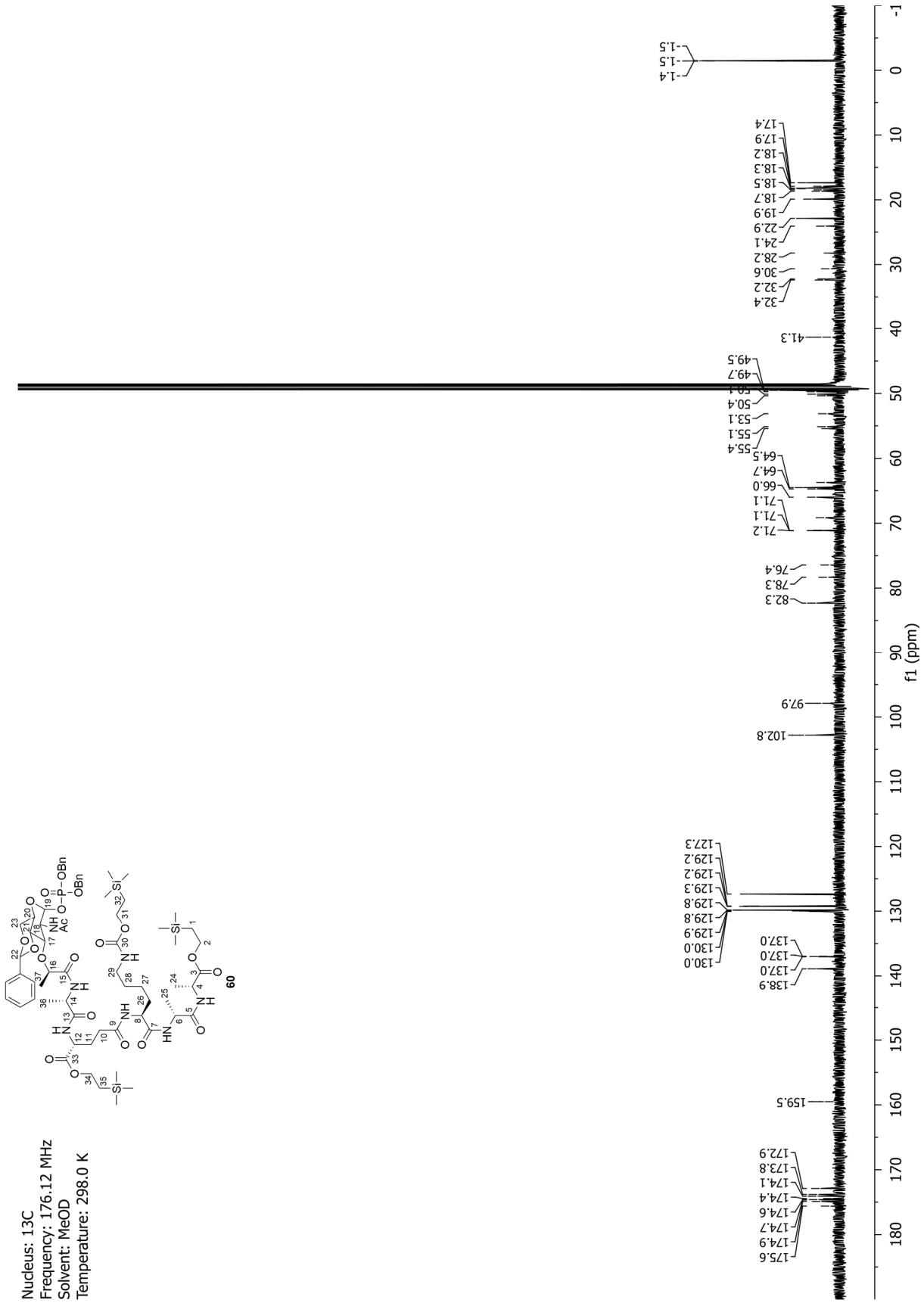

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: DMSO
Temperature: 298.0 K
45
f1 (ppm)

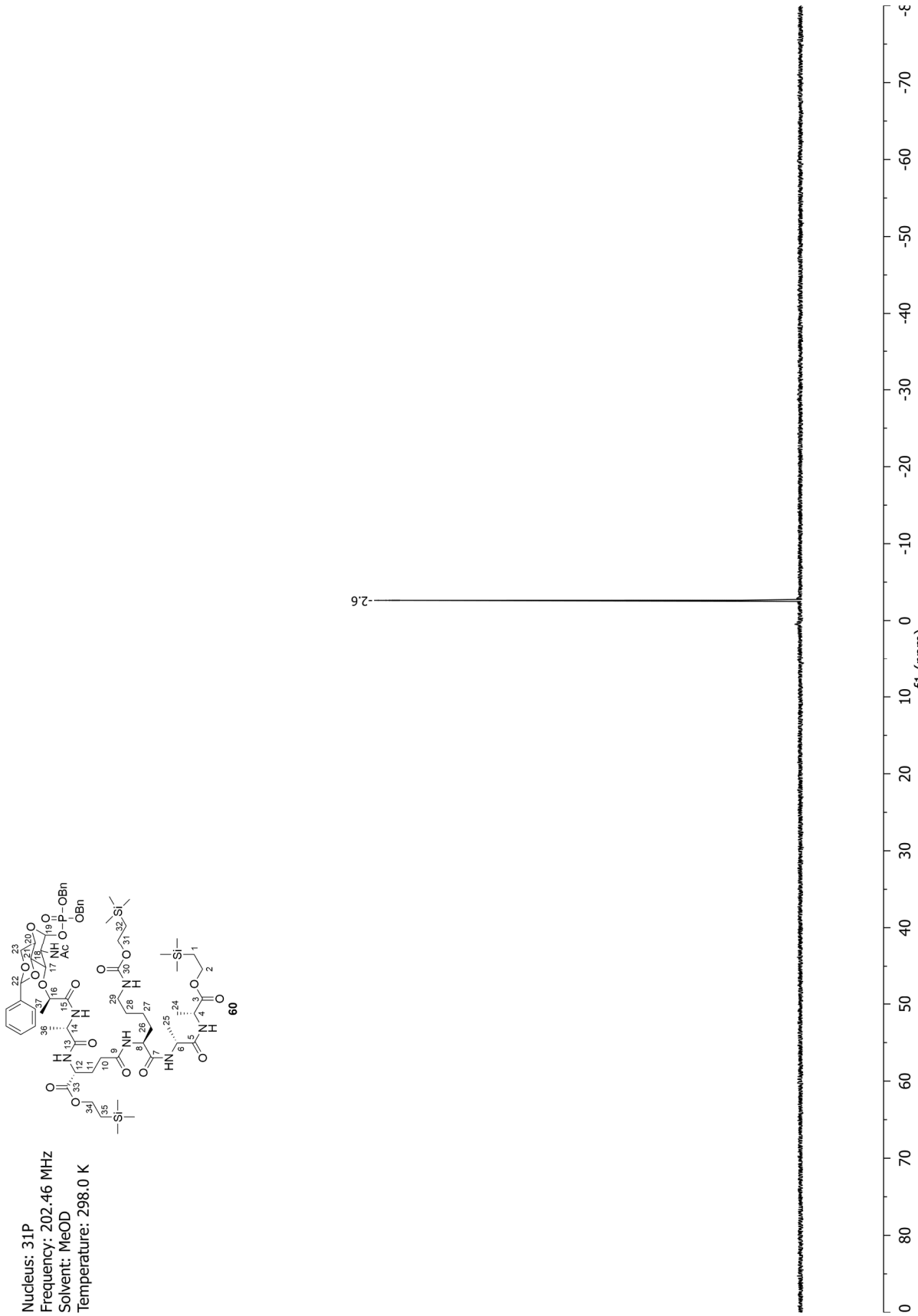

Nucleus: 1H
Frequency: 500.07 MHz
Solvent: D2O
Temperature: 298.0 K
8
4.79 D2O
f1 (ppm)

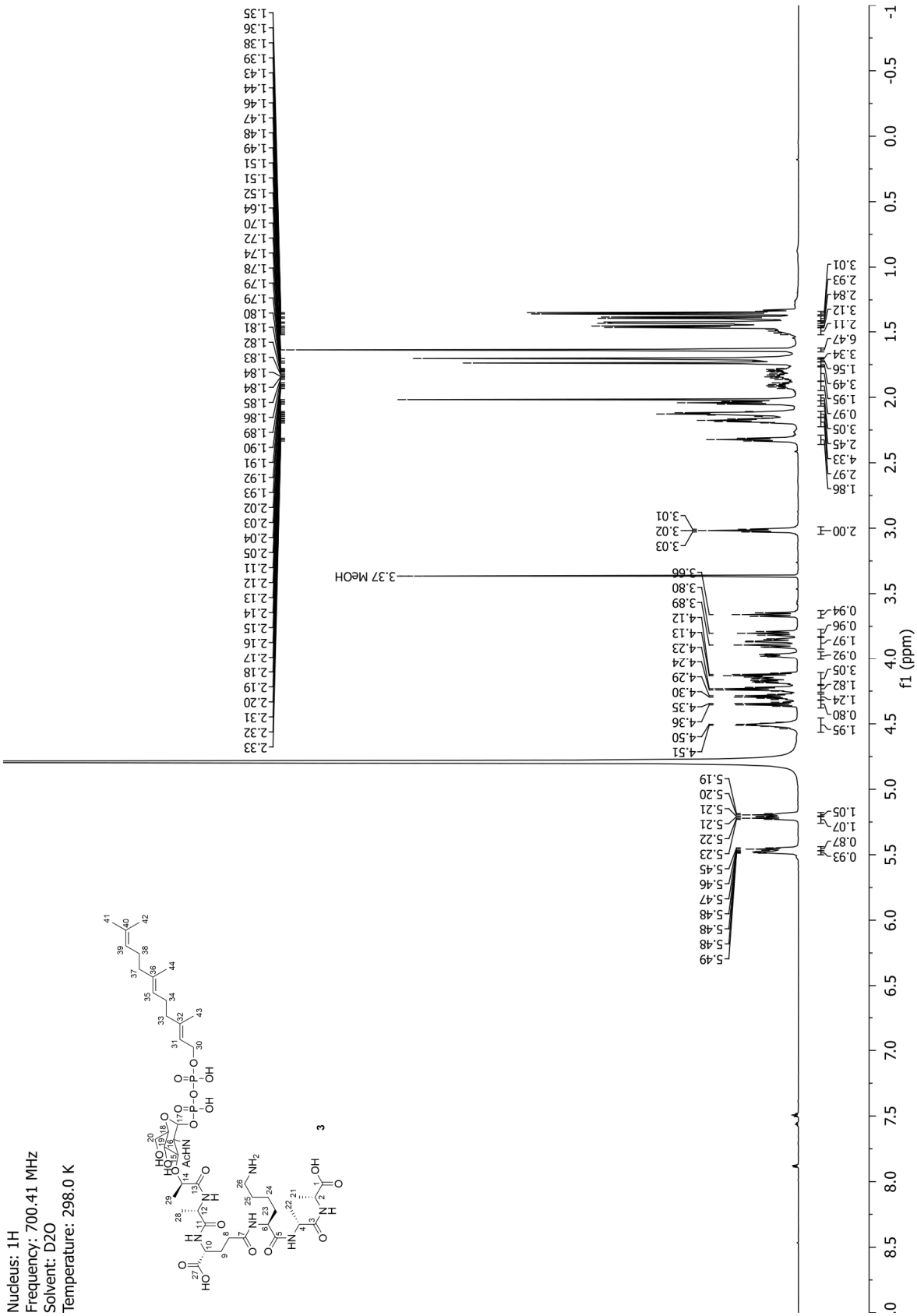

Nucleus: 13C
Frequency: 125.76 MHz
Solvent: D2O
Temperature: 298.0 K
8
f1 (ppm)
15.6
15.9
17.2
25.2
26.4
26.6
39.5
39.6
61.9
61.9
120.1
120.2
124.1
124.5
130.8
135.0
141.4

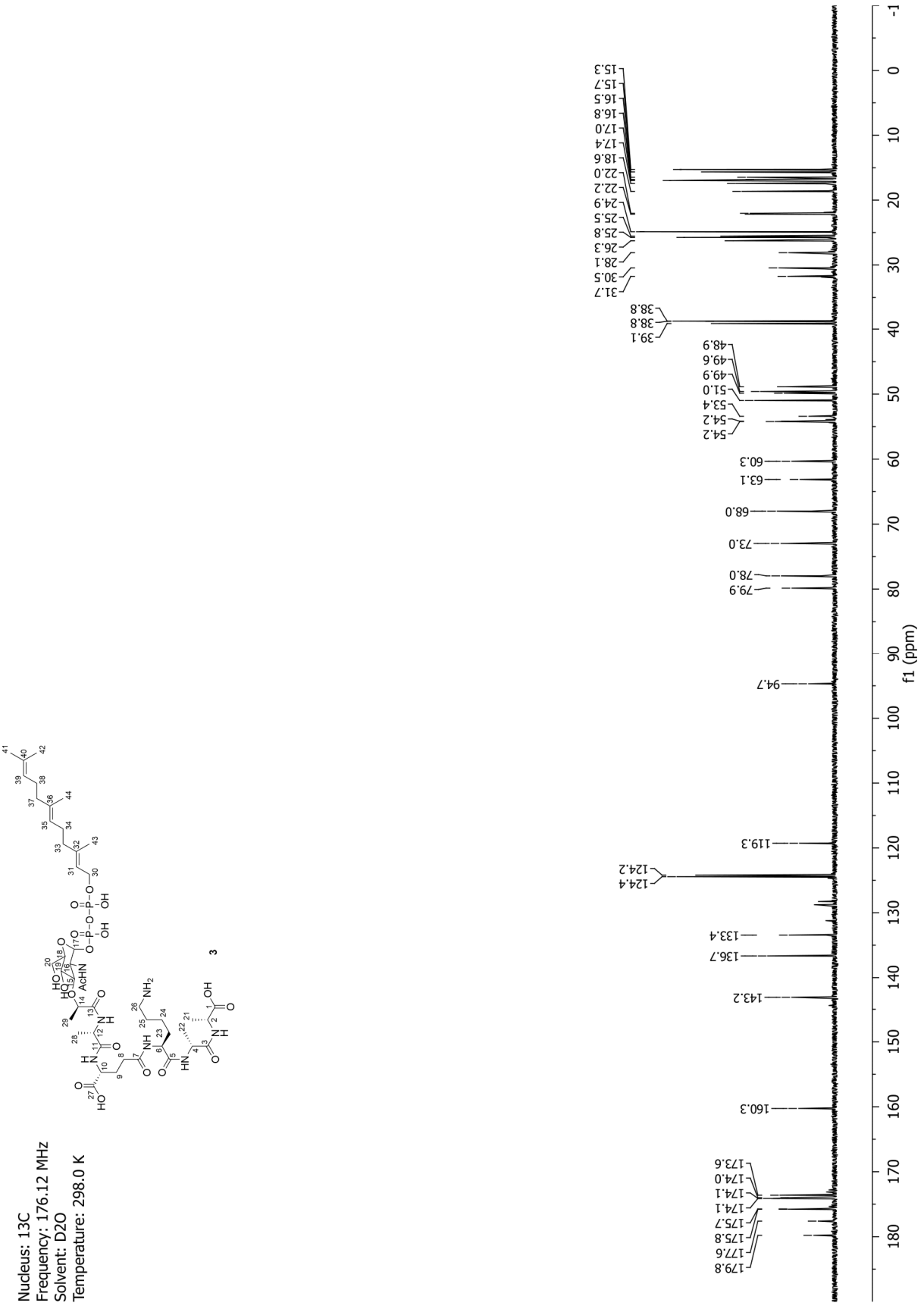

Nucleus: 31P
Frequency: 202.46 MHz
Solvent: D2O
Temperature: 298.0 K
8
0.8
f1 (ppm)

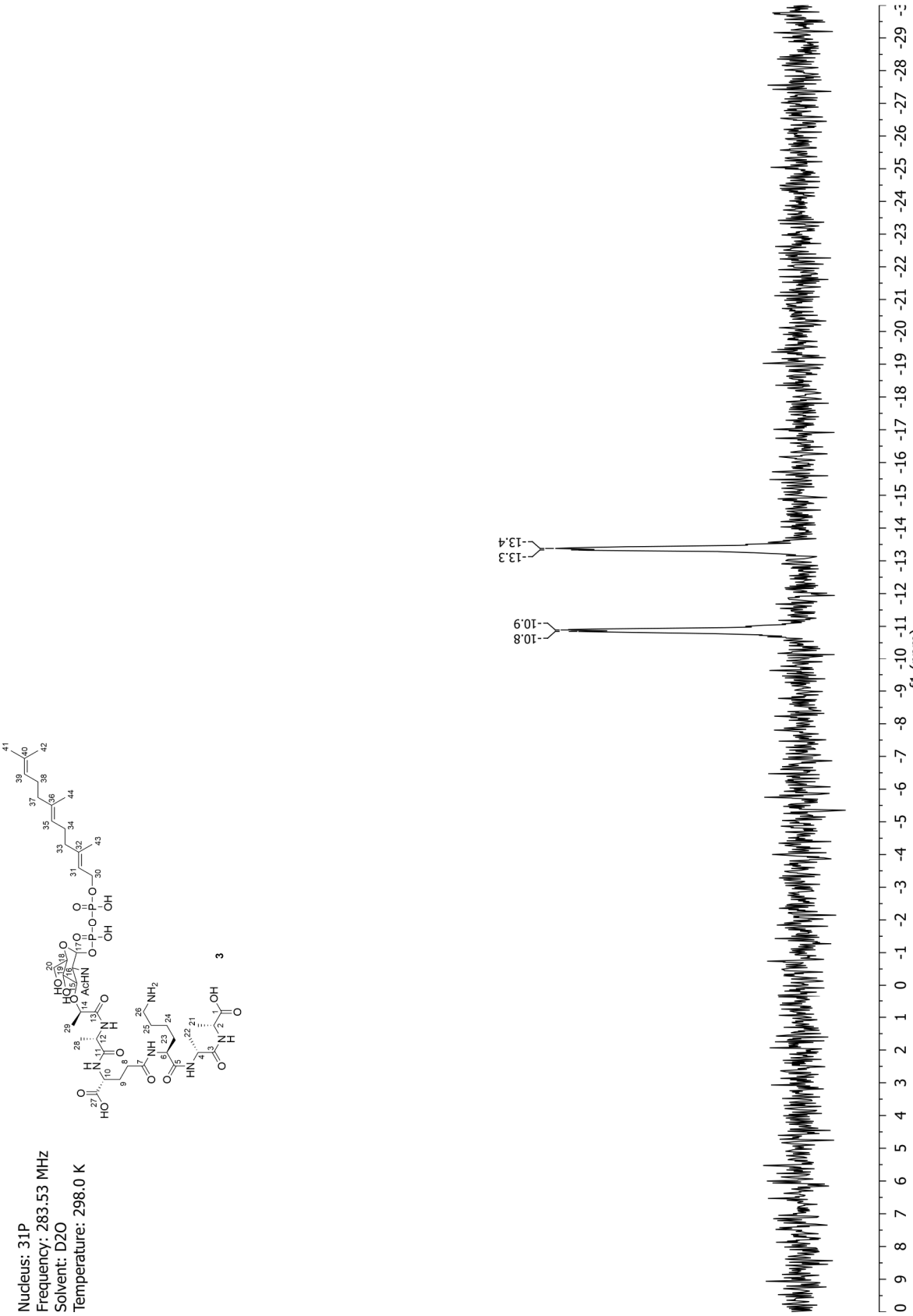

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: MeOD
Temperature: 298.0 K
60
f1 (ppm)

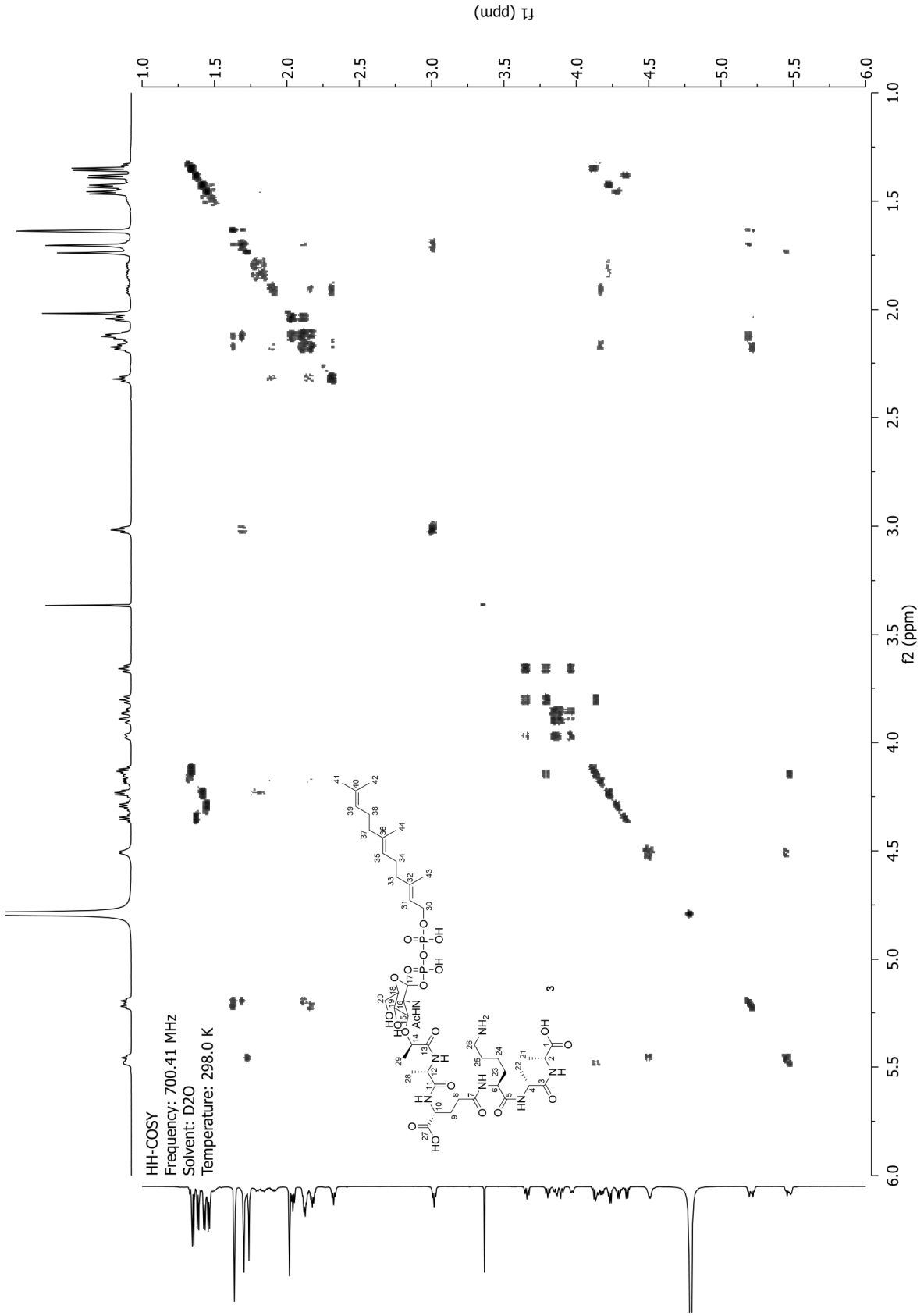

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: MeOD
Temperature: 298.0 K
60
f1 (ppm)

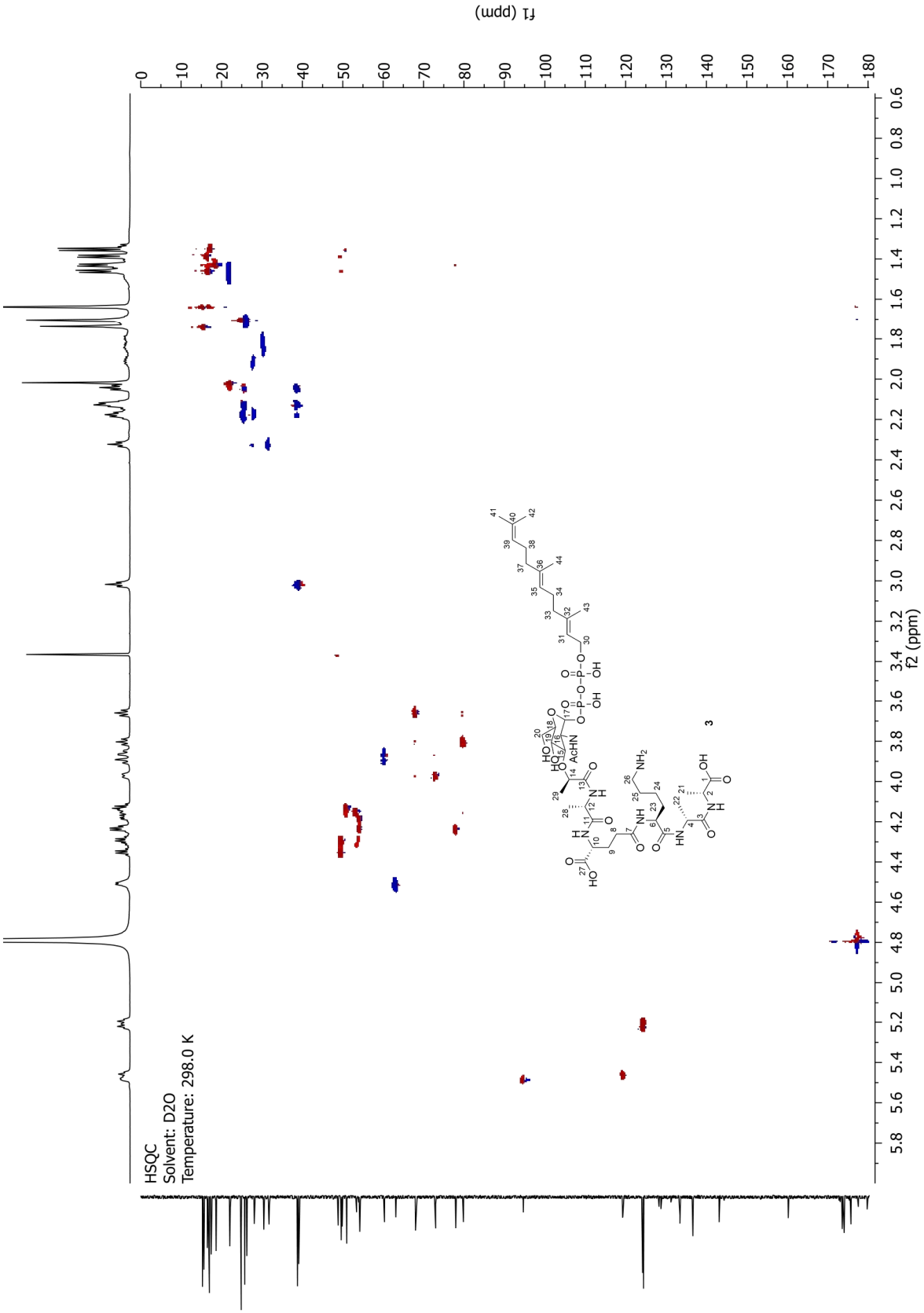

Nucleus: 31P
Frequency: 202.46 MHz
Solvent: MeOD
Temperature: 298.0 K
60
-2.6
f1 (ppm)

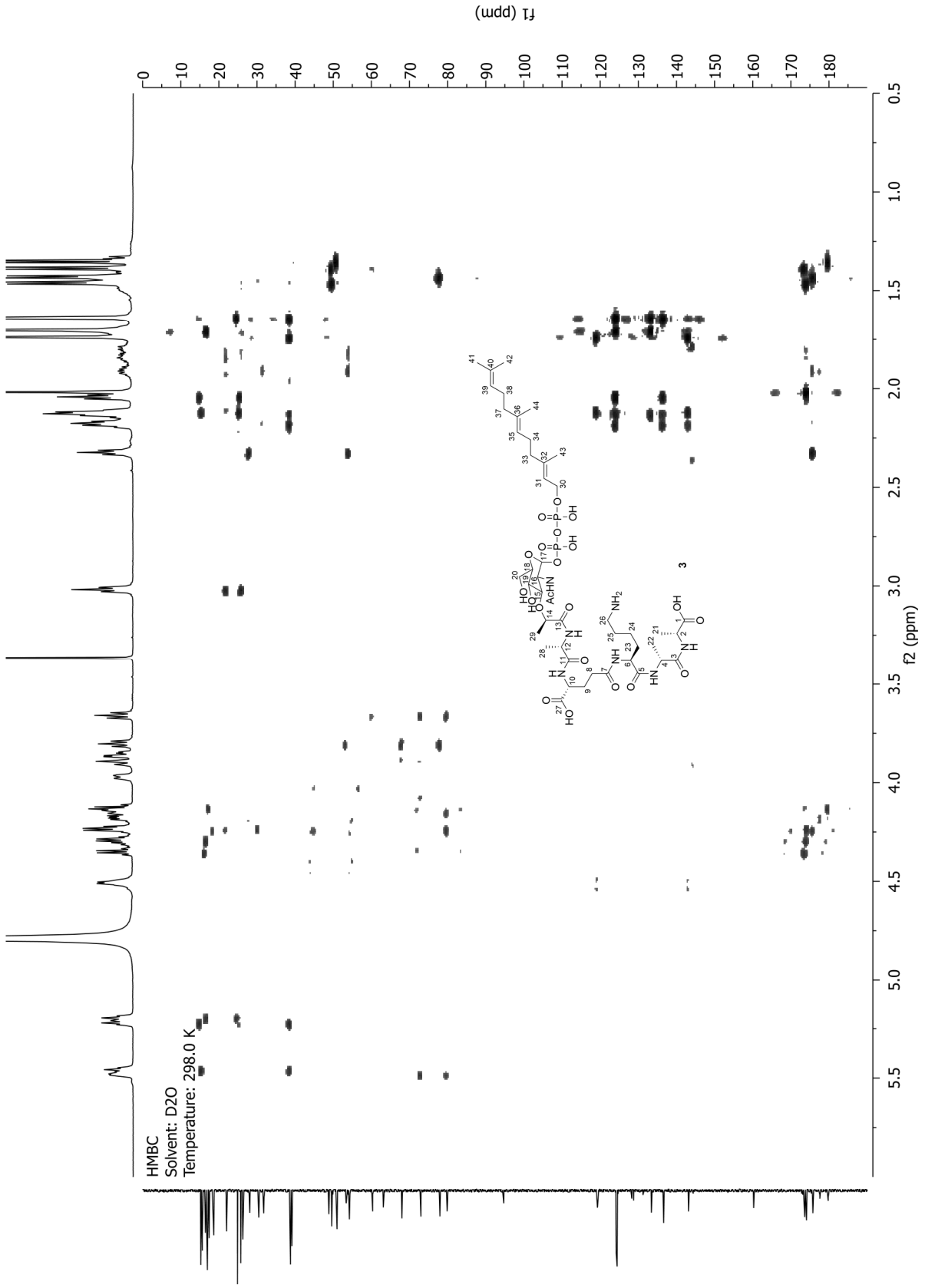

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K
3.37 MeOH
f1 (ppm)

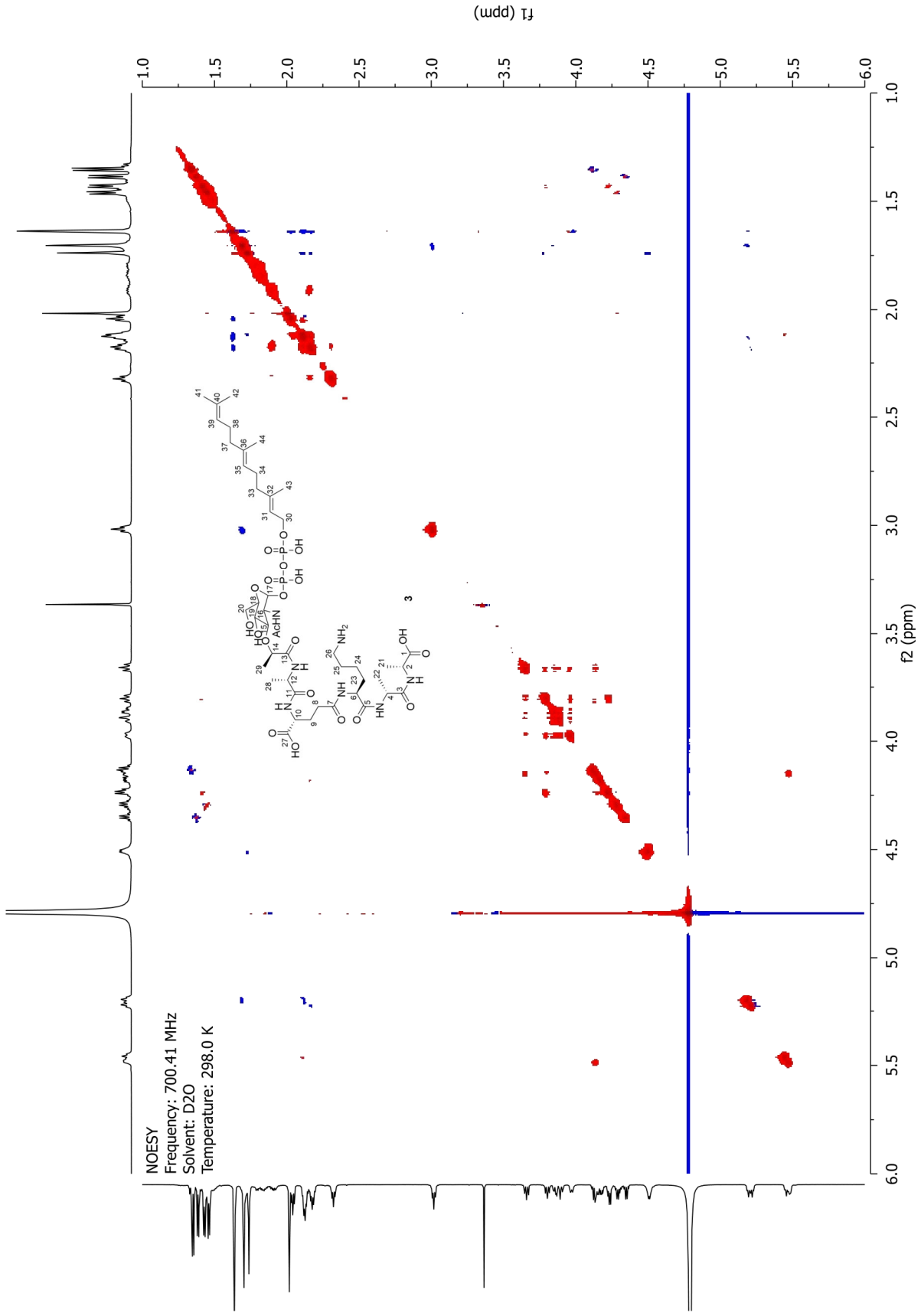

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: D2O
Temperature: 298.0 K
3
f1 (ppm)

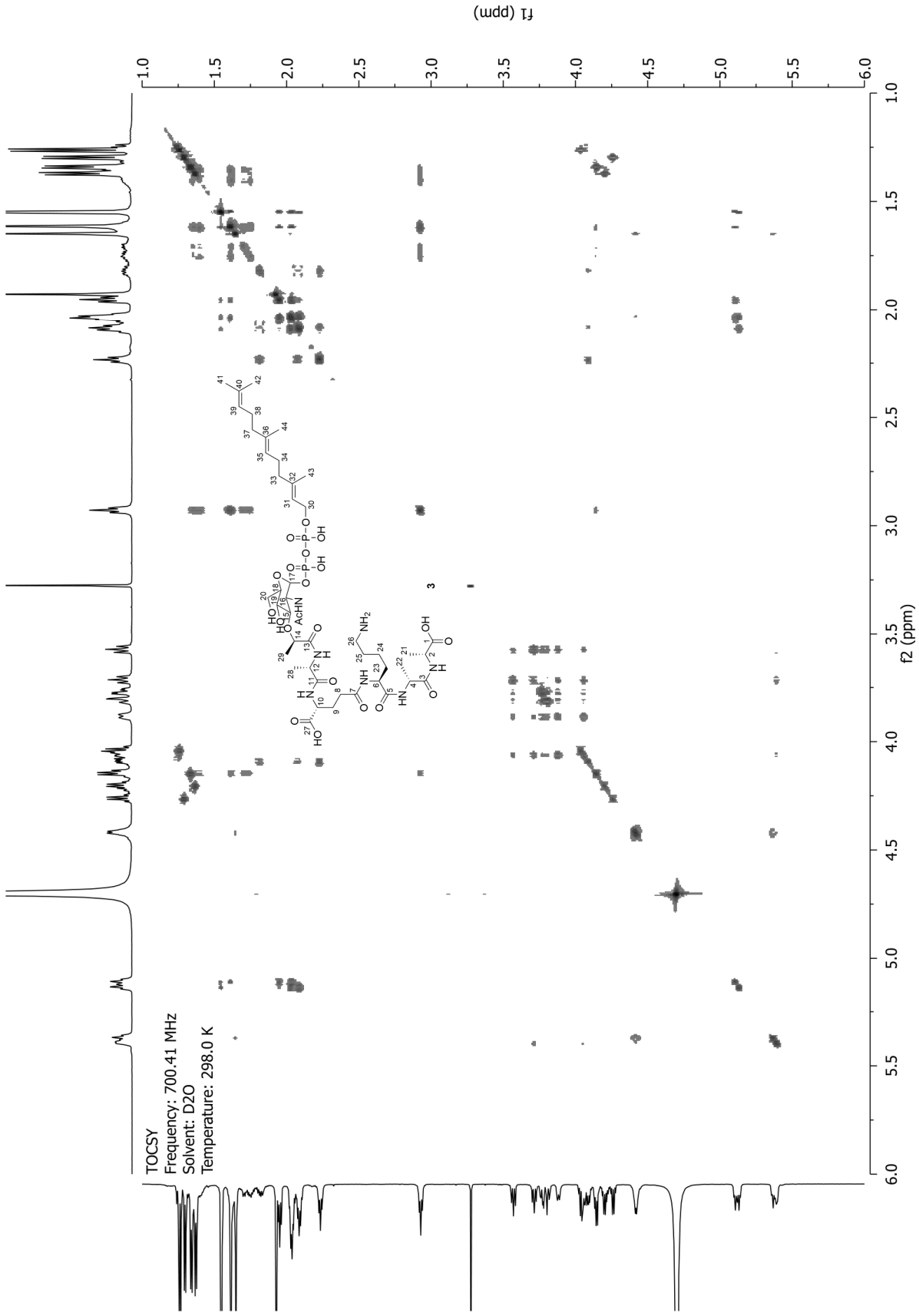

Nucleus: 31P
Frequency: 283.53 MHz
Solvent: D2O
Temperature: 298.0 K
-13.4
-13.3
-10.9
-10.8
f1 (ppm)

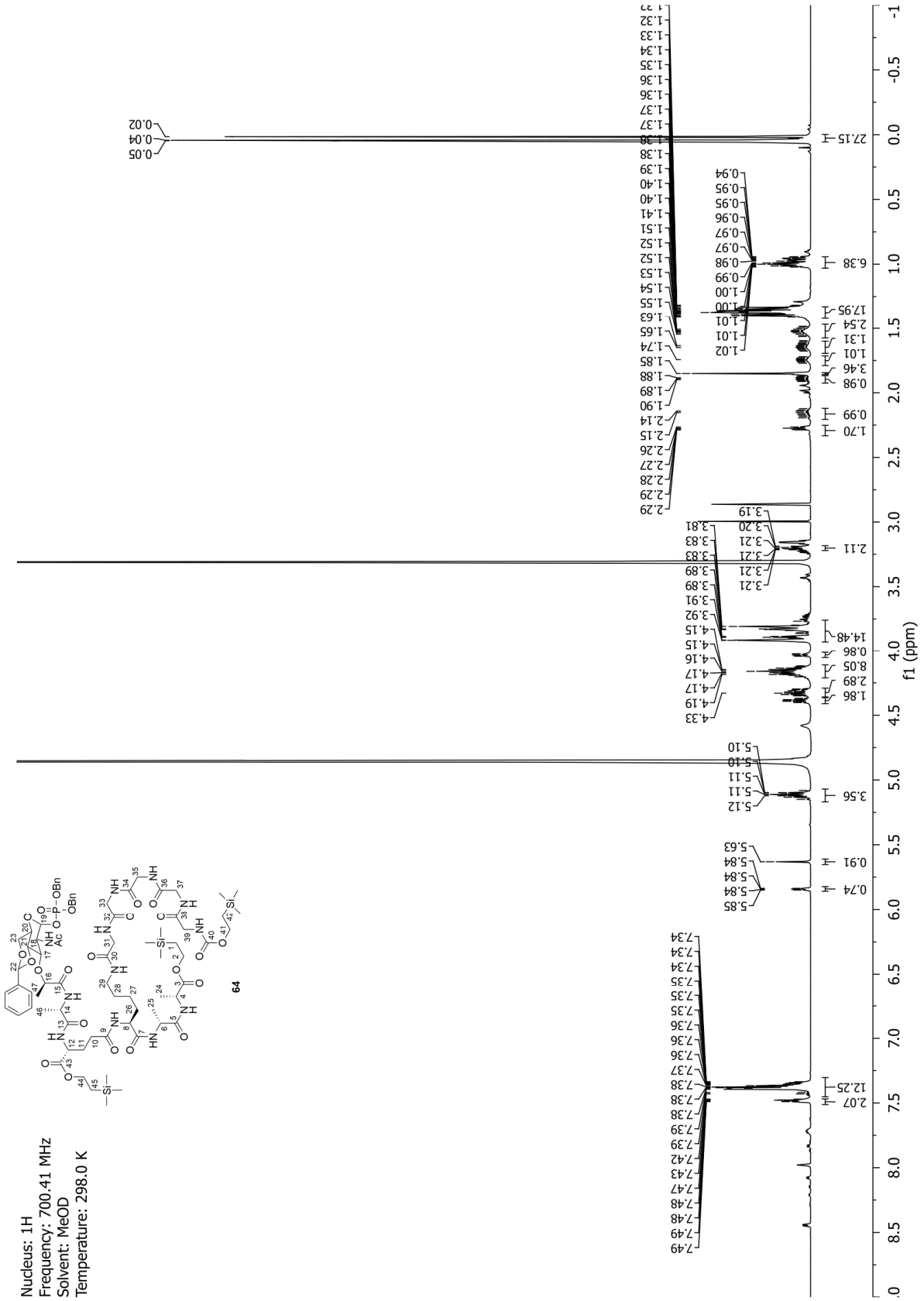

HH-COSY
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K
f2 (ppm)
f1 (ppm)
3

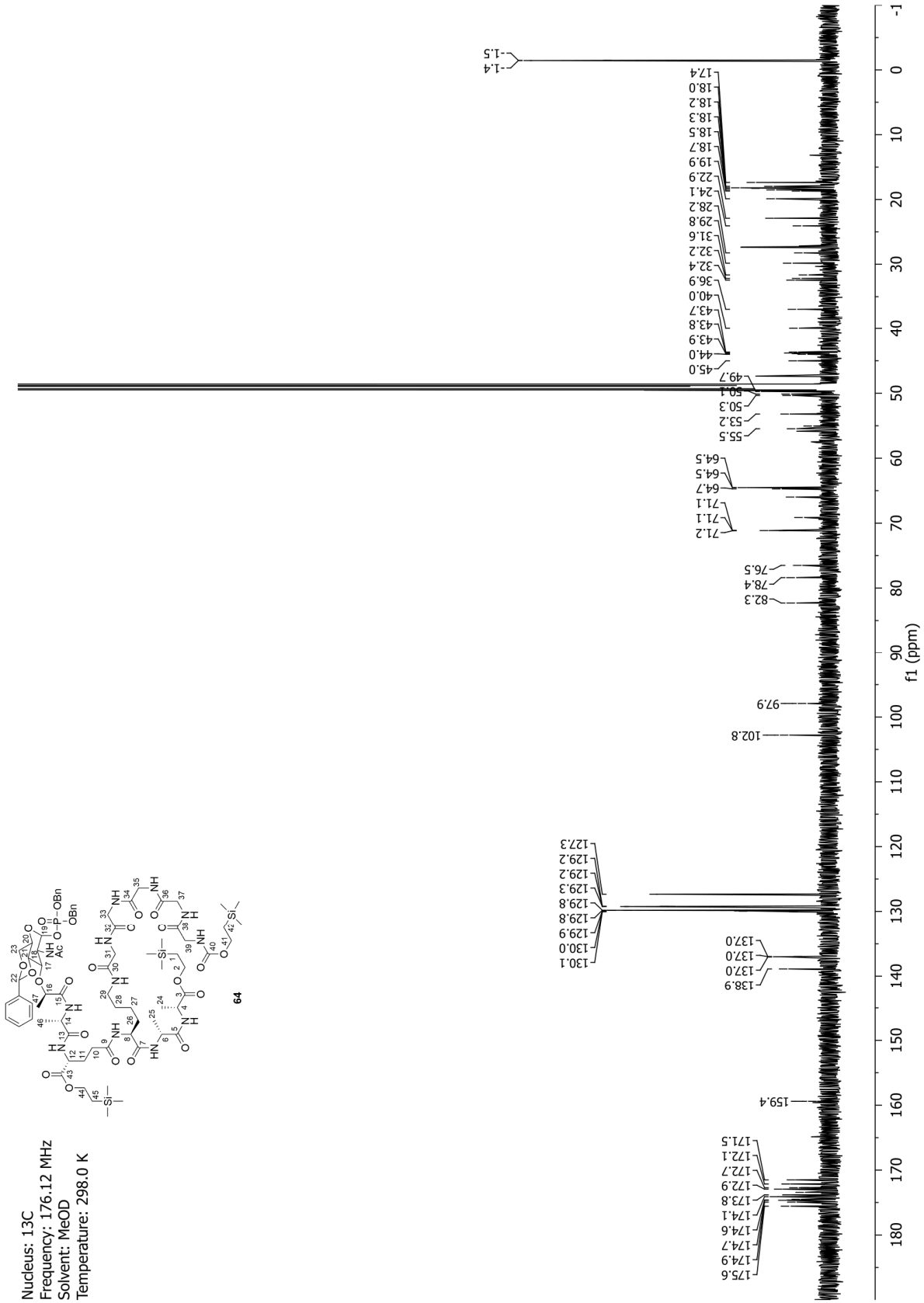

f1 (ppm)
f2 (ppm)
HSQC
Solvent: D2O
Temperature: 298.0 K

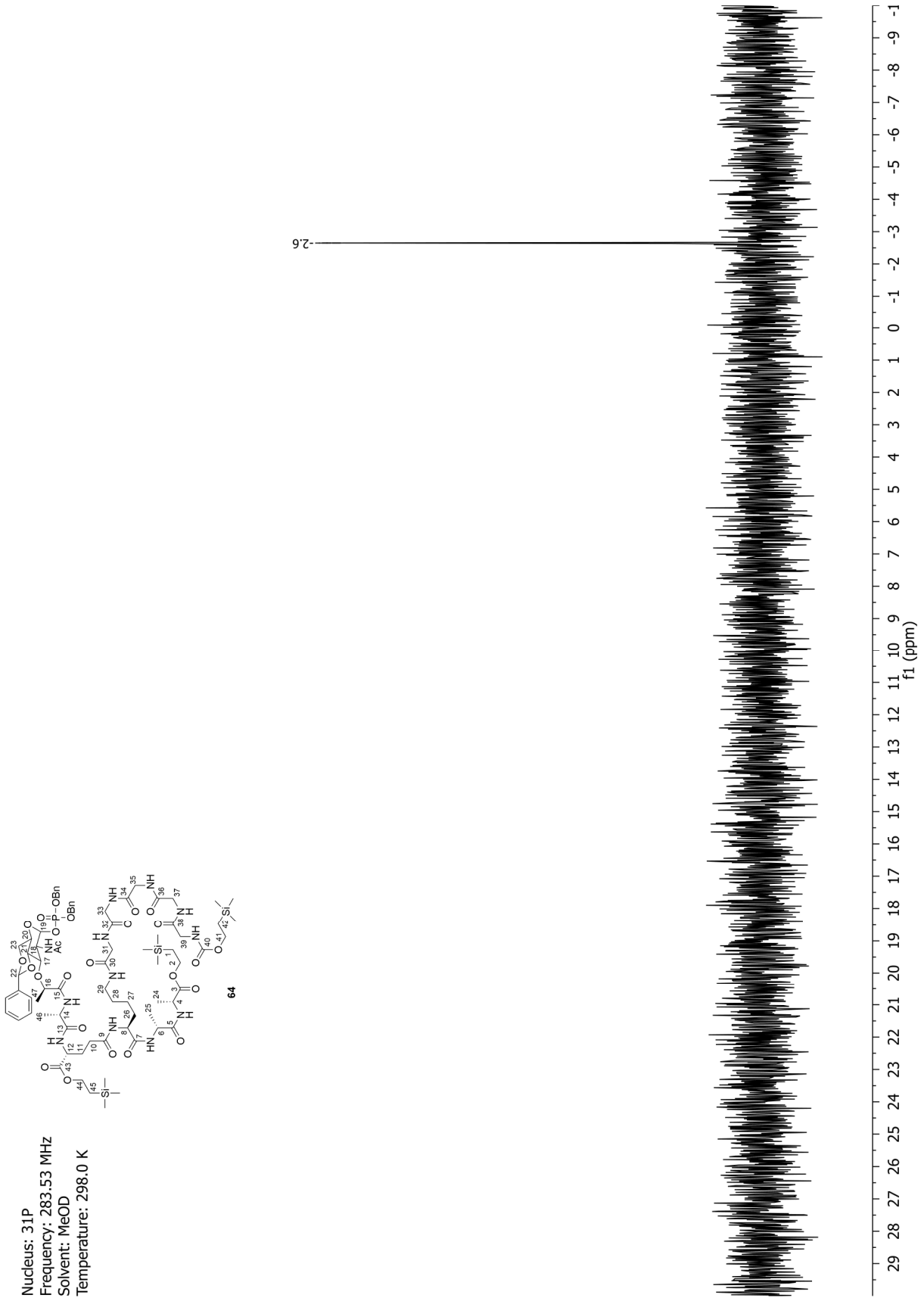

f1 (ppm)
f2 (ppm)
HMBC
Solvent: D2O
Temperature: 298.0 K

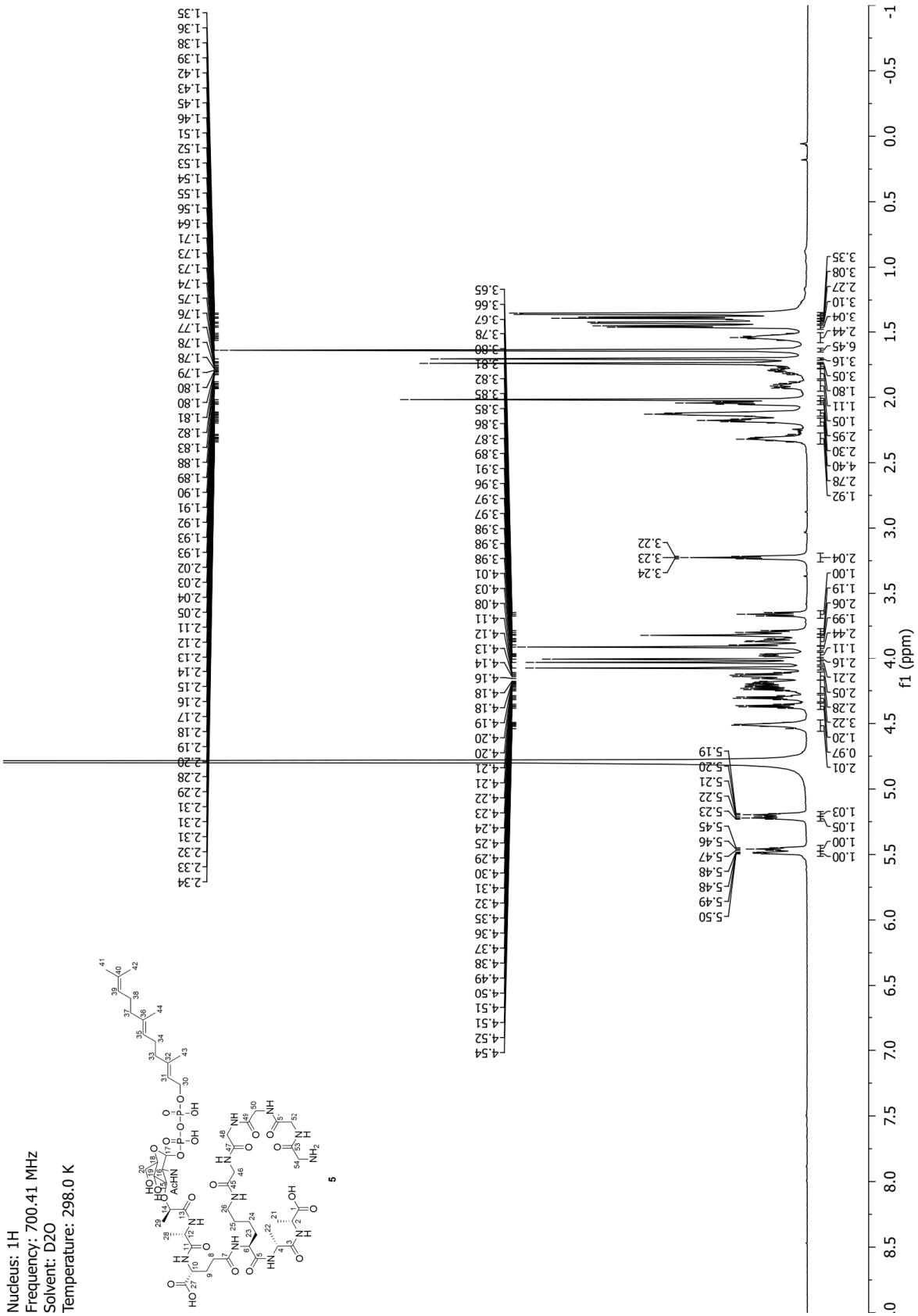

f1 (ppm)
f2 (ppm)
NOESY
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K

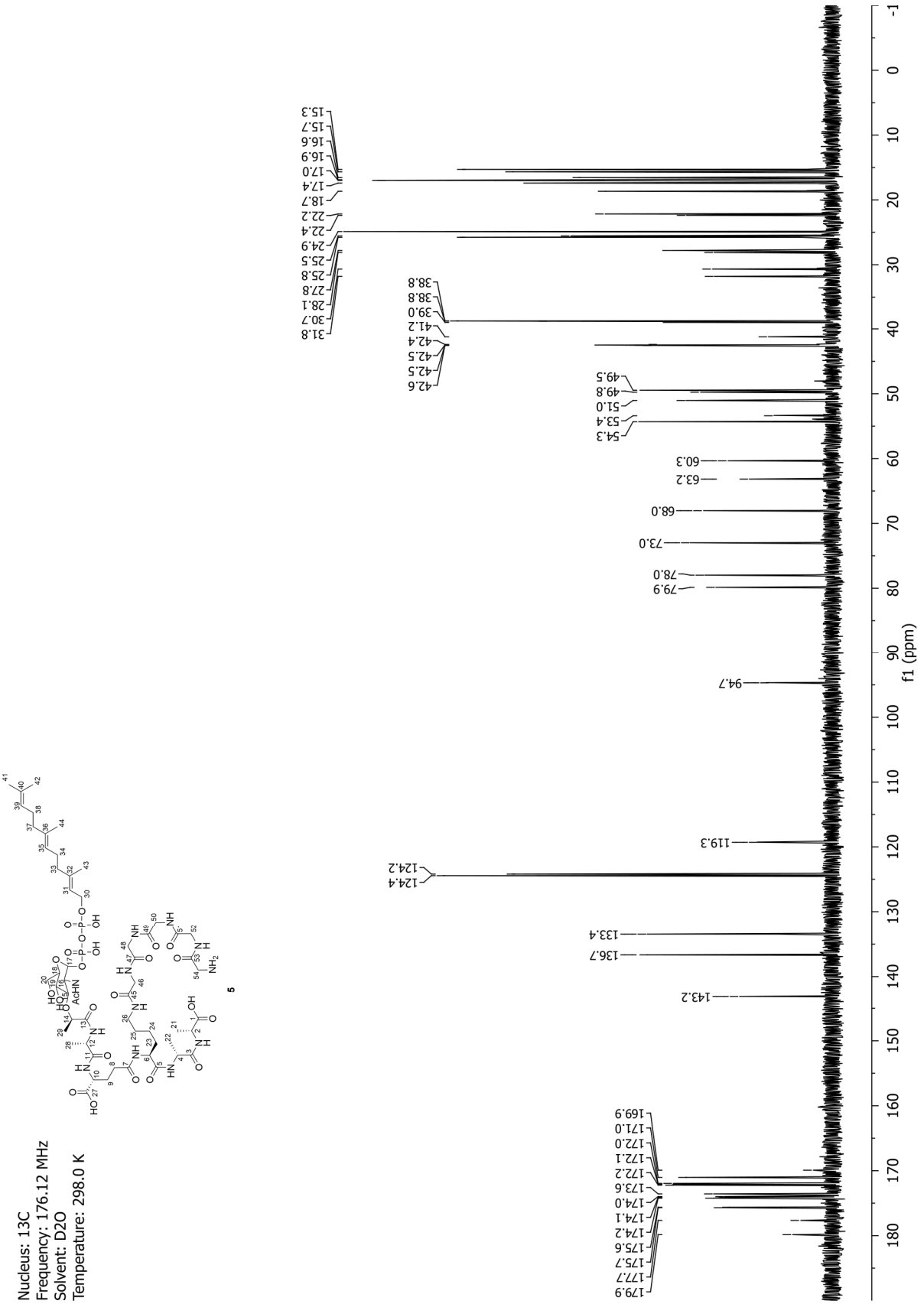

TOCSY
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K
f2 (ppm)
f1 (ppm)

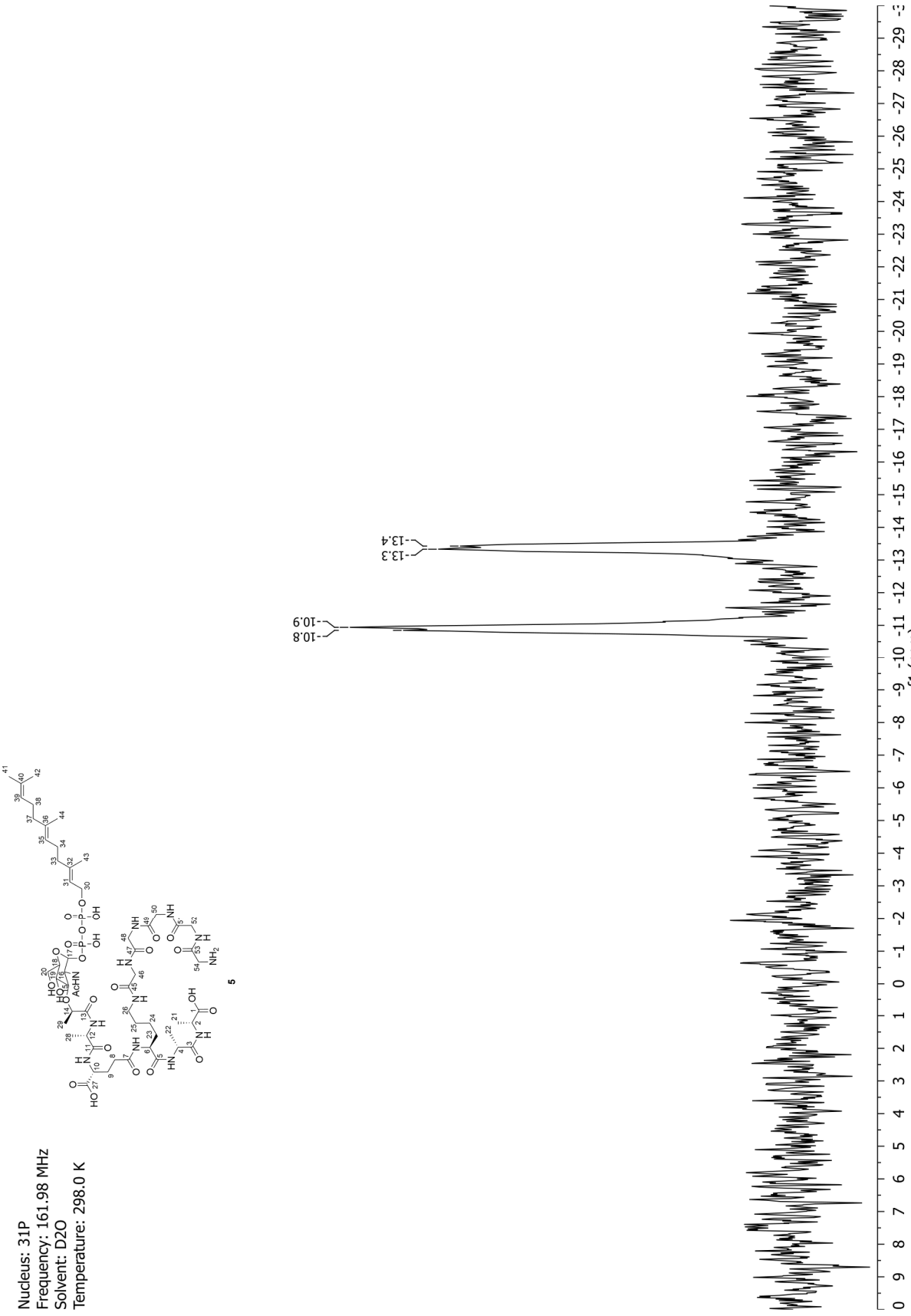

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: MeOD
Temperature: 298.0 K
64
f1 (ppm)

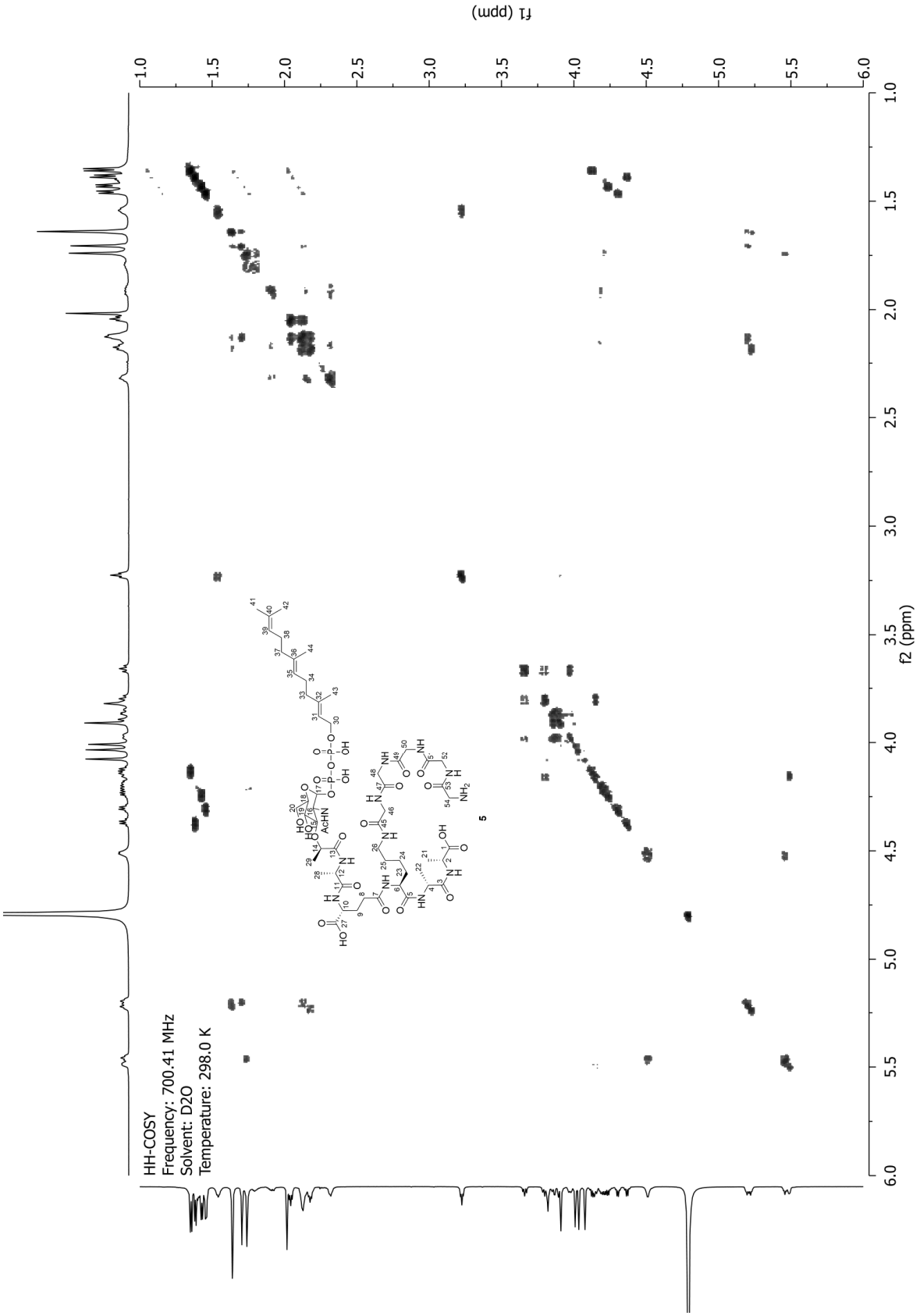

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: MeOD
Temperature: 298.0 K
64
f1 (ppm)

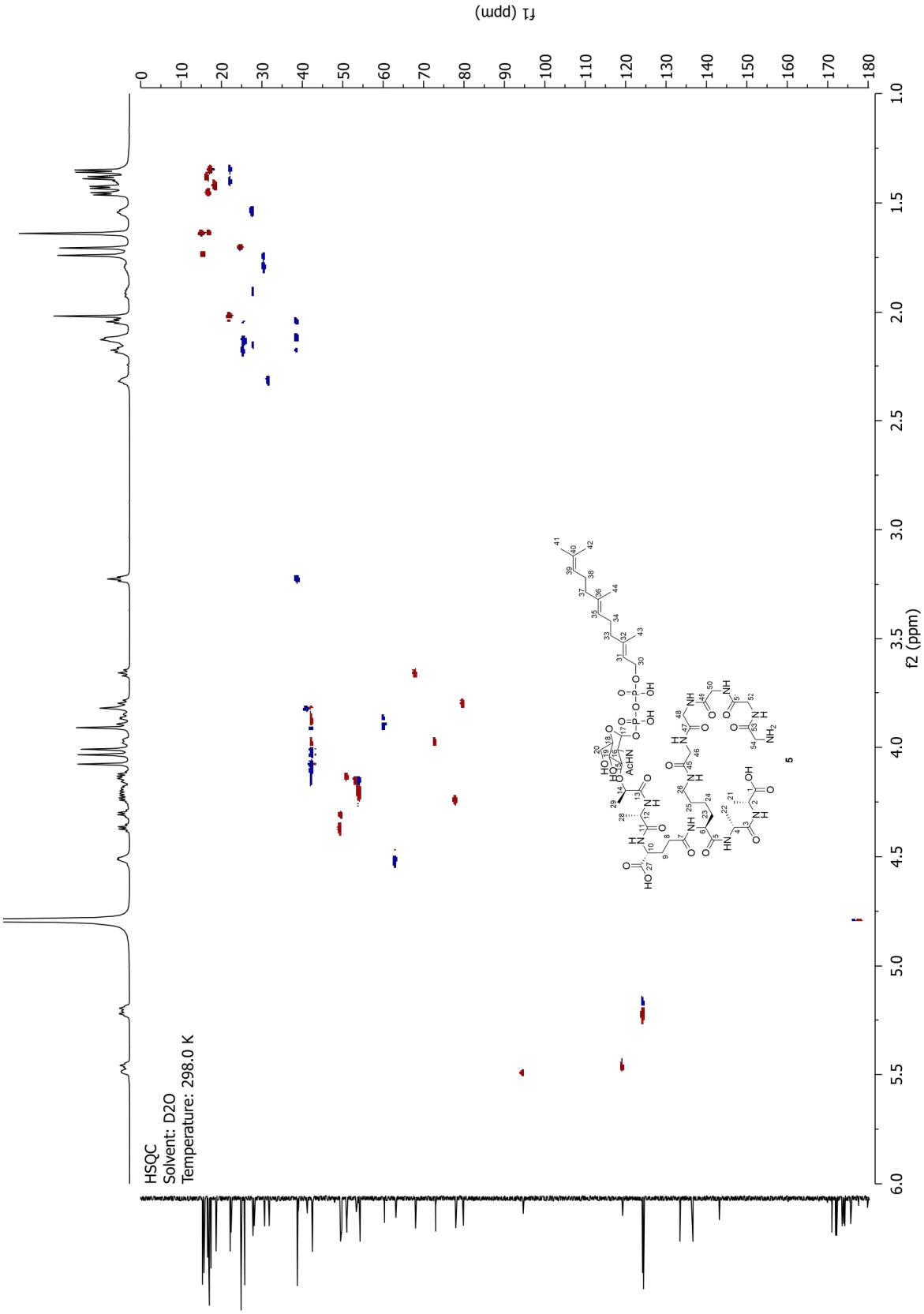

Nucleus: 31P
Frequency: 283.53 MHz
Solvent: MeOD
Temperature: 298.0 K
64
-2.6
f1 (ppm)

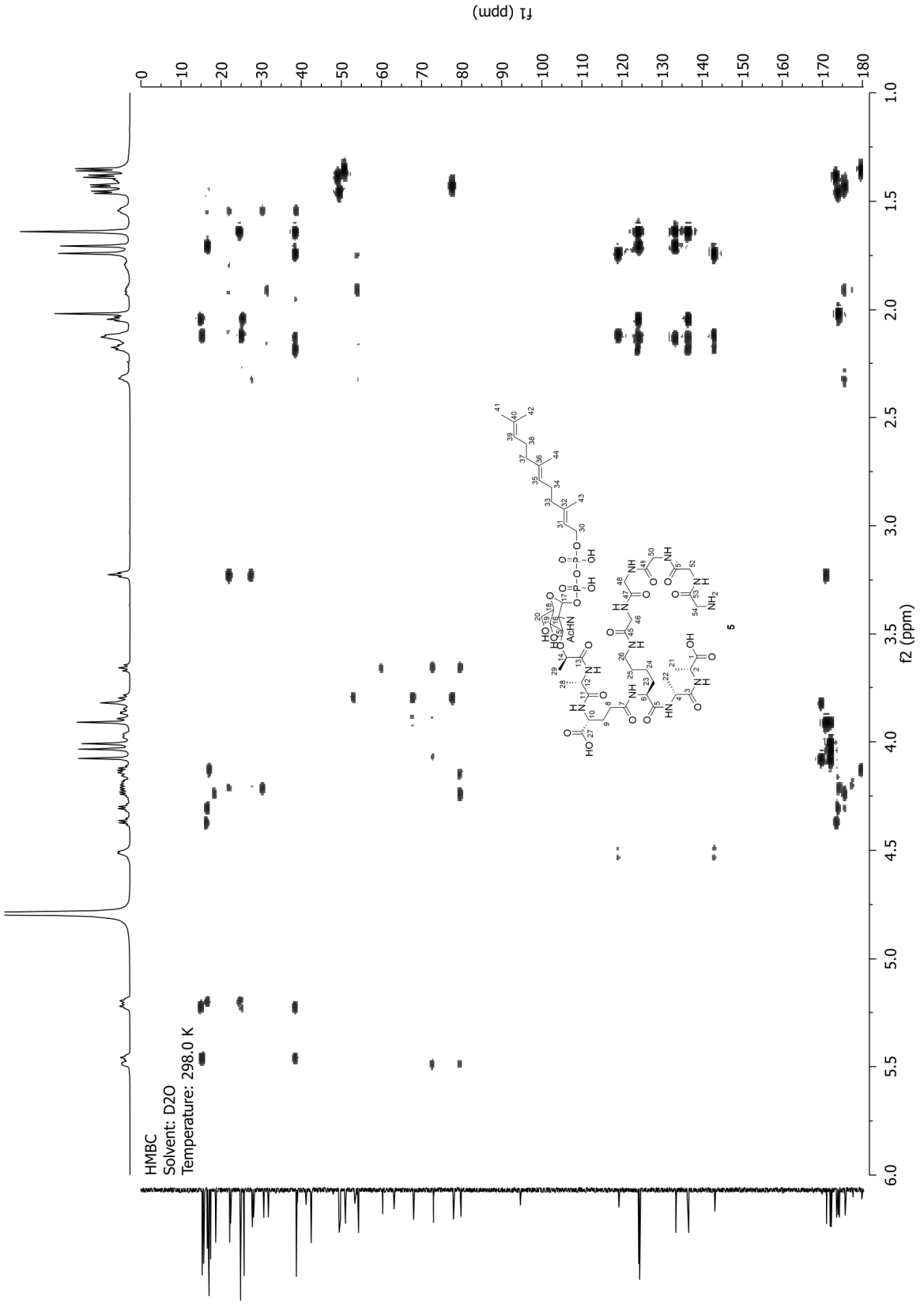

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K
f1 (ppm)

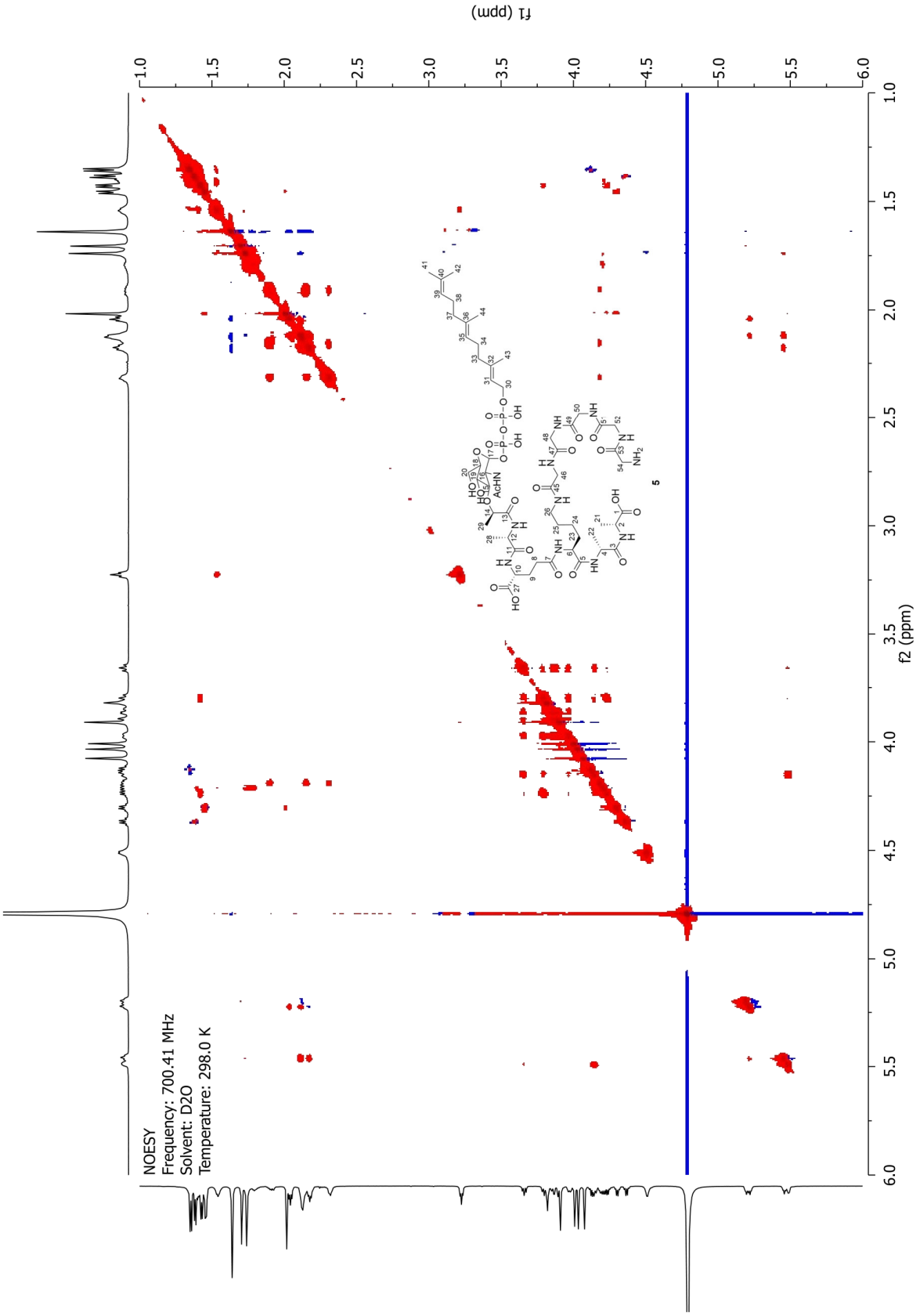

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: D2O
Temperature: 298.0 K
5
f1 (ppm)

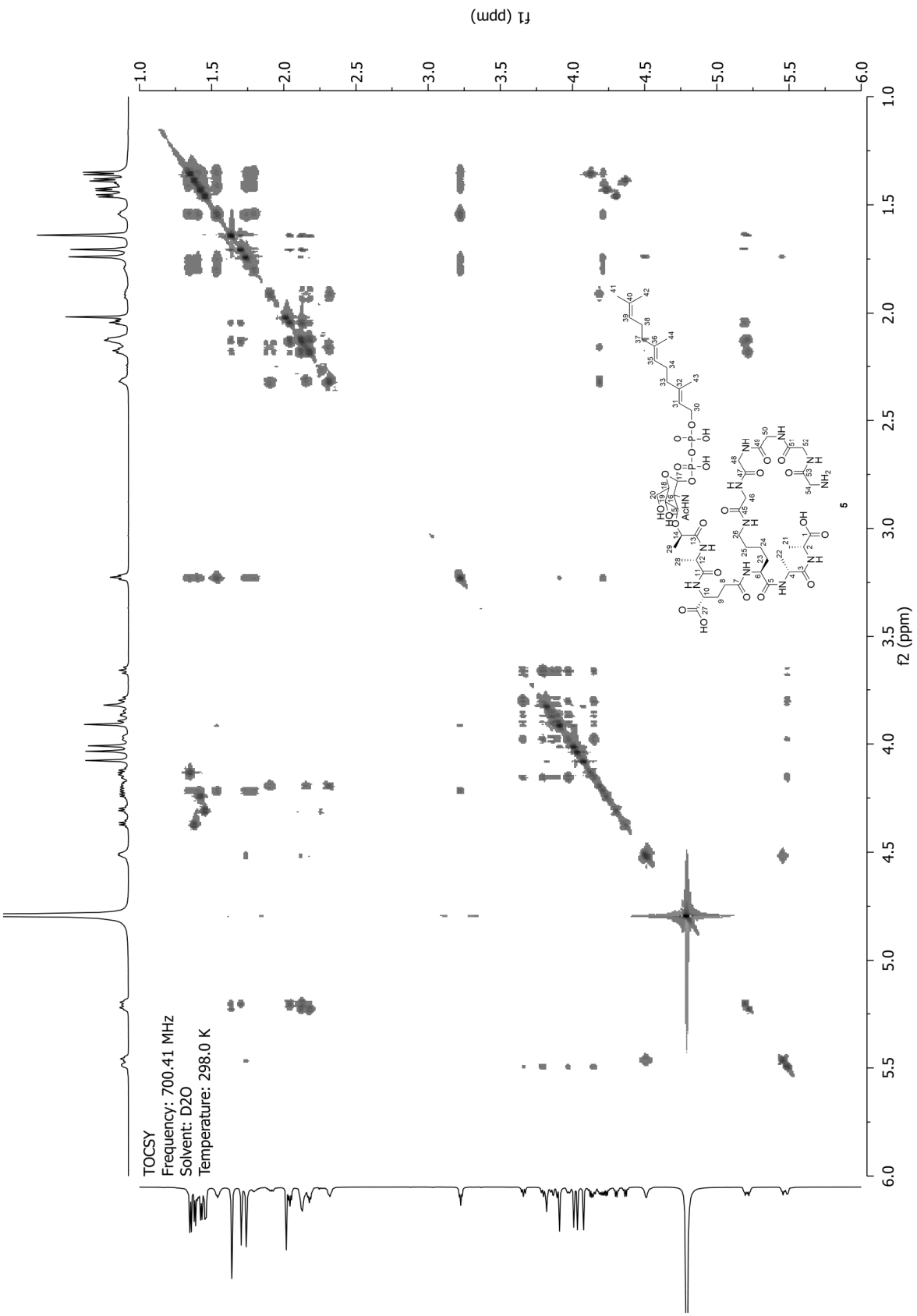

Nucleus: 31P
Frequency: 161.98 MHz
Solvent: D2O
Temperature: 298.0 K
5
-10.8
-10.9
-13.3
-13.4
f1 (ppm)

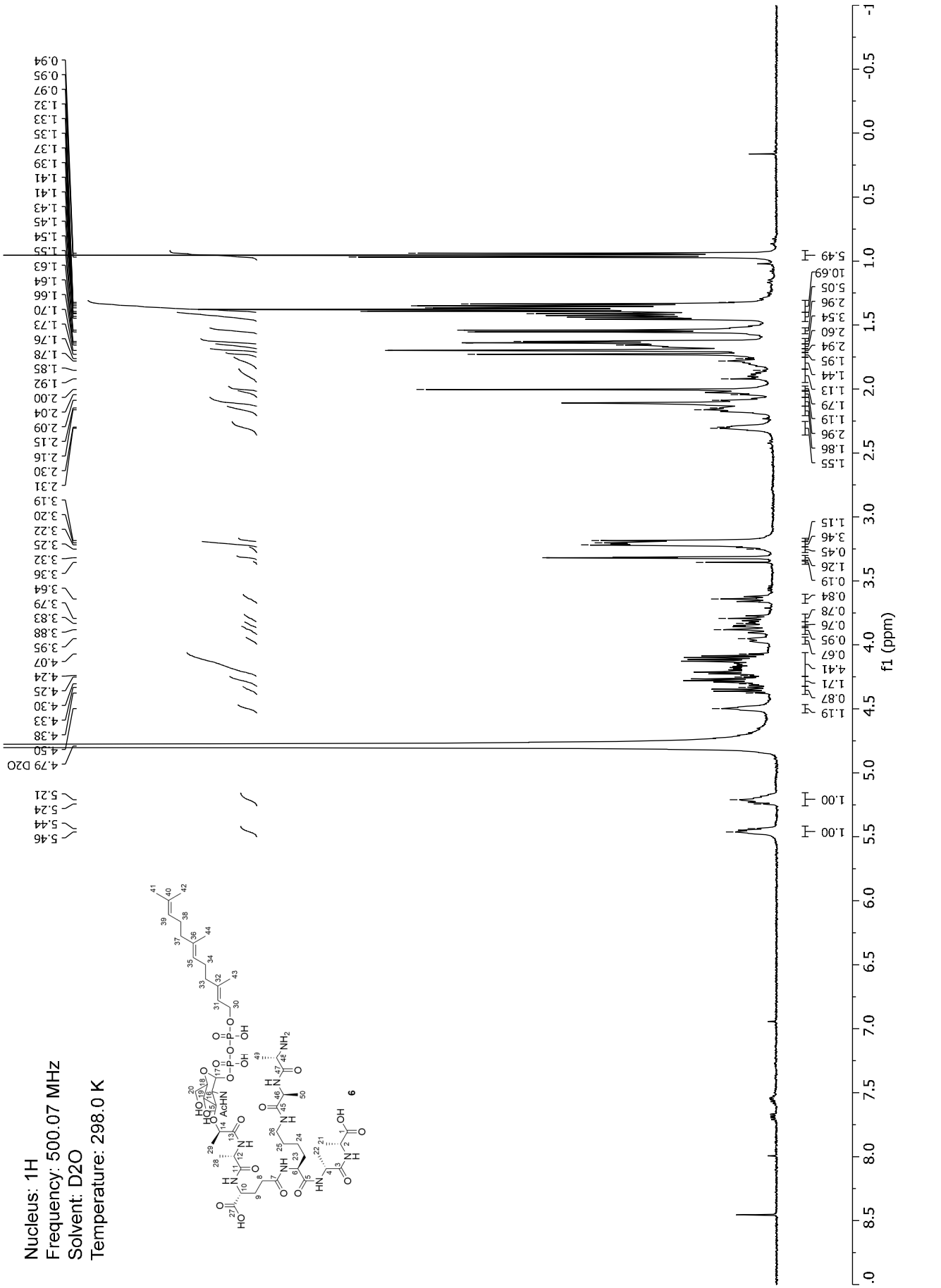

f1 (ppm)
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
f2 (ppm)
HH-COSY
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K
5

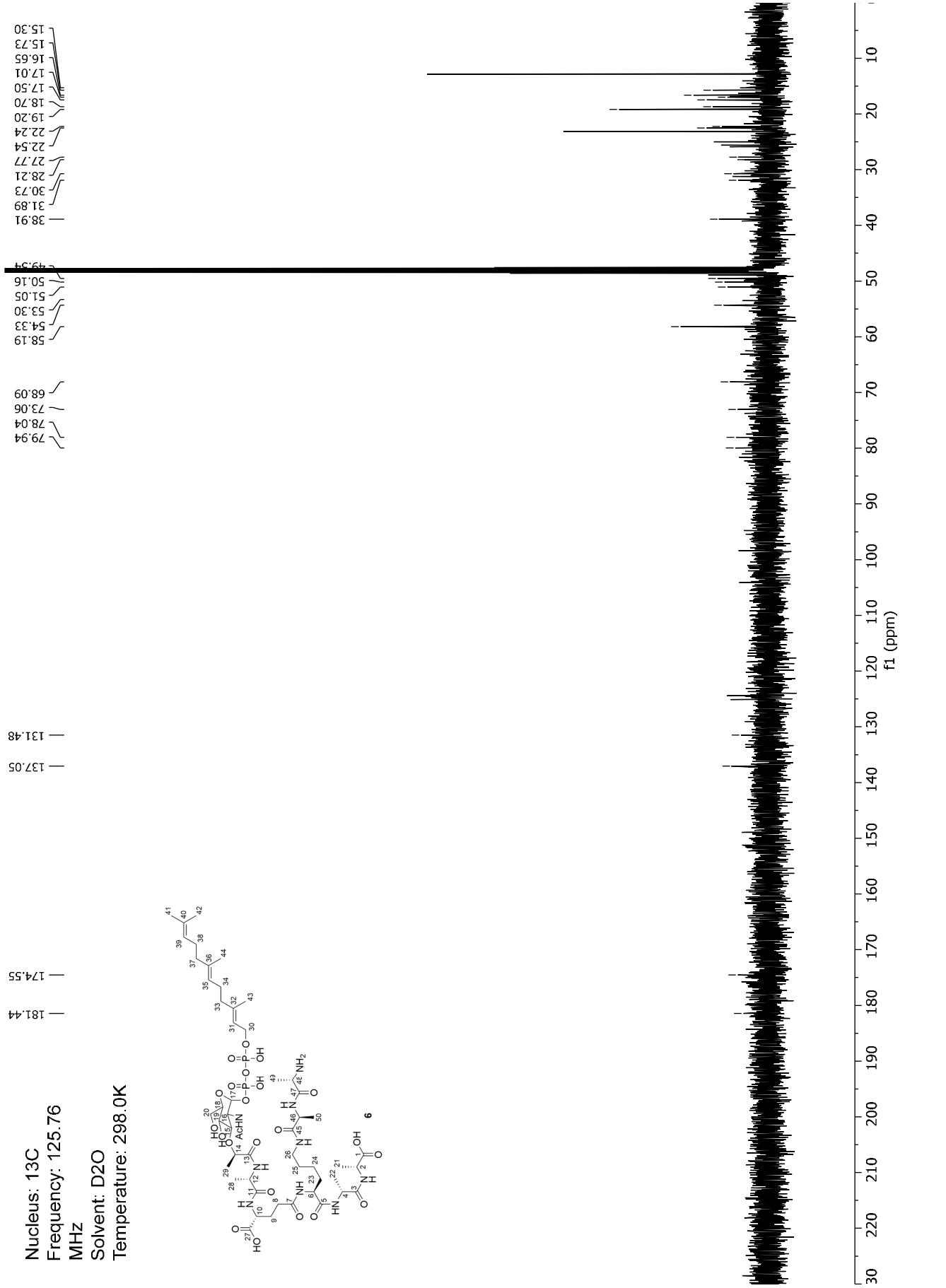

f1 (ppm)
f2 (ppm)
HSQC
Solvent: D2O
Temperature: 298.0 K
5

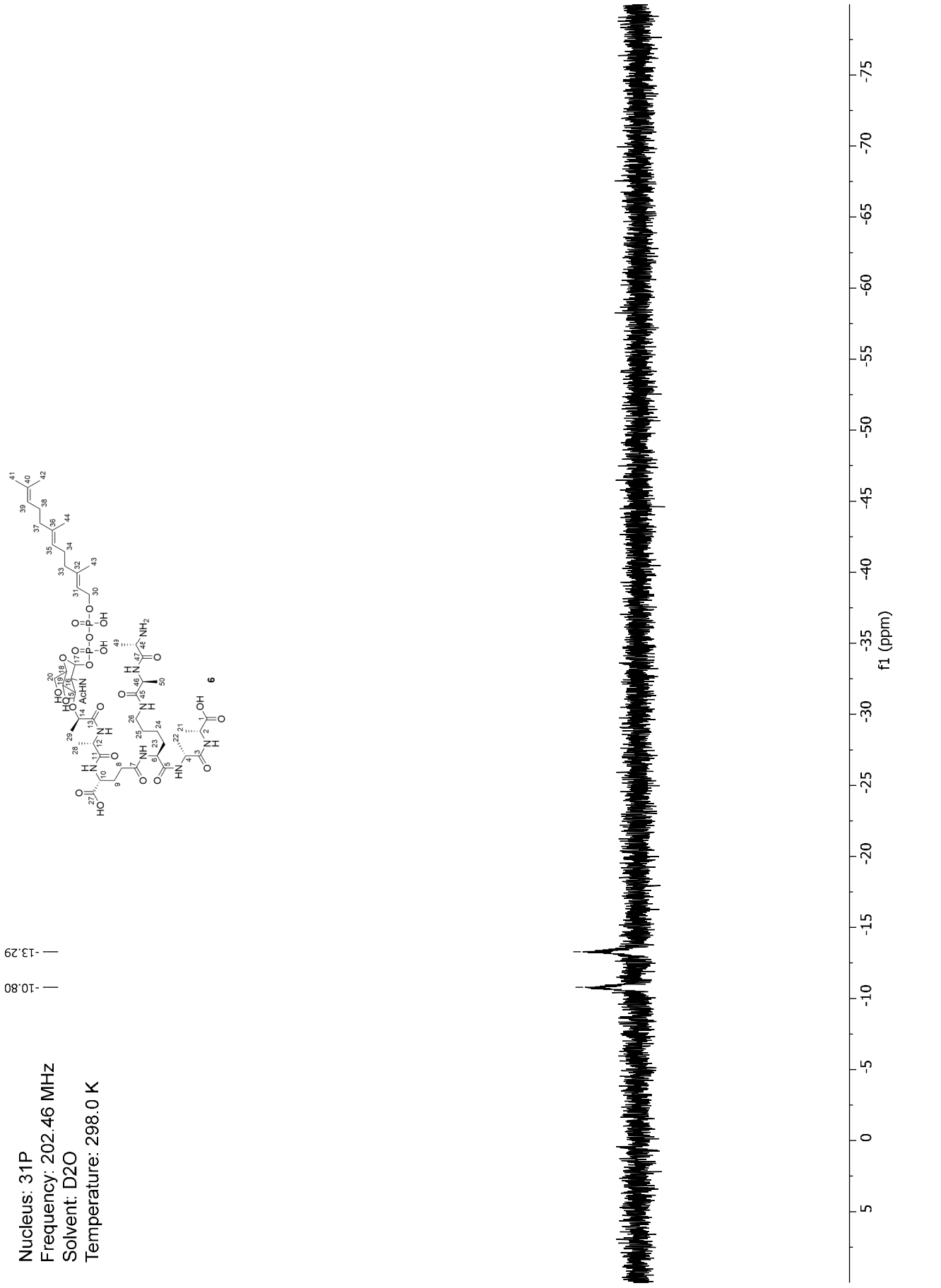

f1 (ppm)
f2 (ppm)
HMBC
Solvent: D2O
Temperature: 298.0 K
5

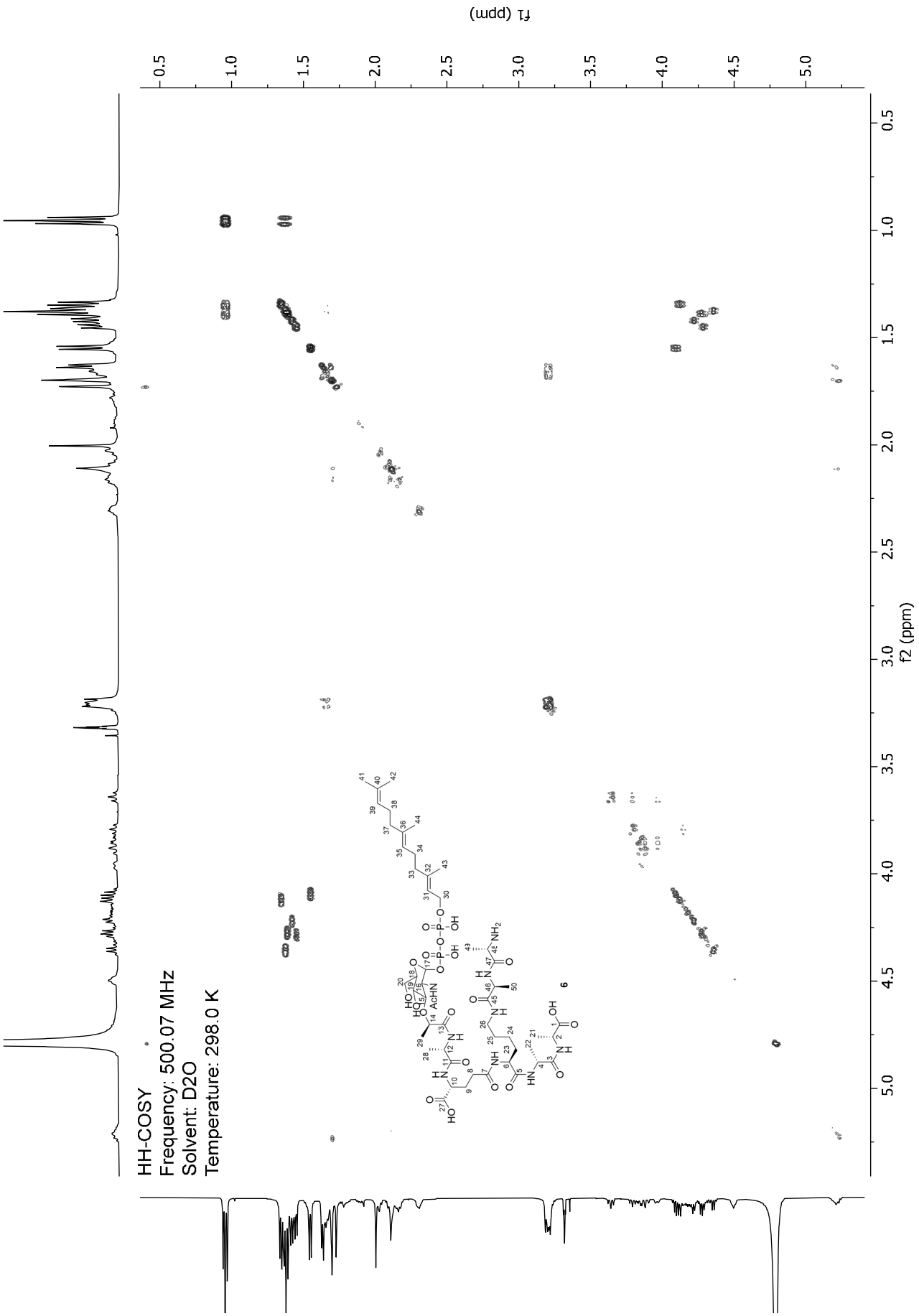

f1 (ppm)
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
f2 (ppm)
NOESY
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K

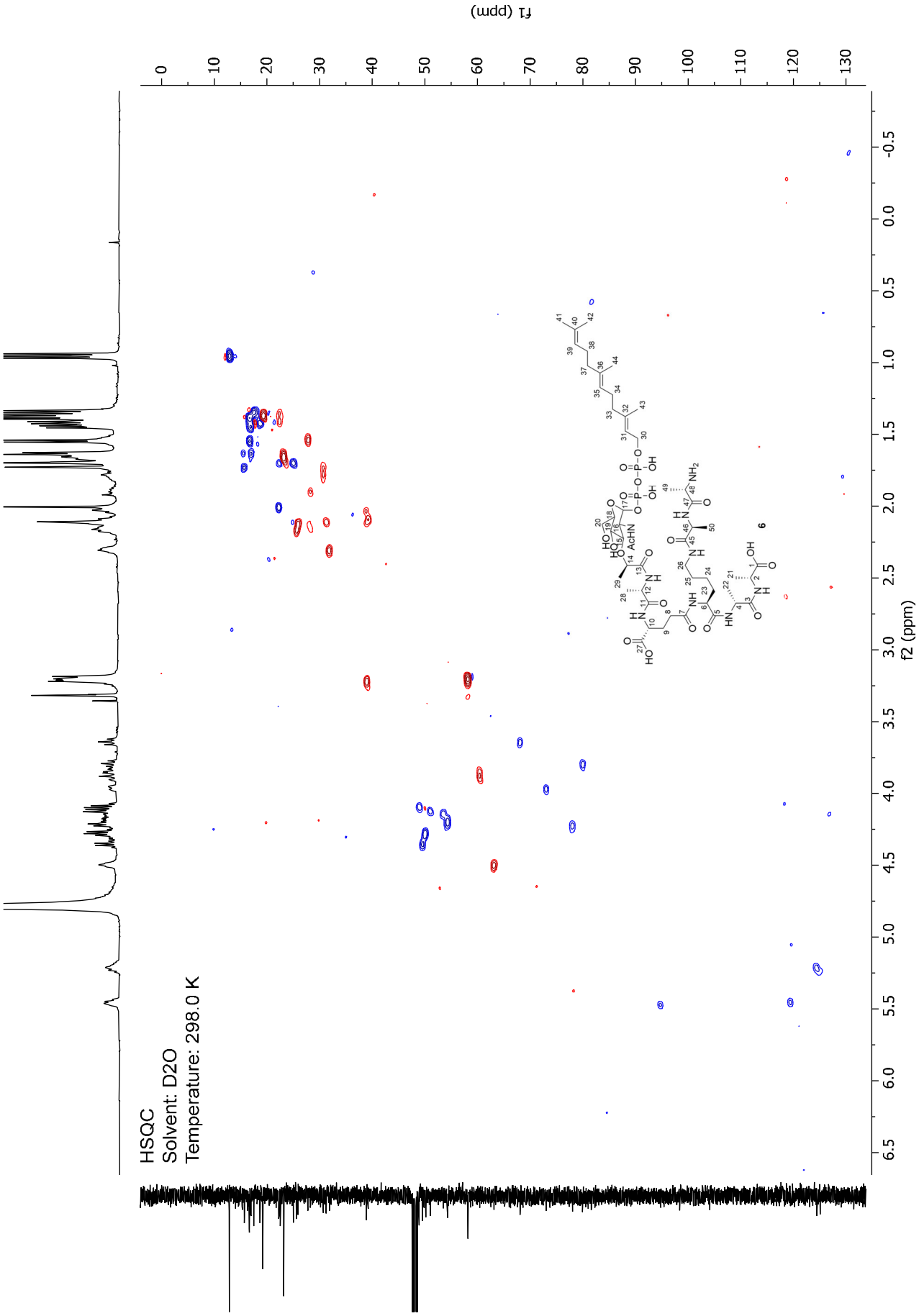

f1 (ppm)
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
f2 (ppm)
TOCSY
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K

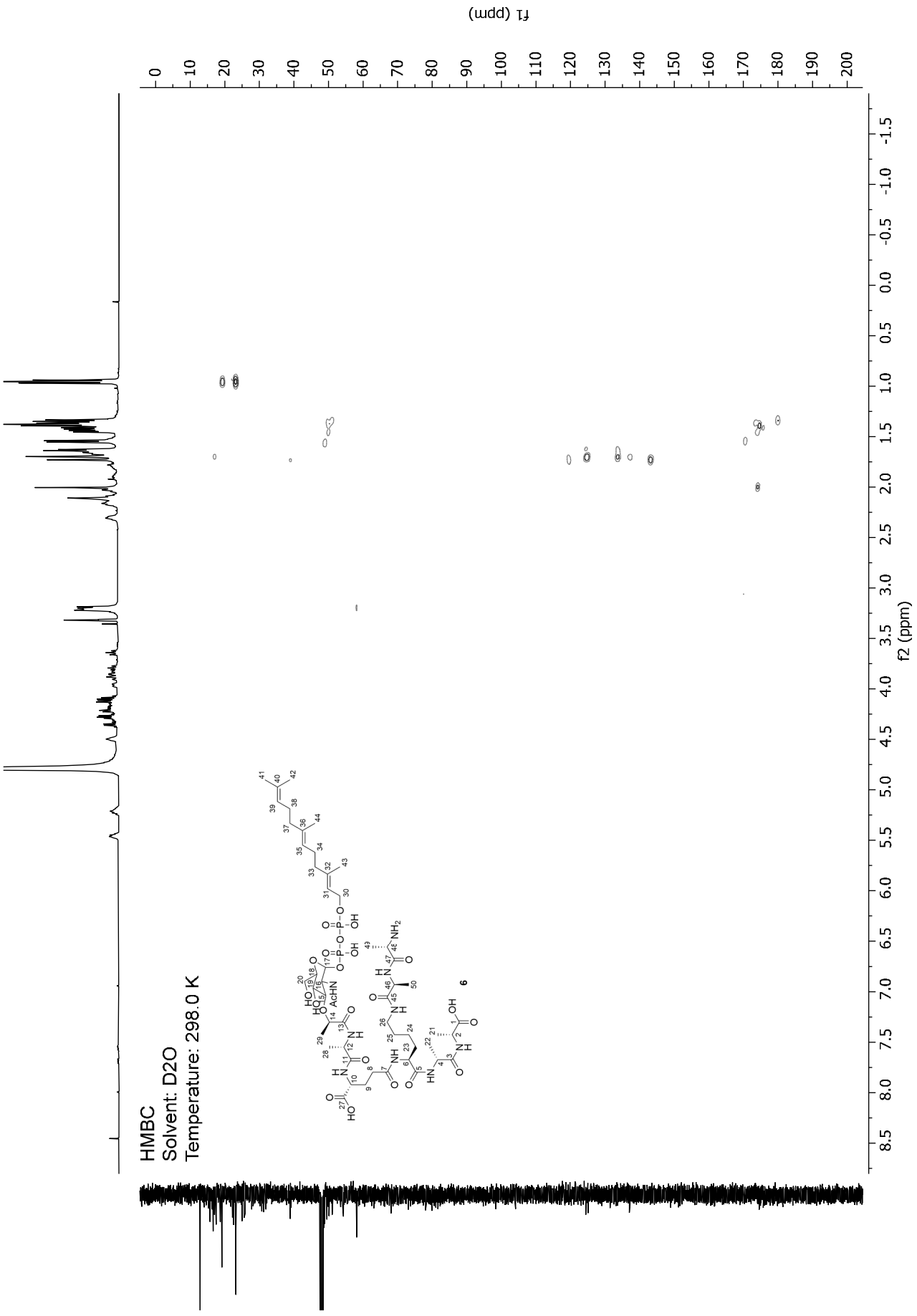

Nucleus: 1H
Frequency: 500.07 MHz
Solvent: D2O
Temperature: 298.0 K
f1 (ppm)
4.79 D2O
6

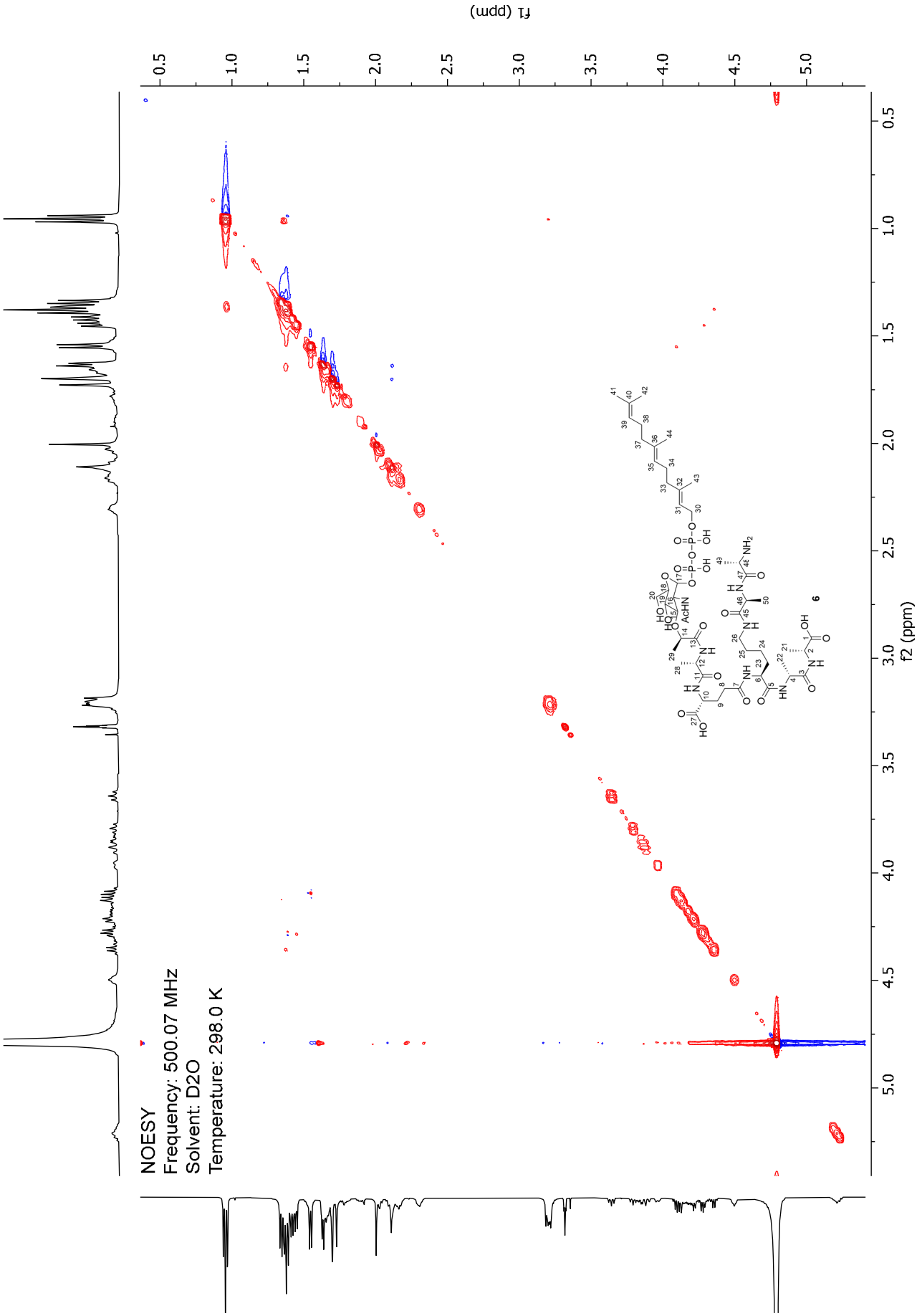

Nucleus: 13C
Frequency: 125.76 MHz
Solvent: D2O
Temperature: 298.0K
15.30
15.73
16.65
17.01
17.50
18.70
19.20
22.24
22.54
27.77
28.21
30.73
31.89
38.91
49.54
50.16
51.05
53.30
54.33
58.19
68.09
73.06
78.04
79.94
131.48
137.05
174.55
181.44
f1 (ppm)
6

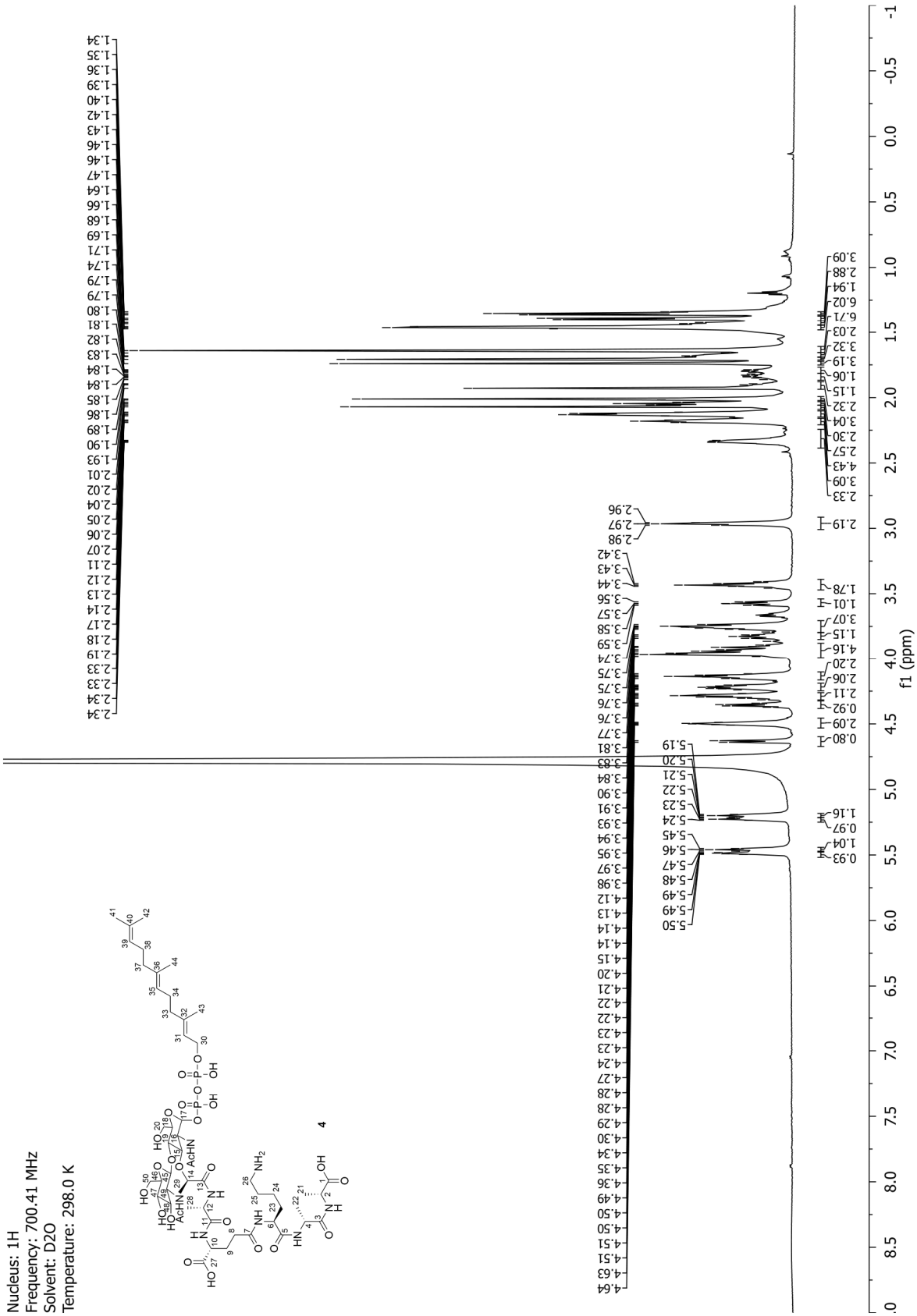

Nucleus: 31P
Frequency: 202.46 MHz
Solvent: D2O
Temperature: 298.0 K
-13.29
-10.80
6
f1 (ppm)

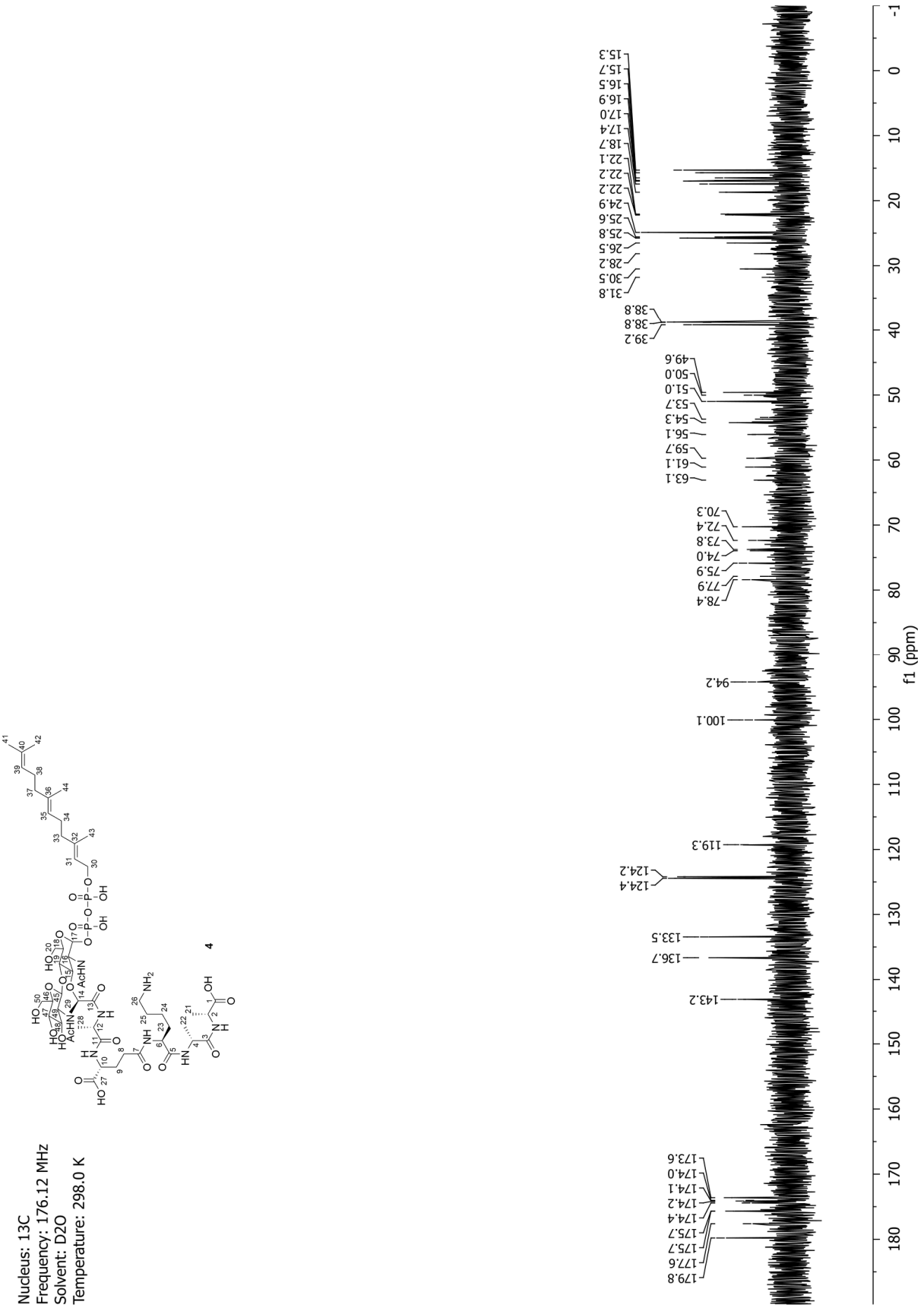

HH-COSY
Frequency: 500.07 MHz
Solvent: D2O
Temperature: 298.0 K
f2 (ppm)
f1 (ppm)
6

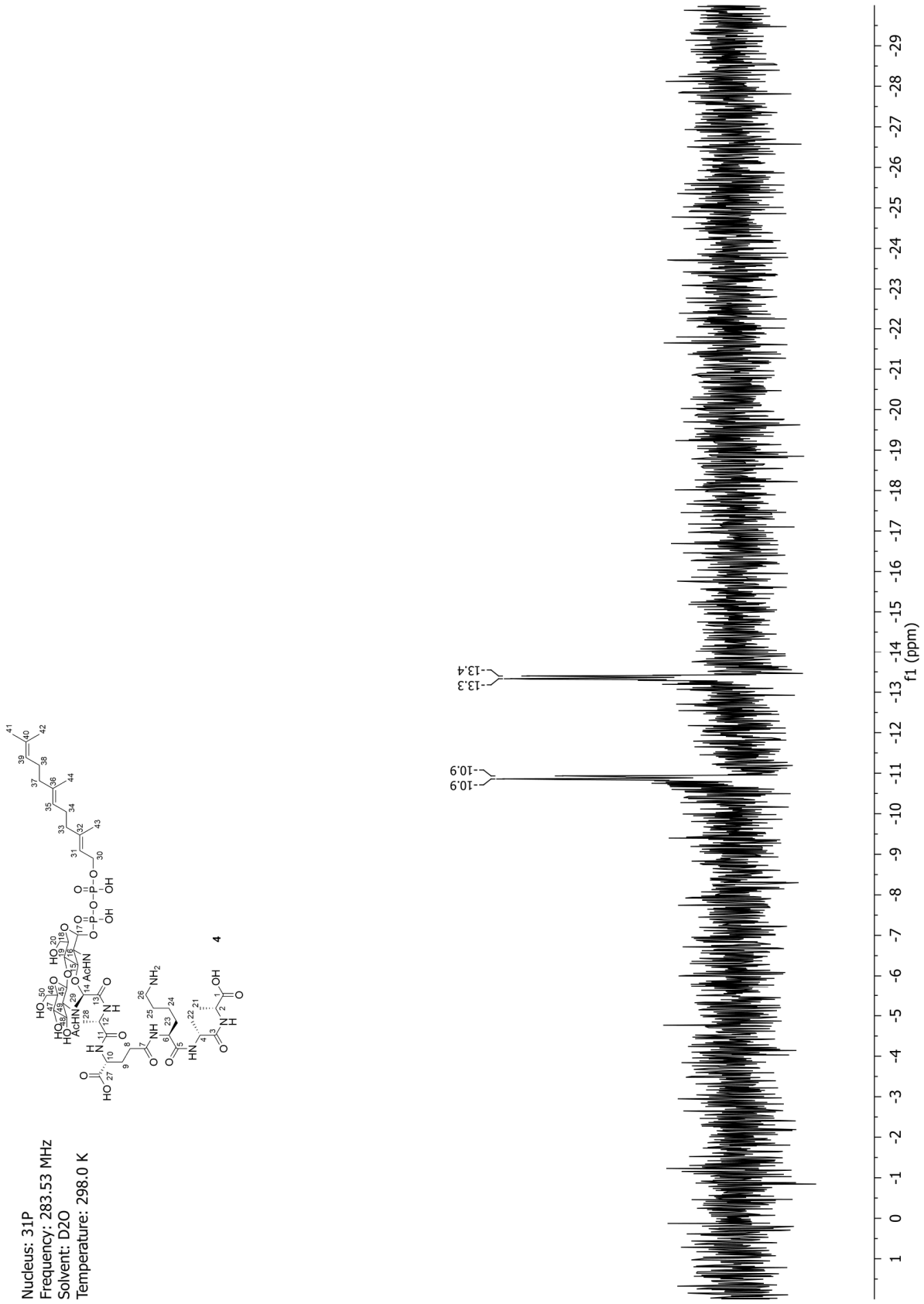

HSQC
Solvent: D2O
Temperature: 298.0 K
f1 (ppm)
f2 (ppm)
6

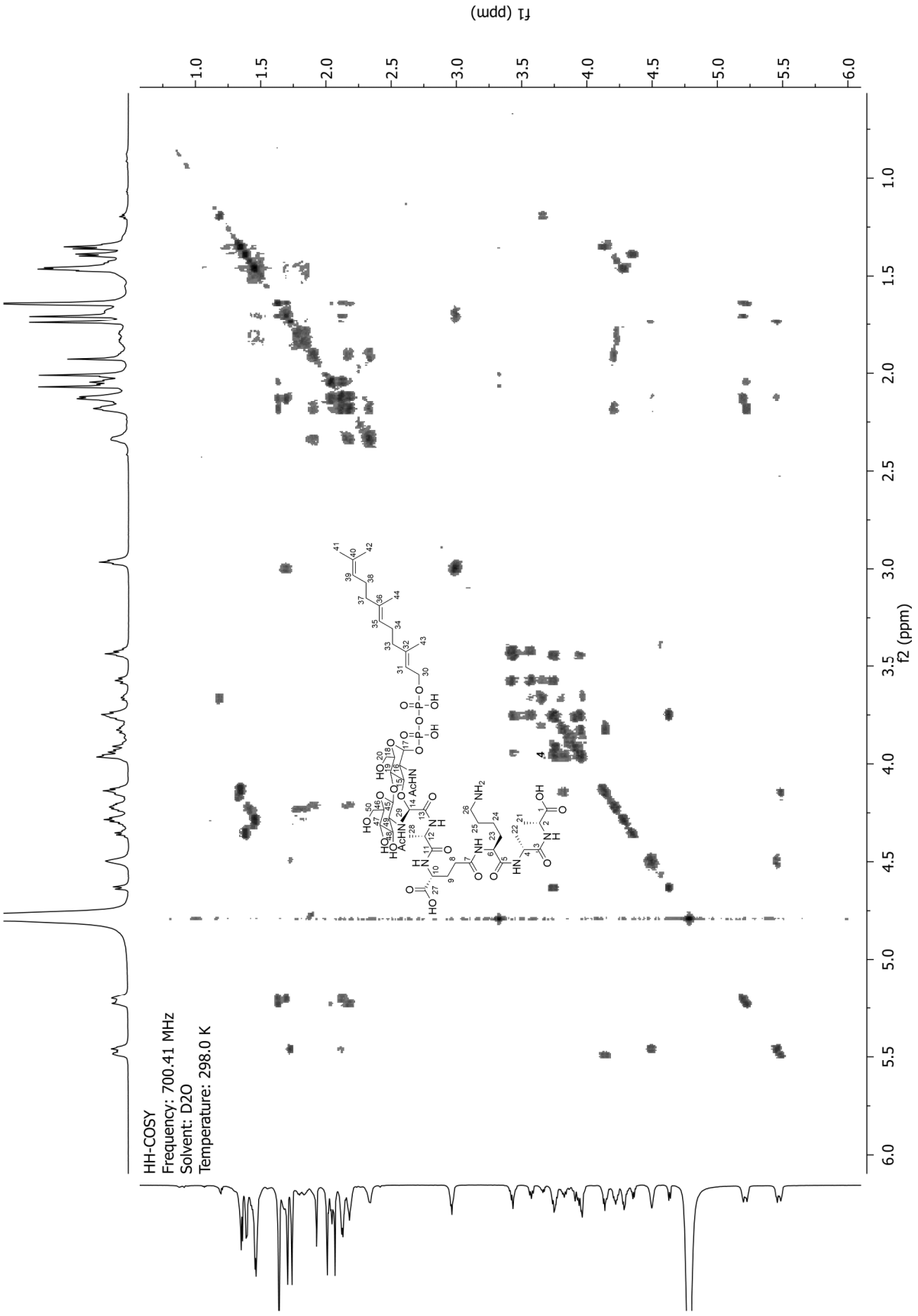

HMBC
Solvent: D2O
Temperature: 298.0 K
f2 (ppm)
f1 (ppm)
6

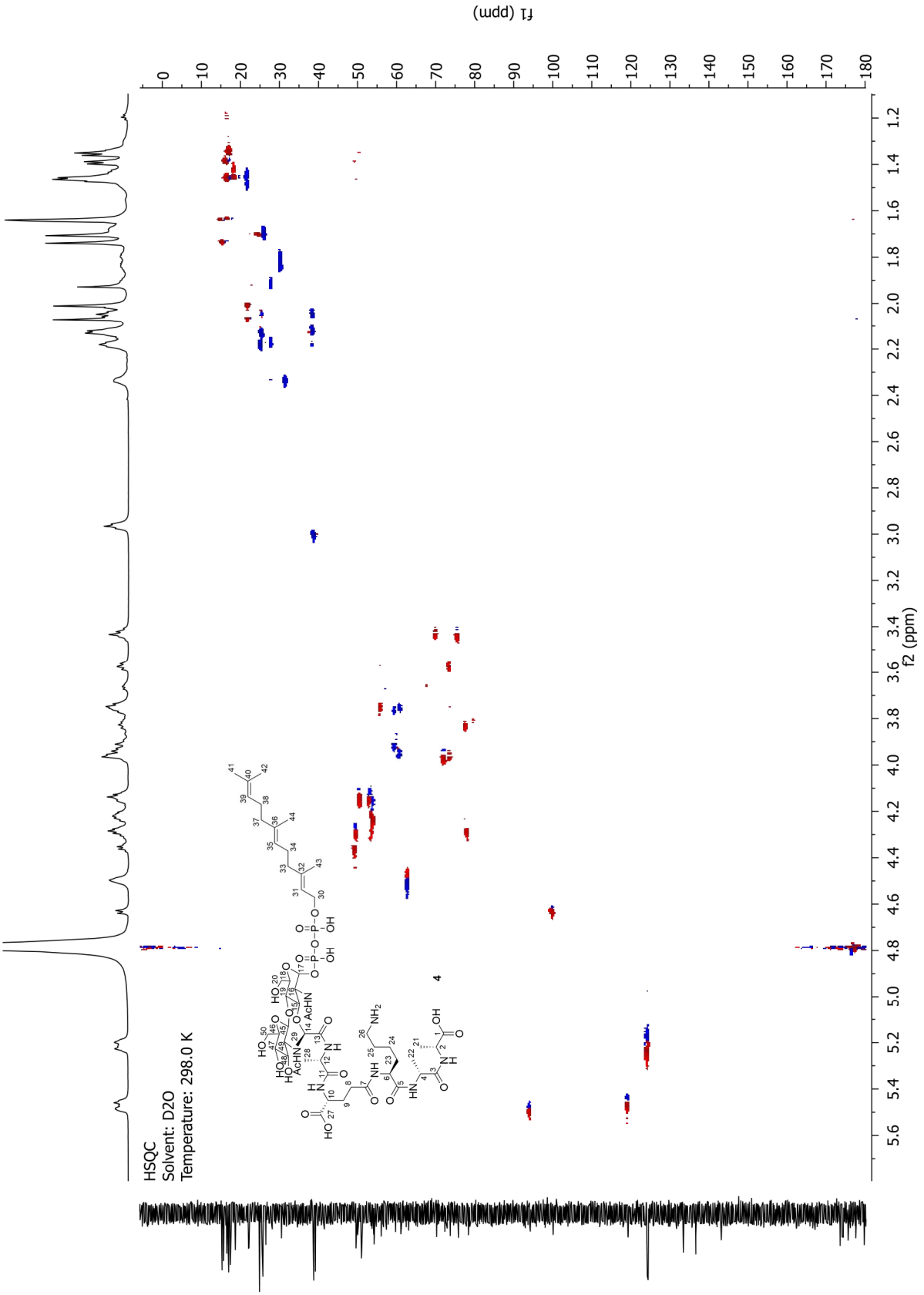

NOESY
Frequency: 500.07 MHz
Solvent: D2O
Temperature: 298.0 K
f1 (ppm)
f2 (ppm)
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
6

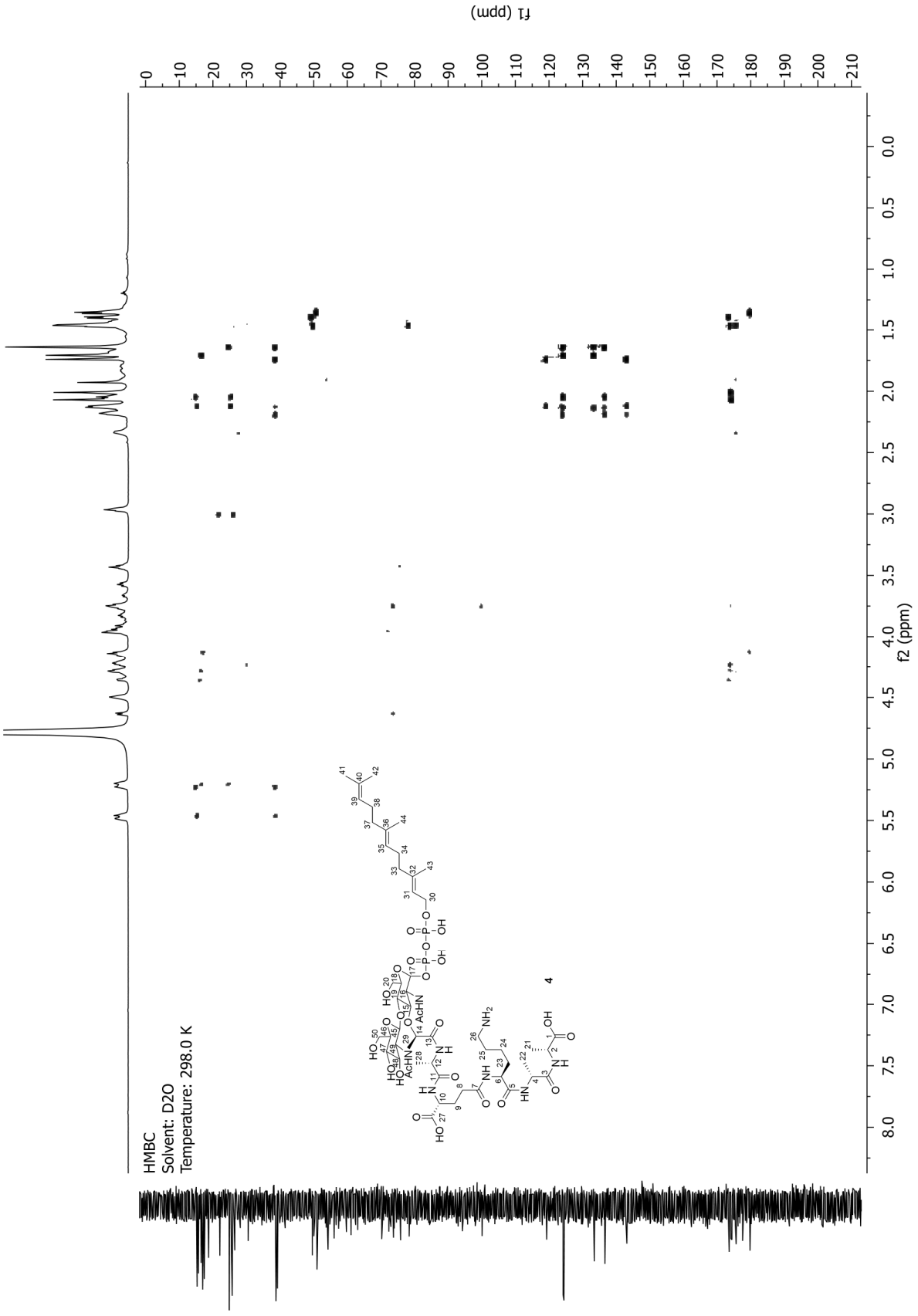

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K
f1 (ppm)
4

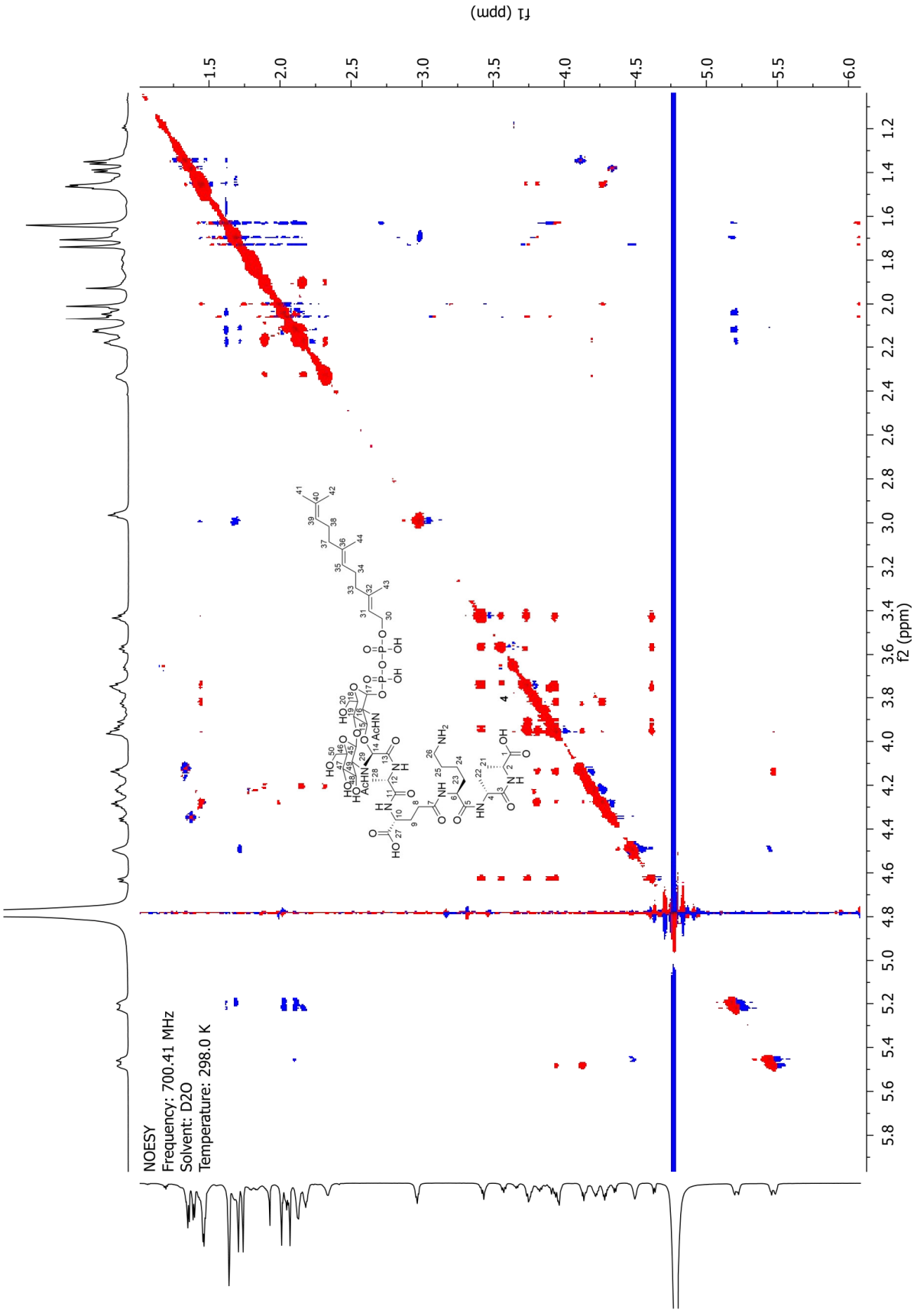

Nucleus: 13C
Frequency: 176.12 MHz
Solvent: D2O
Temperature: 298.0 K
4
f1 (ppm)

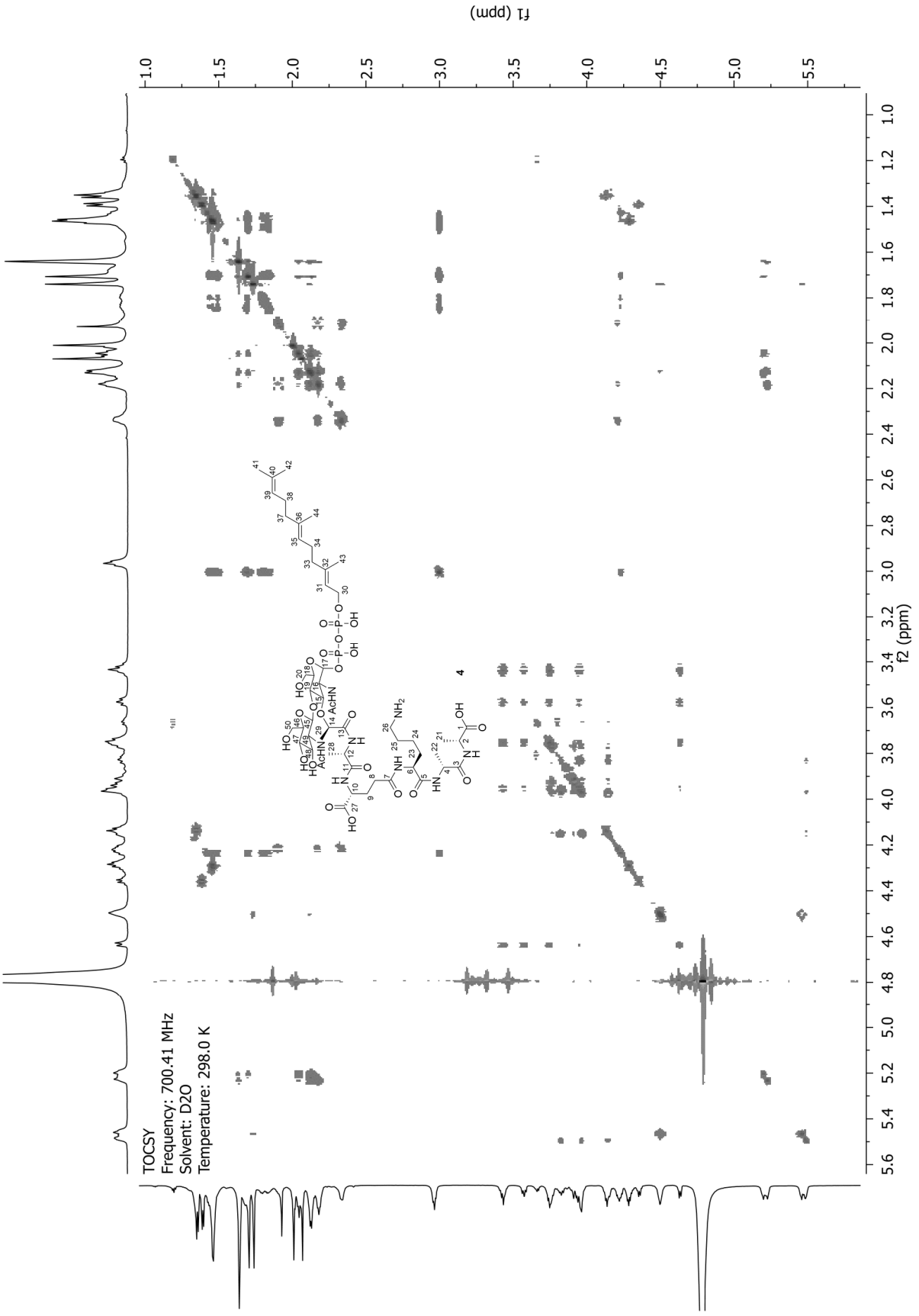

Nucleus: 31P
Frequency: 283.53 MHz
Solvent: D2O
Temperature: 298.0 K
4
-10.9
-10.9
-13.3
-13.4
f1 (ppm)

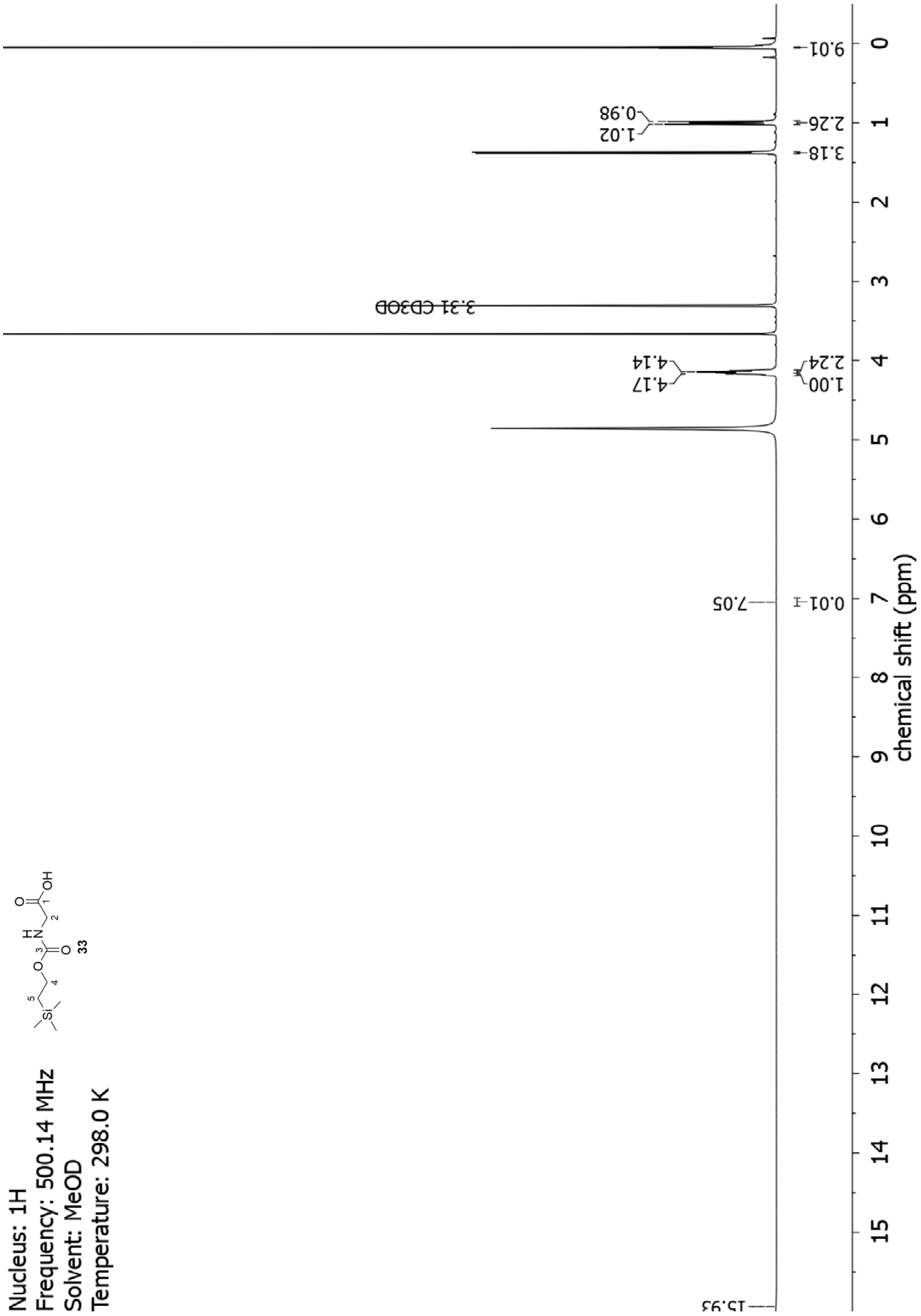

HH-COSY
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K
f1 (ppm)
f2 (ppm)
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0

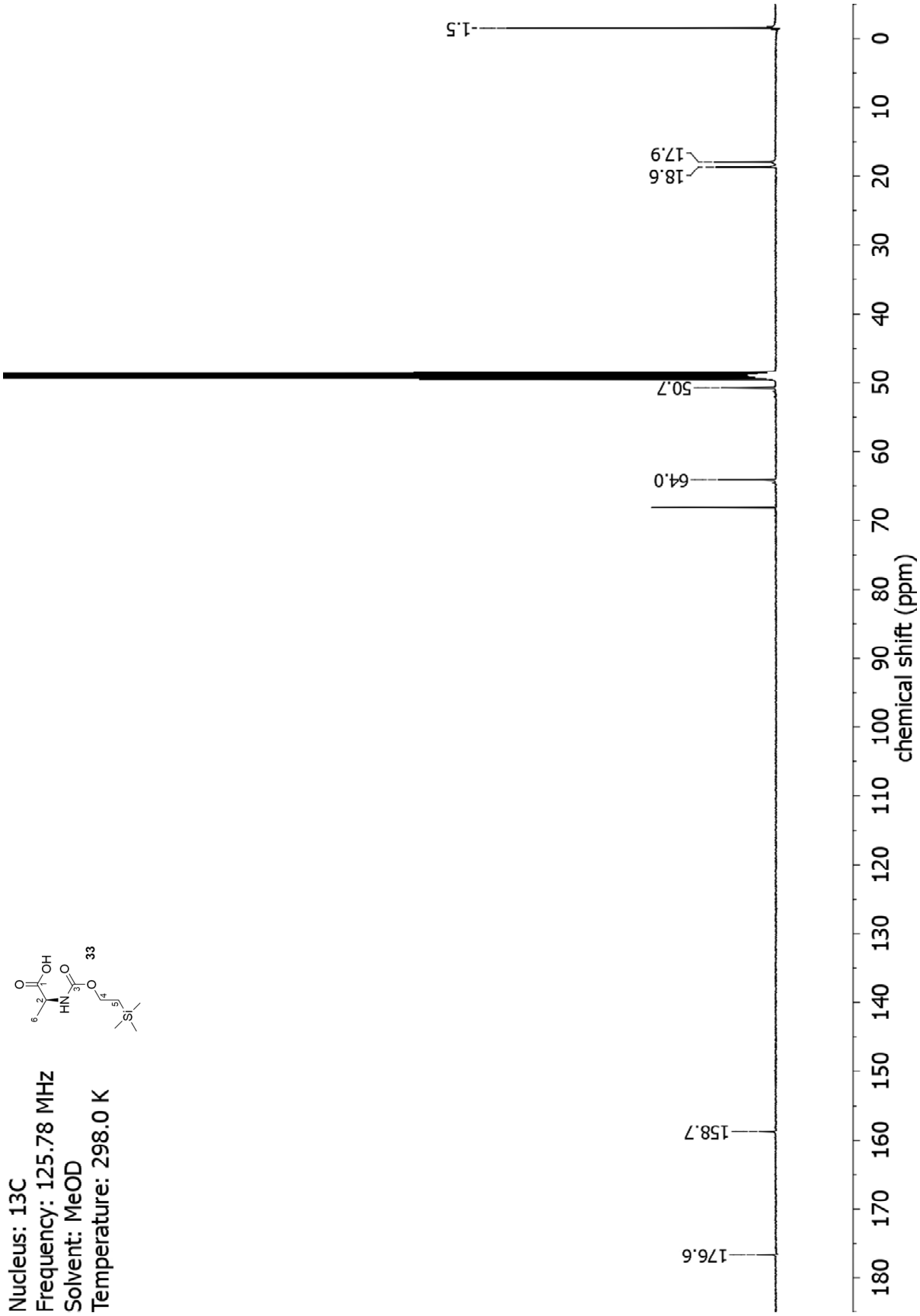

f1 (ppm)
f2 (ppm)
HSQC
Solvent: D2O
Temperature: 298.0 K
4

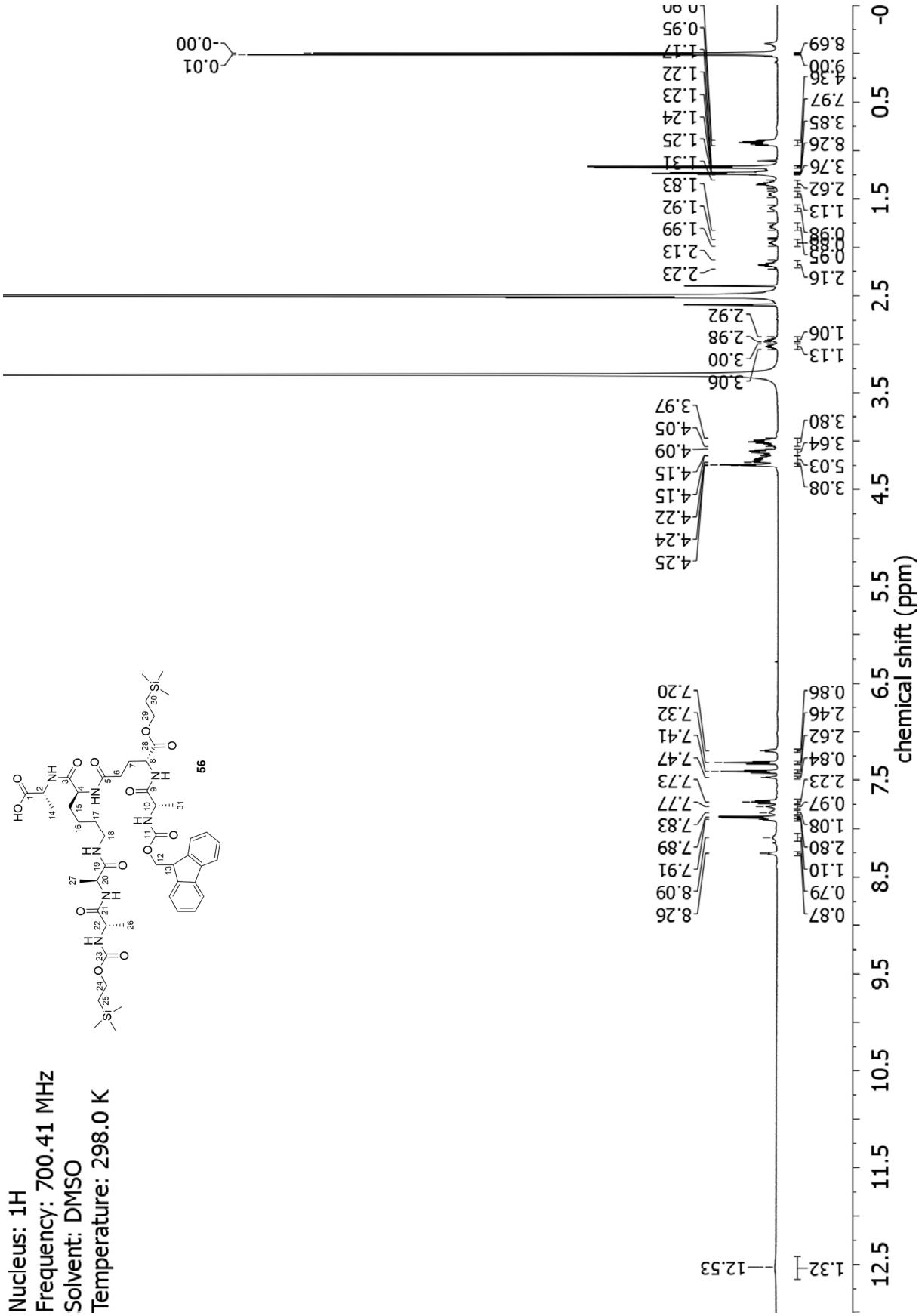

HMBC
Solvent: D2O
Temperature: 298.0 K
f2 (ppm)
f1 (ppm)
4

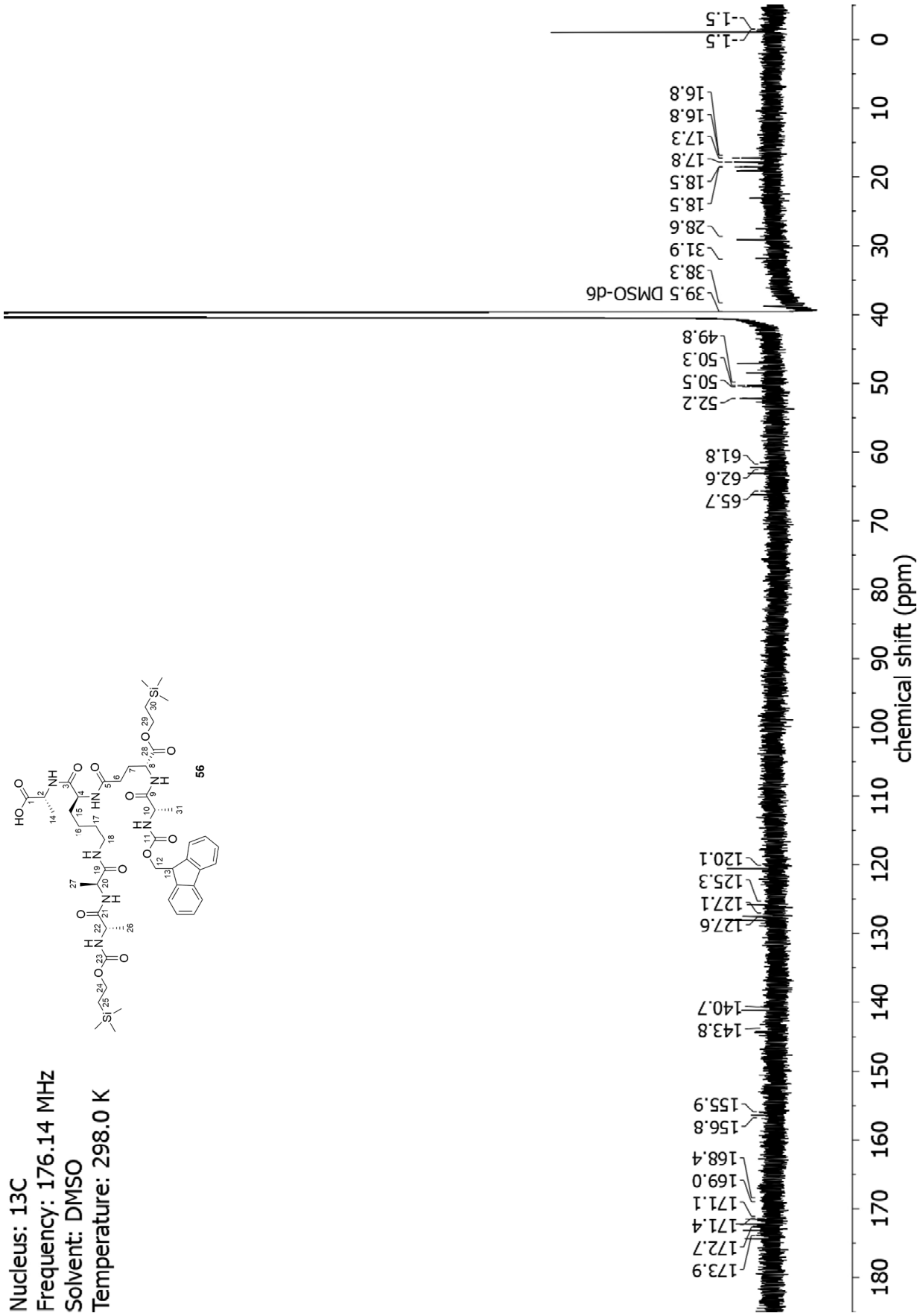

f1 (ppm)
f2 (ppm)
NOESY
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K

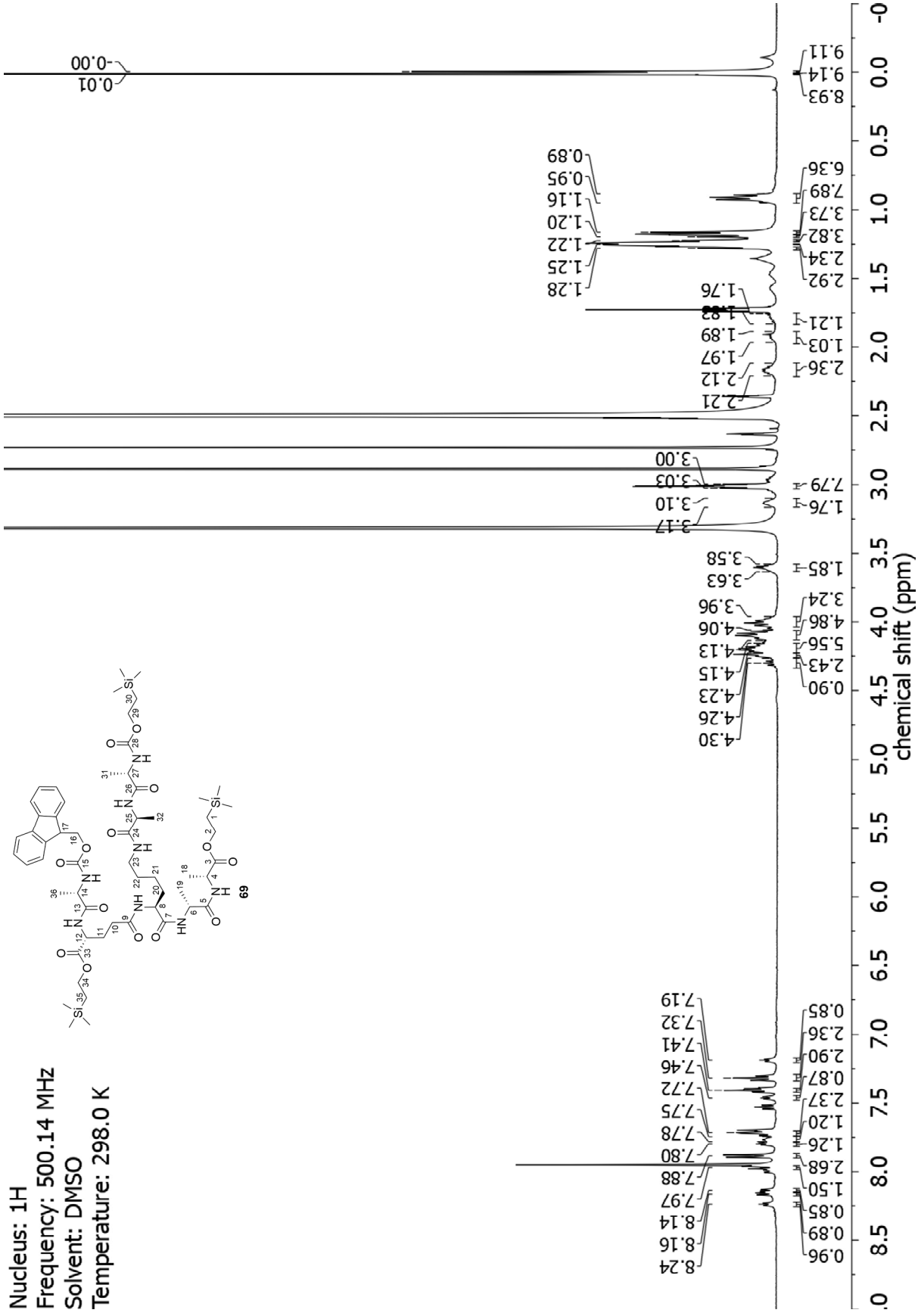

TOCSY
Frequency: 700.41 MHz
Solvent: D2O
Temperature: 298.0 K
f1 (ppm)
f2 (ppm)

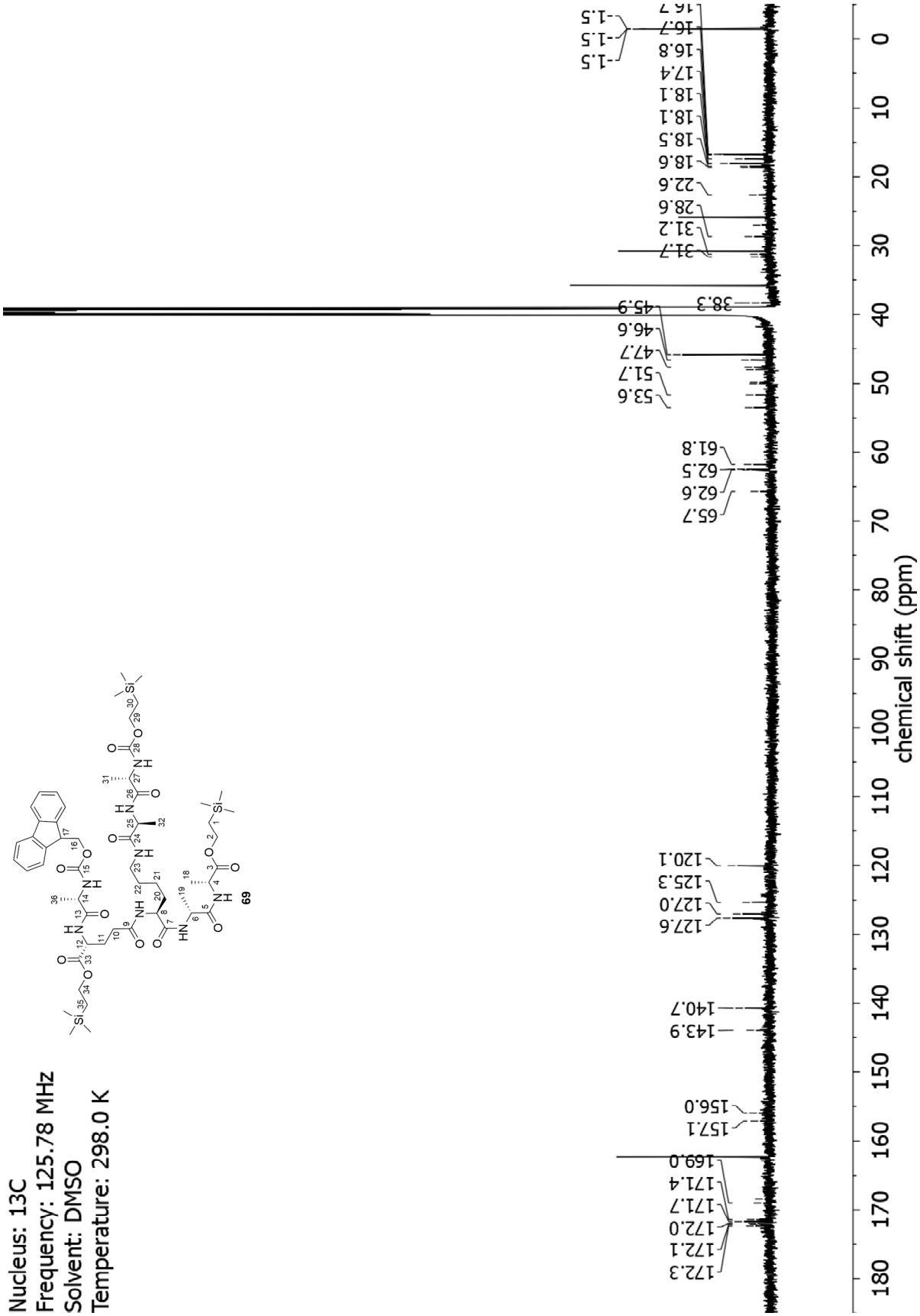

Nucleus: 1H
Frequency: 500.14 MHz
Solvent: MeOD
Temperature: 298.0 K
chemical shift (ppm)
9.01
1.02
0.98
2.26
3.18
3.31 CD3OD
4.17
4.14
2.24
1.00
7.05
0.01
15.93
33

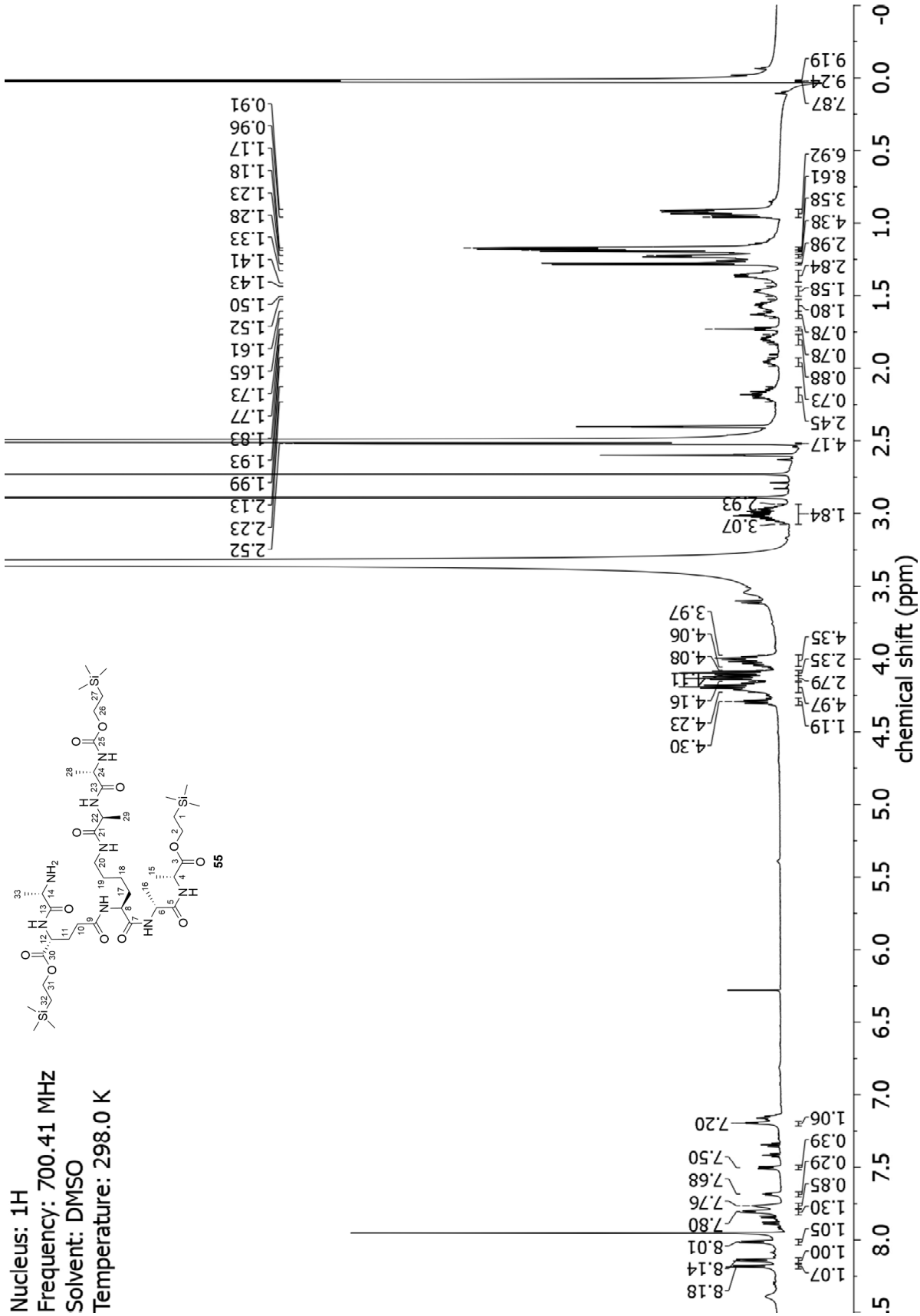

-1.5
17.9
18.6
50.7
64.0
158.7
176.6
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
chemical shift (ppm)
Nucleus: 13C
Frequency: 125.78 MHz
Solvent: MeOD
Temperature: 298.0 K
OH
O
HN
O
O
Si
1
2
3
4
5
6
33

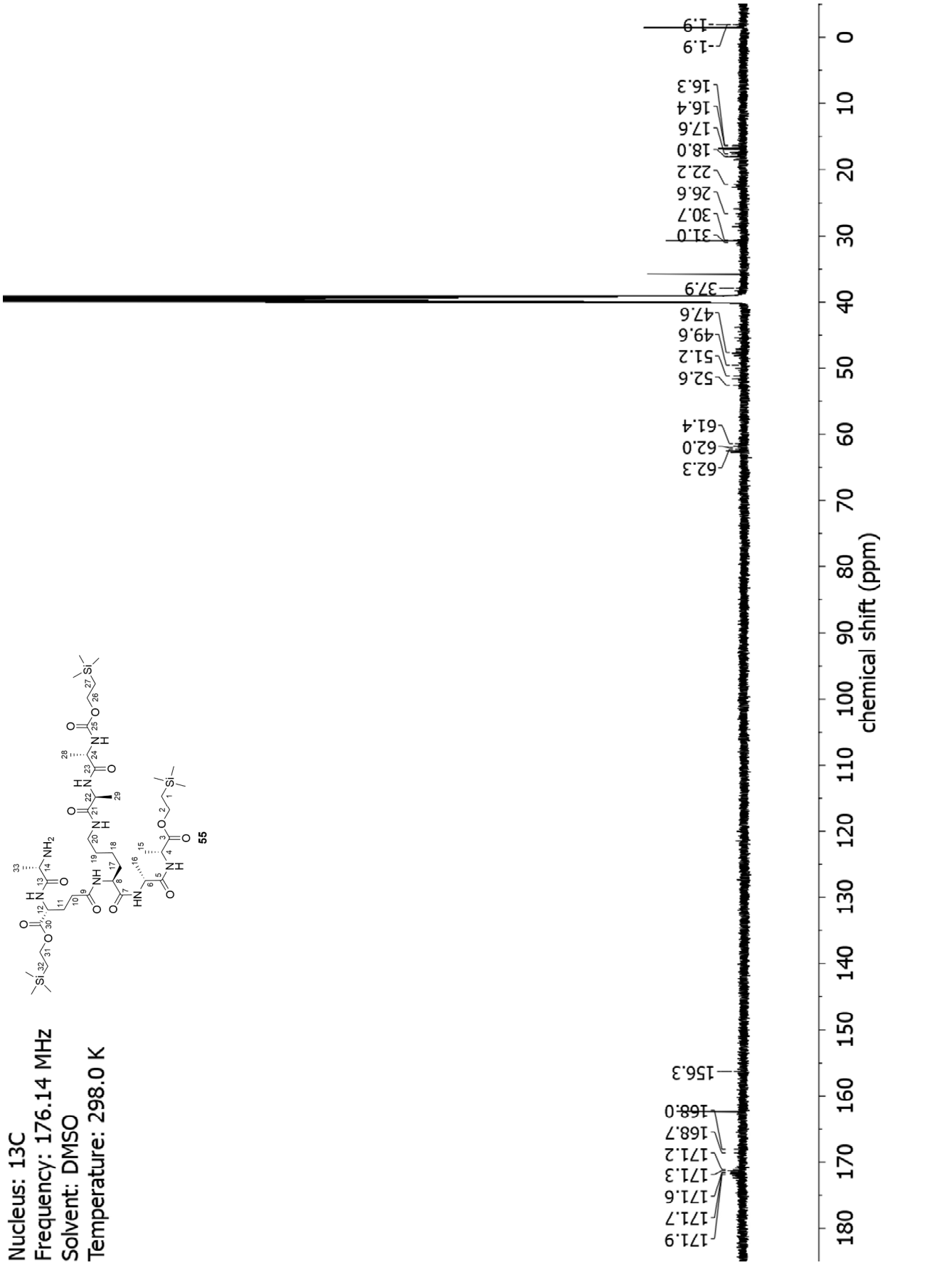

Nucleus: 1H
Frequency: 700.41 MHz
Solvent: DMSO
Temperature: 298.0 K
chemical shift (ppm)
56

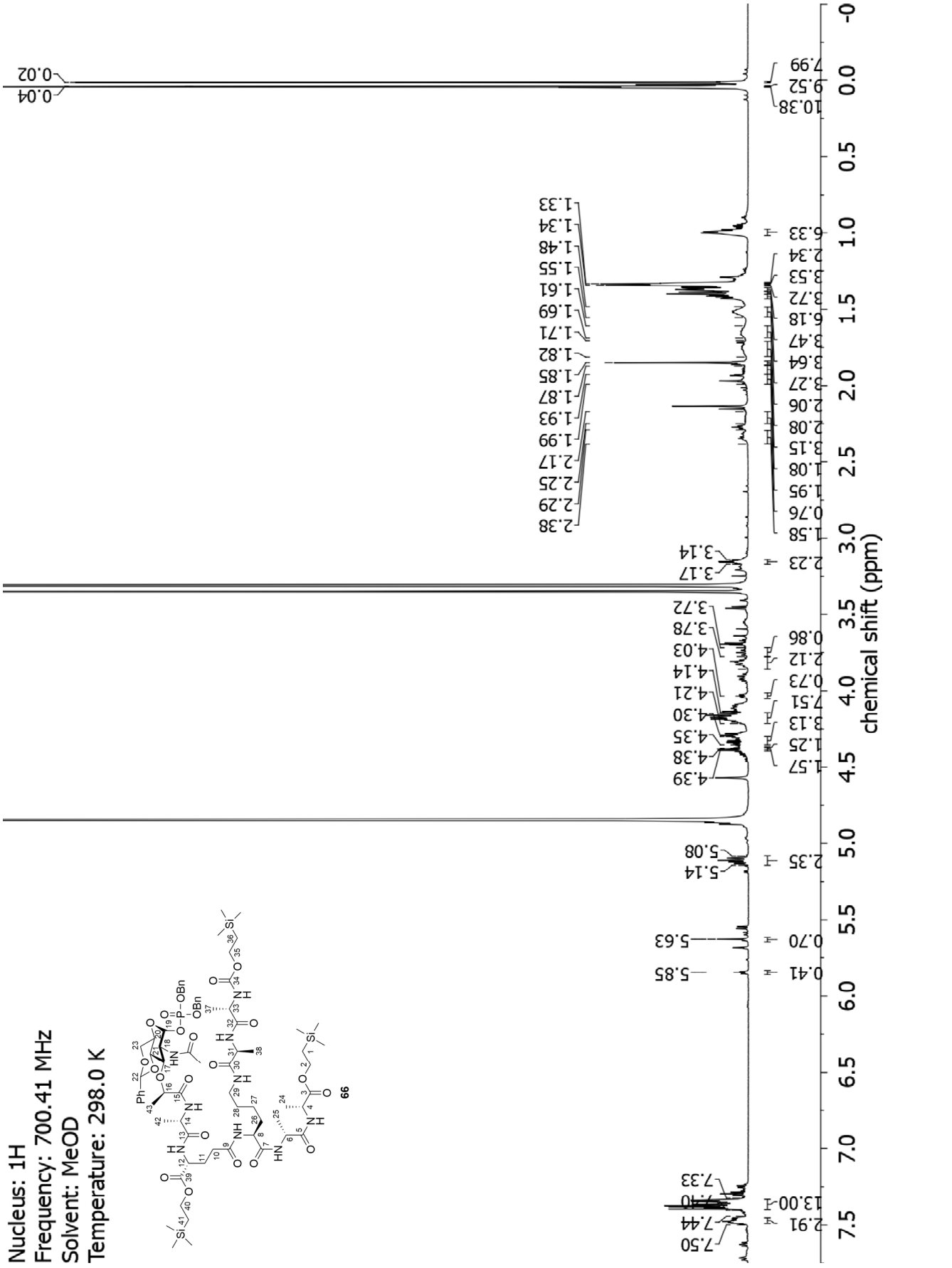

Nucleus: 13C
Frequency: 176.14 MHz
Solvent: DMSO
Temperature: 298.0 K
56
chemical shift (ppm)
-1.5
-1.5
16.8
16.8
17.3
17.8
18.5
18.5
28.6
31.9
38.3
39.5 DMSO-d6
49.8
50.3
50.5
52.2
61.8
62.6
65.7
120.1
125.3
127.1
127.6
140.7
143.8
155.9
156.8
168.4
169.0
171.1
171.4
172.7
173.9

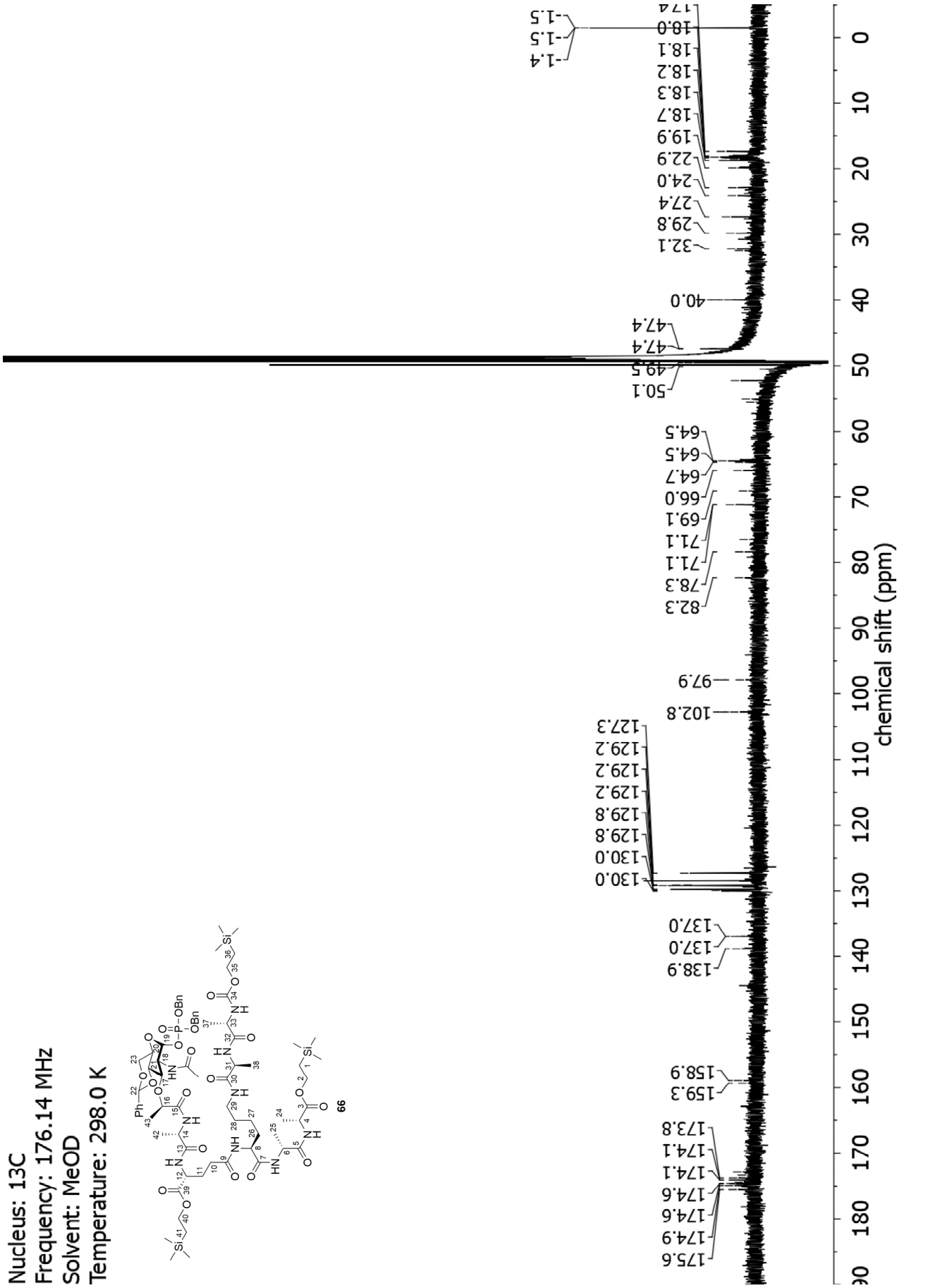

Nucleus: 1H
Frequency: 500.14 MHz
Solvent: DMSO
Temperature: 298.0 K
chemical shift (ppm)
69


Nucleus: 13C
Frequency: 125.78 MHz
Solvent: DMSO
Temperature: 298.0 K
69
chemical shift (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
-1.5
-1.5
16.7
16.8
17.4
18.1
18.1
18.5
18.6
22.6
28.6
31.2
31.7
38.3
45.9
46.6
47.7
51.7
53.6
61.8
62.5
62.6
65.7
120.1
125.3
127.0
127.6
140.7
143.9
156.0
157.1
169.0
171.4
171.7
172.0
172.1
172.3


Nucleus: 1H
Frequency: 700.41 MHz
Solvent: DMSO
Temperature: 298.0 K
chemical shift (ppm)
55


Nucleus: 13C
Frequency: 176.14 MHz
Solvent: DMSO
Temperature: 298.0 K
55
chemical shift (ppm)
-1.9
16.3
16.4
17.6
18.0
22.2
26.6
30.7
31.0
37.9
47.6
49.6
51.2
52.6
61.4
62.0
62.3
156.3
168.0
168.7
171.2
171.3
171.6
171.7
171.9


Nucleus: 1H
Frequency: 700.41 MHz
Solvent: MeOD
Temperature: 298.0 K
66
chemical shift (ppm)


Nucleus: 13C
Frequency: 176.14 MHz
Solvent: MeOD
Temperature: 298.0 K
chemical shift (ppm)
66