Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPLEMENTARY MATERIAL

3′-Amino modifications enhance antifungal properties of *N*^{4}-alkyl-5-methylcytidines for potential biocides

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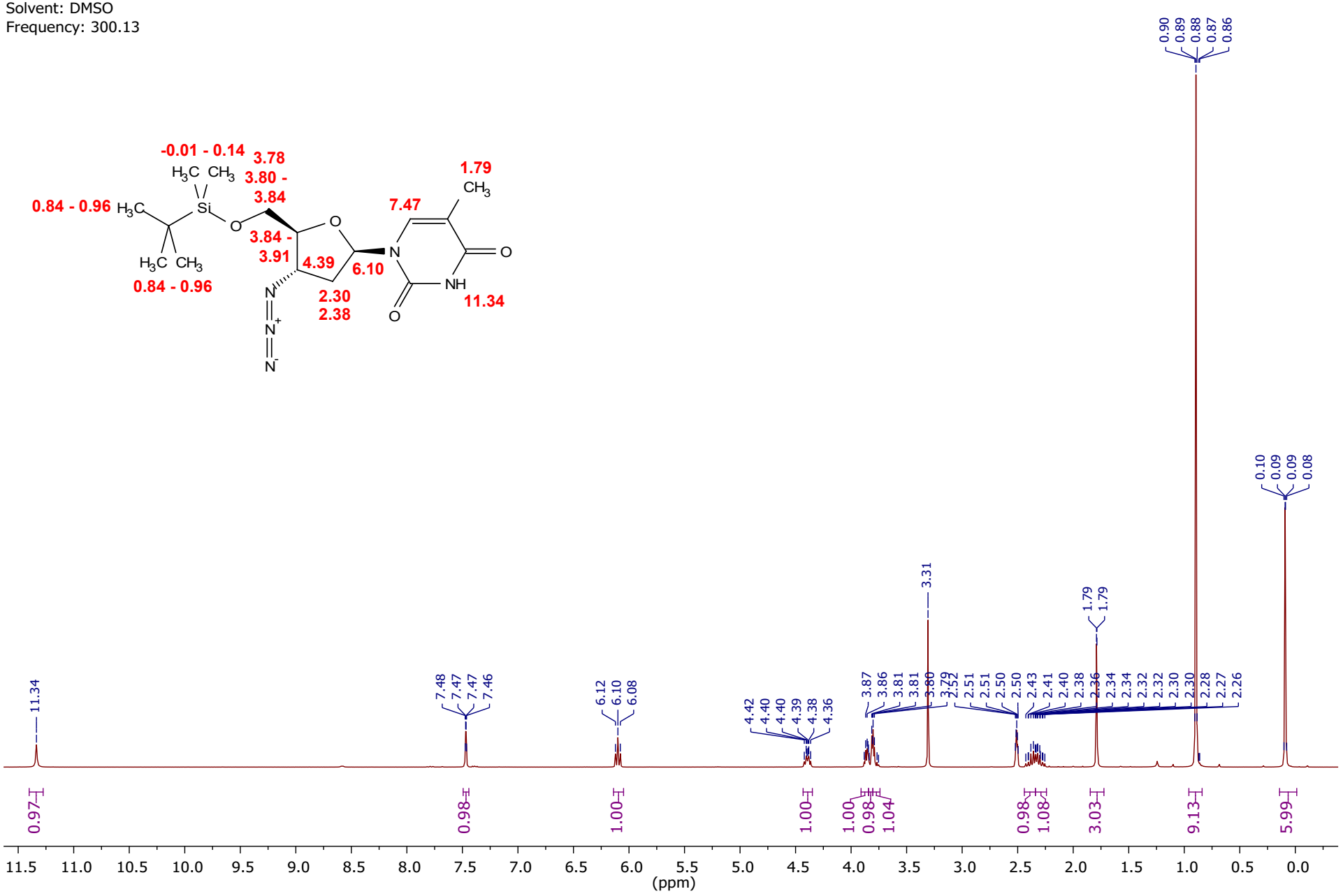
NMR spectra:

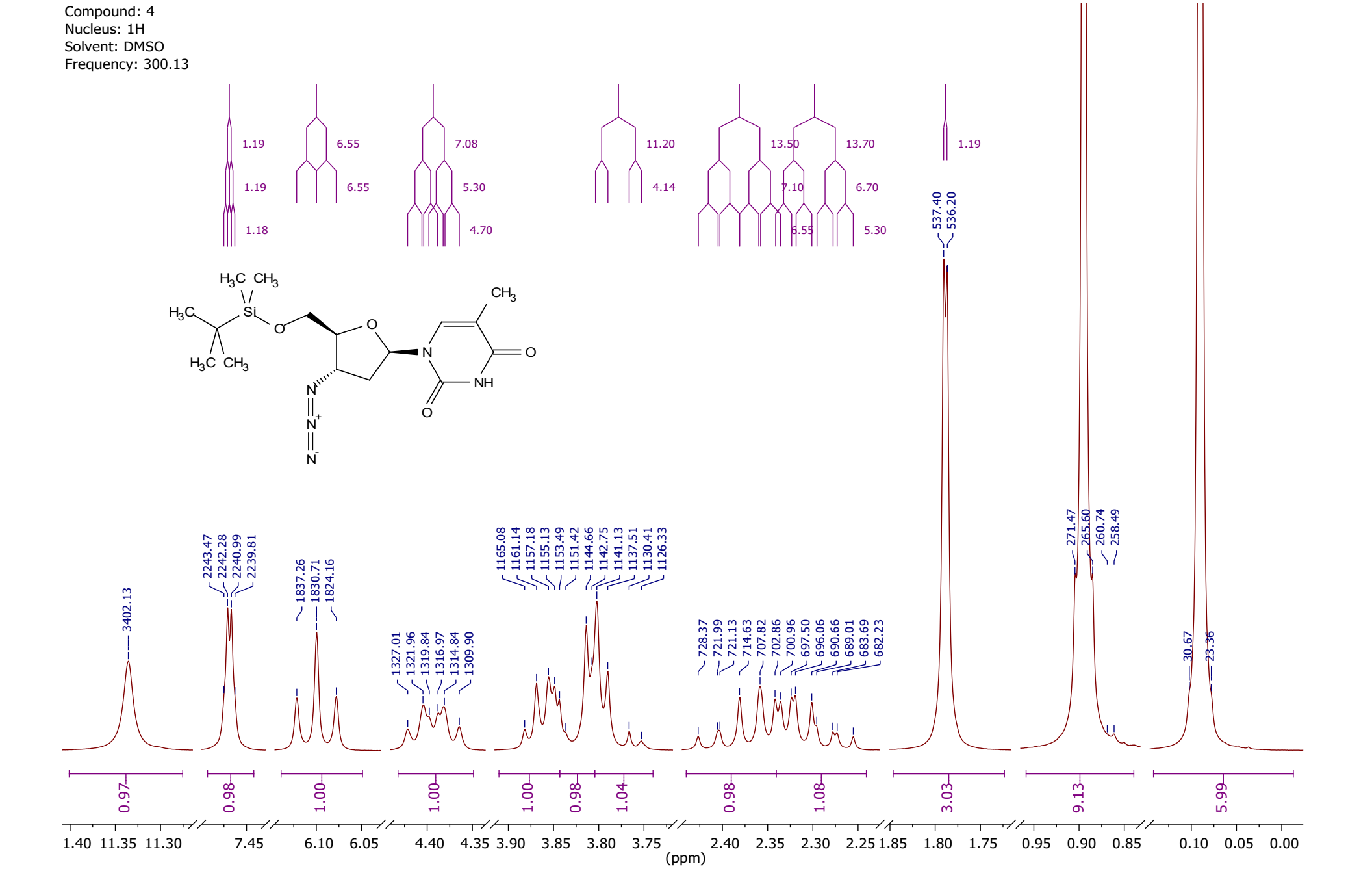
Additional NMR spectra assignment:

HPLC-chromatograms and HRMS spectra:

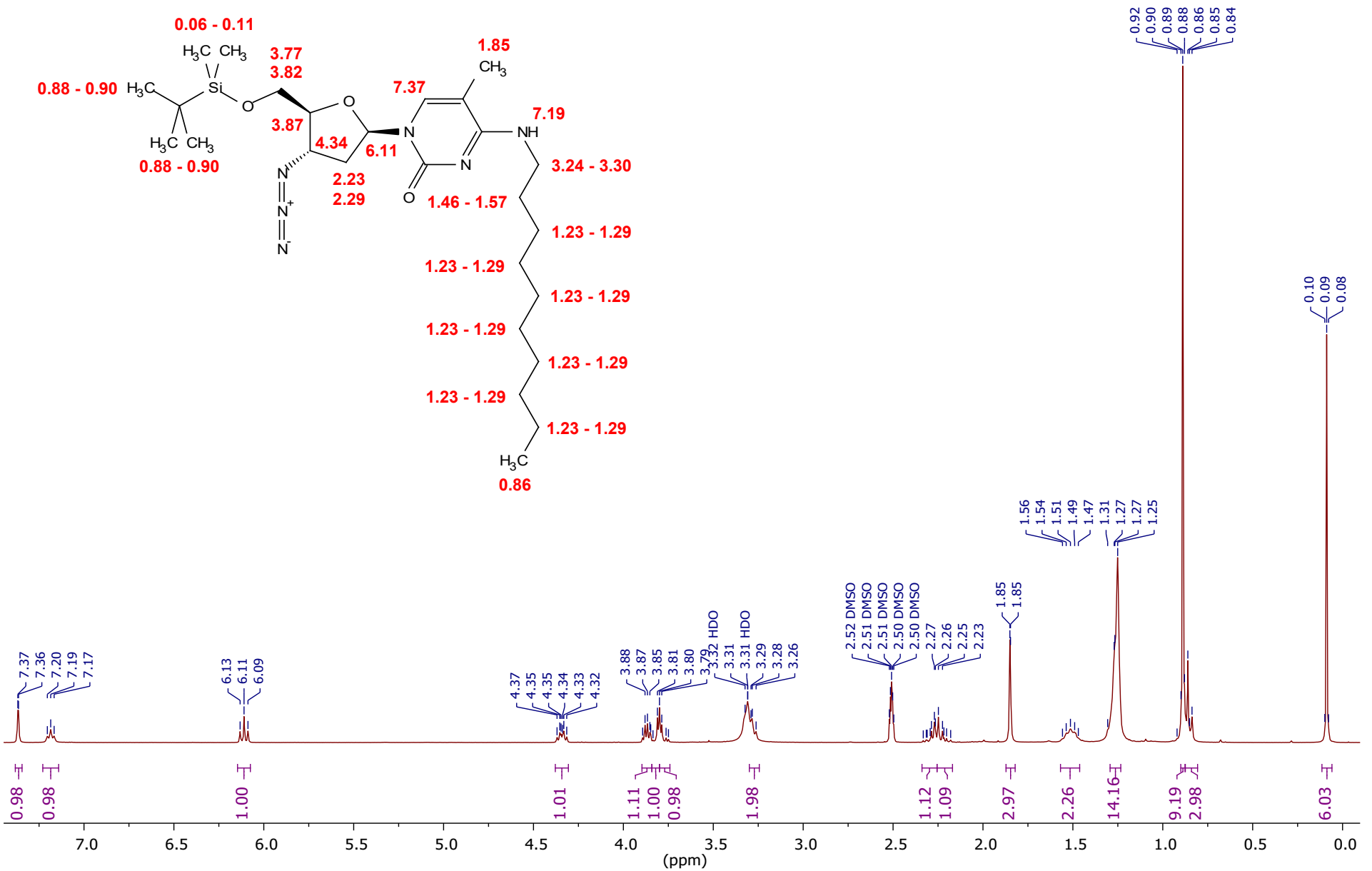
Compound: 4
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

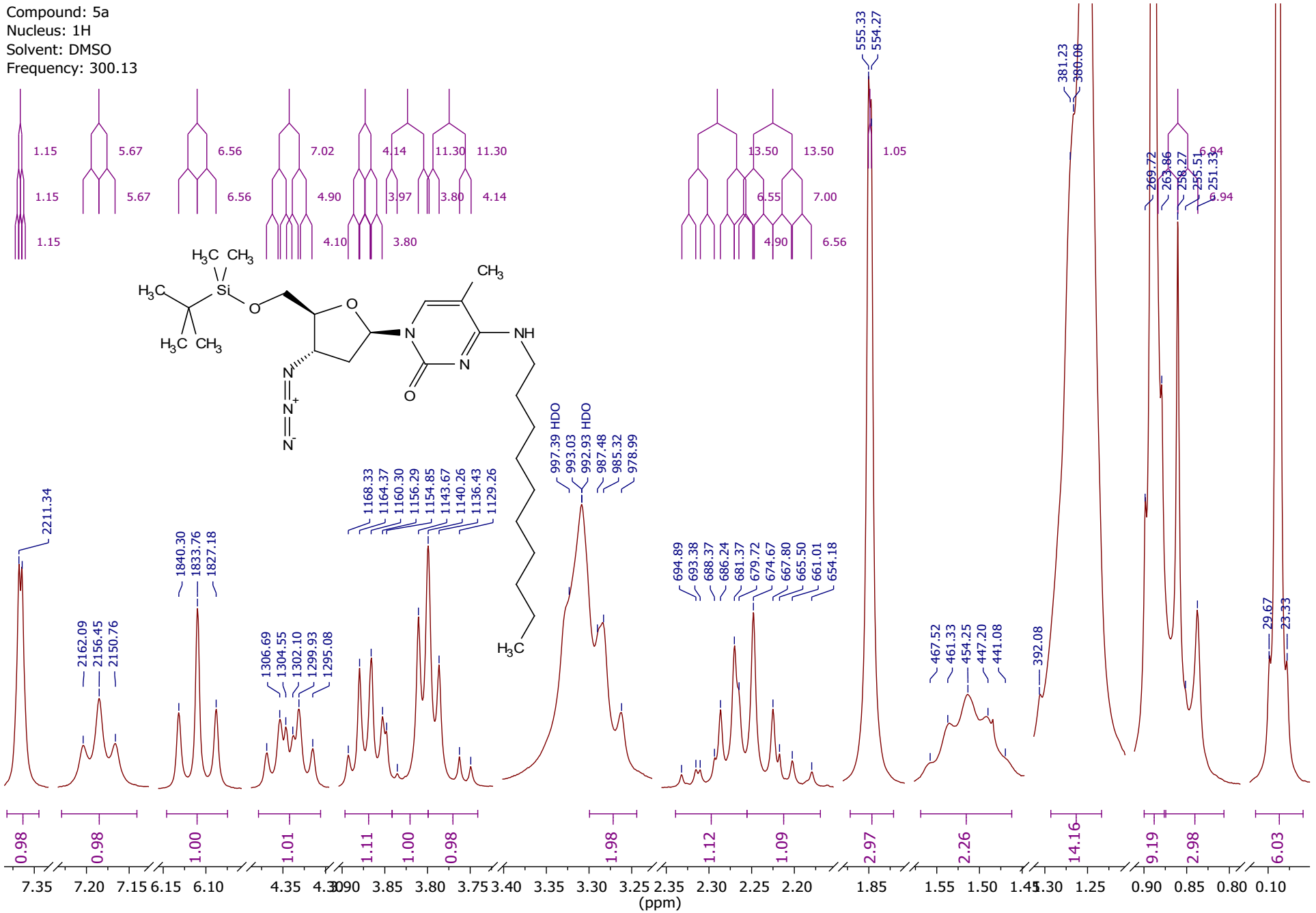


Compound: 4
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

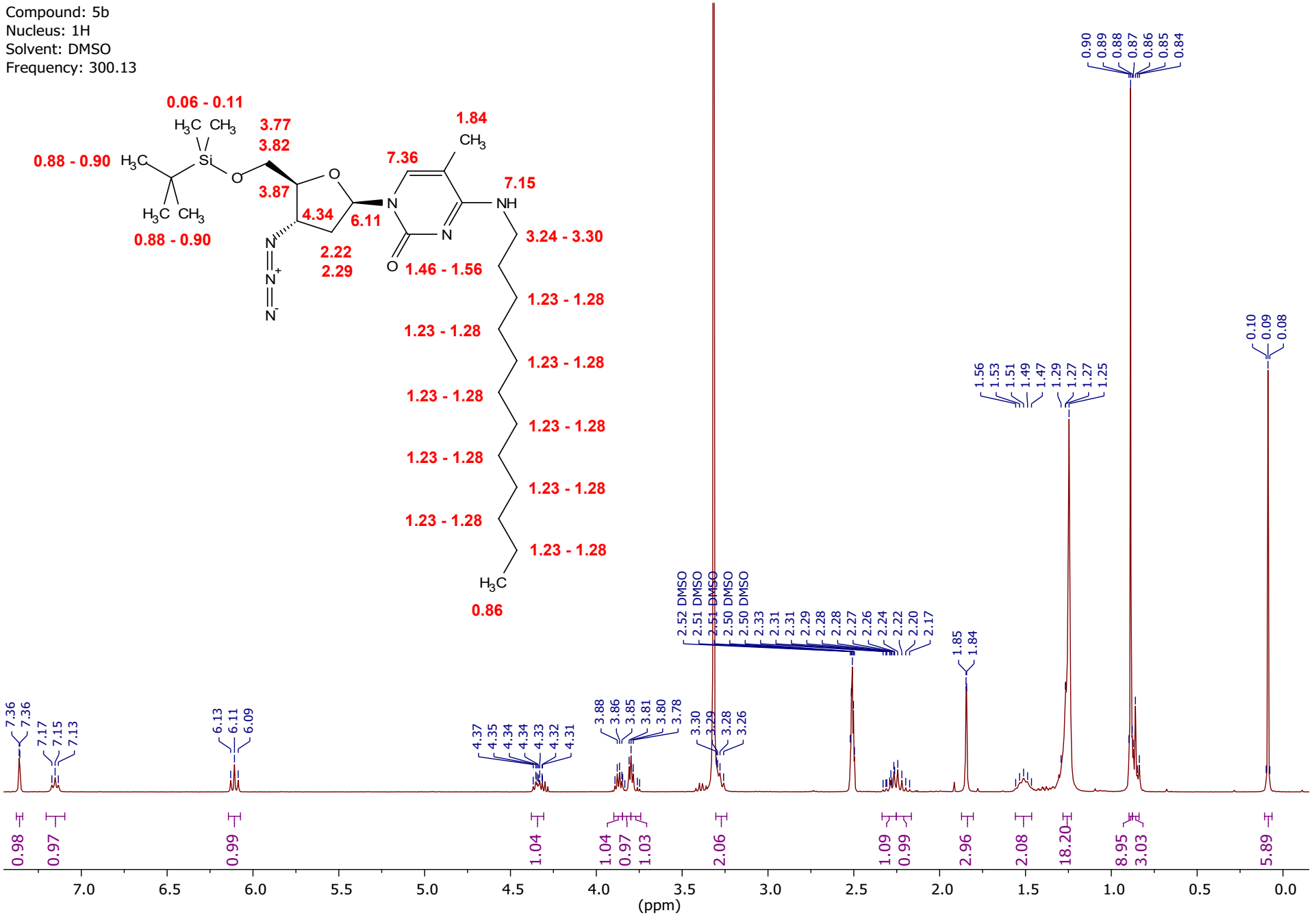


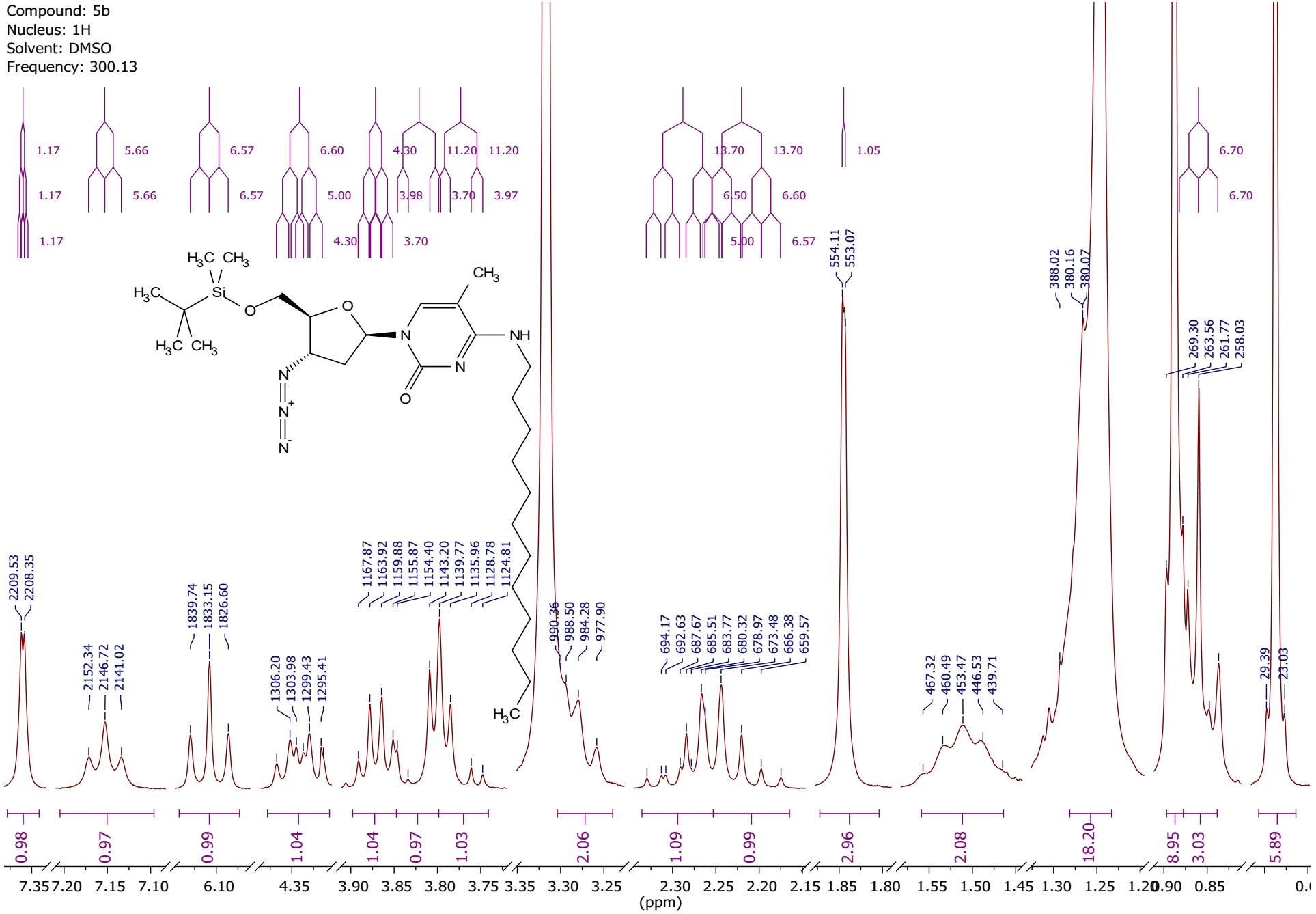
Compound: 5a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13




Compound: 5a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
1.15
1.15
1.15
5.67
5.67
6.56
6.56
7.02
4.90
4.10
4.14
3.97
3.80
11.30
3.80
11.30
4.14
13.50
6.55
4.90
13.50
7.00
6.56
1.05
555.33
554.27
381.23
380.08
269.72
263.86
258.27
255.51
251.33
6.84
6.94
2211.34
2162.09
2156.45
2150.76
1840.30
1833.76
1827.18
1306.69
1304.55
1302.10
1299.93
1295.08
1168.33
1164.37
1160.30
1156.29
1154.85
1143.67
1140.26
1136.43
1129.26
997.39 HDO
993.03
992.93 HDO
987.48
985.32
978.99
694.89
693.38
688.37
686.24
681.37
679.72
674.67
667.80
665.50
661.01
654.18
467.52
461.33
454.25
447.20
441.08
392.08
29.67
23.33
0.98
0.98
1.00
1.01
1.11
1.00
0.98
1.98
1.12
1.09
2.97
2.26
14.16
9.19
2.98
6.03
7.35
7.20
7.15
6.15
6.10
4.35
4.30
3.90
3.85
3.80
3.75
3.40
3.35
3.30
3.25
2.35
2.30
2.25
2.20
1.85
1.55
1.50
1.45
1.30
1.25
0.90
0.85
0.80
0.10
(ppm)

Compound: 5b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13




Compound: 5b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
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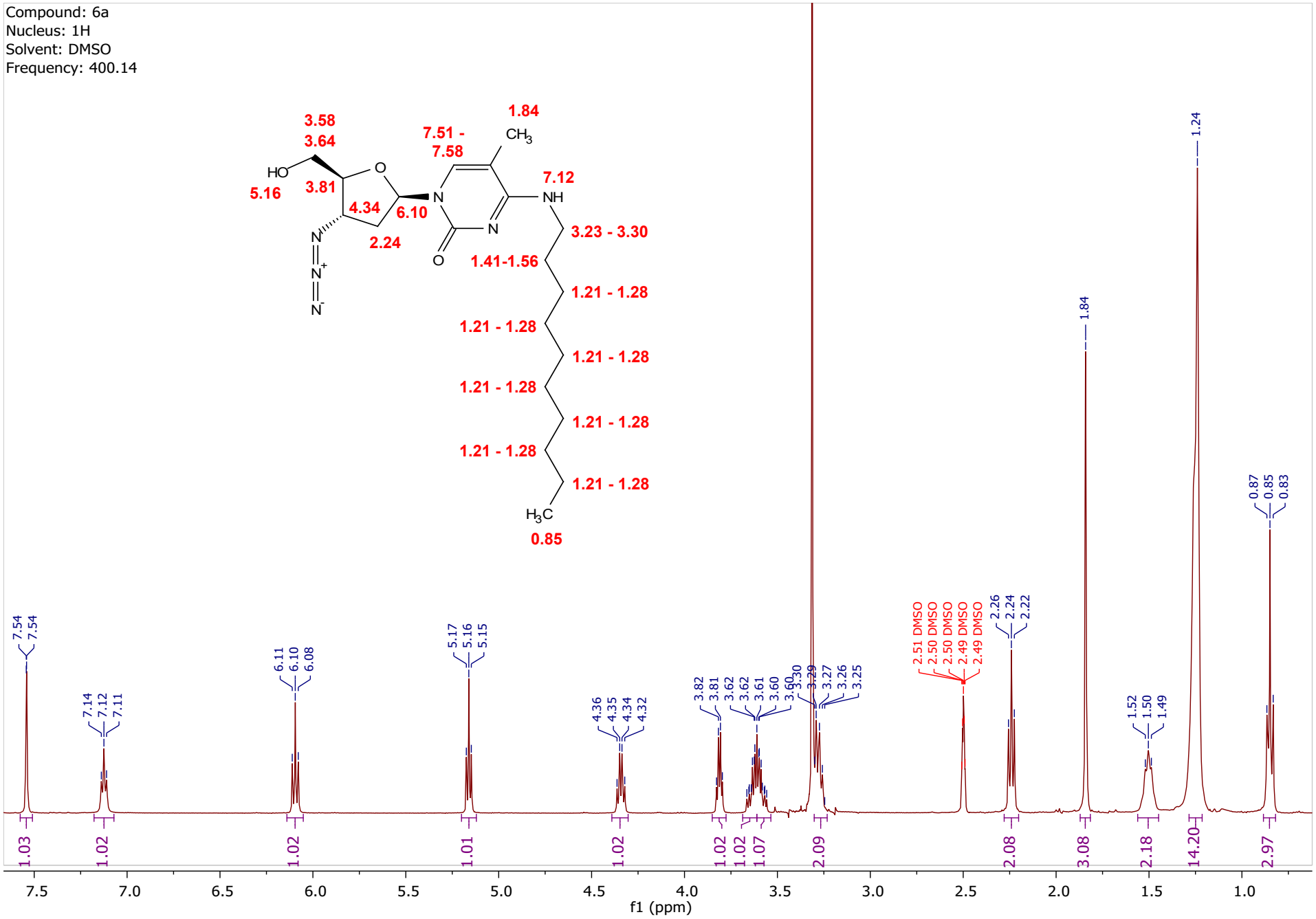
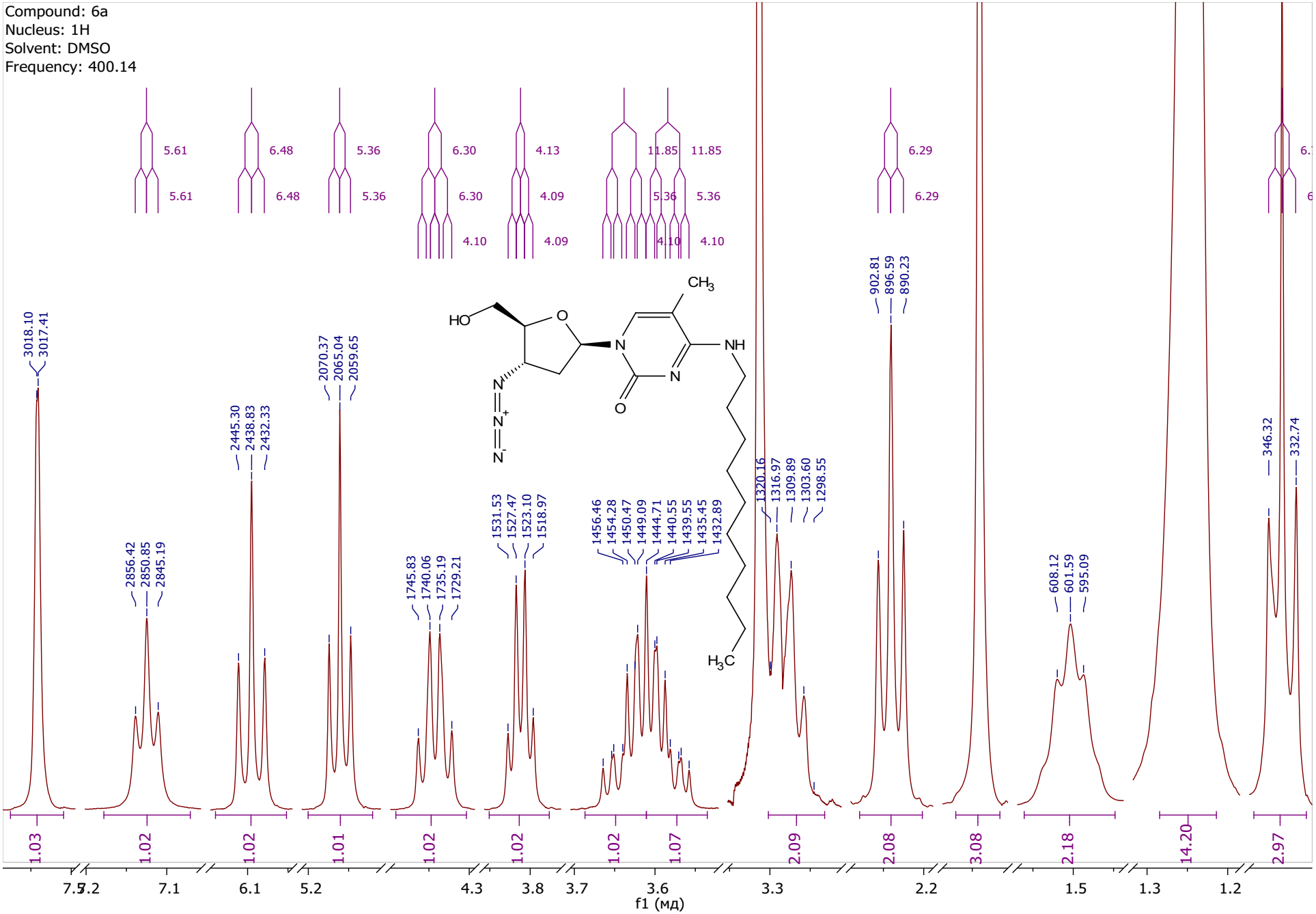
1.17
5.66
5.66
6.57
6.57
6.60
5.00
4.30
4.30
11.20
3.98
3.70
11.20
3.70
3.97
13.70
6.50
5.00
13.70
6.60
6.57
1.05
6.70
6.70
554.11
553.07
388.02
380.16
380.07
269.30
263.56
261.77
258.03
2209.53
2208.35
2152.34
2146.72
2141.02
1839.74
1833.15
1826.60
1306.20
1303.98
1299.43
1295.41
1167.87
1163.92
1159.88
1155.87
1154.40
1143.20
1139.77
1135.96
1128.78
1124.81
990.36
988.50
984.28
977.90
694.17
692.63
687.67
685.51
683.77
680.32
678.97
673.48
666.38
659.57
467.32
460.49
453.47
446.53
439.71
29.39
23.03
0.98
0.97
0.99
1.04
1.04
0.97
1.03
2.06
1.09
0.99
2.96
2.08
18.20
8.95
3.03
5.89
7.35
7.20
7.15
7.10
6.10
4.35
3.90
3.85
3.80
3.75
3.35
3.30
3.25
2.30
2.25
2.20
2.15
1.85
1.80
1.55
1.50
1.45
1.30
1.25
1.20
0.90
0.85
0.(
(ppm)


Compound: 6a
Nucleus: 1H
Solvent: DMSO
Frequency: 400.14
3.58
3.64
1.84
7.51 -
7.58
CH3
HO
O
7.12
5.16
3.81
N
NH
4.34
6.10
N
3.23 - 3.30
2.24
O
1.41-1.56
1.21 - 1.28
1.21 - 1.28
1.21 - 1.28
1.21 - 1.28
1.21 - 1.28
1.21 - 1.28
H3C
0.85
f1 (ppm)


Compound: 6a
Nucleus: 1H
Solvent: DMSO
Frequency: 400.14
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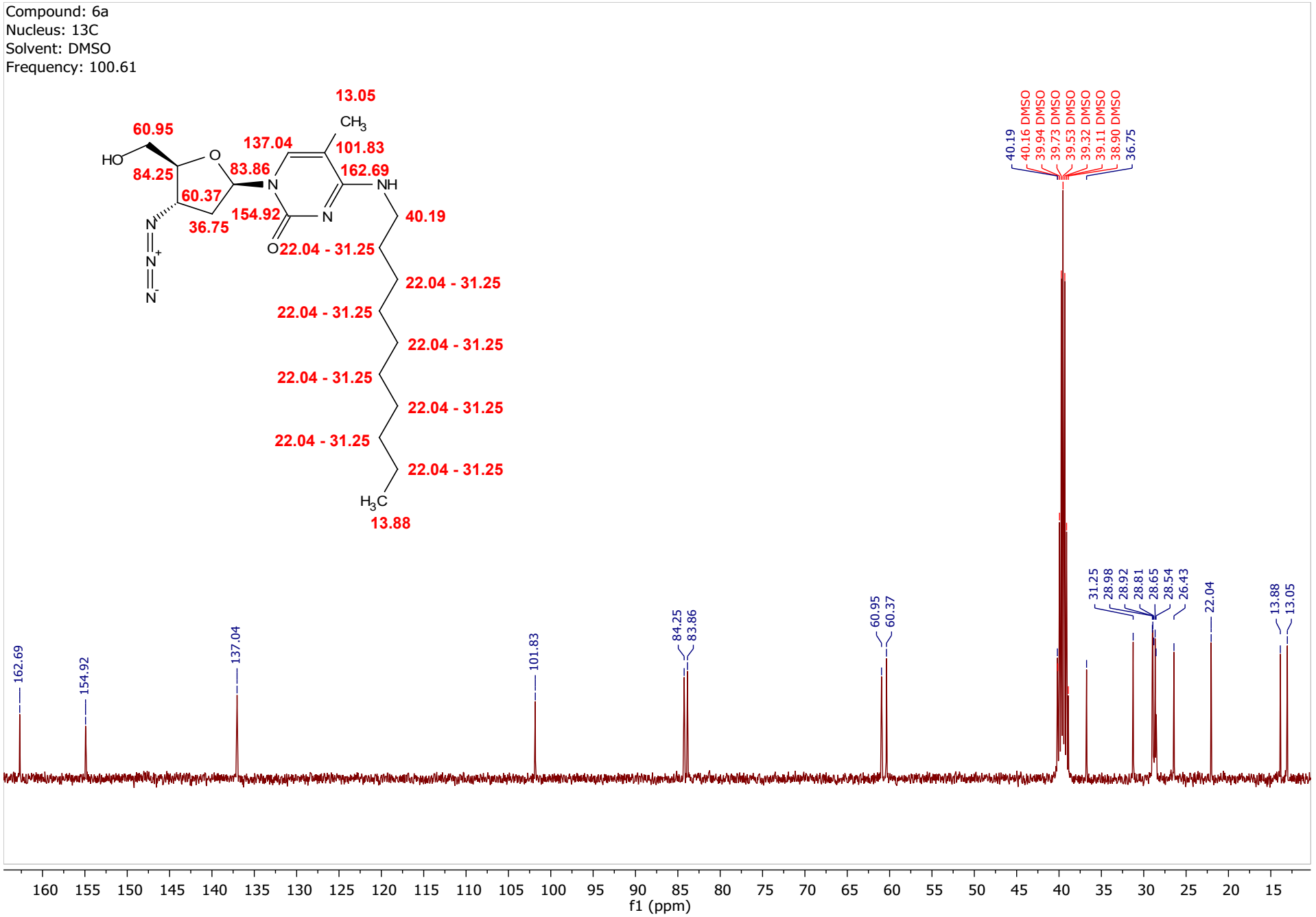
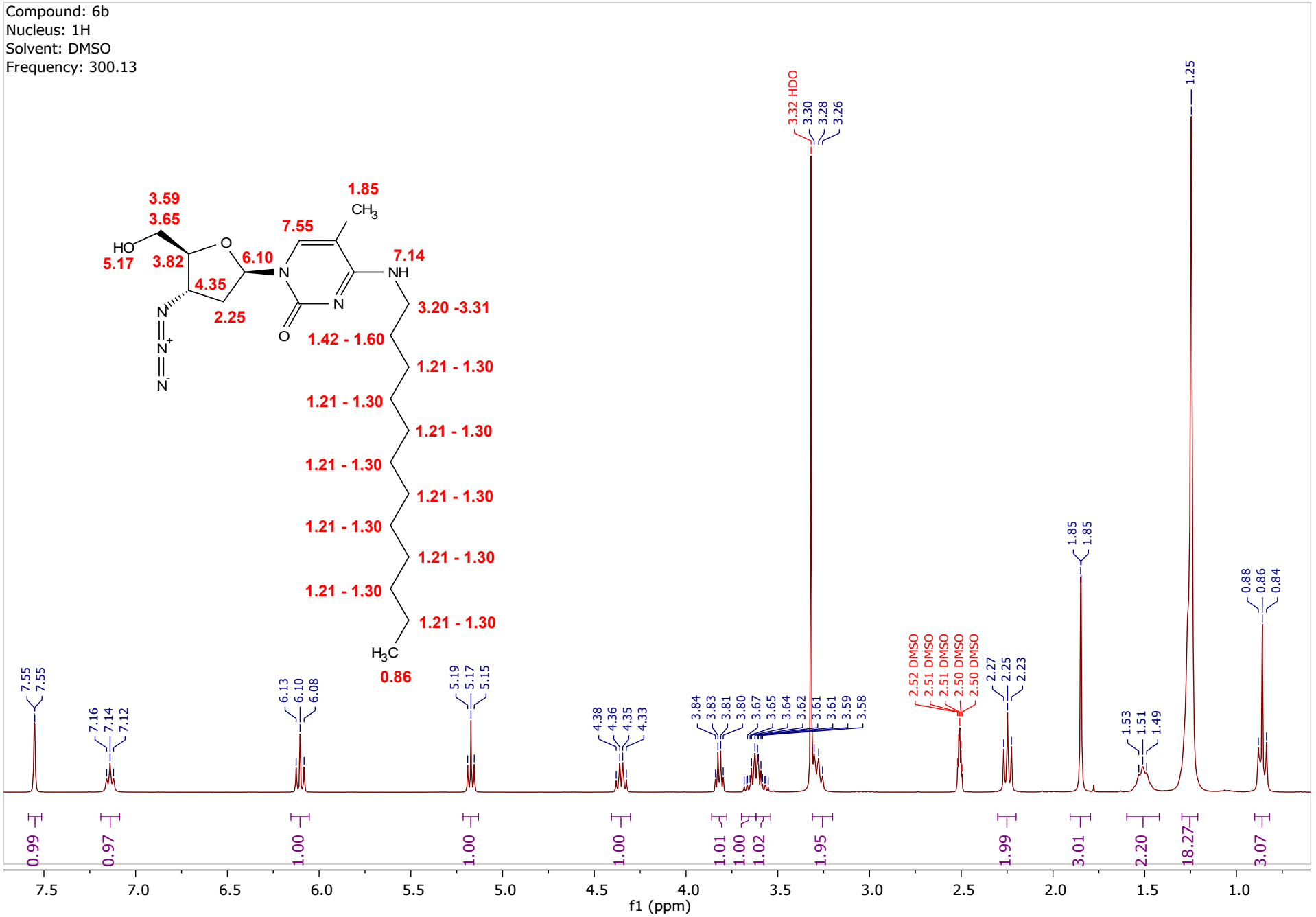
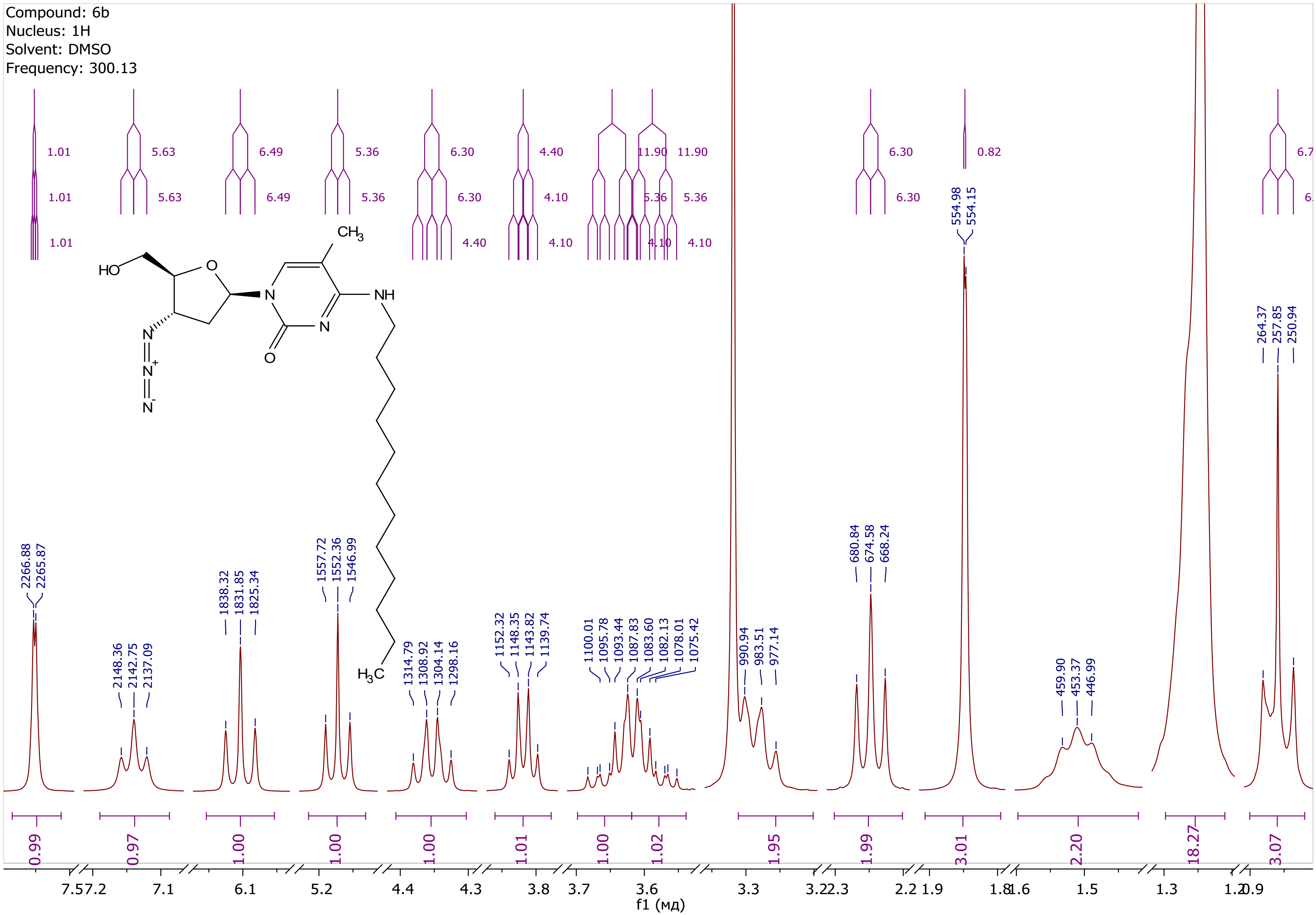
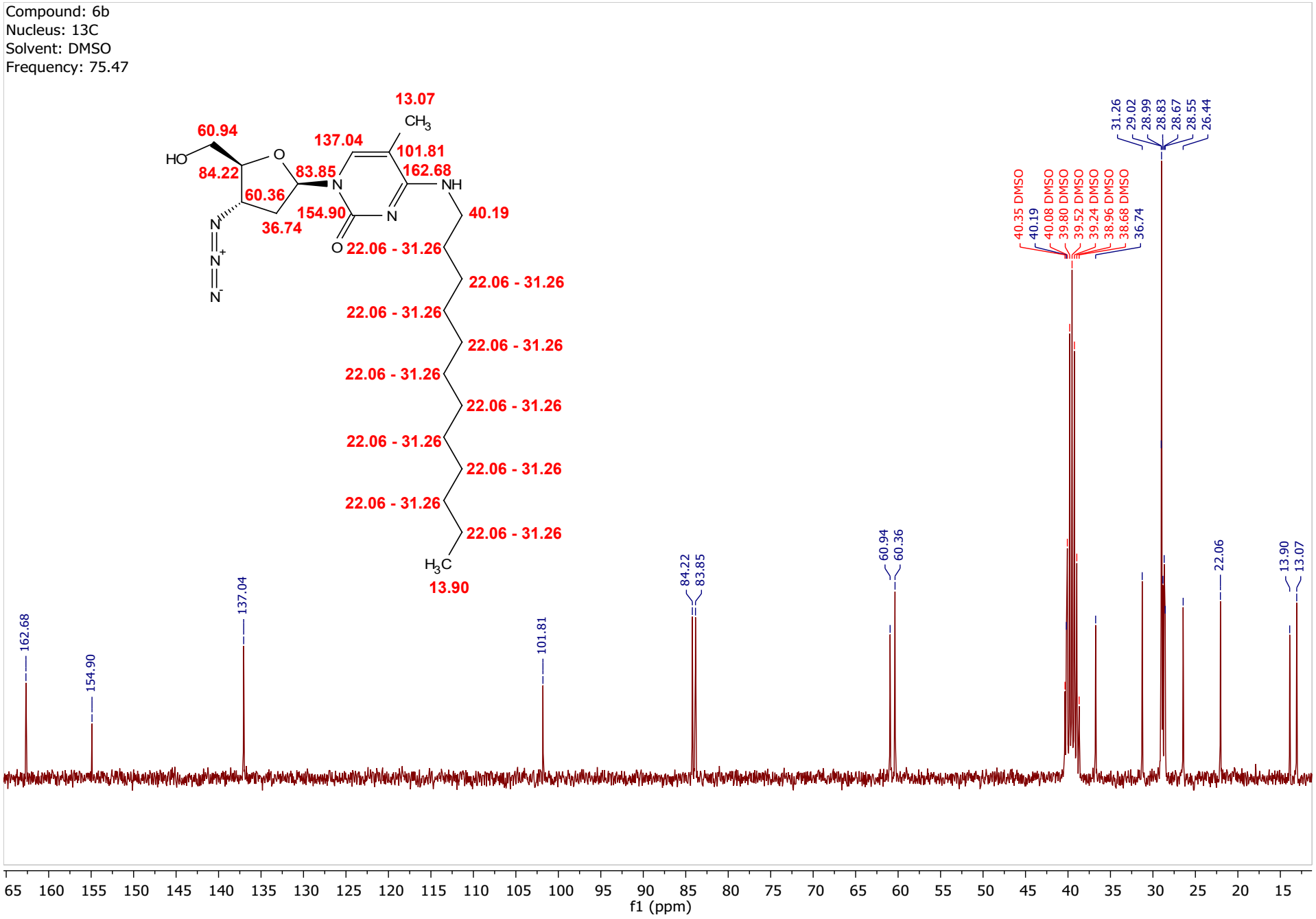
5.61
6.48
6.48
5.36
5.36
6.30
6.30
4.10
4.13
4.09
4.09
11.85
11.85
5.36
5.36
4.10
4.10
6.29
6.29
3018.10
3017.41
2856.42
2850.85
2845.19
2445.30
2438.83
2432.33
2070.37
2065.04
2059.65
1745.83
1740.06
1735.19
1729.21
1531.53
1527.47
1523.10
1518.97
1456.46
1454.28
1450.47
1449.09
1444.71
1440.55
1439.55
1435.45
1432.89
1320.16
1316.97
1309.89
1303.60
1298.55
902.81
896.59
890.23
608.12
601.59
595.09
346.32
332.74
HO
O
N
NH
N
O
CH3
N+
N-
H3C
1.03
1.02
1.02
1.01
1.02
1.02
1.02
1.07
2.09
2.08
3.08
2.18
14.20
2.97
7.5
7.2
7.1
6.1
5.2
4.3
3.8
3.7
3.6
3.3
2.2
1.5
1.3
1.2
f1 (мд)


Compound: 6a
Nucleus: 13C
Solvent: DMSO
Frequency: 100.61
13.05
60.95
137.04
101.83
84.25
83.86
162.69
60.37
154.92
40.19
36.75
22.04 - 31.25
13.88
40.19
40.16 DMSO
39.94 DMSO
39.73 DMSO
39.53 DMSO
39.32 DMSO
39.11 DMSO
38.90 DMSO
36.75
31.25
28.98
28.92
28.81
28.65
28.54
26.43
22.04
13.88
13.05
162.69
154.92
137.04
101.83
84.25
83.86
60.95
60.37
f1 (ppm)


Compound: 6b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
3.59
3.65
HO
5.17
3.82
4.35
2.25
6.10
7.55
1.85
CH3
7.14
NH
3.20 -3.31
1.42 - 1.60
1.21 - 1.30
1.21 - 1.30
1.21 - 1.30
1.21 - 1.30
1.21 - 1.30
1.21 - 1.30
1.21 - 1.30
H3C
0.86
3.32 HDO
3.30
3.28
3.26
1.25
1.85
1.85
0.88
0.86
0.84
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.27
2.25
2.23
1.53
1.51
1.49
7.55
7.55
7.16
7.14
7.12
6.13
6.10
6.08
5.19
5.17
5.15
4.38
4.36
4.35
4.33
3.84
3.83
3.81
3.80
3.67
3.65
3.64
3.62
3.61
3.61
3.59
3.58
0.99
0.97
1.00
1.00
1.00
1.01
1.00
1.02
1.95
1.99
3.01
2.20
18.27
3.07
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
f1 (ppm)


Compound: 6b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
f1 (мд)


Compound: 6b
Nucleus: 13C
Solvent: DMSO
Frequency: 75.47
13.07
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137.04
101.81
84.22
83.85
162.68
60.36
154.90
40.19
36.74
22.06 - 31.26
13.90
162.68
154.90
137.04
101.81
84.22
83.85
60.94
60.36
40.35 DMSO
40.19
40.08 DMSO
39.80 DMSO
39.52 DMSO
39.24 DMSO
38.96 DMSO
38.68 DMSO
36.74
31.26
29.02
28.99
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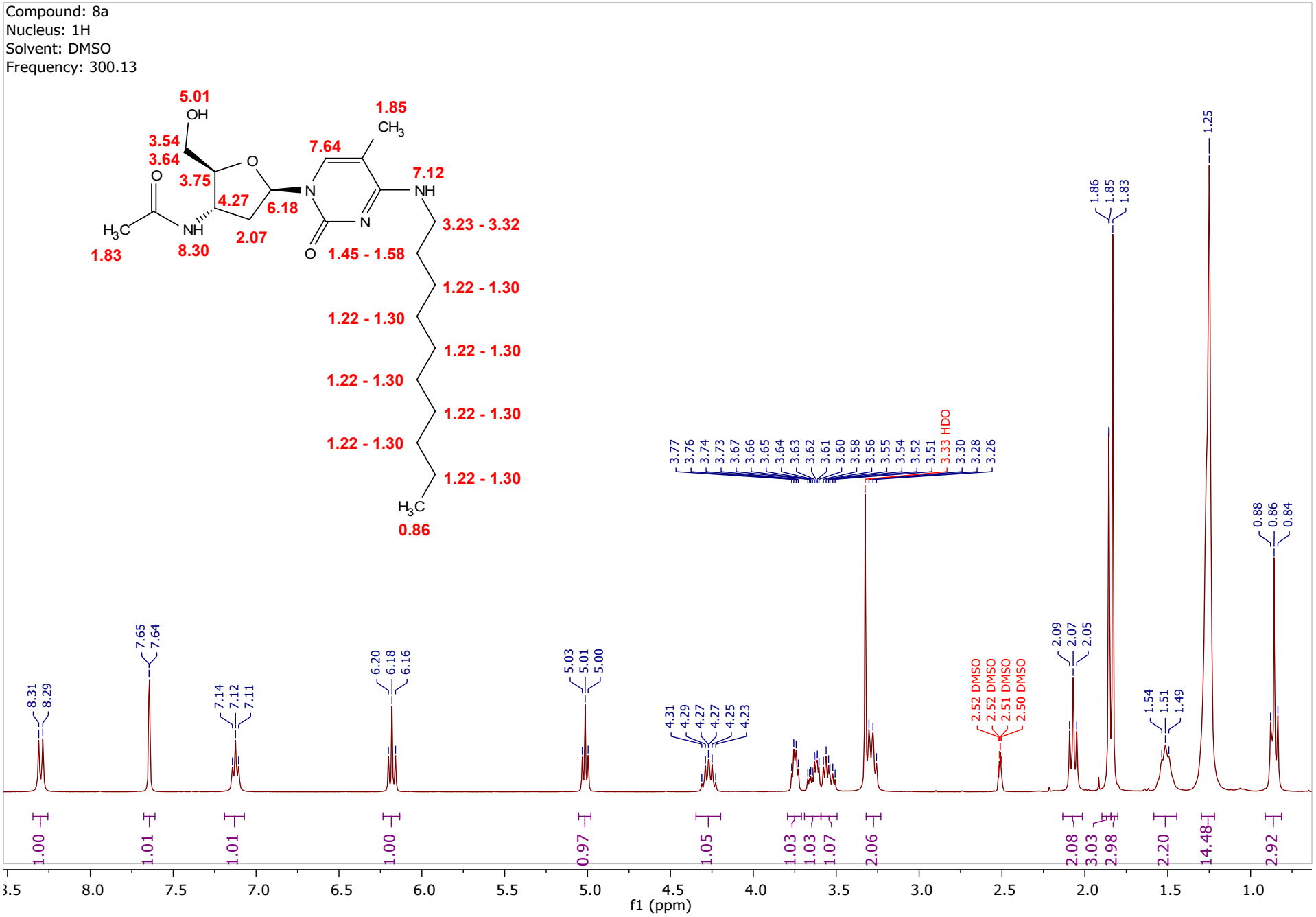
28.67
28.55
26.44
22.06
13.90
13.07
f1 (ppm)


Compound: 8a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
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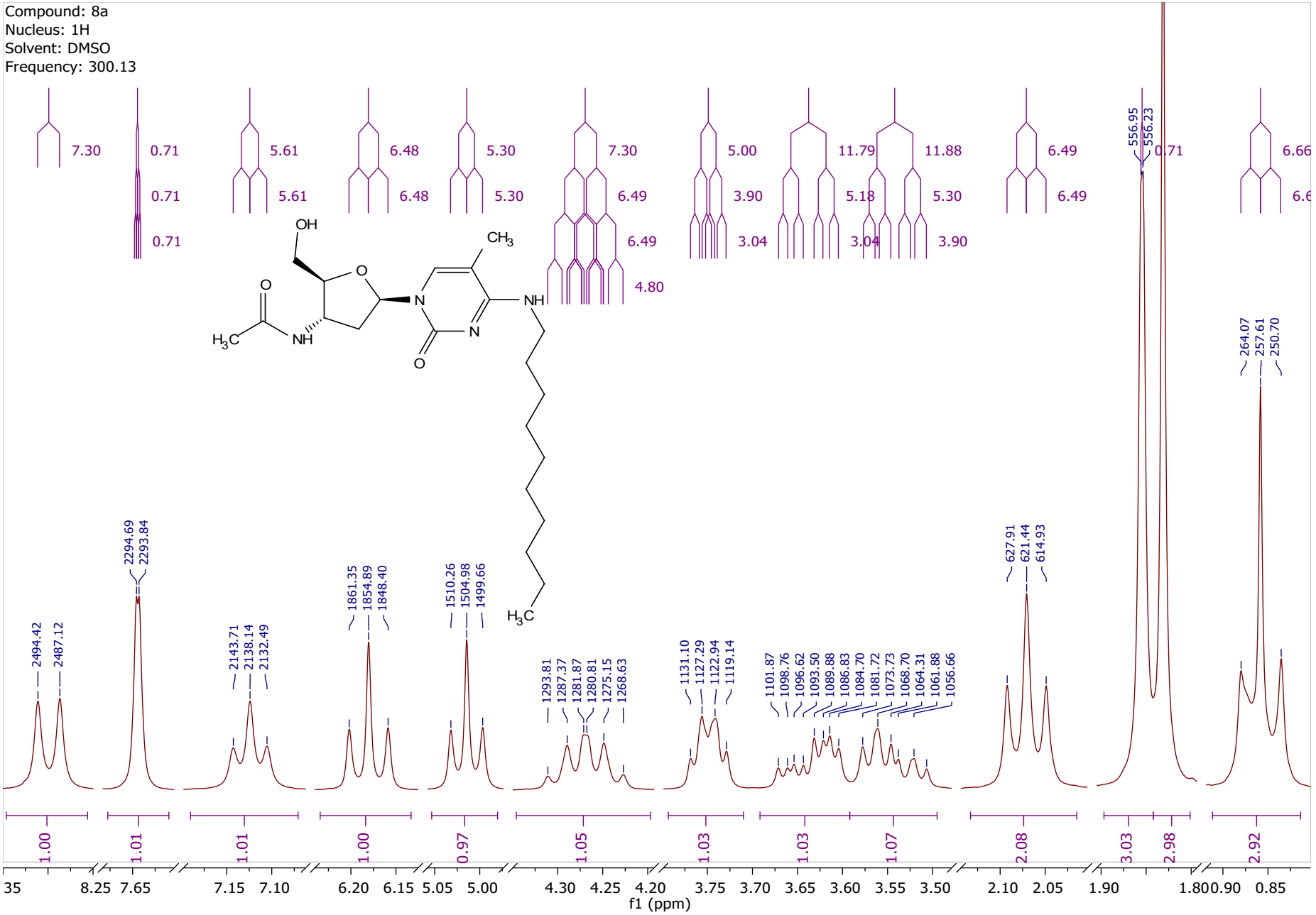
OH
3.54
3.64
3.75
4.27
6.18
2.07
8.30
1.83
1.85
CH3
7.64
7.12
NH
3.23 - 3.32
1.45 - 1.58
1.22 - 1.30
1.22 - 1.30
1.22 - 1.30
1.22 - 1.30
1.22 - 1.30
1.22 - 1.30
0.86
f1 (ppm)


Compound: 8a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
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0.71
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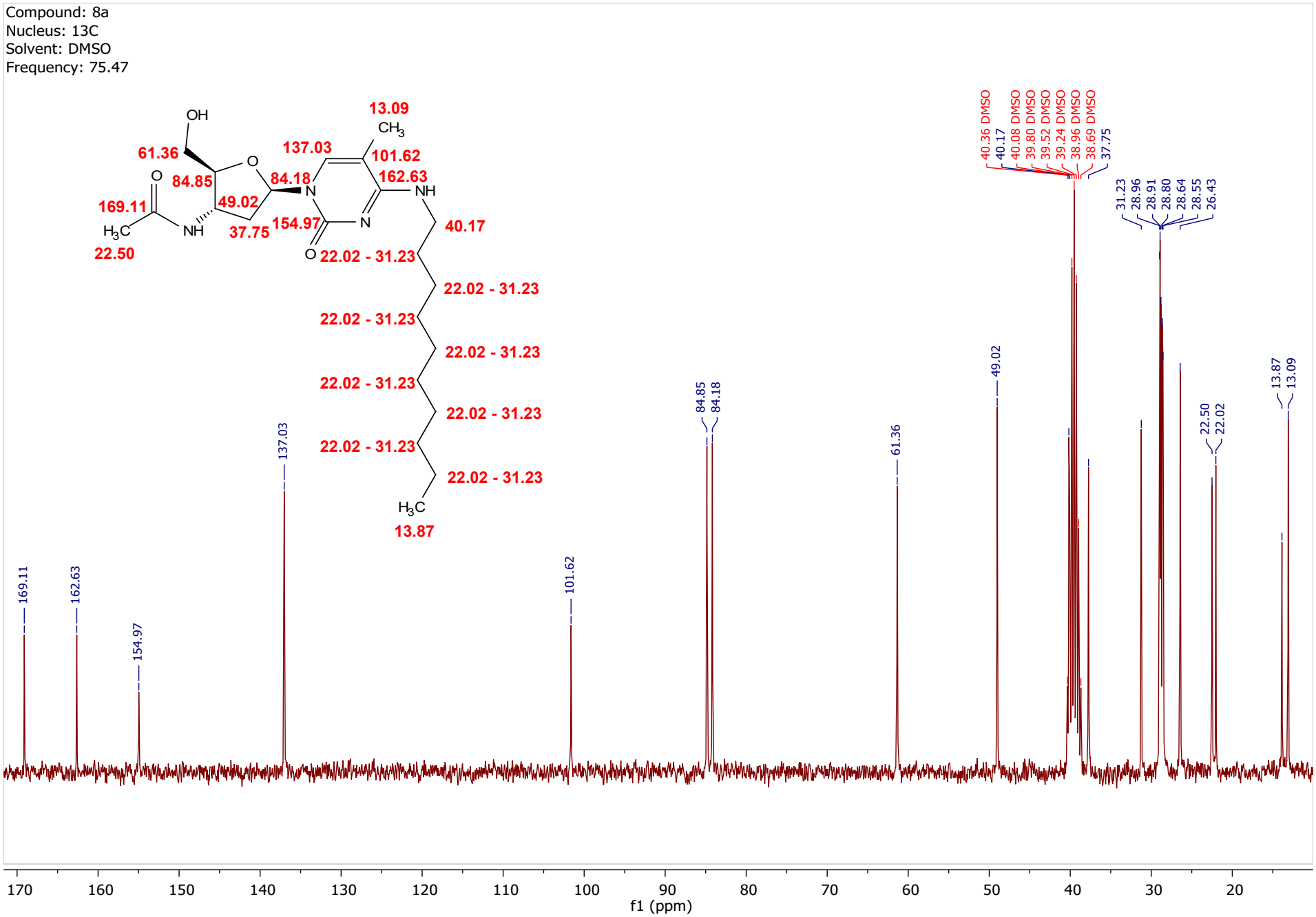
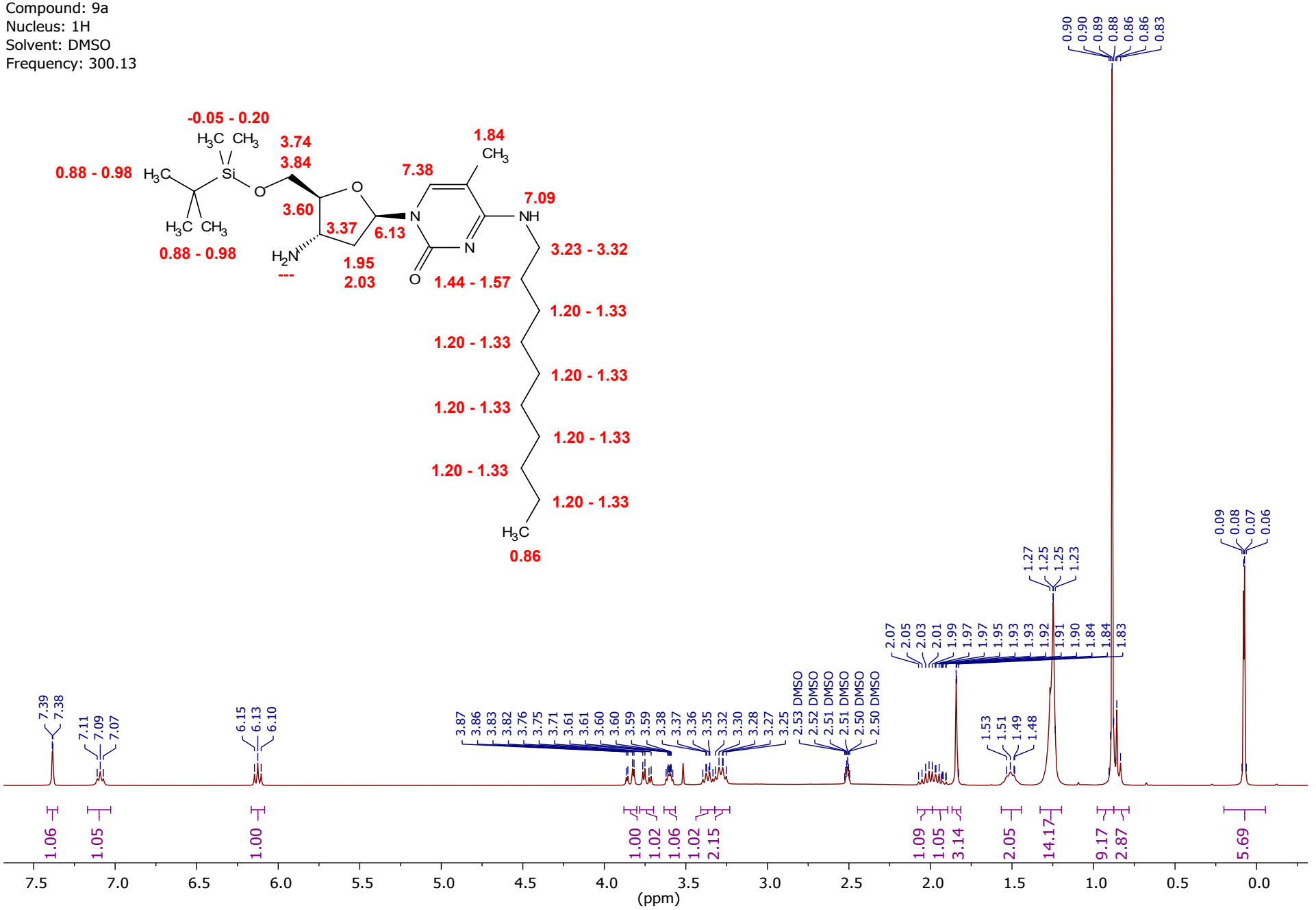
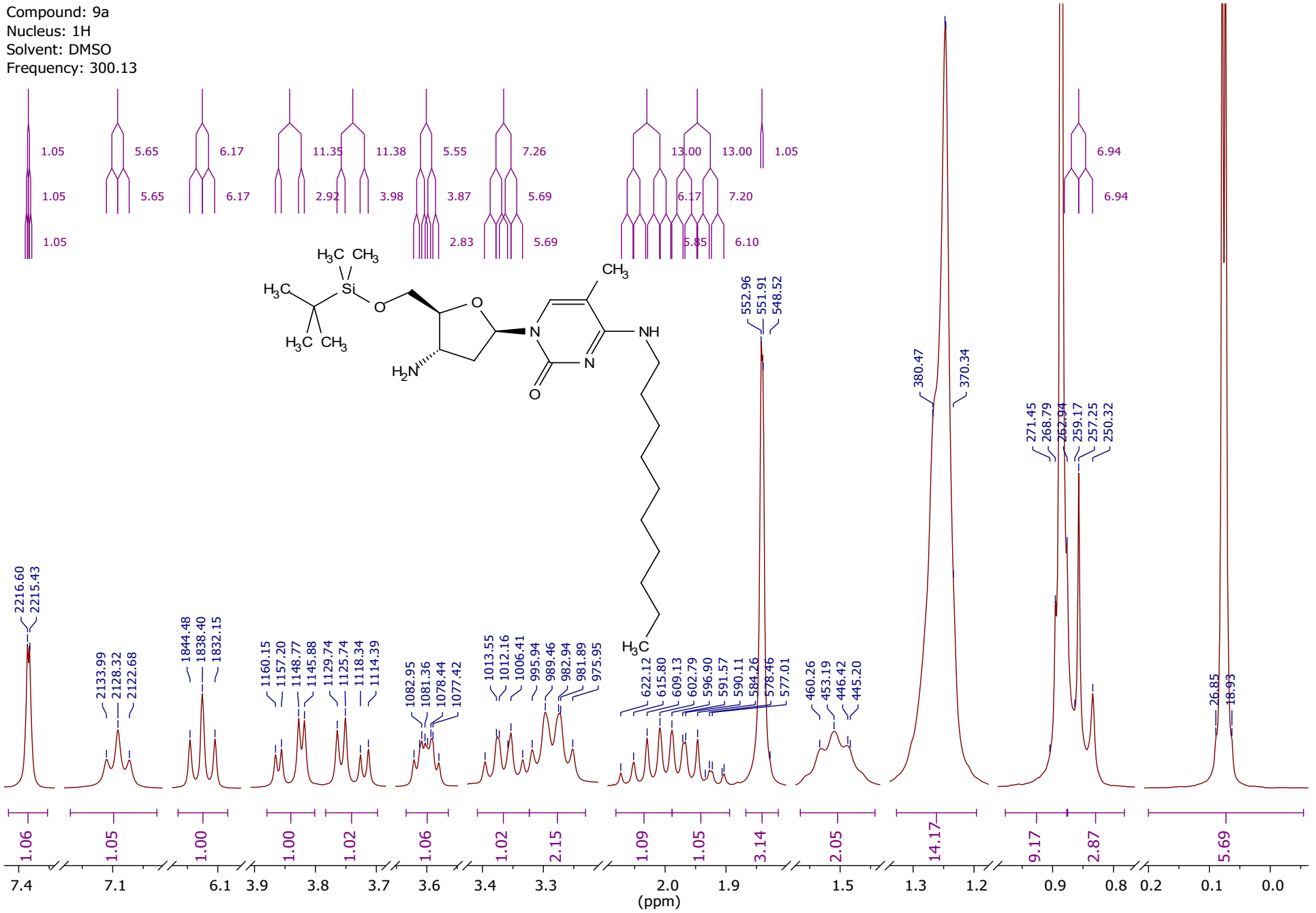
6.48
6.48
5.30
5.30
7.30
6.49
6.49
4.80
5.00
3.90
3.04
11.79
5.18
3.04
11.88
5.30
3.90
6.49
6.49
556.95
556.23
0.71
6.66
6.6
OH
O
O
N
CH3
NH
N
H3C
NH
O
H3C
264.07
257.61
250.70
2494.42
2487.12
2294.69
2293.84
2143.71
2138.14
2132.49
1861.35
1854.89
1848.40
1510.26
1504.98
1499.66
1293.81
1287.37
1281.87
1280.81
1275.15
1268.63
1131.10
1127.29
1122.94
1119.14
1101.87
1098.76
1096.62
1093.50
1089.88
1086.83
1084.70
1081.72
1073.73
1068.70
1064.31
1061.88
1056.66
627.91
621.44
614.93
1.00
1.01
1.01
1.00
0.97
1.05
1.03
1.03
1.07
2.08
3.03
2.98
2.92
35
8.25
7.65
7.15
7.10
6.20
6.15
5.05
5.00
4.30
4.25
4.20
3.75
3.70
3.65
3.60
3.55
3.50
2.10
2.05
1.90
1.80
0.90
0.85
f1 (ppm)

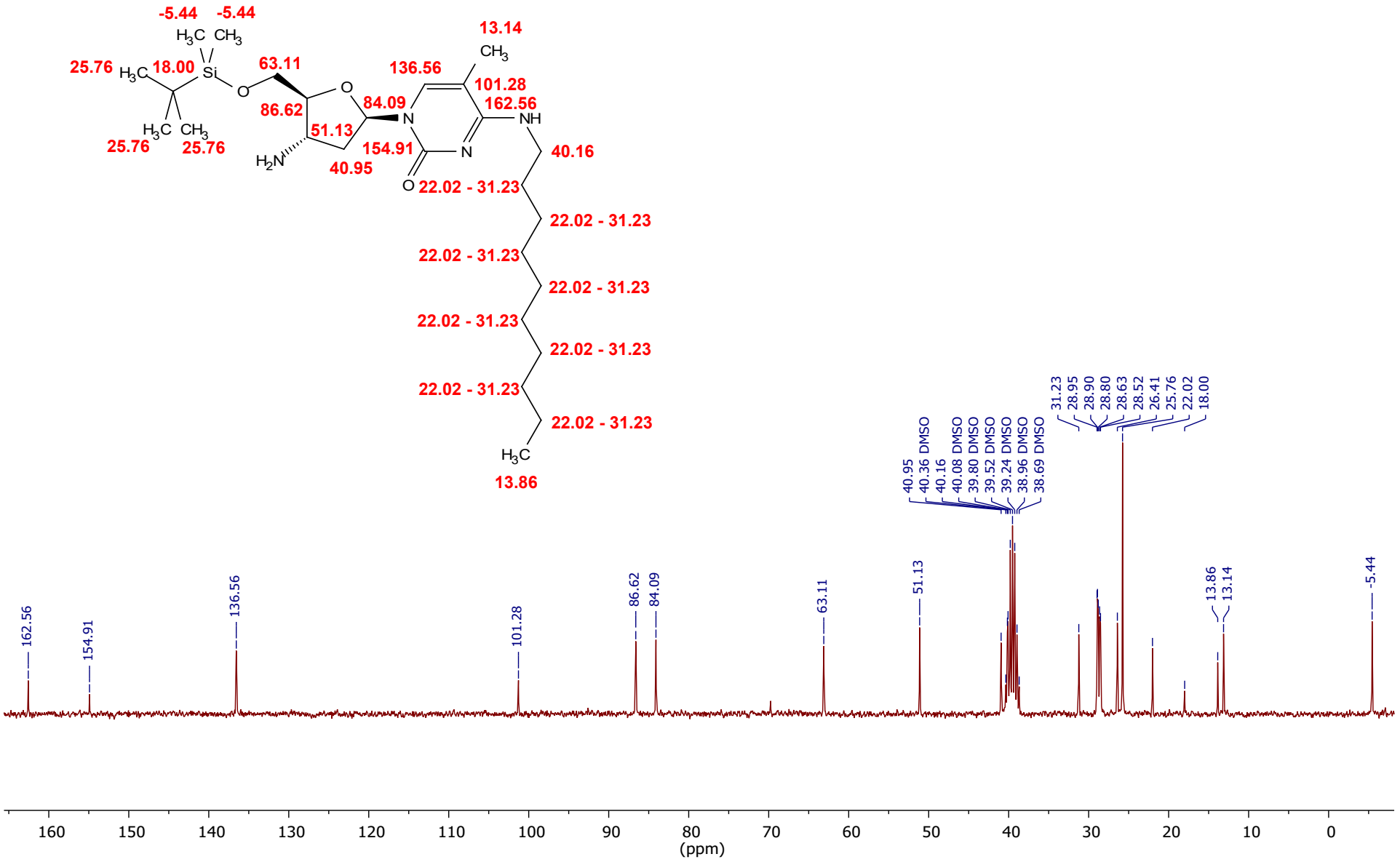

Compound: 8a
Nucleus: 13C
Solvent: DMSO
Frequency: 75.47
OH
61.36
O
84.85
84.18
O
N
NH
169.11
49.02
13.09
CH3
137.03
101.62
162.63
H3C
NH
37.75
154.97
N
22.50
O
22.02 - 31.23
40.17
22.02 - 31.23
22.02 - 31.23
22.02 - 31.23
22.02 - 31.23
22.02 - 31.23
22.02 - 31.23
H3C
13.87
40.36 DMSO
40.17
40.08 DMSO
39.80 DMSO
39.52 DMSO
39.24 DMSO
38.96 DMSO
38.69 DMSO
37.75
31.23
28.96
28.91
28.80
28.64
28.55
26.43
169.11
162.63
154.97
137.03
101.62
84.85
84.18
61.36
49.02
22.50
22.02
13.87
13.09
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

Compound: 9a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

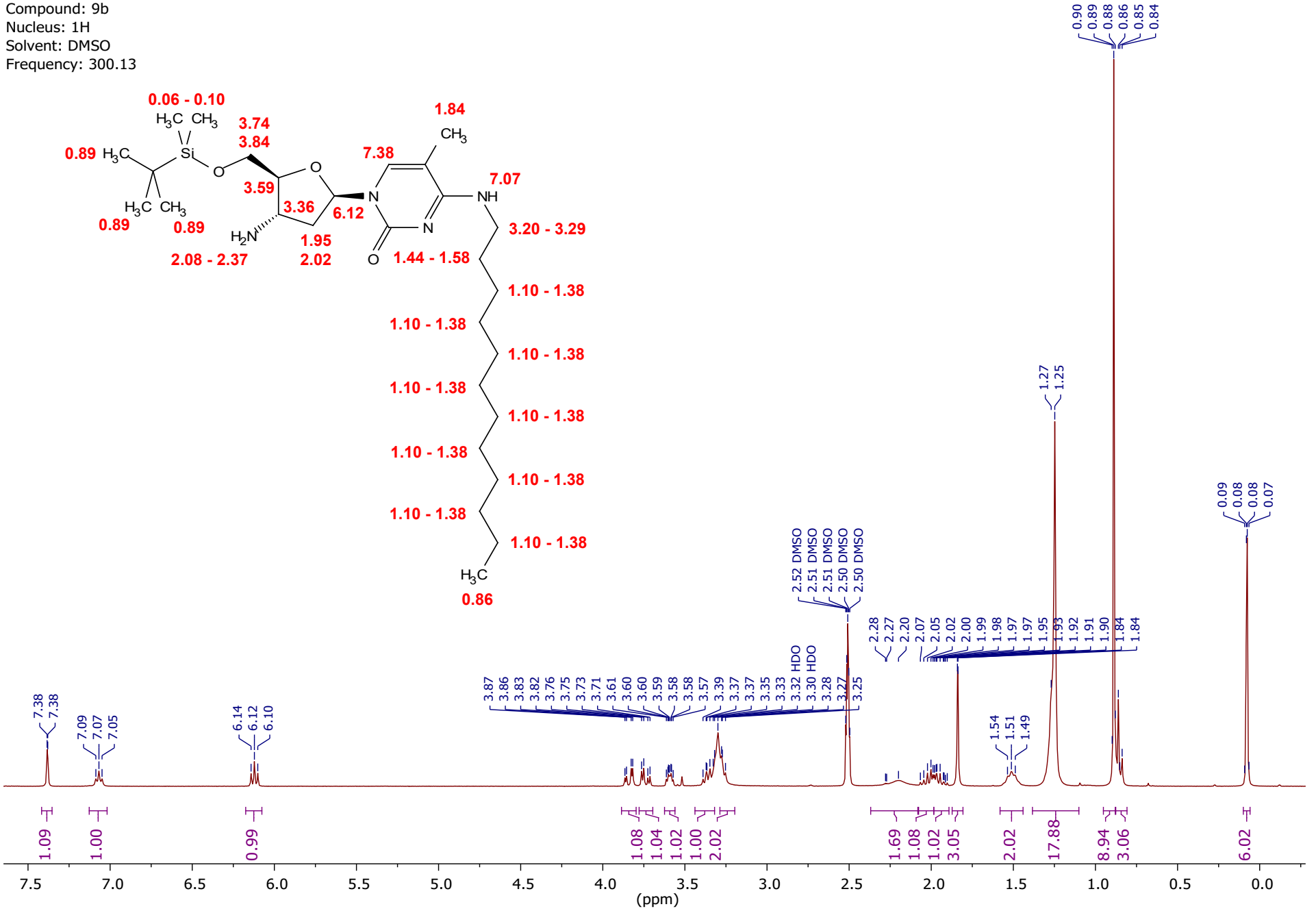



Compound: 9a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
1.05
1.05
1.05
5.65
5.65
6.17
6.17
11.35
2.92
11.38
3.98
5.55
3.87
2.83
7.26
5.69
5.69
13.00
6.17
5.85
13.00
7.20
6.10
1.05
6.94
6.94
H3C CH3
H3C
Si
H3C CH3
O
O
H2N
N
N
NH
O
CH3
H3C
2216.60
2215.43
2133.99
2128.32
2122.68
1844.48
1838.40
1832.15
1160.15
1157.20
1148.77
1145.88
1129.74
1125.74
1118.34
1114.39
1082.95
1081.36
1078.44
1077.42
1013.55
1012.16
1006.41
995.94
989.46
982.94
981.89
975.95
622.12
615.80
609.13
602.79
596.90
591.57
590.11
584.26
578.46
577.01
552.96
551.91
548.52
460.26
453.19
446.42
445.20
380.47
370.34
271.45
268.79
262.94
259.17
257.25
250.32
26.85
18.93
1.06
1.05
1.00
1.00
1.02
1.06
1.02
2.15
1.09
1.05
3.14
2.05
14.17
9.17
2.87
5.69
7.4
7.1
6.1
3.9
3.8
3.7
3.6
3.4
3.3
2.0
1.9
1.5
1.3
1.2
0.9
0.8
0.2
0.1
0.0
(ppm)

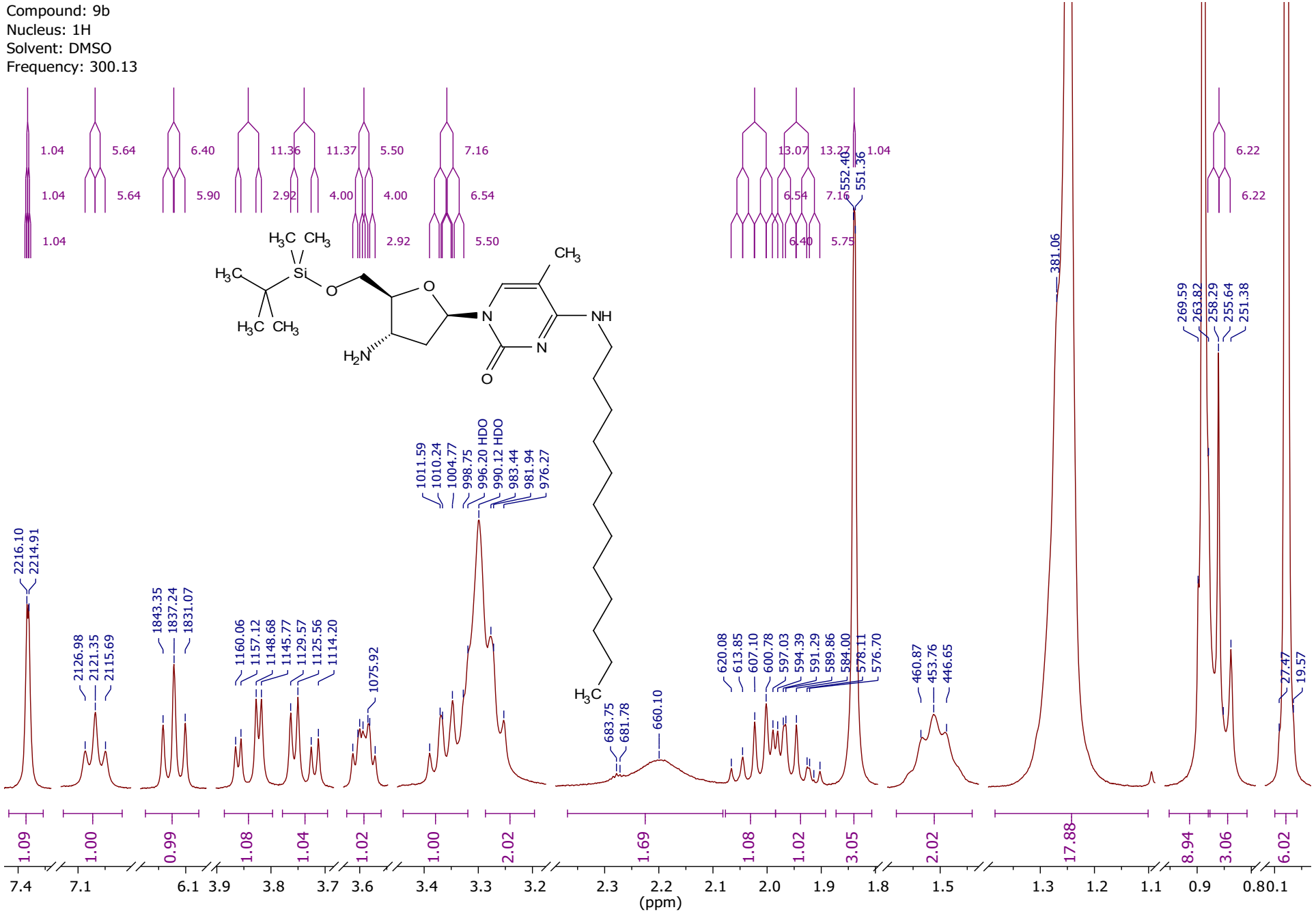
Compound: 9a
Nucleus: 13C
Solvent: DMSO
Frequency: 75.47

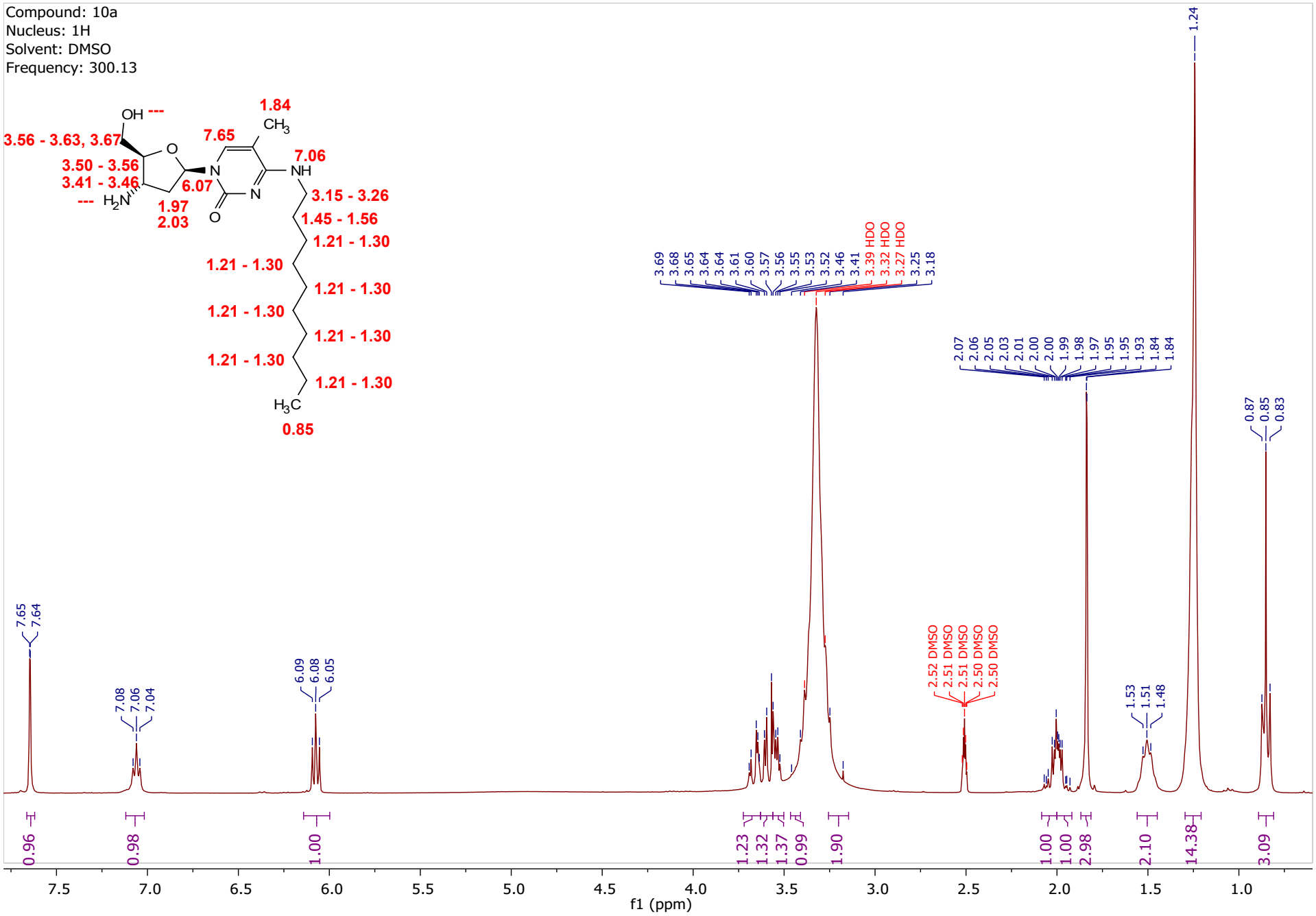


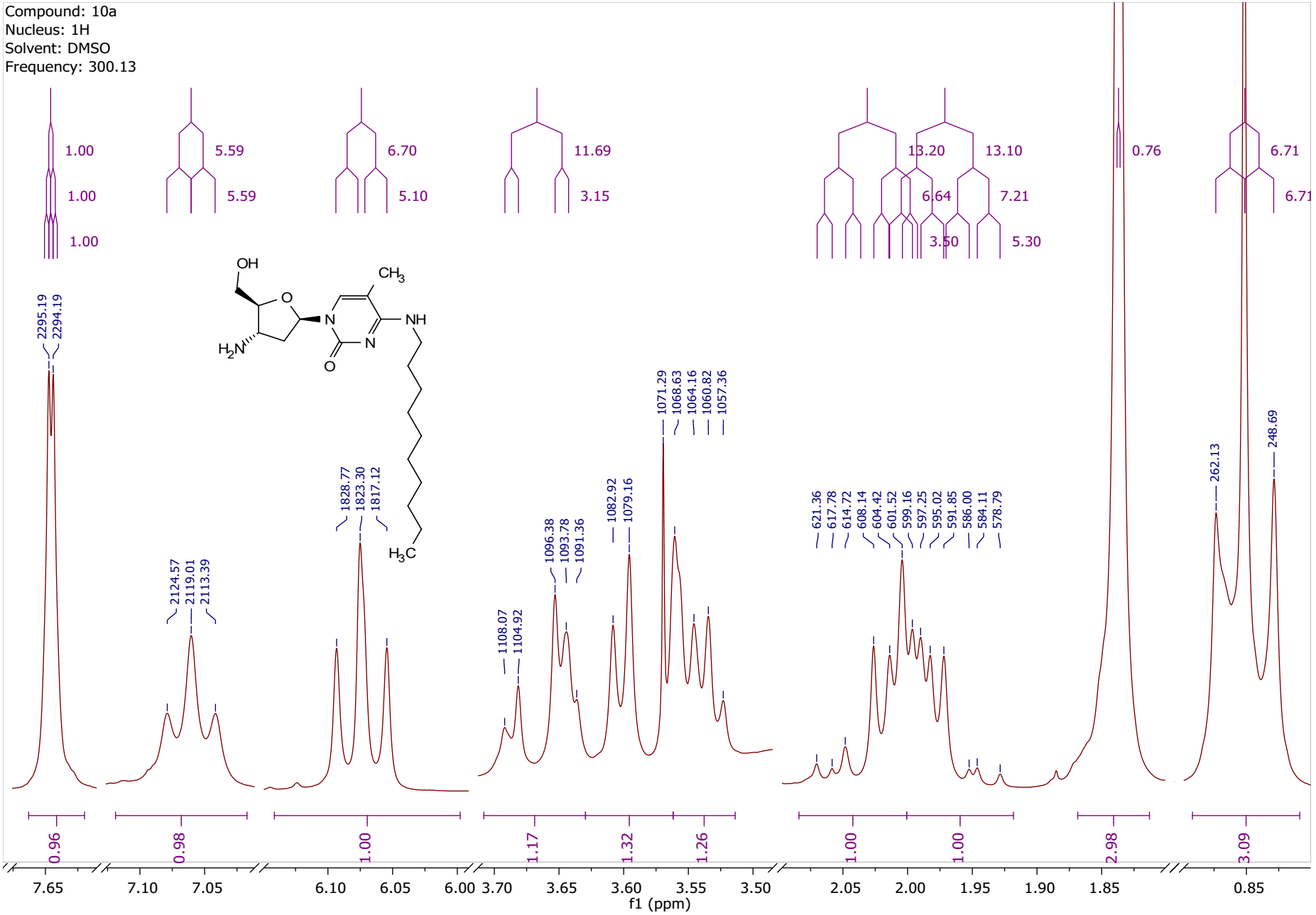
Compound: 9b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

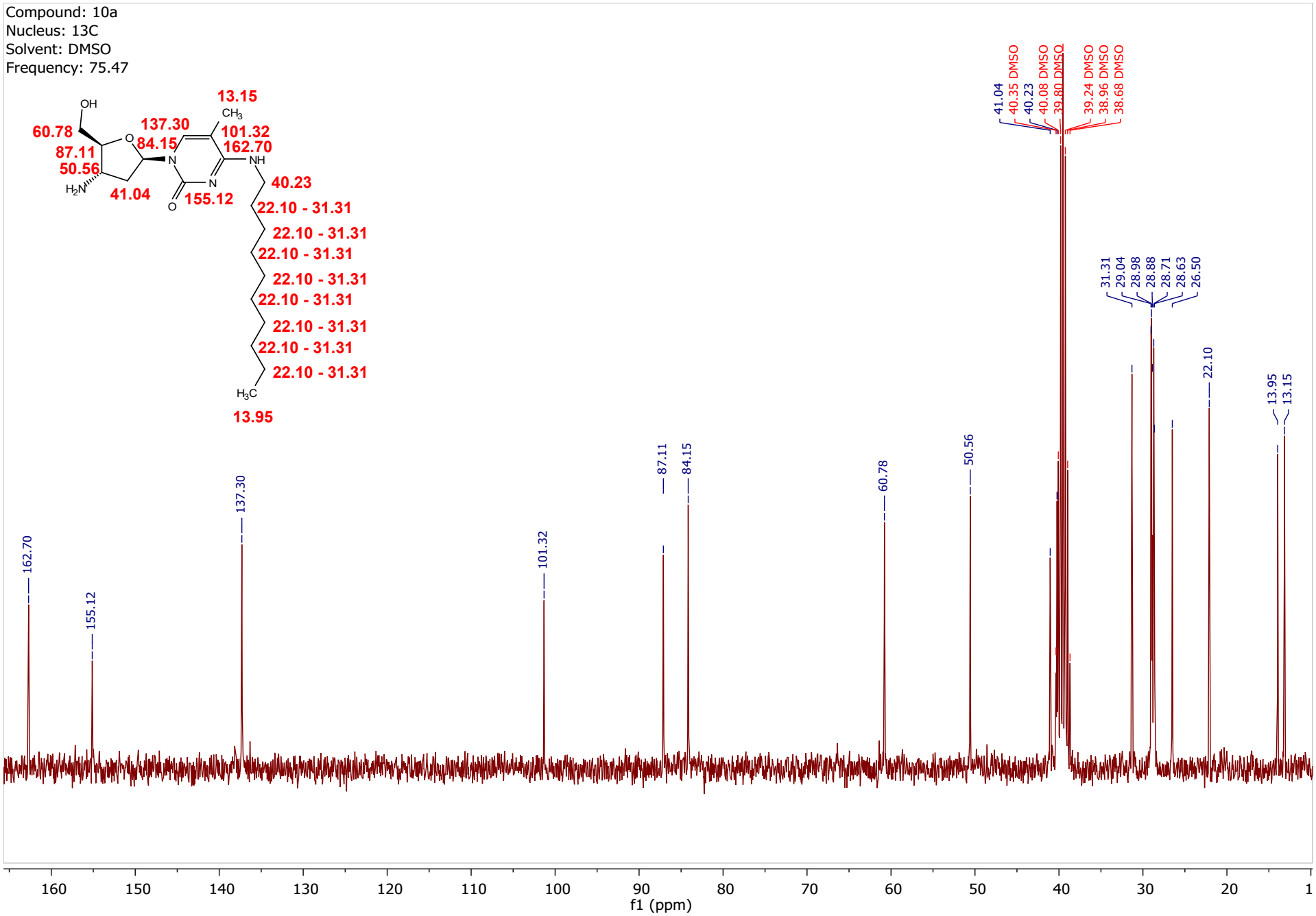


Compound: 9b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

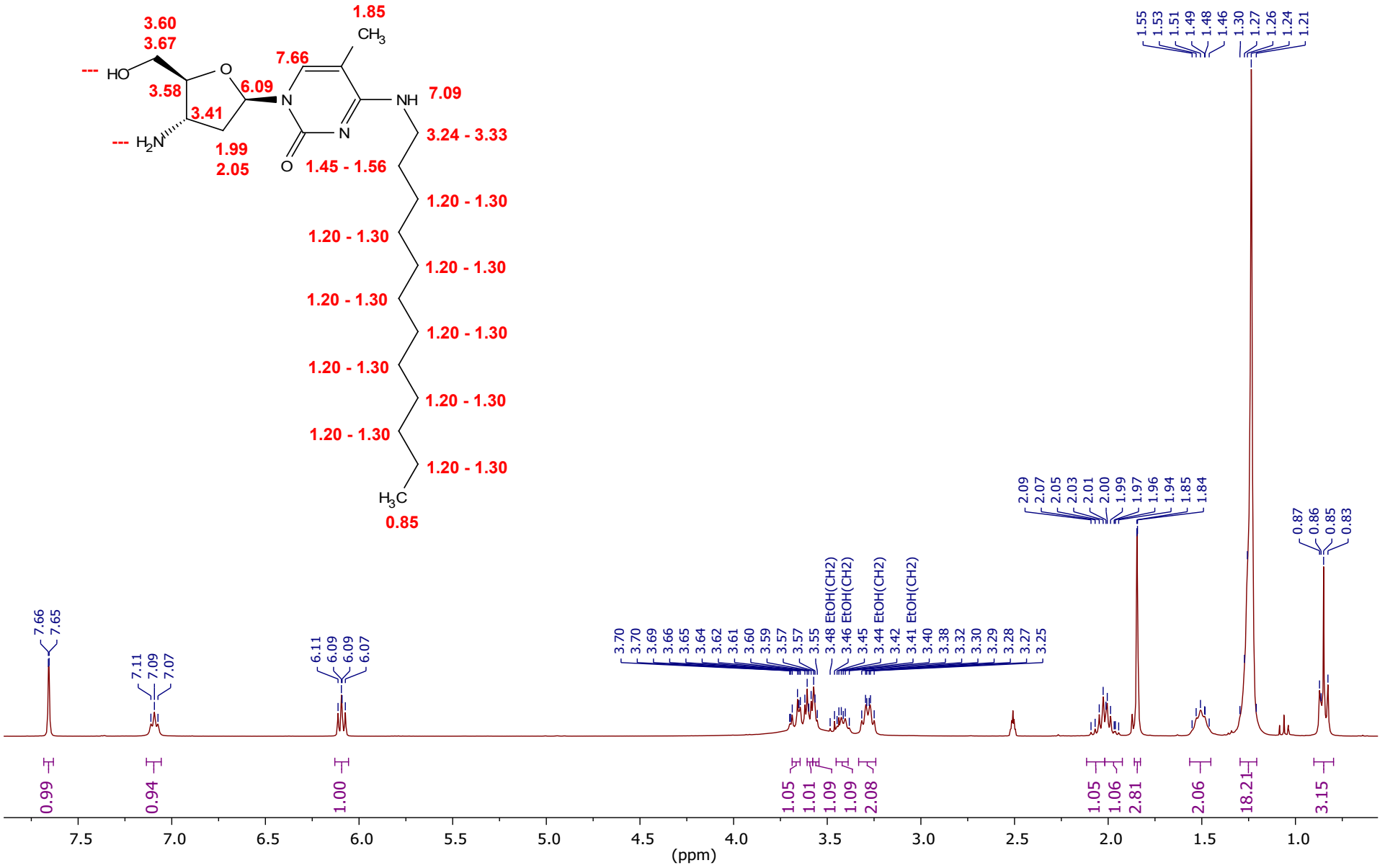



Compound: 10a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
OH ---
3.56 - 3.63, 3.67
3.50 - 3.56
3.41 - 3.46
--- H2N
1.97
2.03
7.65
6.07
1.84
CH3
7.06
NH
3.15 - 3.26
1.45 - 1.56
1.21 - 1.30
1.21 - 1.30
1.21 - 1.30
1.21 - 1.30
1.21 - 1.30
1.21 - 1.30
H3C
0.85
f1 (ppm)

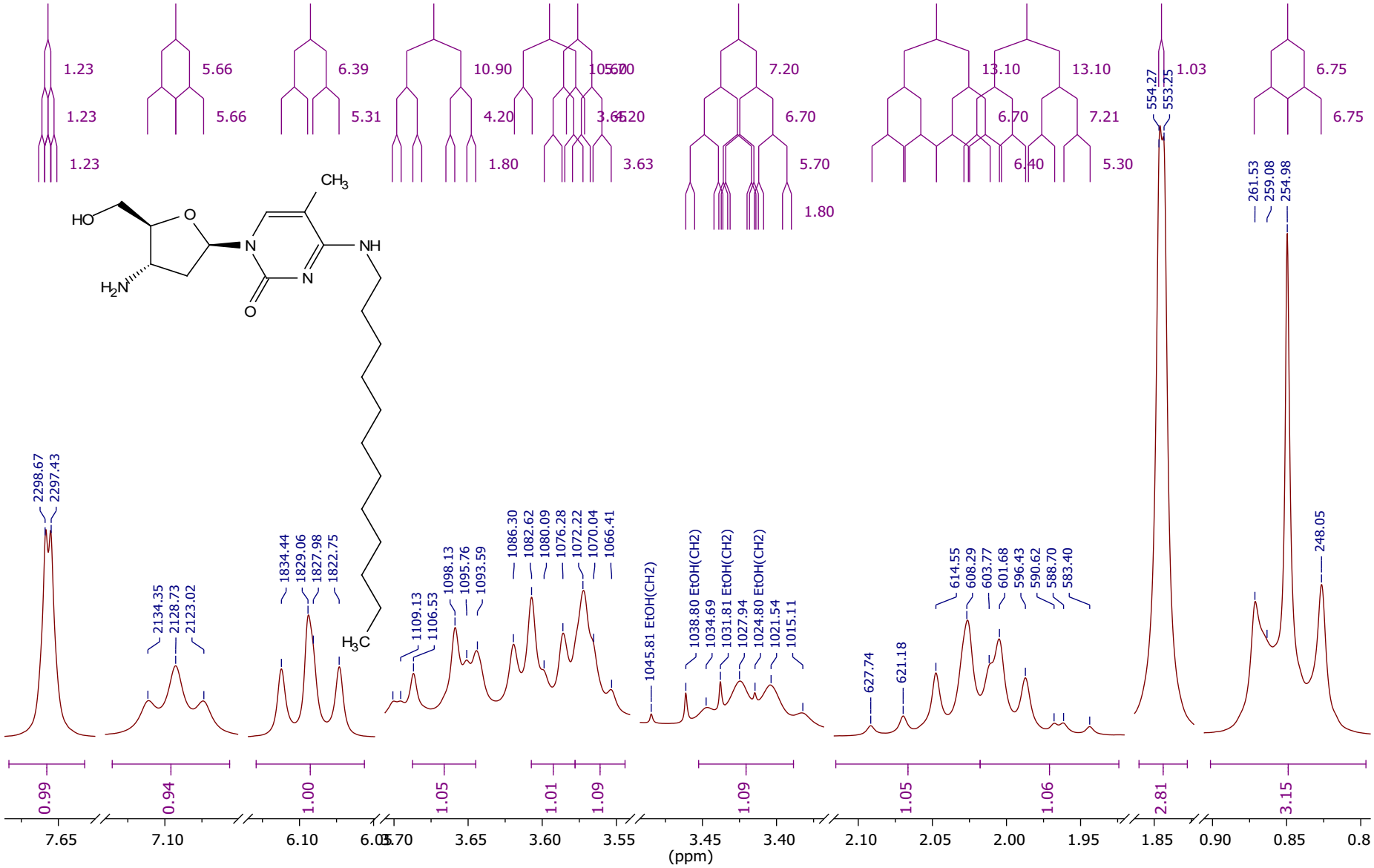

Compound: 10a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
1.00
1.00
1.00
5.59
5.59
6.70
5.10
11.69
3.15
13.20
13.10
6.64
7.21
3.50
5.30
0.76
6.71
6.71
OH
CH3
O
N
NH
H2N
N
O
H3C
2295.19
2294.19
2124.57
2119.01
2113.39
1828.77
1823.30
1817.12
1108.07
1104.92
1096.38
1093.78
1091.36
1082.92
1079.16
1071.29
1068.63
1064.16
1060.82
1057.36
621.36
617.78
614.72
608.14
604.42
601.52
599.16
597.25
595.02
591.85
586.00
584.11
578.79
262.13
248.69
0.96
0.98
1.00
1.17
1.32
1.26
1.00
1.00
2.98
3.09
7.65
7.10
7.05
6.10
6.05
6.00
3.70
3.65
3.60
3.55
3.50
2.05
2.00
1.95
1.90
1.85
0.85
f1 (ppm)


Compound: 10a
Nucleus: 13C
Solvent: DMSO
Frequency: 75.47
13.15
137.30
101.32
60.78
84.15
162.70
87.11
50.56
40.23
41.04
155.12
22.10 - 31.31
13.95
41.04
40.35 DMSO
40.23
40.08 DMSO
39.80 DMSO
39.24 DMSO
38.96 DMSO
38.68 DMSO
31.31
29.04
28.98
28.88
28.71
28.63
26.50
22.10
13.95
13.15
162.70
155.12
137.30
101.32
87.11
84.15
60.78
50.56
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
1
f1 (ppm)

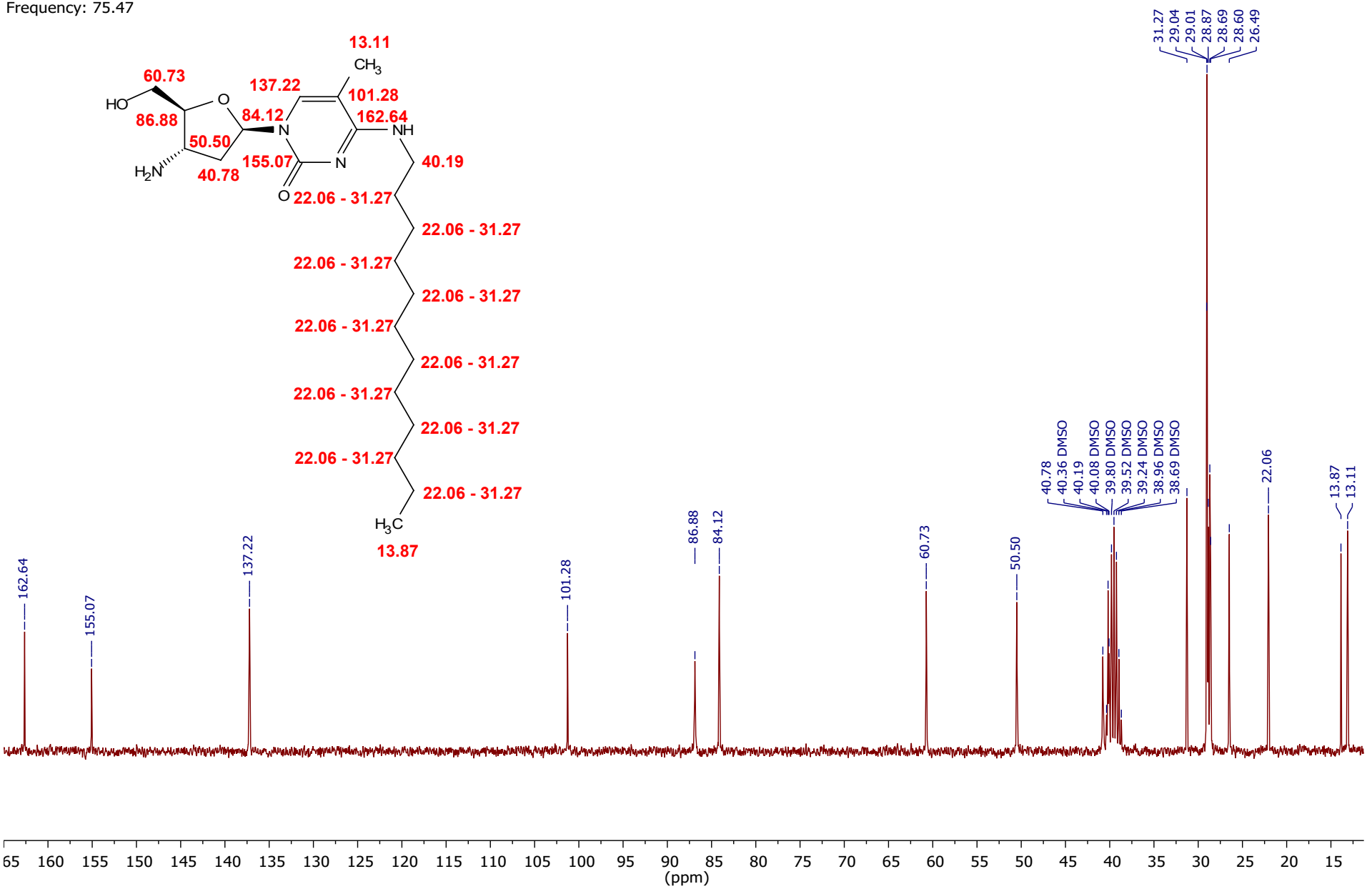
Compound: 10b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

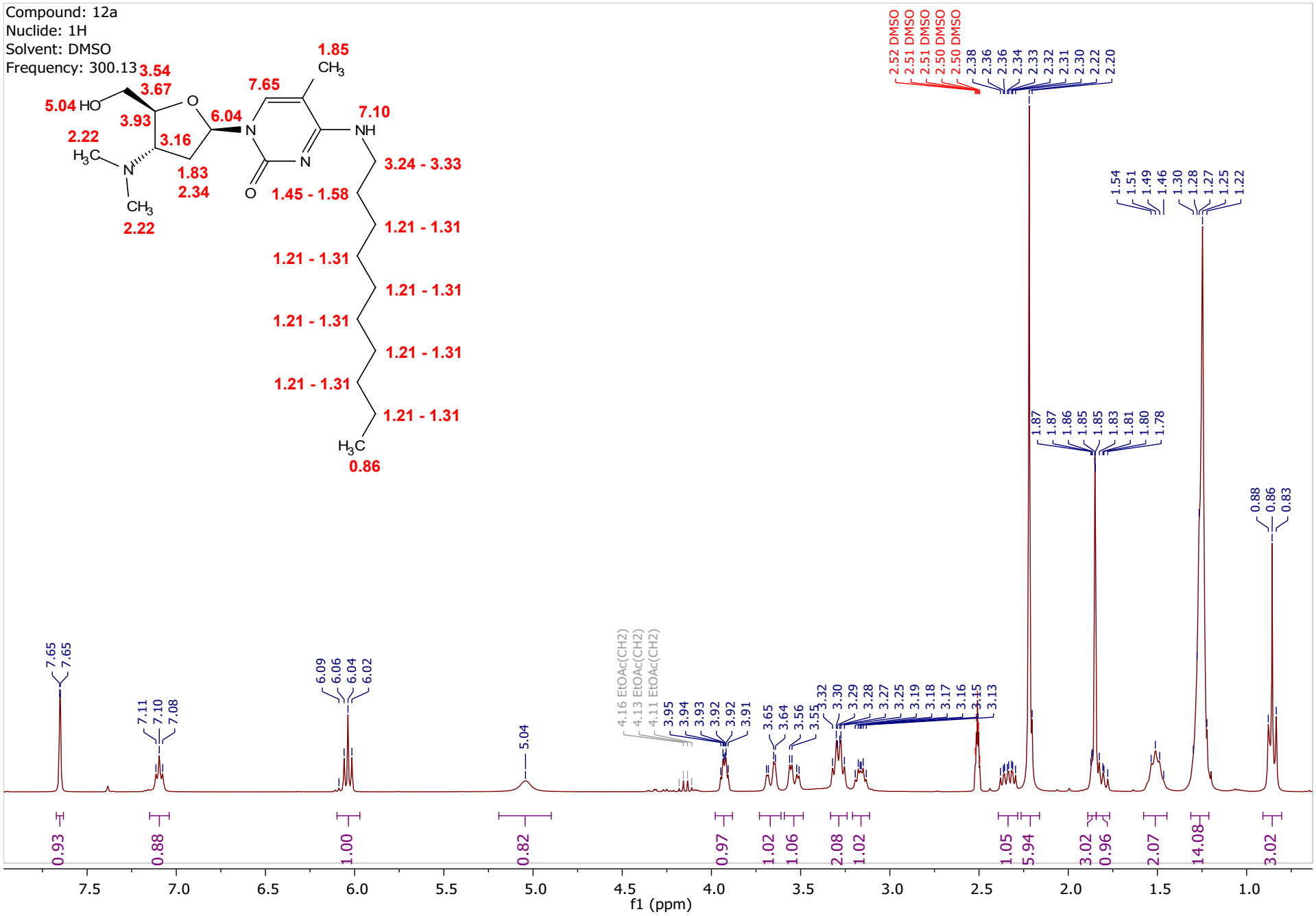


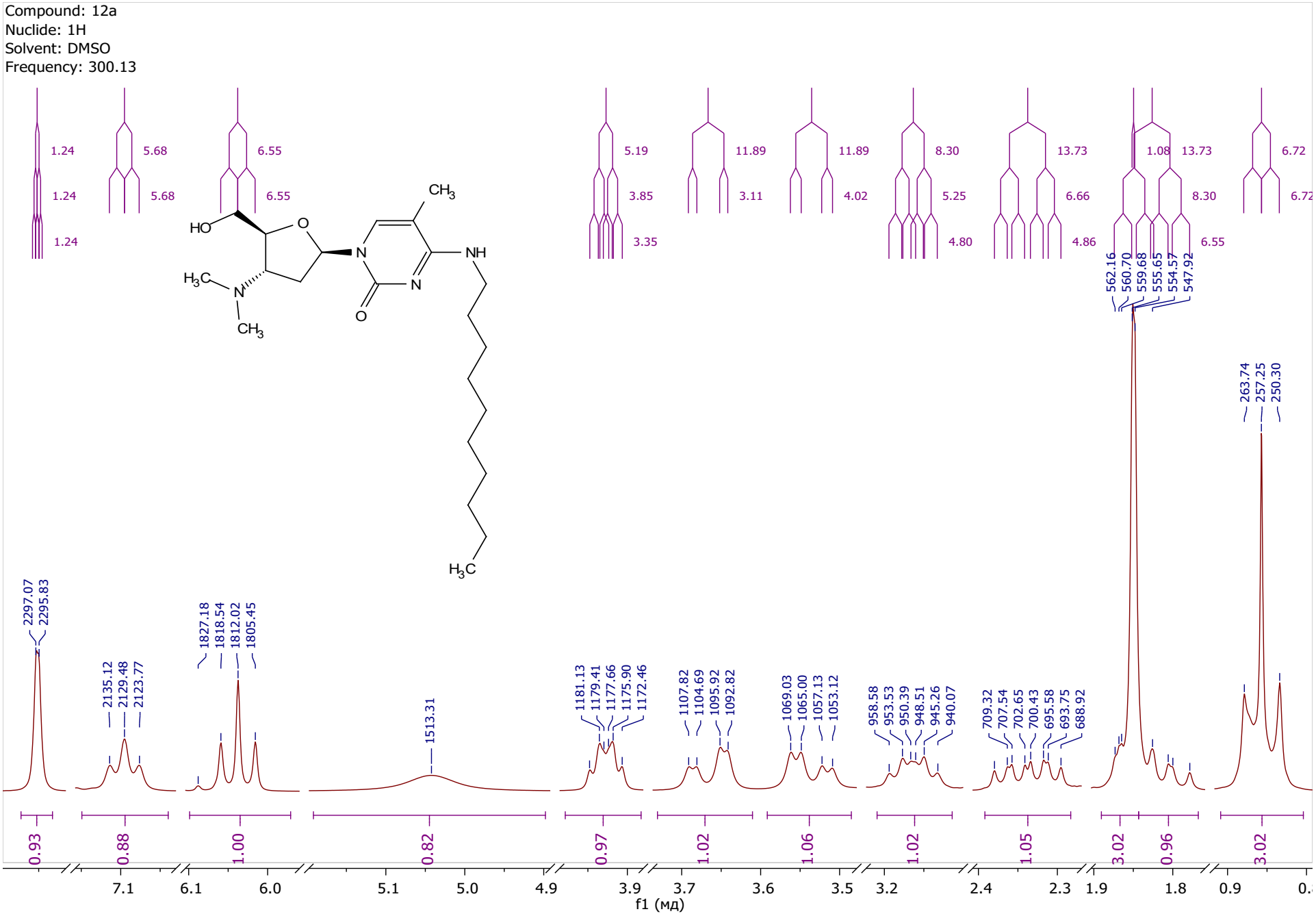
Compound: 10b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

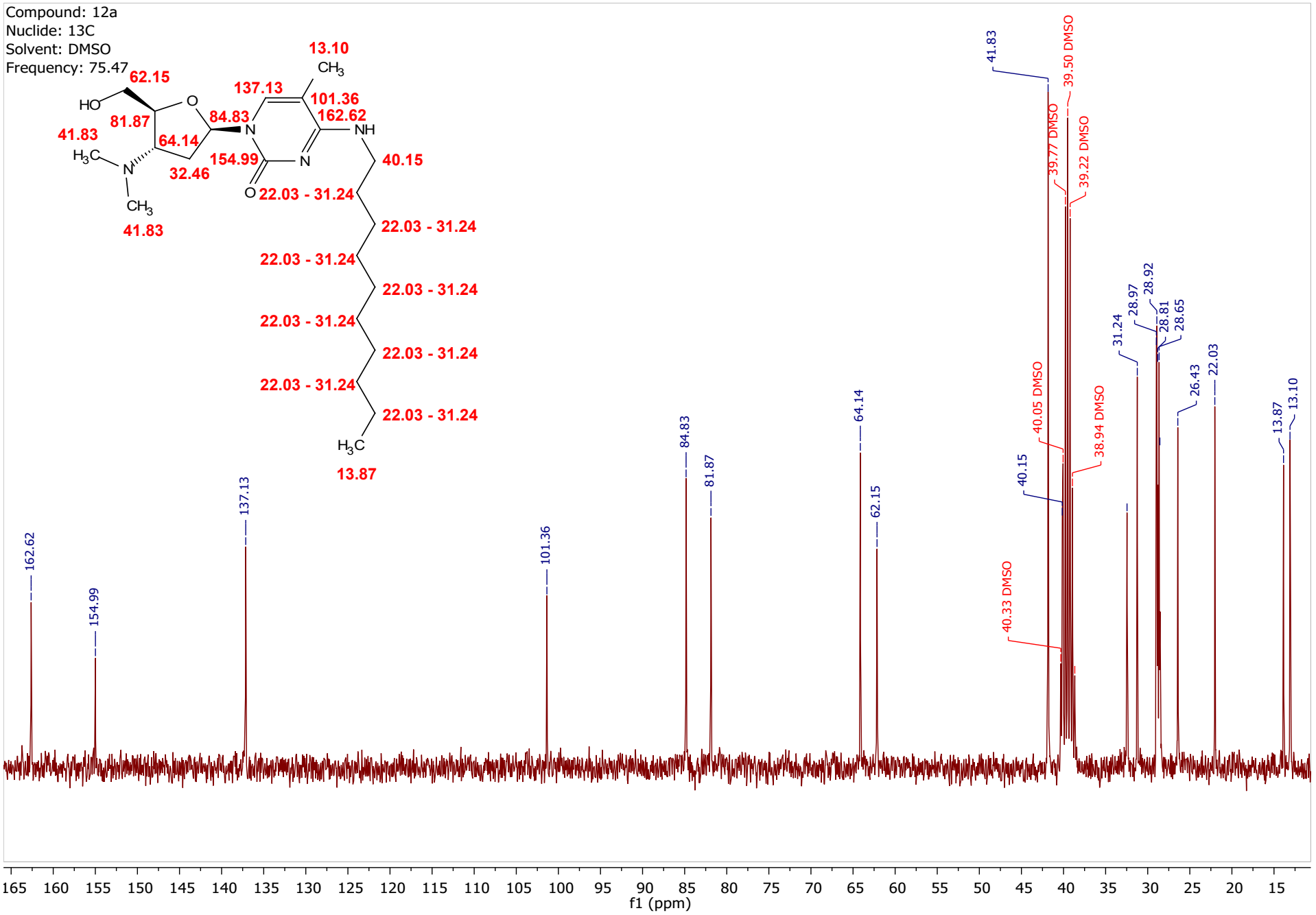


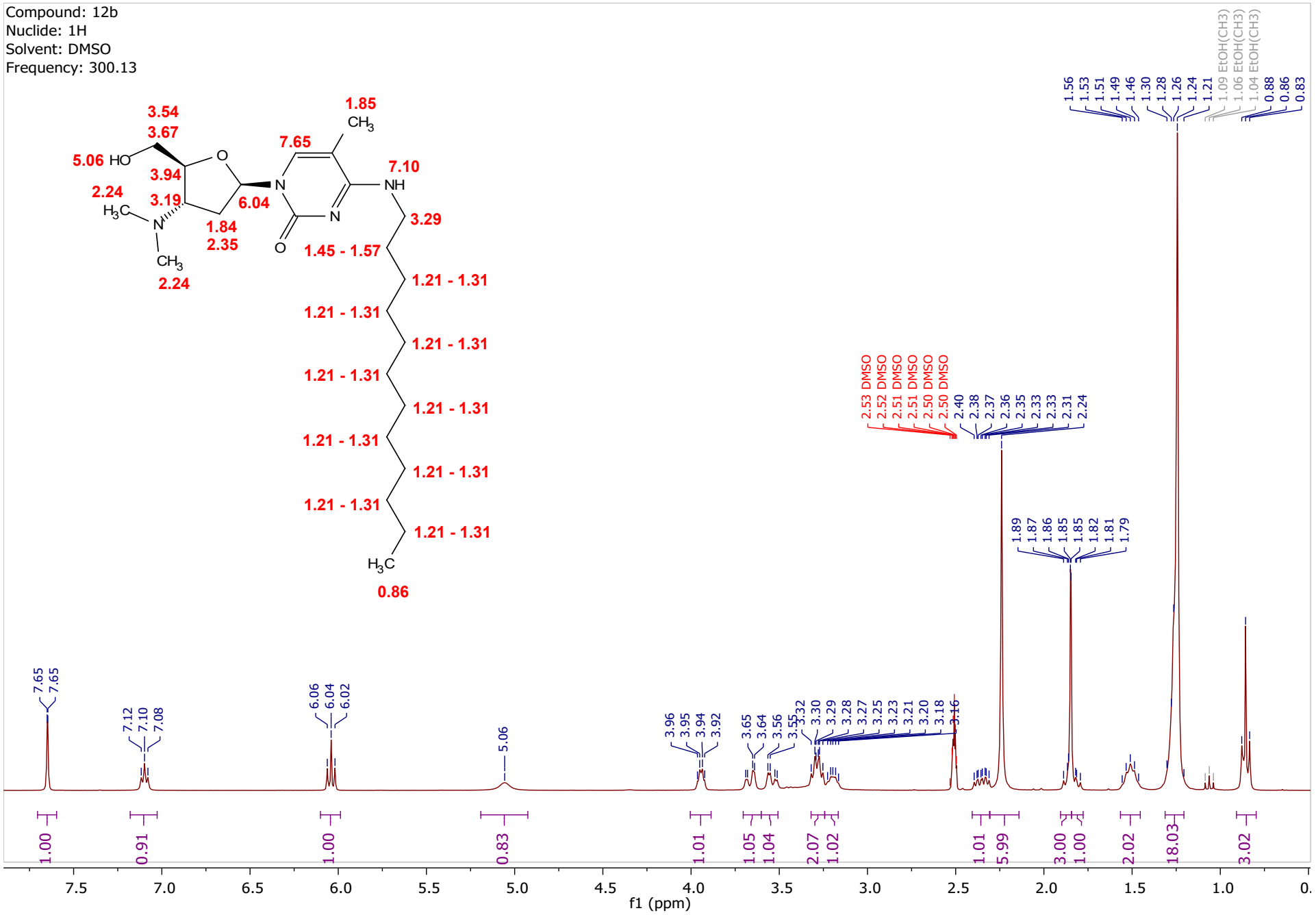
Compound: 10b
Nucleus: 13C
Solvent: DMSO
Frequency: 75.47

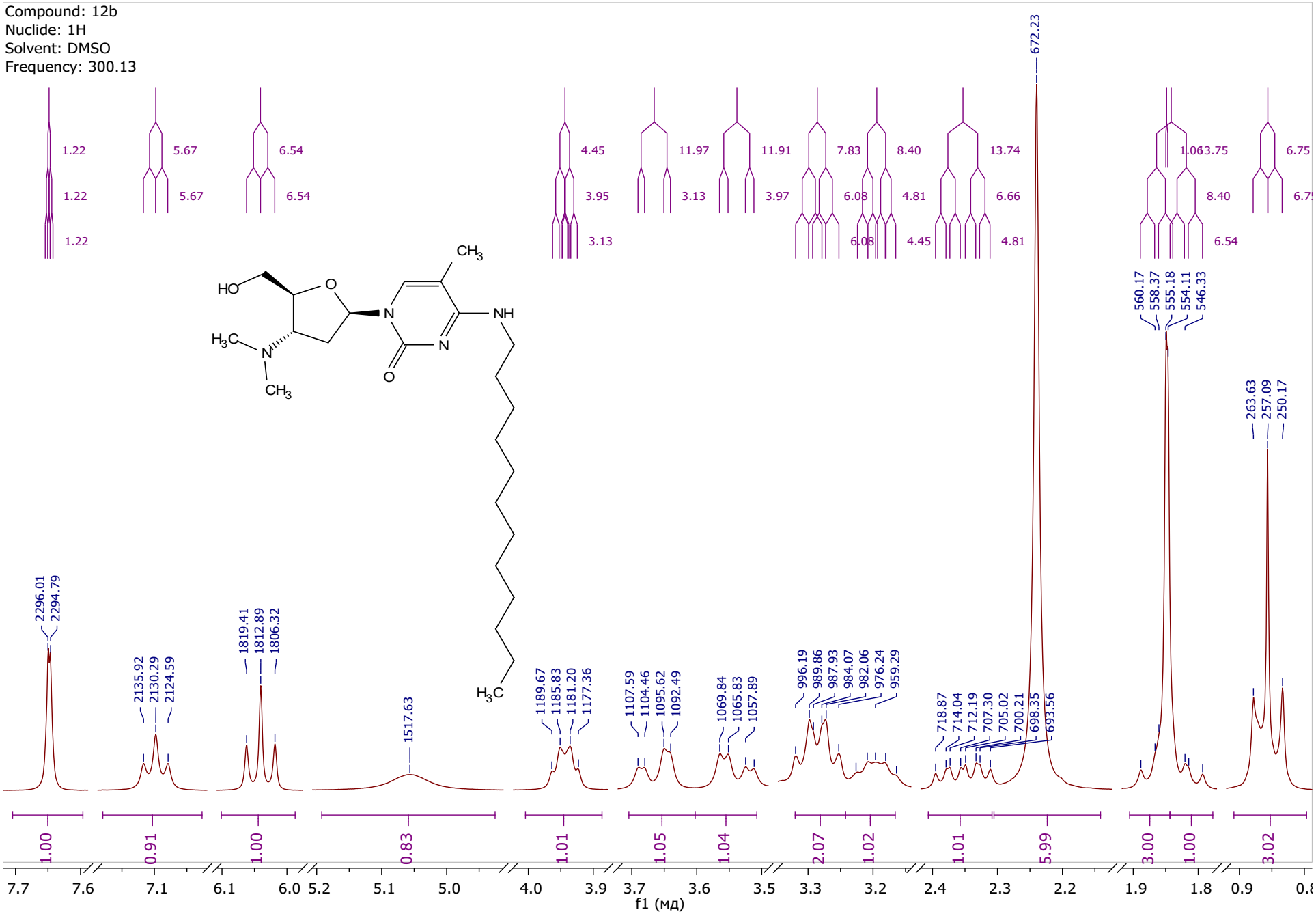


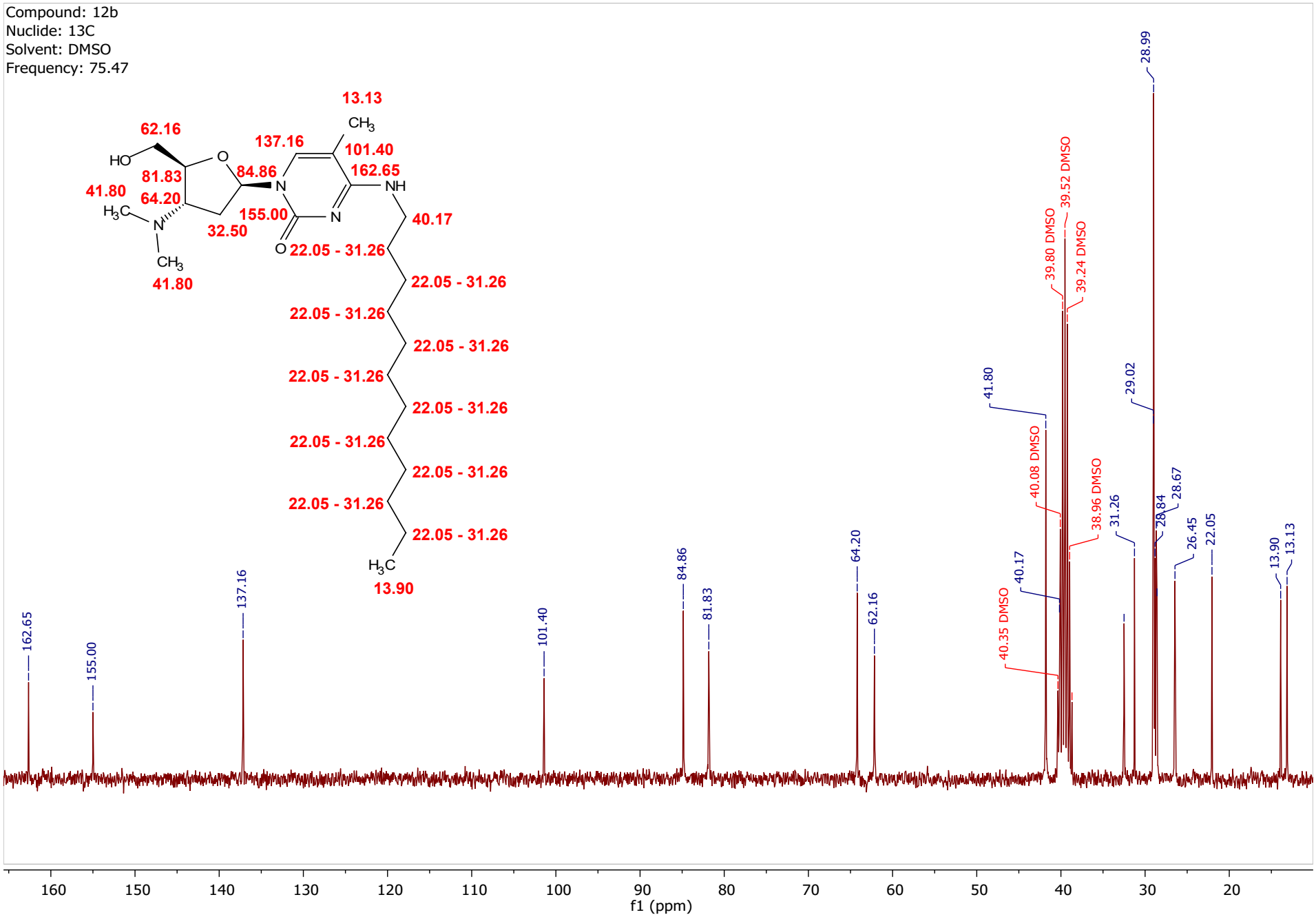

Compound: 12a
Nuclide: 1H
Solvent: DMSO
Frequency: 300.13
f1 (ppm)


Compound: 12a
Nuclide: 1H
Solvent: DMSO
Frequency: 300.13
1.24
1.24
1.24
5.68
5.68
6.55
6.55
5.19
3.85
3.35
11.89
3.11
11.89
4.02
8.30
5.25
4.80
13.73
6.66
4.86
1.08
13.73
8.30
6.55
6.72
6.72
HO
O
N
NH
H_3C
N
CH_3
N
CH_3
O
H_3C
562.16
560.70
559.68
555.65
554.57
547.92
263.74
257.25
250.30
2297.07
2295.83
2135.12
2129.48
2123.77
1827.18
1818.54
1812.02
1805.45
1513.31
1181.13
1179.41
1177.66
1175.90
1172.46
1107.82
1104.69
1095.92
1092.82
1069.03
1065.00
1057.13
1053.12
958.58
953.53
950.39
948.51
945.26
940.07
709.32
707.54
702.65
700.43
695.58
693.75
688.92
0.93
0.88
1.00
0.82
0.97
1.02
1.06
1.02
1.05
3.02
0.96
3.02
7.1
6.1
6.0
5.1
5.0
4.9
3.9
3.7
3.6
3.5
3.2
2.4
2.3
1.9
1.8
0.9
f1 (мд)

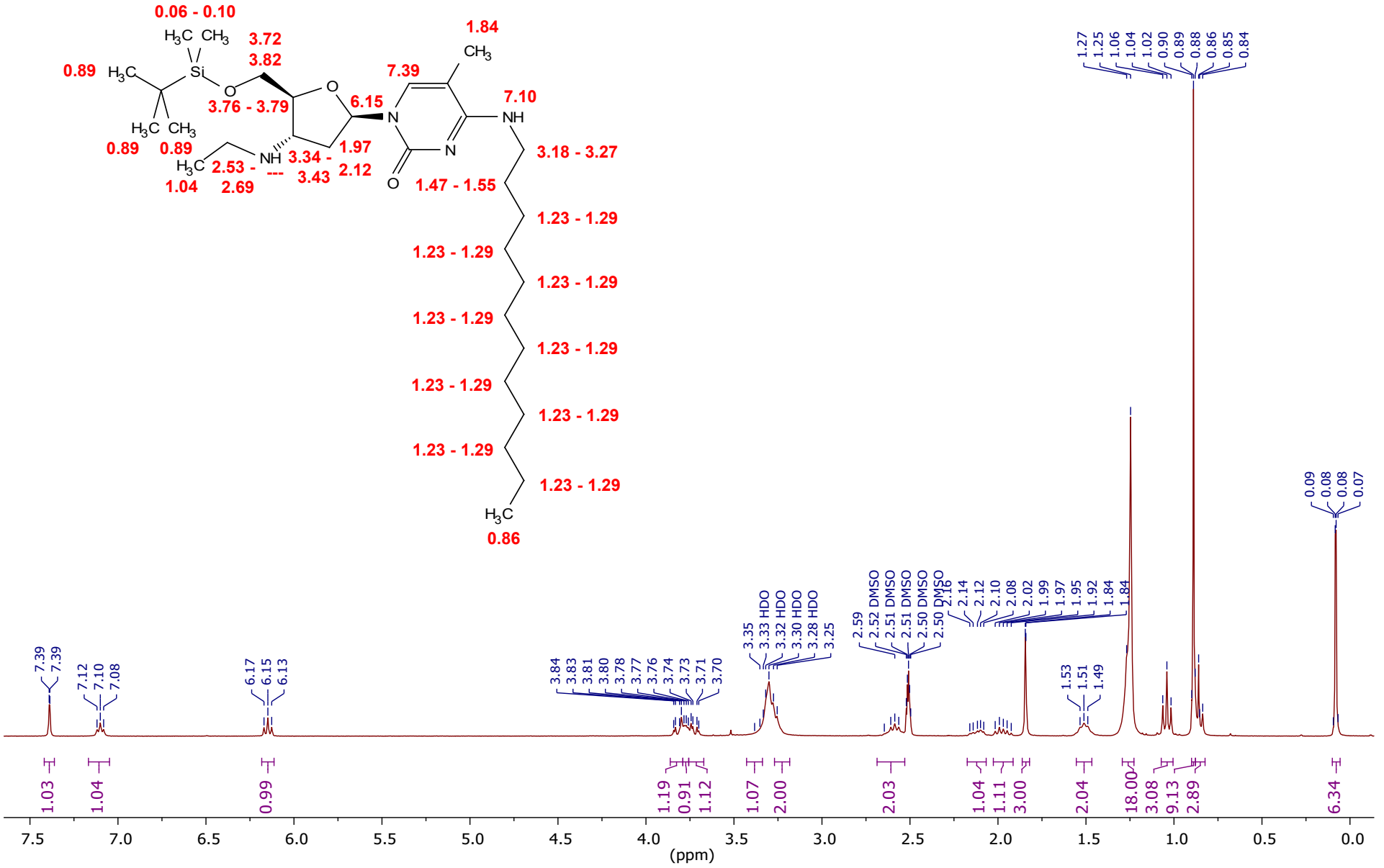

Compound: 12a
Nuclide: 13C
Solvent: DMSO
Frequency: 75.47
13.10
62.15
137.13
101.36
162.62
84.83
81.87
41.83
64.14
154.99
40.15
32.46
22.03 - 31.24
41.83
22.03 - 31.24
22.03 - 31.24
22.03 - 31.24
22.03 - 31.24
22.03 - 31.24
22.03 - 31.24
13.87
41.83
39.50 DMSO
39.77 DMSO
39.22 DMSO
28.92
28.97
28.81
28.65
31.24
26.43
22.03
40.05 DMSO
38.94 DMSO
13.87
13.10
64.14
84.83
81.87
40.15
62.15
137.13
101.36
162.62
154.99
40.33 DMSO
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)

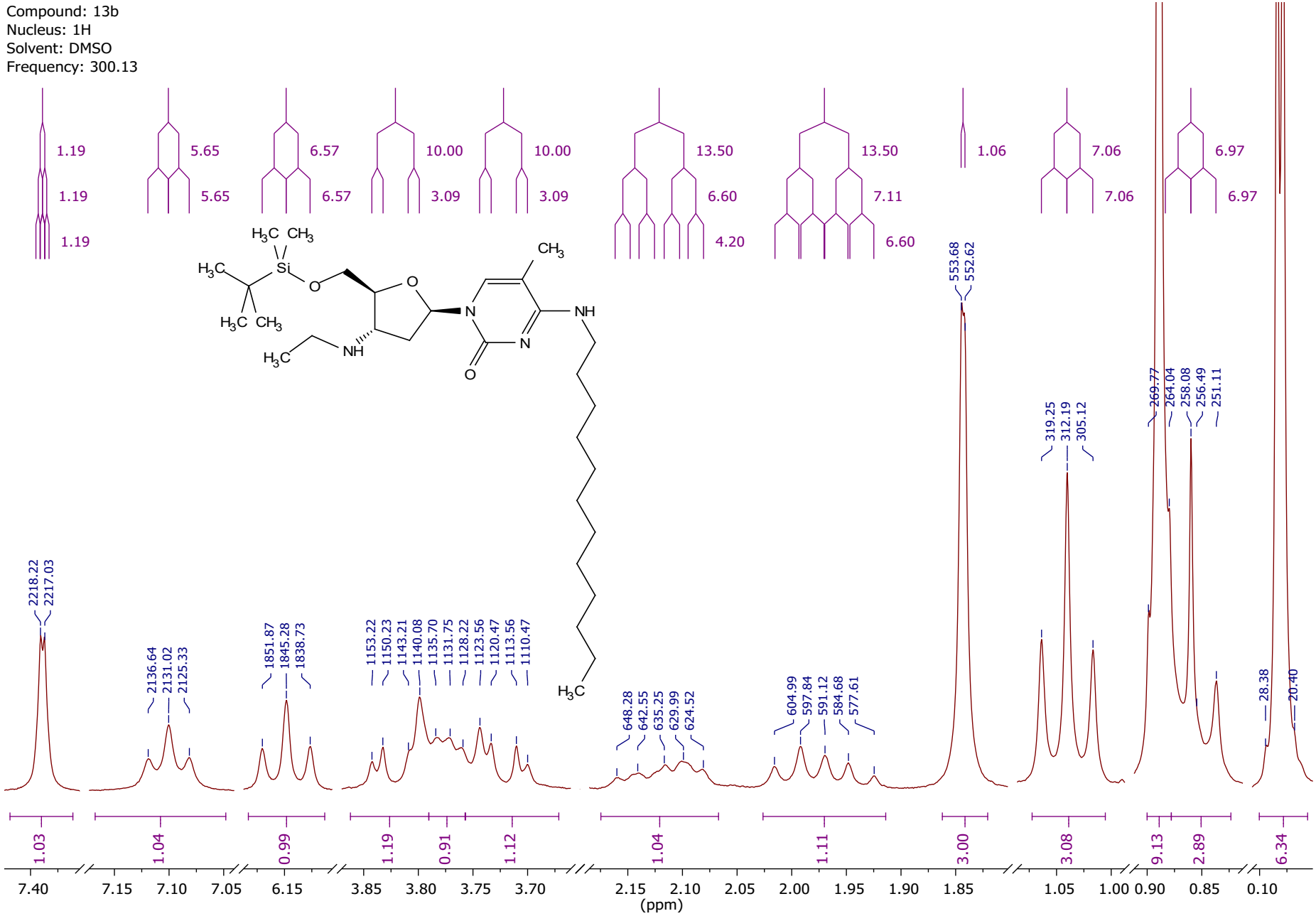

Compound: 12b
Nuclide: 1H
Solvent: DMSO
Frequency: 300.13
f1 (ppm)

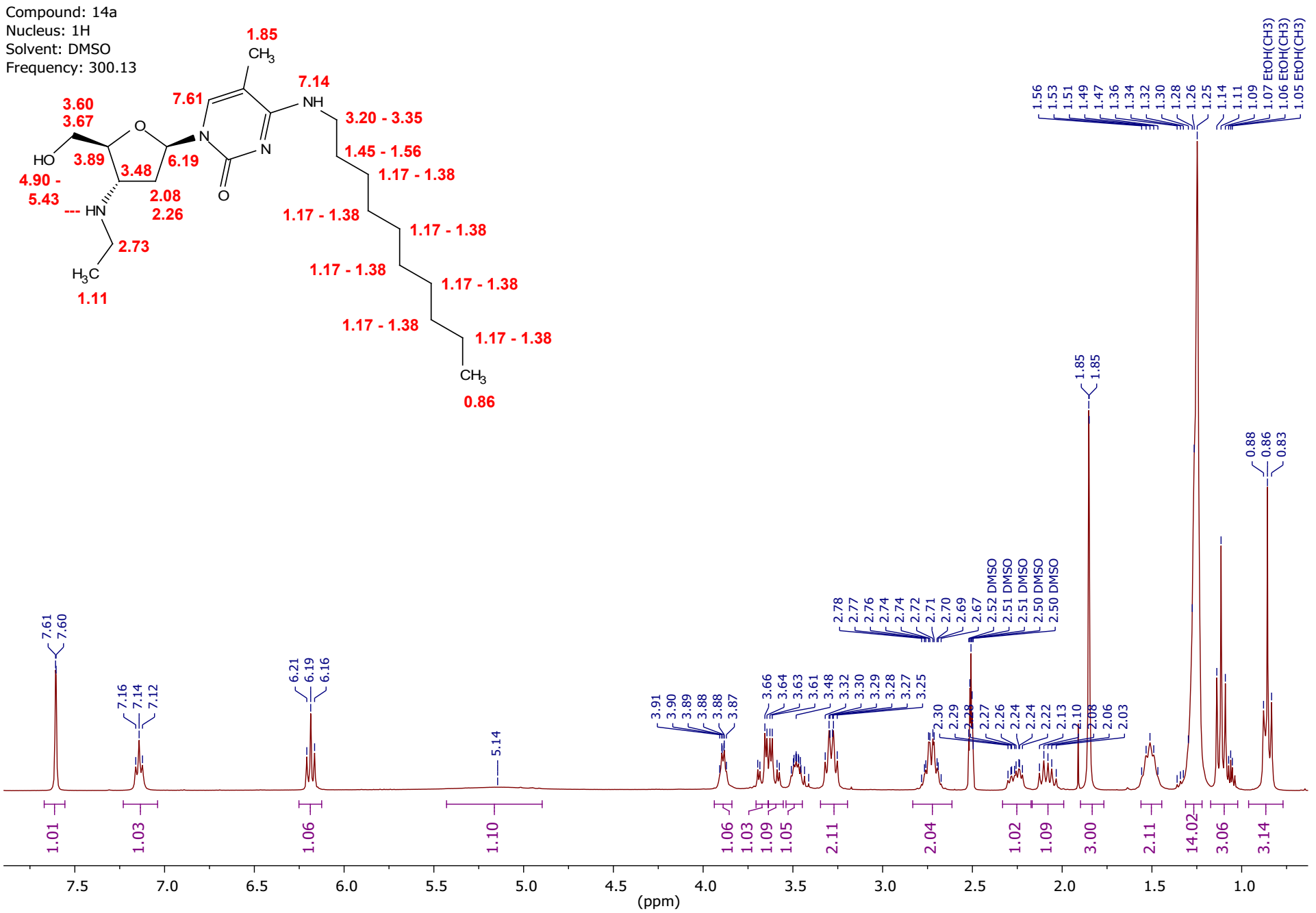

Compound: 12b
Nuclide: 1H
Solvent: DMSO
Frequency: 300.13
1.22
1.22
1.22
5.67
5.67
6.54
6.54
4.45
3.95
3.13
11.97
3.13
11.91
3.97
7.83
6.08
6.08
8.40
4.81
4.45
13.74
6.66
4.81
1.06
13.75
8.40
6.54
6.75
6.7
672.23
560.17
558.37
555.18
554.11
546.33
263.63
257.09
250.17
2296.01
2294.79
2135.92
2130.29
2124.59
1819.41
1812.89
1806.32
1517.63
1189.67
1185.83
1181.20
1177.36
1107.59
1104.46
1095.62
1092.49
1069.84
1065.83
1057.89
996.19
989.86
987.93
984.07
982.06
976.24
959.29
718.87
714.04
712.19
707.30
705.02
700.21
698.35
693.56
1.00
0.91
1.00
0.83
1.01
1.05
1.04
2.07
1.02
1.01
5.99
3.00
1.00
3.02
7.7
7.6
7.1
6.1
6.0
5.2
5.1
5.0
4.0
3.9
3.7
3.6
3.5
3.3
3.2
2.4
2.3
2.2
1.9
1.8
0.9
f1 (мд)


Compound: 12b
Nuclide: 13C
Solvent: DMSO
Frequency: 75.47
13.13
62.16
137.16
101.40
162.65
81.83
84.86
41.80
64.20
155.00
40.17
32.50
22.05 - 31.26
41.80
13.90
162.65
155.00
137.16
101.40
84.86
81.83
64.20
62.16
41.80
40.35 DMSO
40.17
40.08 DMSO
39.80 DMSO
39.52 DMSO
39.24 DMSO
38.96 DMSO
31.26
29.02
28.99
28.84
28.67
26.45
22.05
13.90
13.13
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

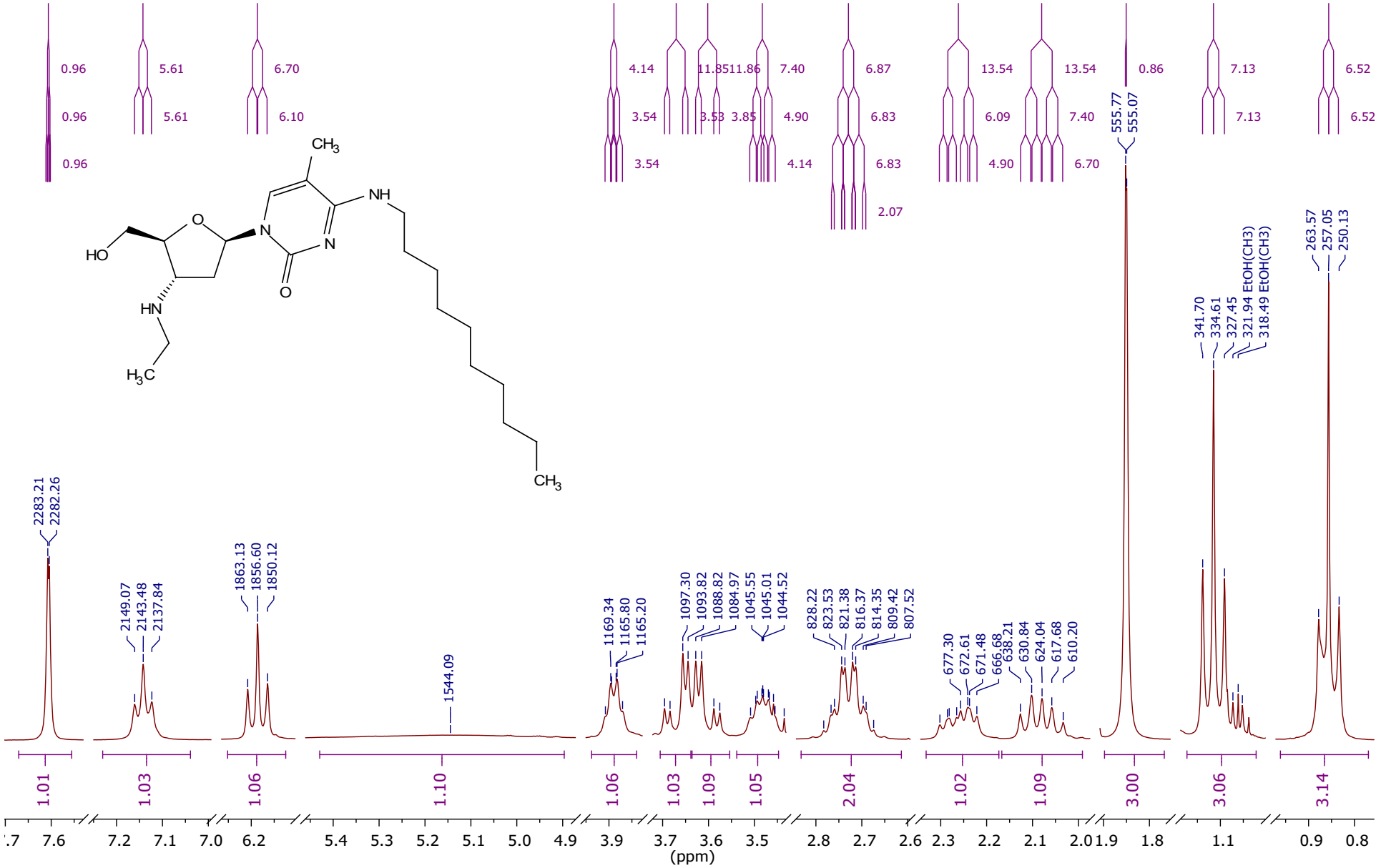
Compound: 13b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

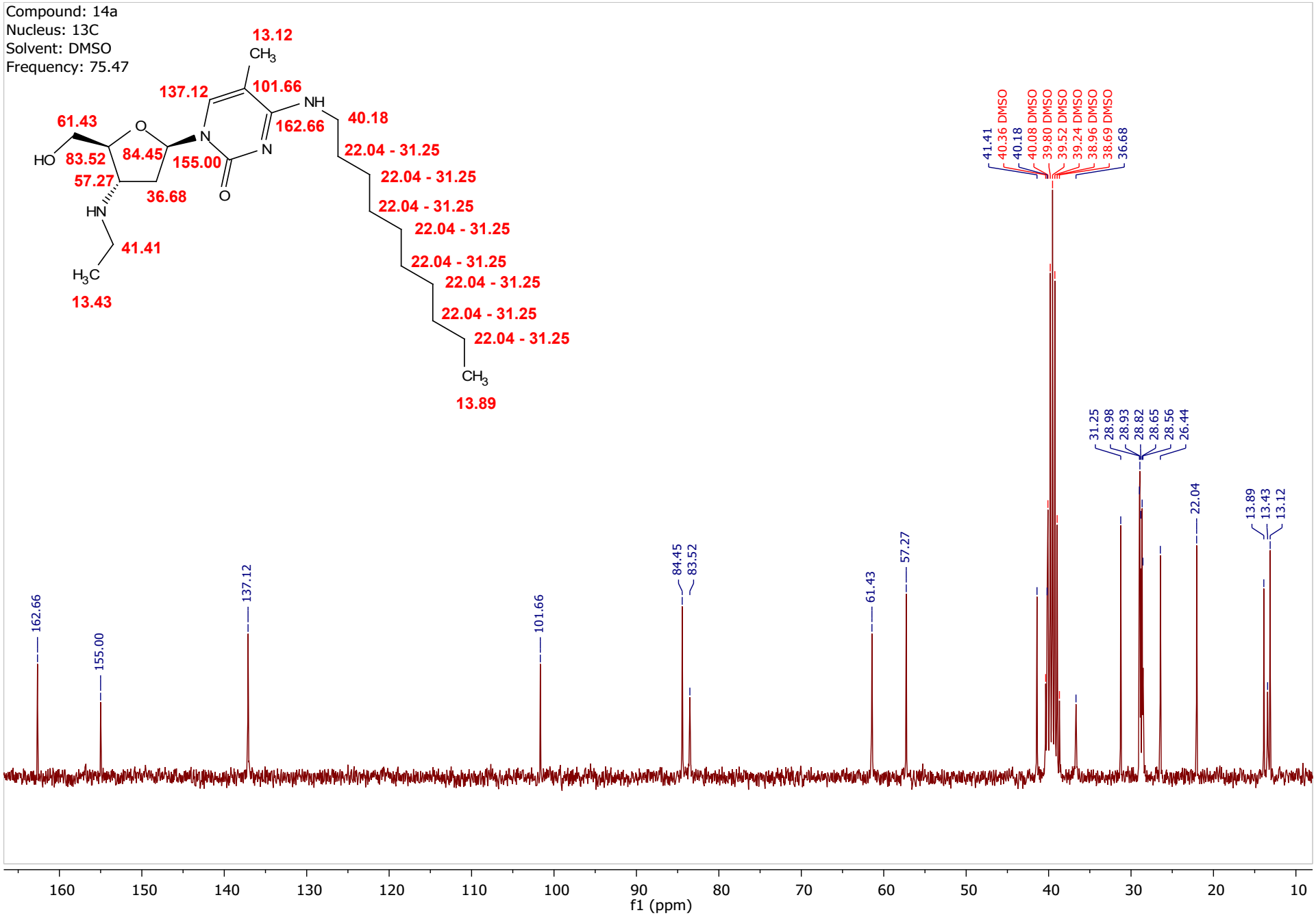



Compound: 13b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
1.19
1.19
1.19
5.65
5.65
6.57
6.57
10.00
3.09
10.00
3.09
13.50
6.60
4.20
13.50
7.11
6.60
1.06
7.06
7.06
6.97
6.97
2218.22
2217.03
2136.64
2131.02
2125.33
1851.87
1845.28
1838.73
1153.22
1150.23
1143.21
1140.08
1135.70
1131.75
1128.22
1123.56
1120.47
1113.56
1110.47
648.28
642.55
635.25
629.99
624.52
604.99
597.84
591.12
584.68
577.61
553.68
552.62
319.25
312.19
305.12
269.77
264.04
258.08
256.49
251.11
28.38
20.40
1.03
1.04
0.99
1.19
0.91
1.12
1.04
1.11
3.00
3.08
9.13
2.89
6.34
7.40
7.15
7.10
7.05
6.15
3.85
3.80
3.75
3.70
2.15
2.10
2.05
2.00
1.95
1.90
1.85
1.05
1.00
0.90
0.85
0.10
(ppm)

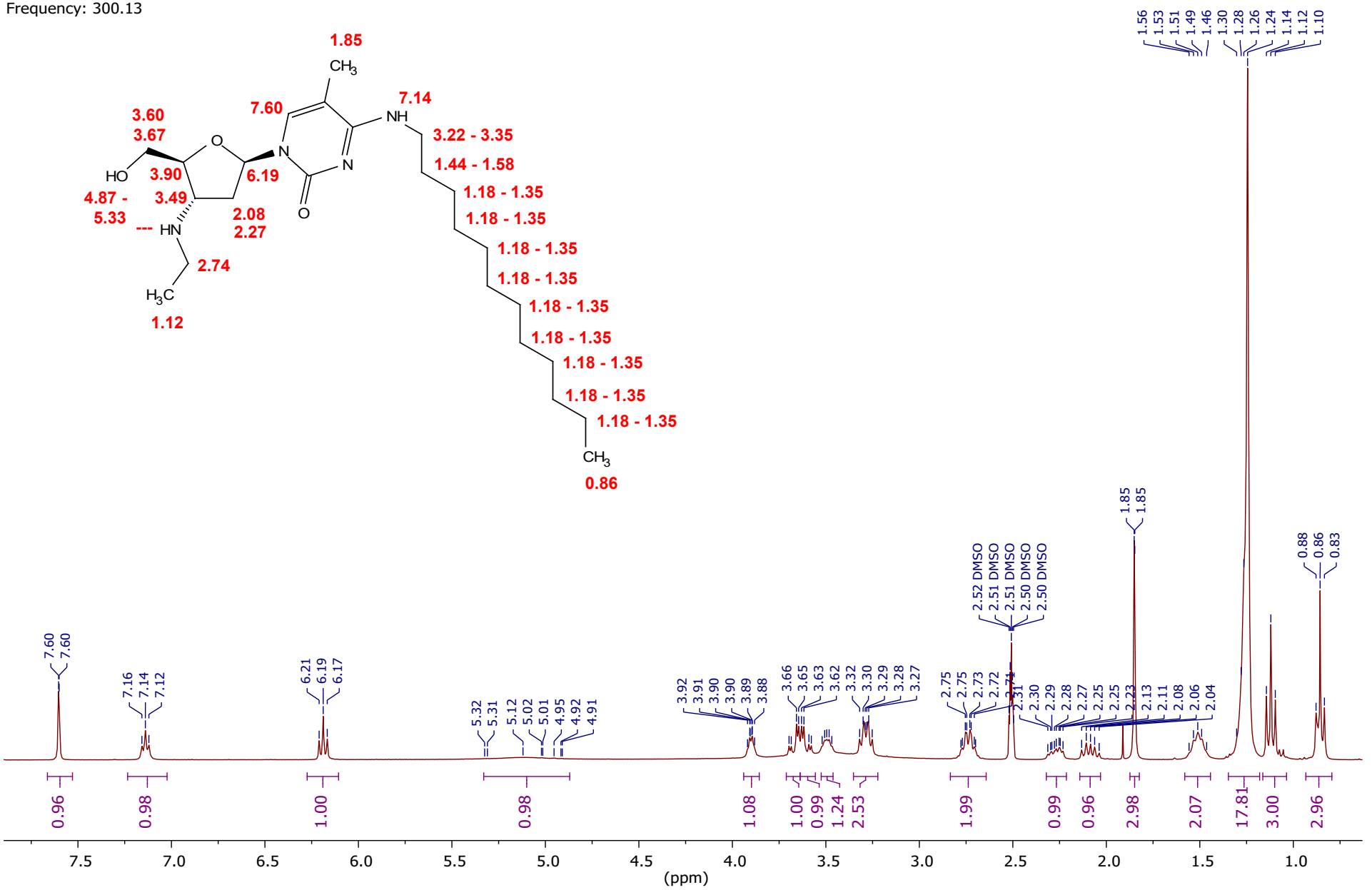

Compound: 14a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13
1.85
CH3
7.14
NH
7.61
3.60
3.67
HO
3.89
3.48
6.19
4.90 -
5.43
2.08
2.26
--- HN
2.73
H3C
1.11
3.20 - 3.35
1.45 - 1.56
1.17 - 1.38
1.17 - 1.38
1.17 - 1.38
1.17 - 1.38
1.17 - 1.38
1.17 - 1.38
CH3
0.86
(ppm)

Compound: 14a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

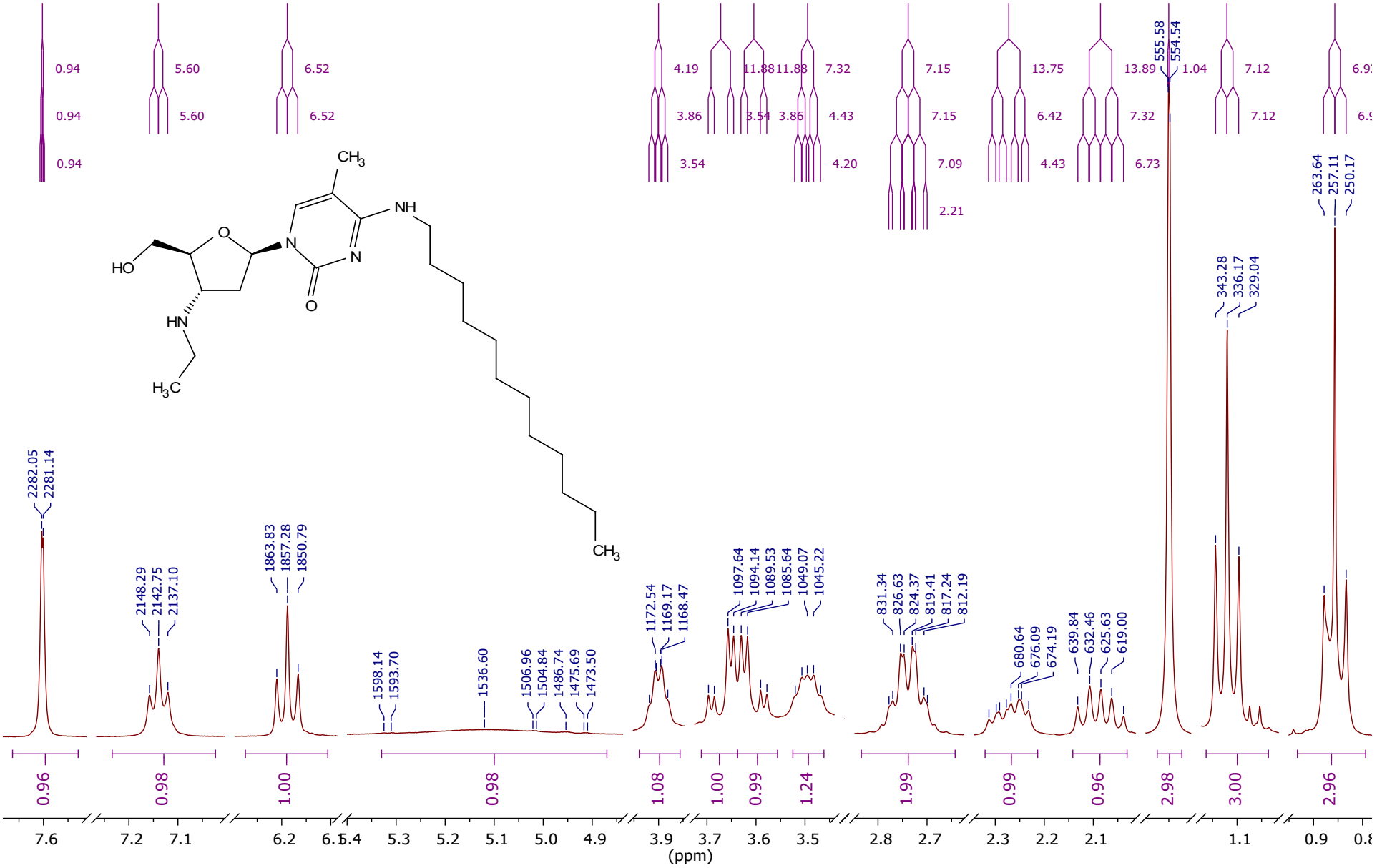


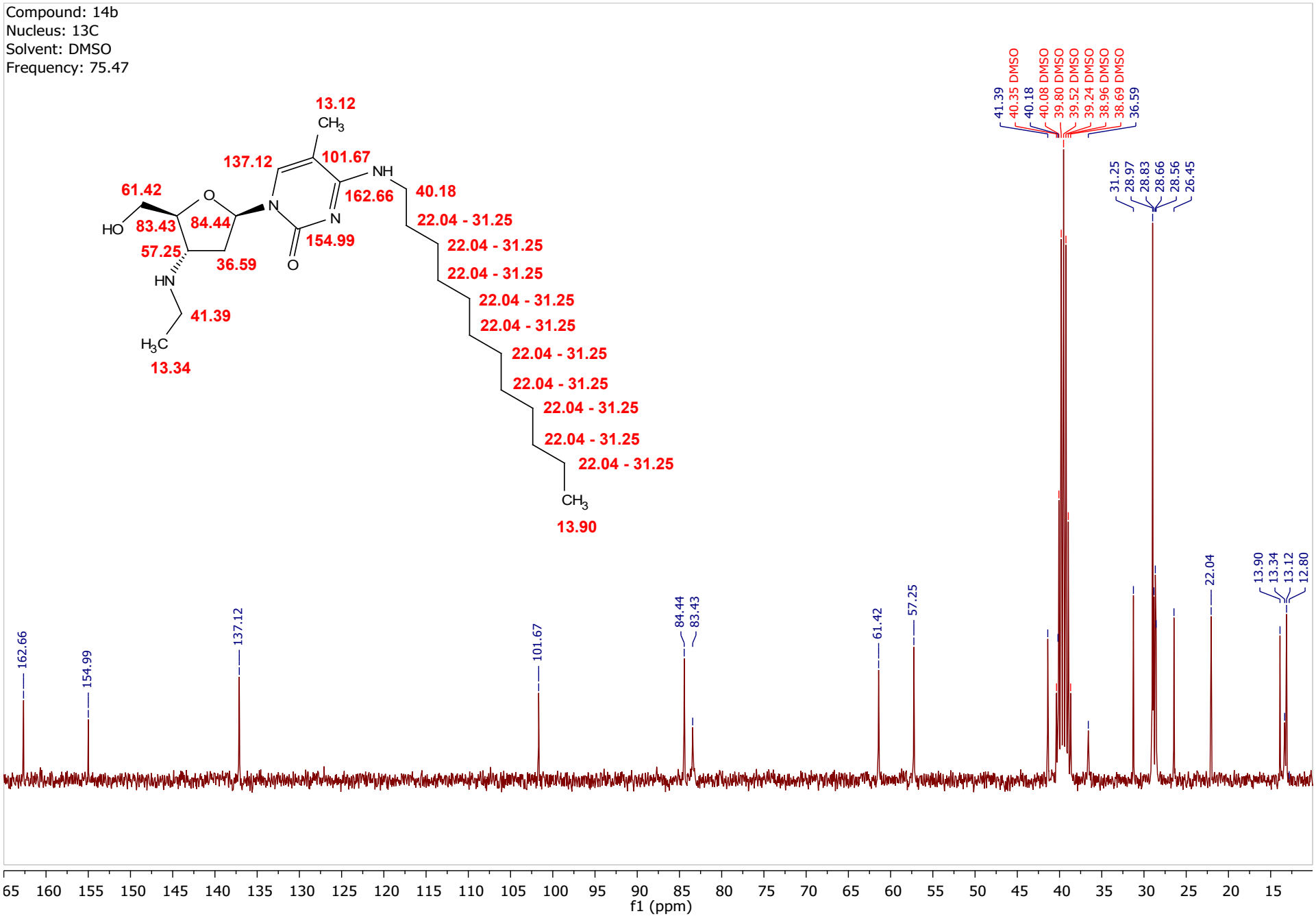

Compound: 14a
Nucleus: 13C
Solvent: DMSO
Frequency: 75.47
13.12
137.12
101.66
61.43
162.66
40.18
22.04 - 31.25
84.45
155.00
83.52
57.27
36.68
41.41
13.43
13.89
41.41
40.36 DMSO
40.18
40.08 DMSO
39.80 DMSO
39.52 DMSO
39.24 DMSO
38.96 DMSO
38.69 DMSO
36.68
31.25
28.98
28.93
28.82
28.65
28.56
26.44
22.04
13.89
13.43
13.12
162.66
155.00
137.12
101.66
84.45
83.52
61.43
57.27
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Compound: 14b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

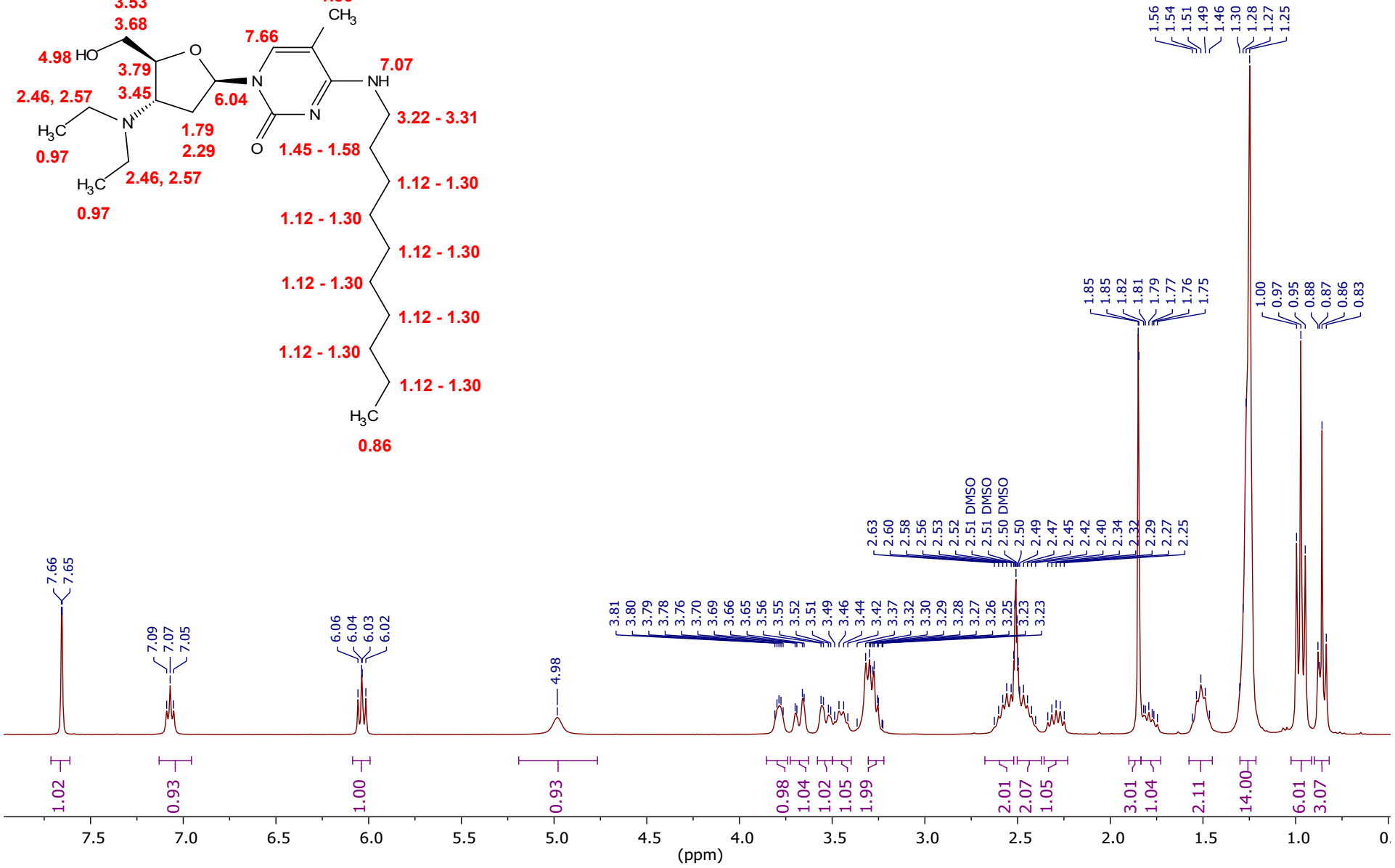


Compound: 14b
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

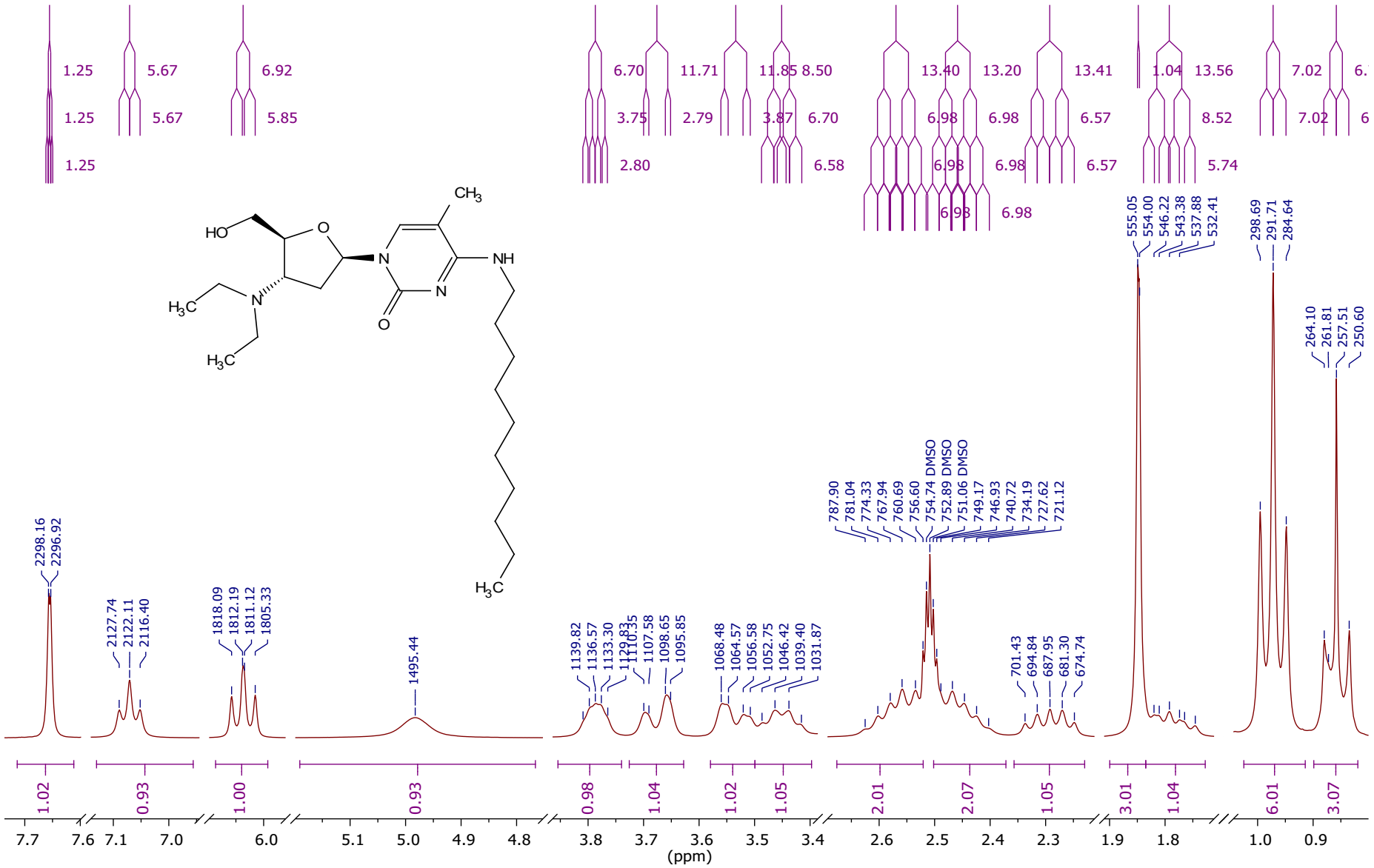


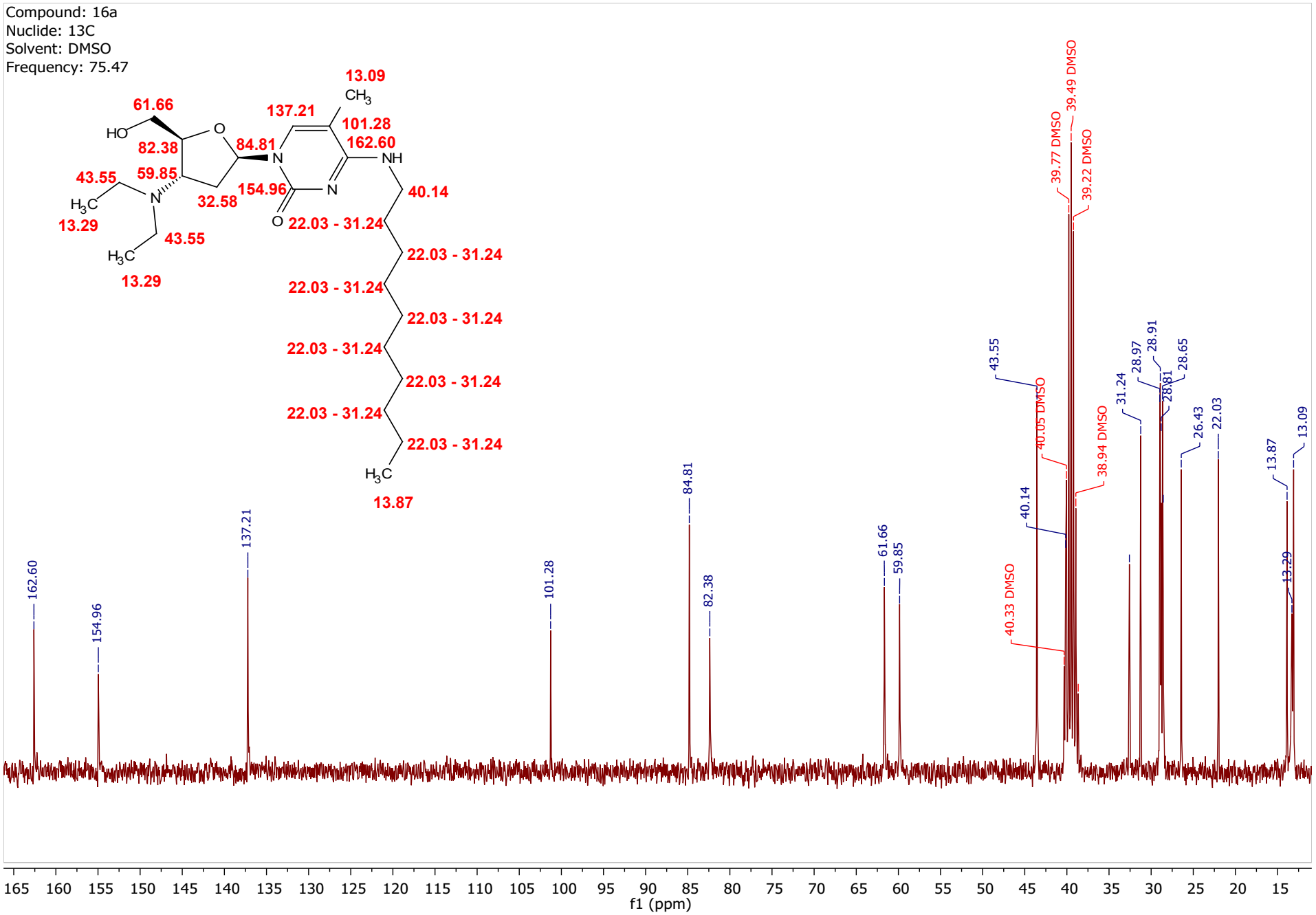

Compound: 14b
Nucleus: 13C
Solvent: DMSO
Frequency: 75.47
13.12
137.12
101.67
NH
61.42
162.66
40.18
HO
83.43
84.44
154.99
22.04 - 31.25
57.25
36.59
HN
41.39
13.34
13.90
41.39
40.35 DMSO
40.18
40.08 DMSO
39.80 DMSO
39.52 DMSO
39.24 DMSO
38.96 DMSO
38.69 DMSO
36.59
31.25
28.97
28.83
28.66
28.56
26.45
22.04
13.90
13.34
13.12
12.80
162.66
154.99
137.12
101.67
84.44
83.43
61.42
57.25
65 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)

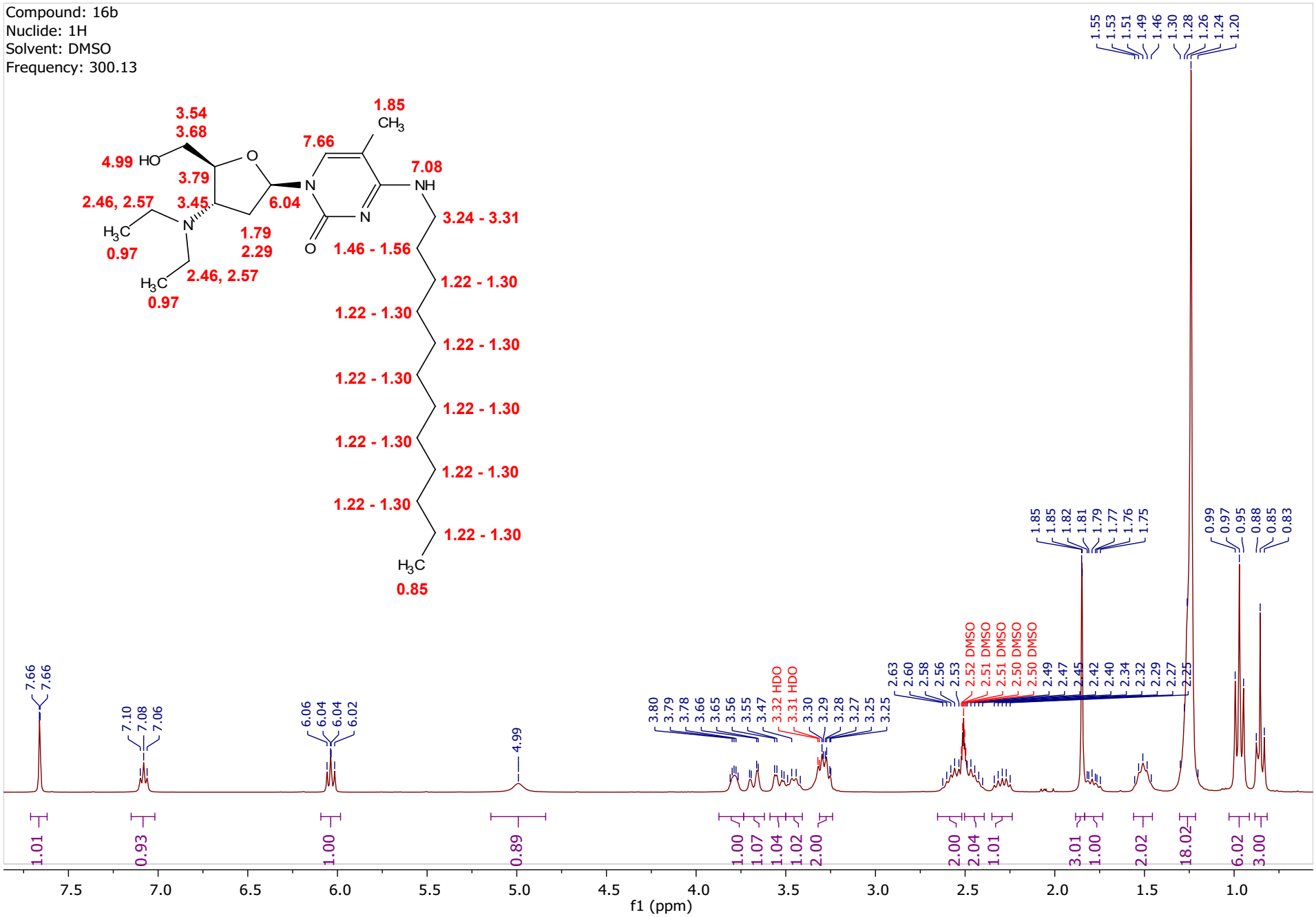
Compound: 16a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

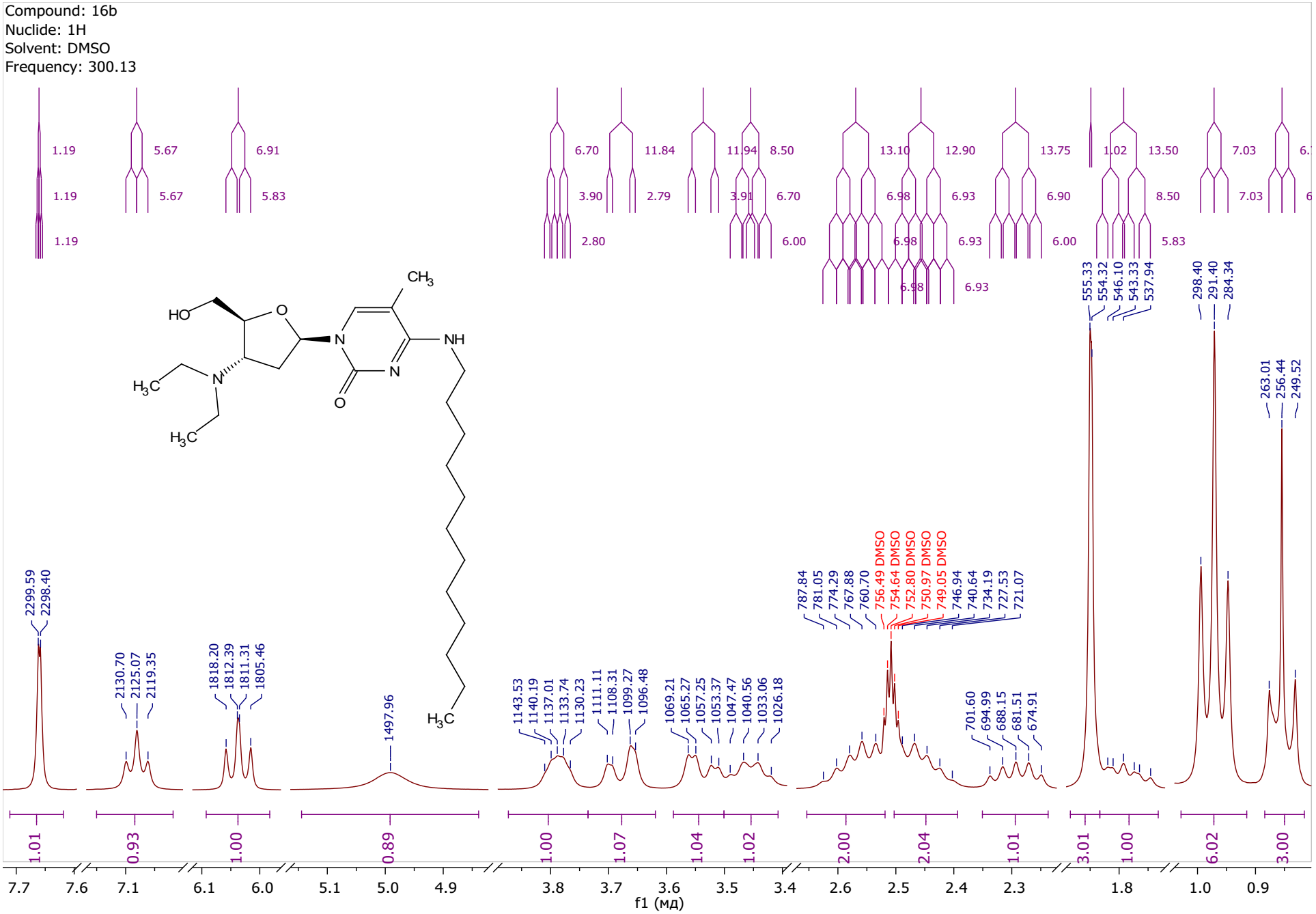


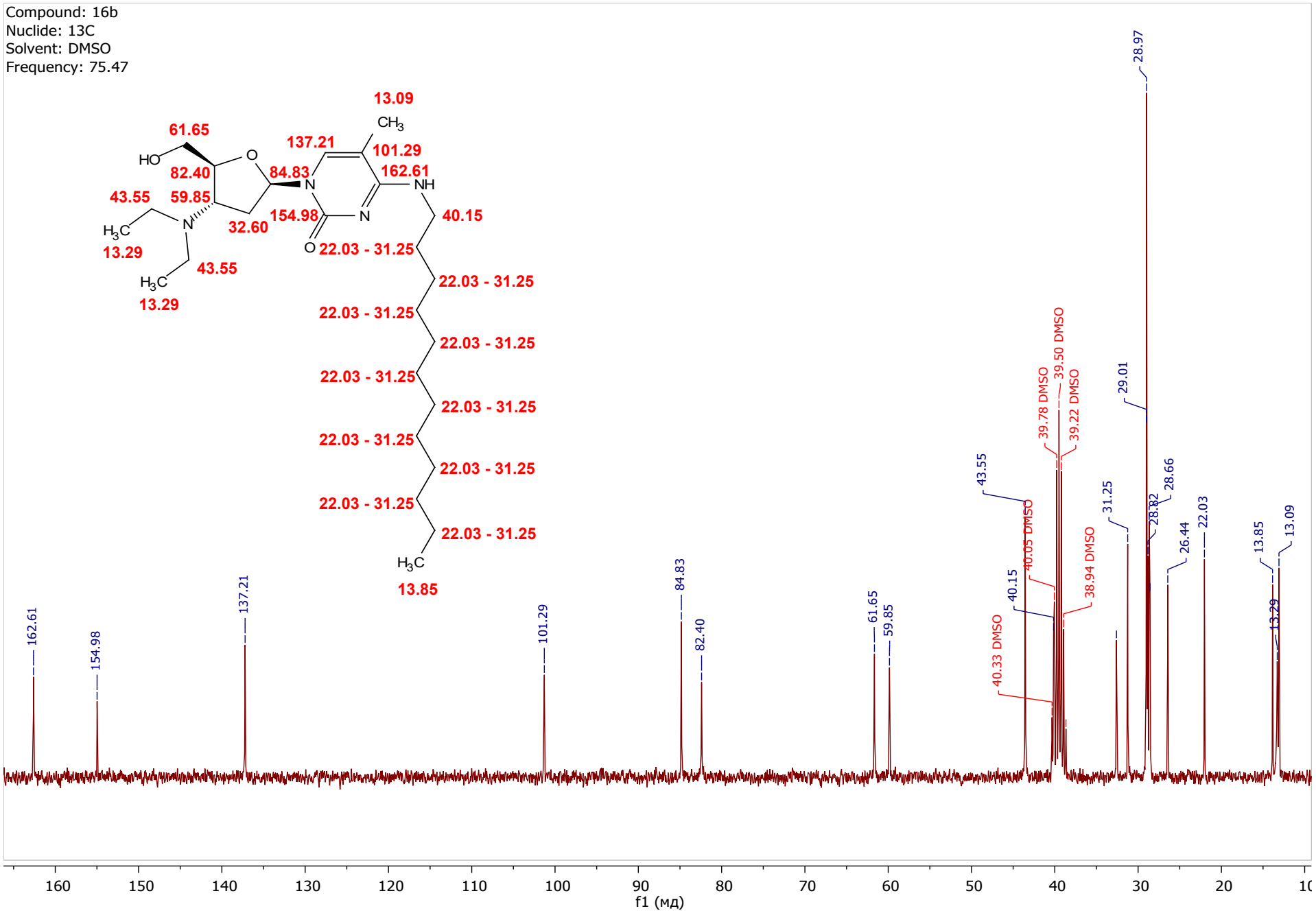
Compound: 16a
Nucleus: 1H
Solvent: DMSO
Frequency: 300.13

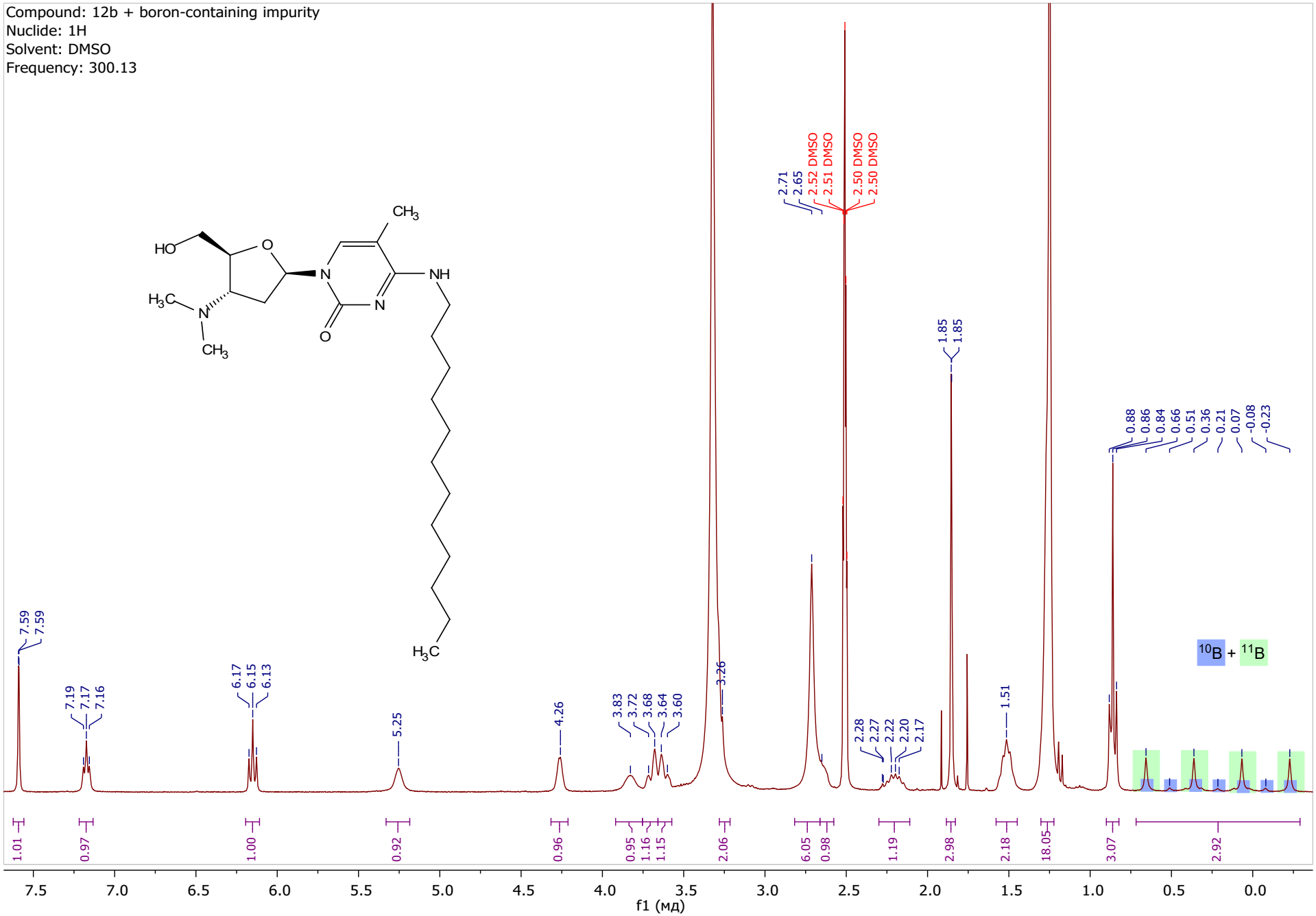


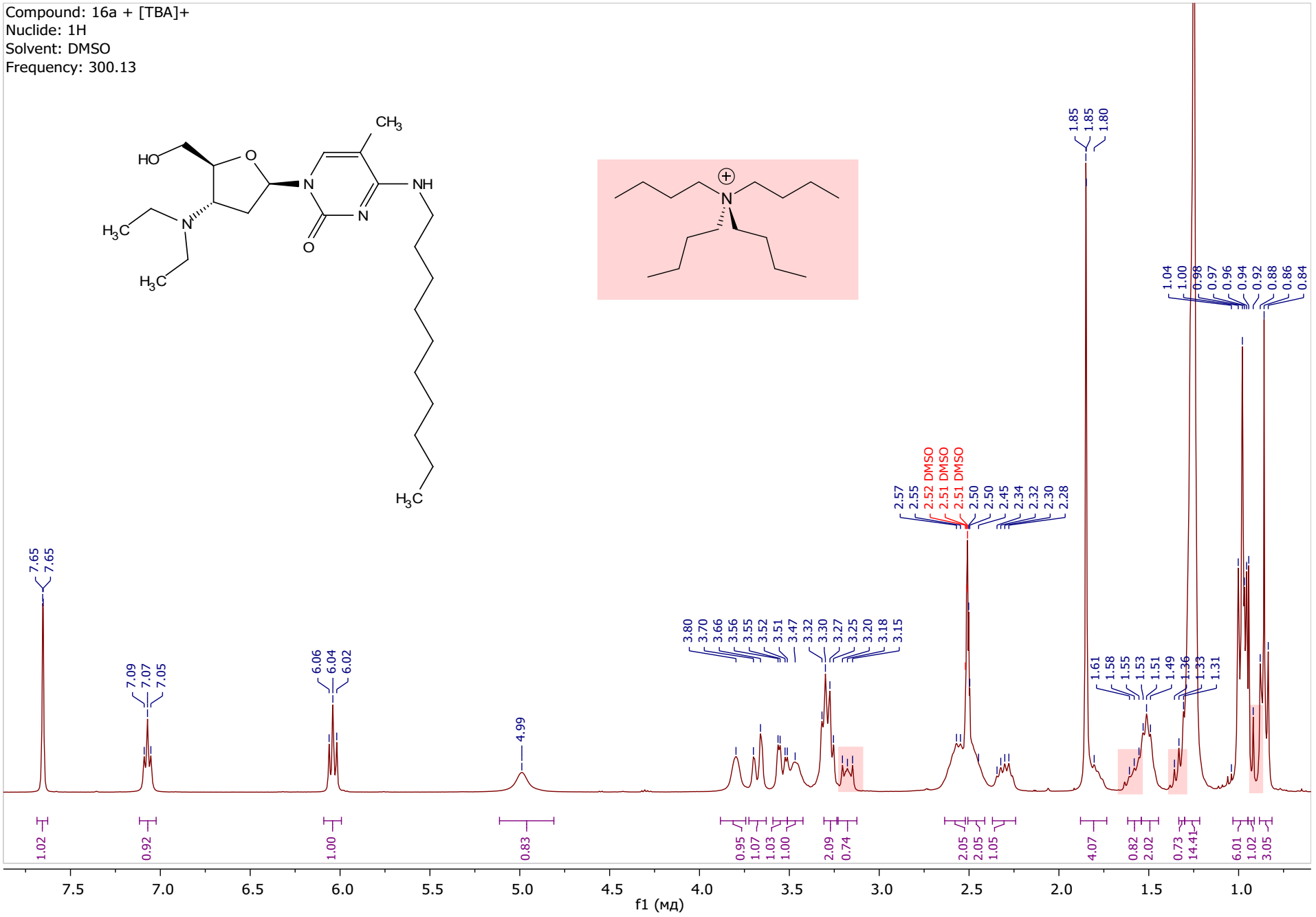

Compound: 16a
Nuclide: 13C
Solvent: DMSO
Frequency: 75.47
13.09
61.66
137.21
101.28
82.38
84.81
162.60
43.55
59.85
154.96
40.14
32.58
13.29
43.55
22.03 - 31.24
13.29
22.03 - 31.24
22.03 - 31.24
22.03 - 31.24
22.03 - 31.24
22.03 - 31.24
22.03 - 31.24
13.87
162.60
154.96
137.21
101.28
84.81
82.38
61.66
59.85
43.55
40.33 DMSO
40.14
40.05 DMSO
39.77 DMSO
39.49 DMSO
39.22 DMSO
38.94 DMSO
31.24
28.97
28.91
28.81
28.65
26.43
22.03
13.87
13.29
13.09
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)

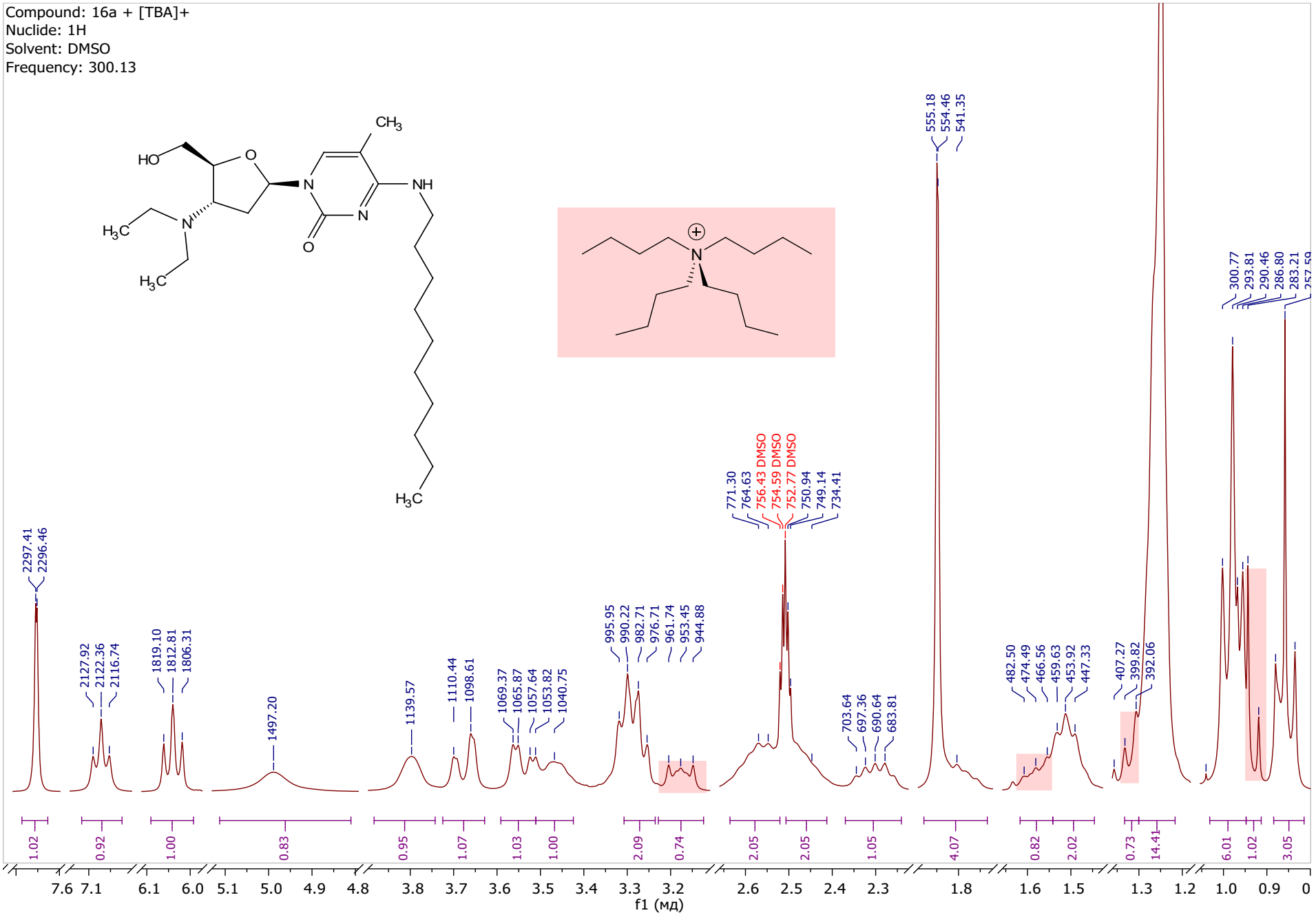

Compound: 16b
Nuclide: 1H
Solvent: DMSO
Frequency: 300.13
f1 (ppm)

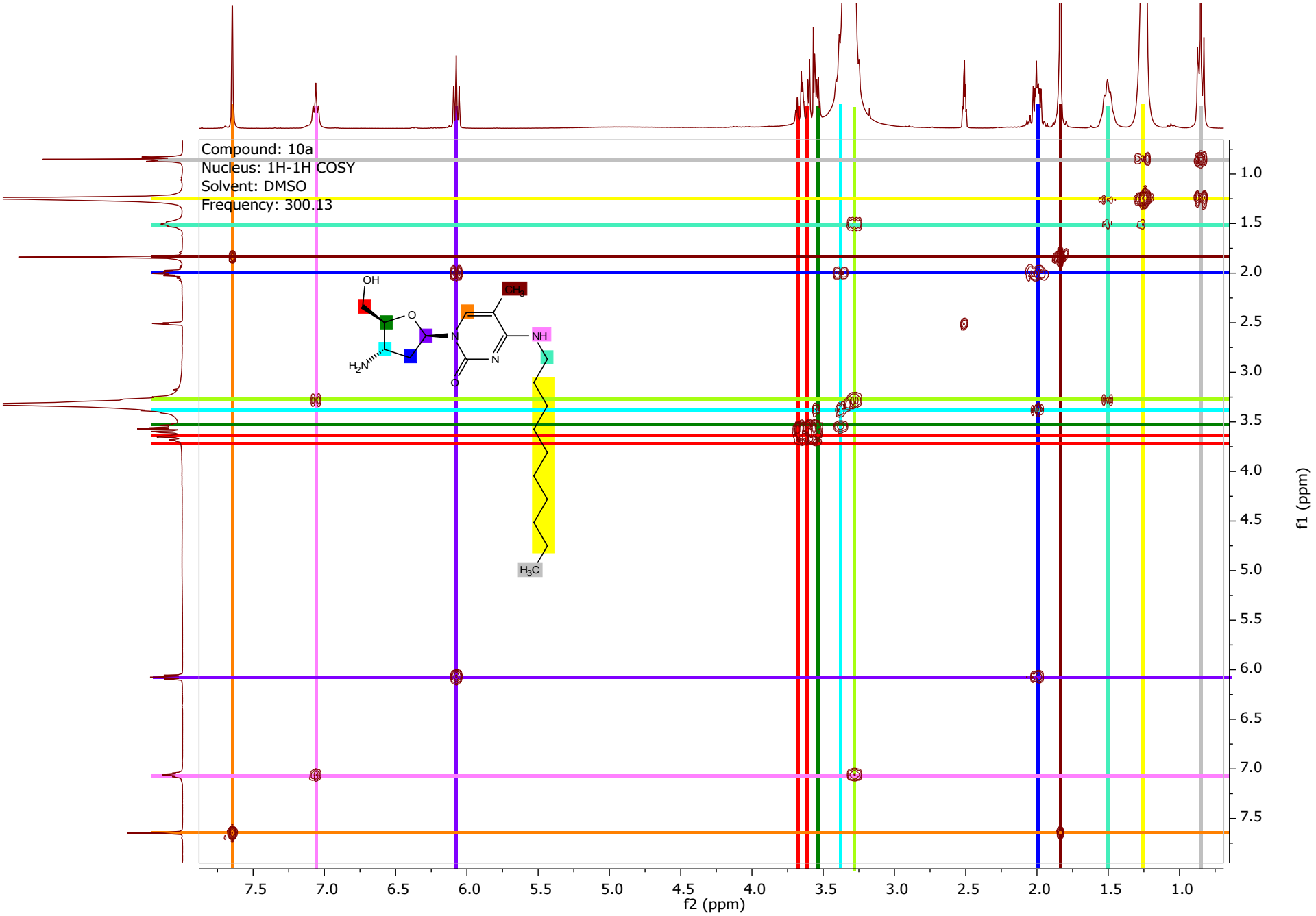

Compound: 16b
Nuclide: 1H
Solvent: DMSO
Frequency: 300.13
1.19
1.19
1.19
5.67
5.67
6.91
5.83
6.70
3.90
2.80
11.84
2.79
11.94
3.91
8.50
6.70
6.00
13.10
6.98
6.98
6.98
12.90
6.93
6.93
6.93
13.75
6.90
6.00
1.02
8.50
5.83
13.50
7.03
7.03
HO
O
N
N
NH
CH_3
H_3C
N
H_3C
O
H_3C
555.33
554.32
546.10
543.33
537.94
298.40
291.40
284.34
263.01
256.44
249.52
2299.59
2298.40
2130.70
2125.07
2119.35
1818.20
1812.39
1811.31
1805.46
1497.96
1143.53
1140.19
1137.01
1133.74
1130.23
1111.11
1108.31
1099.27
1096.48
1069.21
1065.27
1057.25
1053.37
1047.47
1040.56
1033.06
1026.18
787.84
781.05
774.29
767.88
760.70
756.49 DMSO
754.64 DMSO
752.80 DMSO
750.97 DMSO
749.05 DMSO
746.94
740.64
734.19
727.53
721.07
701.60
694.99
688.15
681.51
674.91
1.01
0.93
1.00
0.89
1.00
1.07
1.04
1.02
2.00
2.04
1.01
3.01
1.00
6.02
3.00
7.7
7.6
7.1
6.1
6.0
5.1
5.0
4.9
3.8
3.7
3.6
3.5
3.4
2.6
2.5
2.4
2.3
1.8
1.0
0.9
f1 (мд)

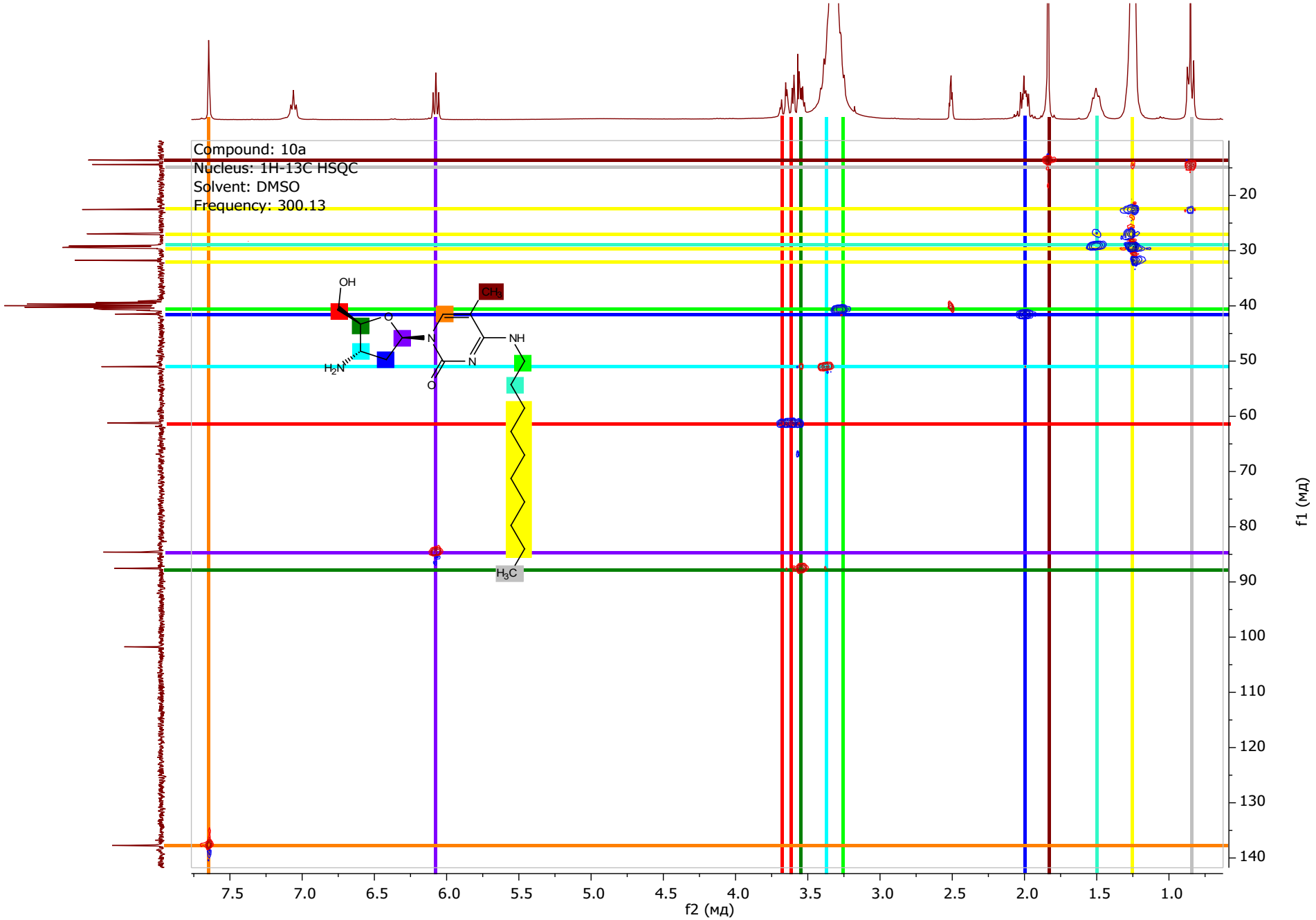

Compound: 16b
Nuclide: 13C
Solvent: DMSO
Frequency: 75.47
13.09
61.65
137.21
101.29
82.40
84.83
162.61
43.55
59.85
154.98
40.15
32.60
13.29
22.03 - 31.25
43.55
13.29
13.85
162.61
154.98
137.21
101.29
84.83
82.40
61.65
59.85
43.55
40.33 DMSO
40.15
40.05 DMSO
39.78 DMSO
39.50 DMSO
39.22 DMSO
38.94 DMSO
31.25
29.01
28.97
28.82
28.66
26.44
22.03
13.85
13.29
13.09
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (мд)

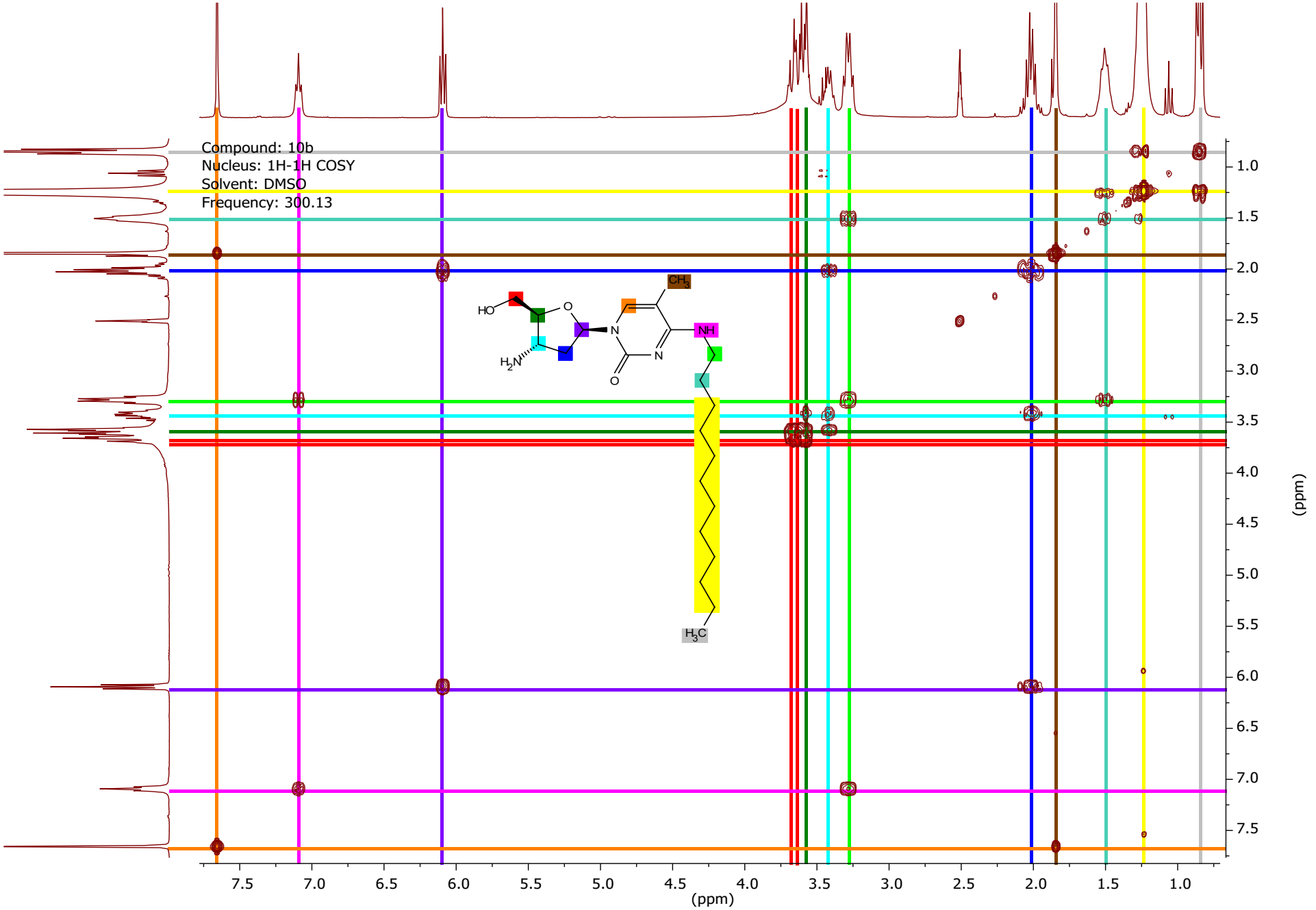

Compound: 12b + boron-containing impurity
Nuclide: 1H
Solvent: DMSO
Frequency: 300.13
HO
O
N
NH
H_3C
N
CH_3
CH_3
N
O
H_3C
2.71
2.65
2.52 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
1.85
1.85
0.88
0.86
0.84
0.66
0.51
0.36
0.21
0.07
-0.08
-0.23
7.59
7.59
7.19
7.17
7.16
6.17
6.15
6.13
5.25
4.26
3.83
3.72
3.68
3.64
3.60
3.26
2.28
2.27
2.22
2.20
2.17
1.51
^{10}B + ^{11}B
1.01
0.97
1.00
0.92
0.96
0.95
1.16
1.15
2.06
6.05
0.98
1.19
2.98
2.18
18.05
3.07
2.92
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 (мд)

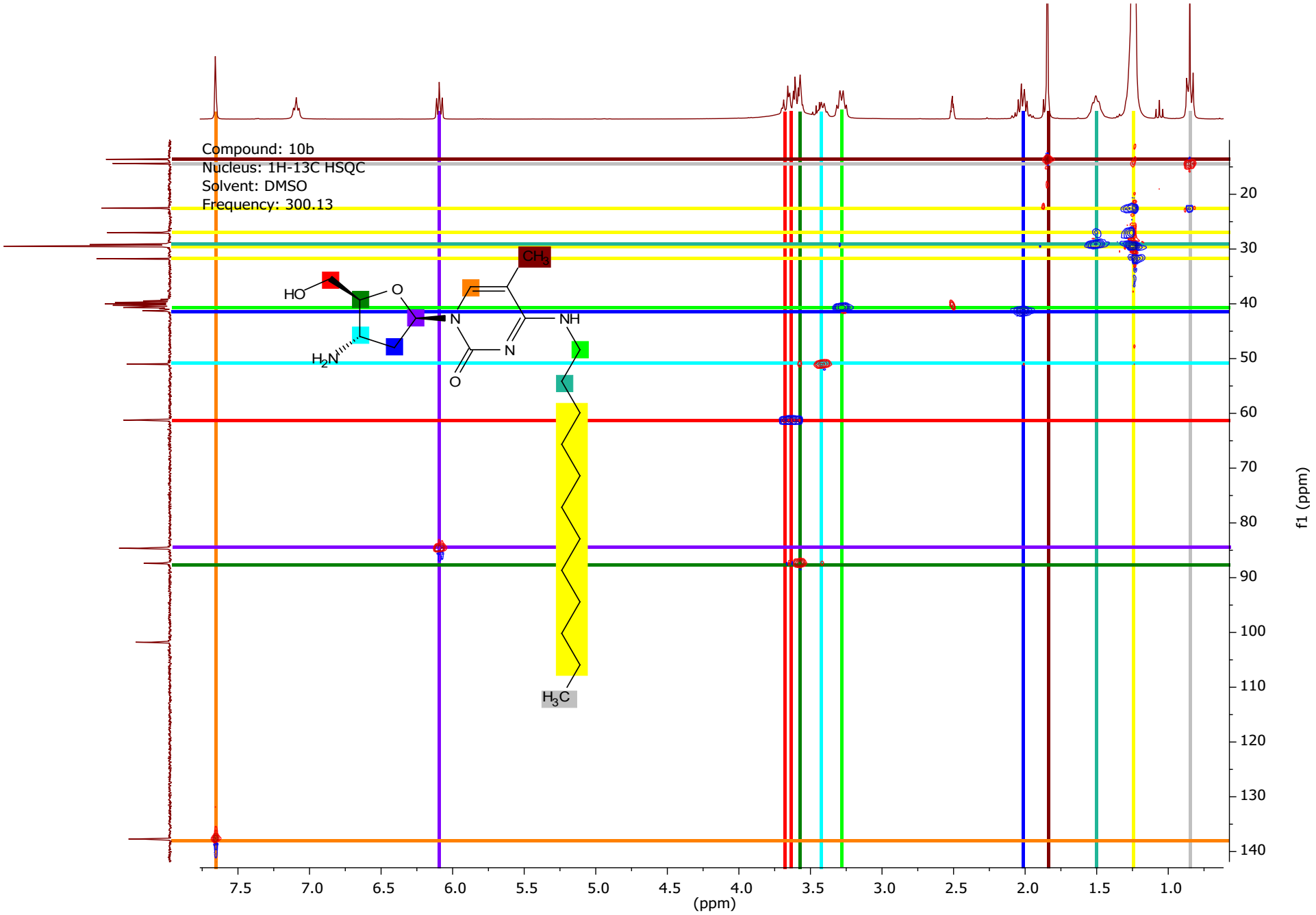

Compound: 16a + [TBA]+
Nuclide: 1H
Solvent: DMSO
Frequency: 300.13
f1 (мд)

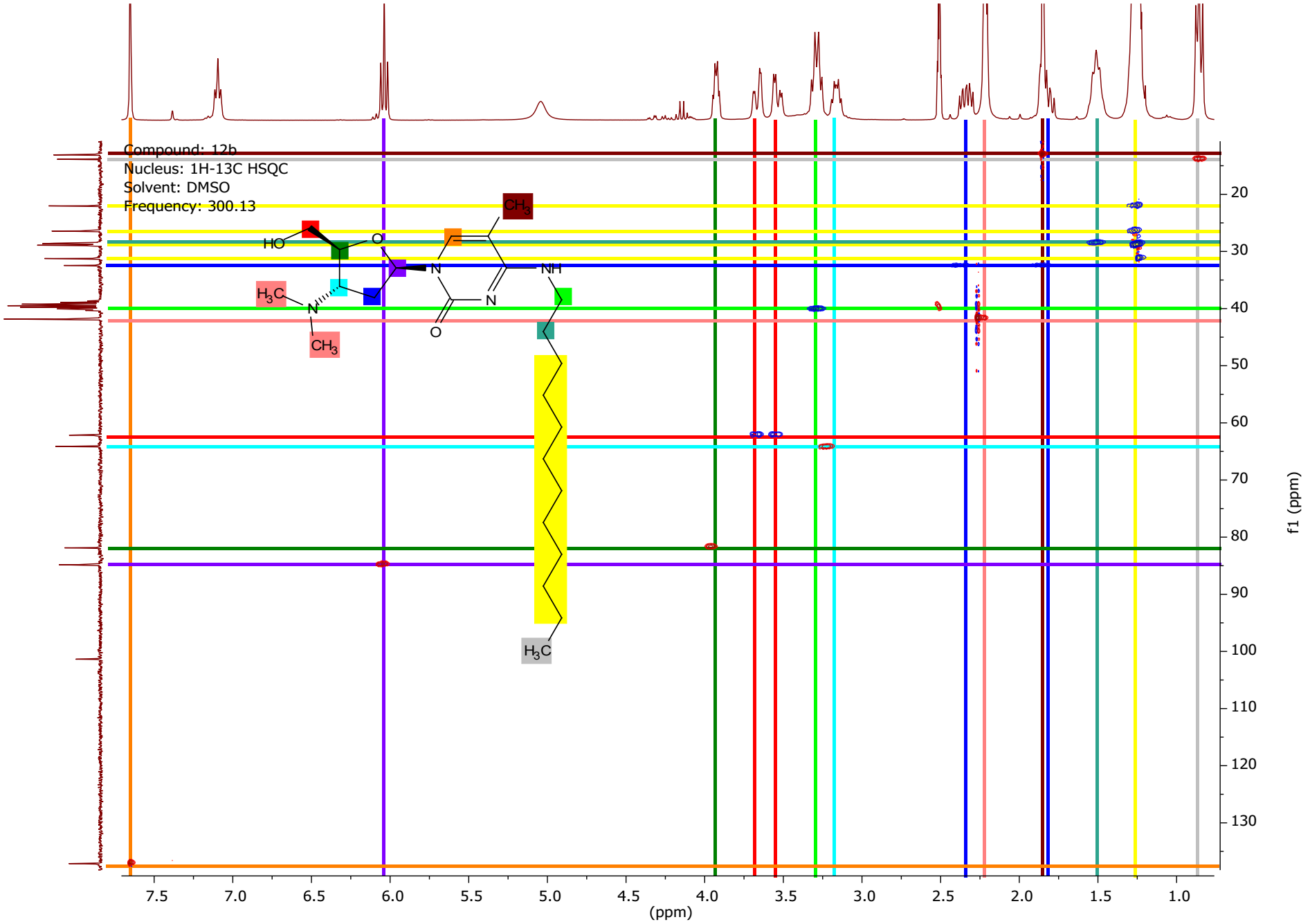

Compound: 16a + [TBA]+
Nuclide: 1H
Solvent: DMSO
Frequency: 300.13
HO
O
N
NH
N
O
CH3
H3C
N
H3C
H3C
N
555.18
554.46
541.35
300.77
293.81
290.46
286.80
283.21
257.59
2297.41
2296.46
2127.92
2122.36
2116.74
1819.10
1812.81
1806.31
1497.20
1139.57
1110.44
1098.61
1069.37
1065.87
1057.64
1053.82
1040.75
995.95
990.22
982.71
976.71
961.74
953.45
944.88
771.30
764.63
756.43 DMSO
754.59 DMSO
752.77 DMSO
750.94
749.14
734.41
703.64
697.36
690.64
683.81
482.50
474.49
466.56
459.63
453.92
447.33
407.27
399.82
392.06
1.02
0.92
1.00
0.83
0.95
1.07
1.03
1.00
2.09
0.74
2.05
2.05
1.05
4.07
0.82
2.02
0.73
14.41
6.01
1.02
3.05
7.6 7.1 6.1 6.0 5.1 5.0 4.9 4.8 3.8 3.7 3.6 3.5 3.4 3.3 3.2 2.6 2.5 2.4 2.3 1.8 1.6 1.5 1.3 1.2 1.0 0.9 0
f1 (мд)

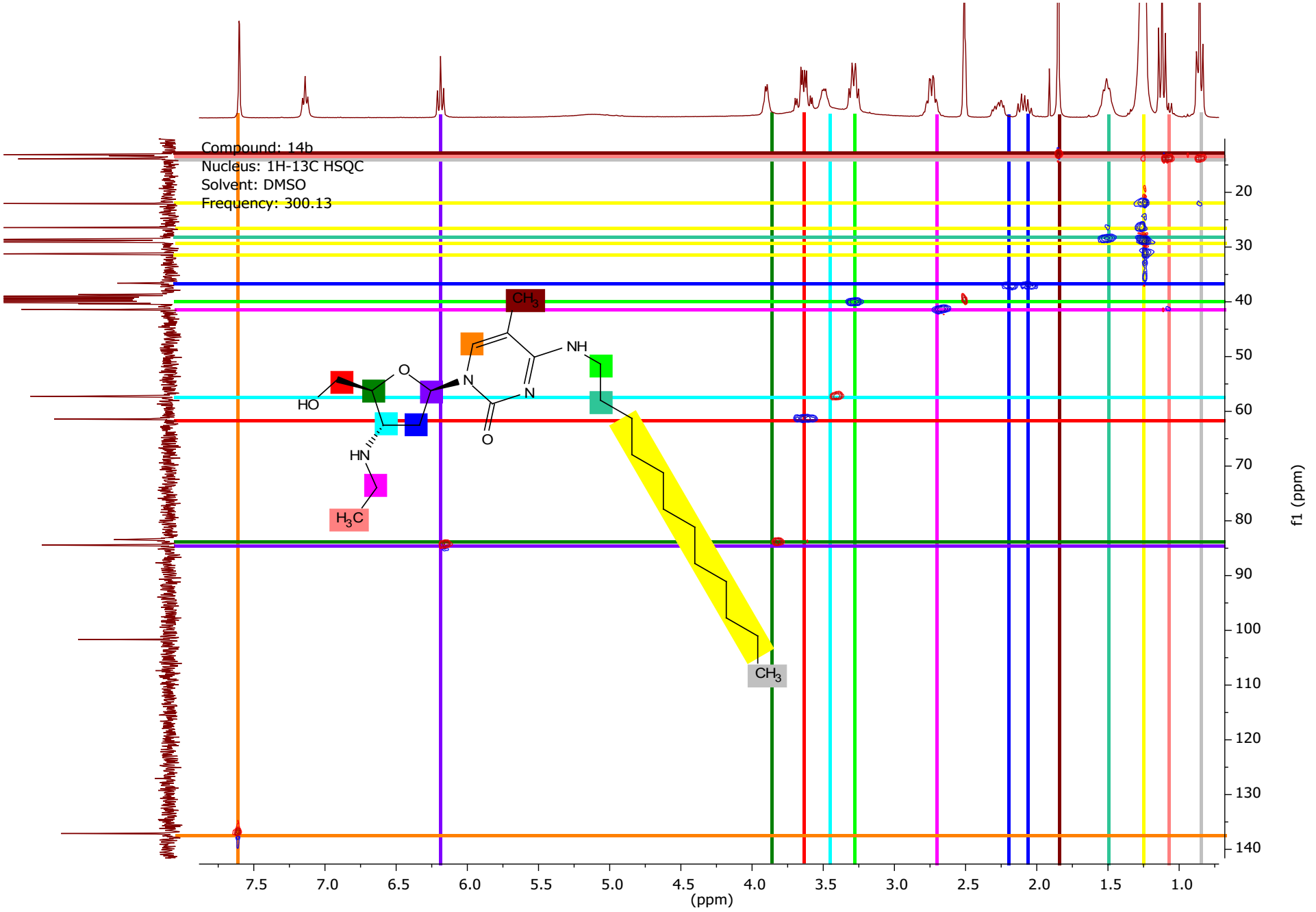

Compound: 10a
Nucleus: 1H-1H COSY
Solvent: DMSO
Frequency: 300.13
OH
O
N
NH
N
O
CH3
H2N
H3C
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
f1 (ppm)

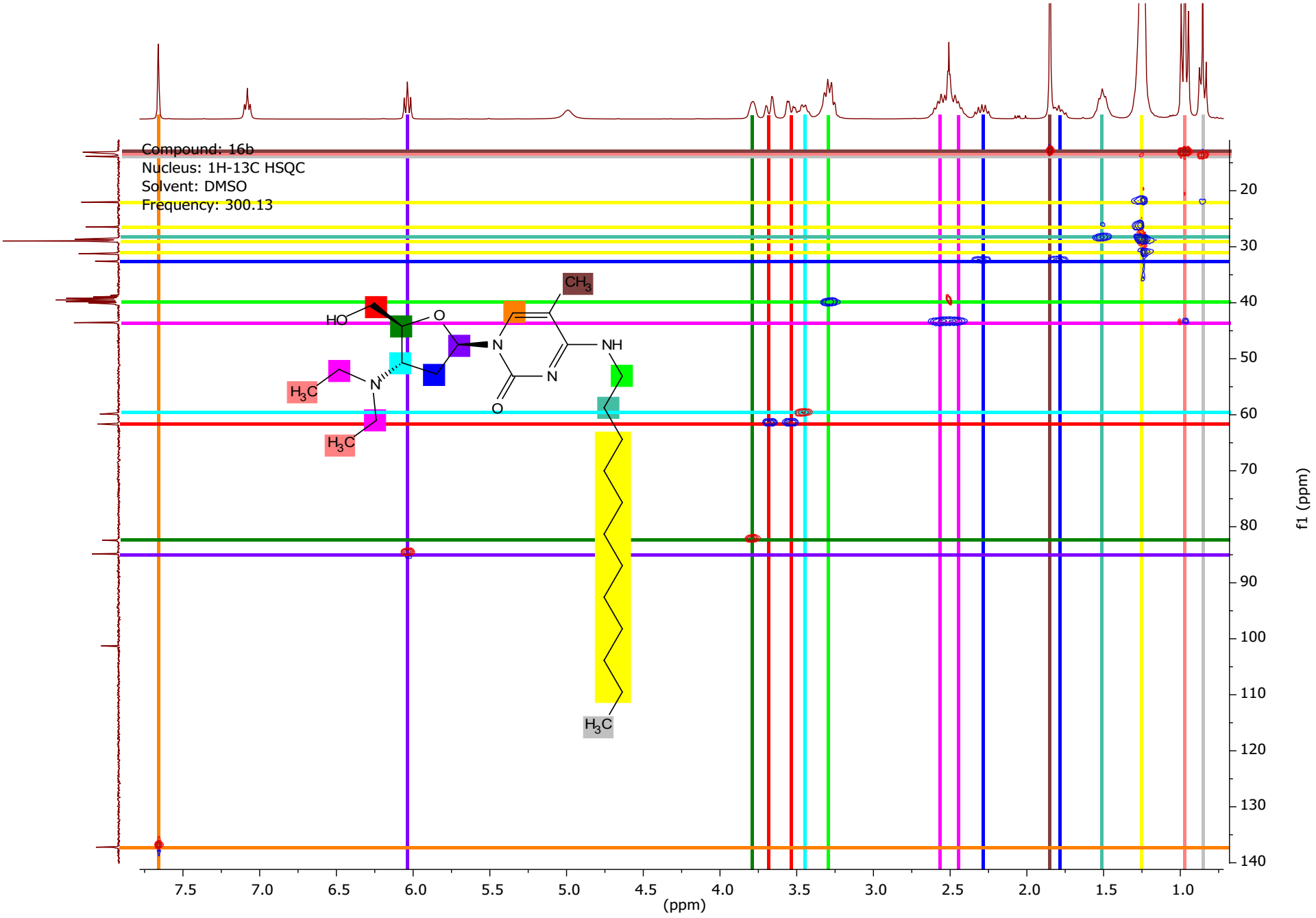

Compound: 10a
Nucleus: 1H-13C HSQC
Solvent: DMSO
Frequency: 300.13
OH
CH3
NH
N
O
H2N
H3C
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (мд)
20
30
40
50
60
70
80
90
100
110
120
130
140
f1 (мд)


Compound: 10b
Nucleus: 1H-1H COSY
Solvent: DMSO
Frequency: 300.13
HO
O
N
NH
CH3
H2N
N
O
H3C
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
(ppm)


Compound: 10b
Nucleus: 1H-13C HSQC
Solvent: DMSO
Frequency: 300.13
HO
O
N
NH
N
O
CH_3
H_2N
H_3C
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
(ppm)
20
30
40
50
60
70
80
90
100
110
120
130
140
f1 (ppm)


Compound: 12b
Nucleus: 1H-13C HSQC
Solvent: DMSO
Frequency: 300.13
HO
O
CH3
N
NH
N
O
H3C
N
CH3
H3C
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
(ppm)
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)


Compound: 14b
Nucleus: 1H-13C HSQC
Solvent: DMSO
Frequency: 300.13
CH3
NH
O
N
N
HO
O
HN
H3C
CH3
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
(ppm)
20
30
40
50
60
70
80
90
100
110
120
130
140
f1 (ppm)


Compound: 16b
Nucleus: 1H-13C HSQC
Solvent: DMSO
Frequency: 300.13
HO
O
N
NH
N
O
CH3
H3C
N
H3C
H3C
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
(ppm)
20
30
40
50
60
70
80
90
100
110
120
130
140
f1 (ppm)

HPLC-chromatogram and HRMS spectrum of **6b**

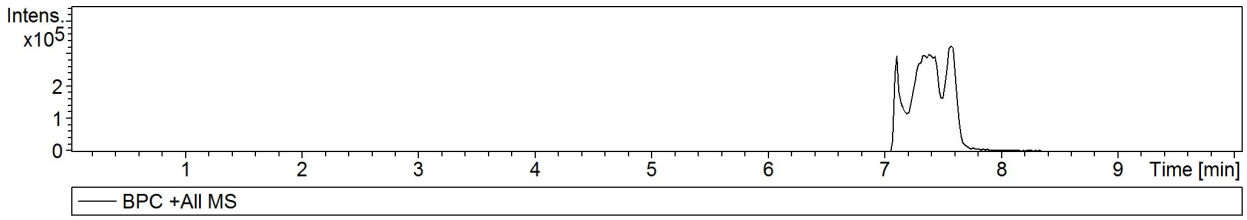
Display Report

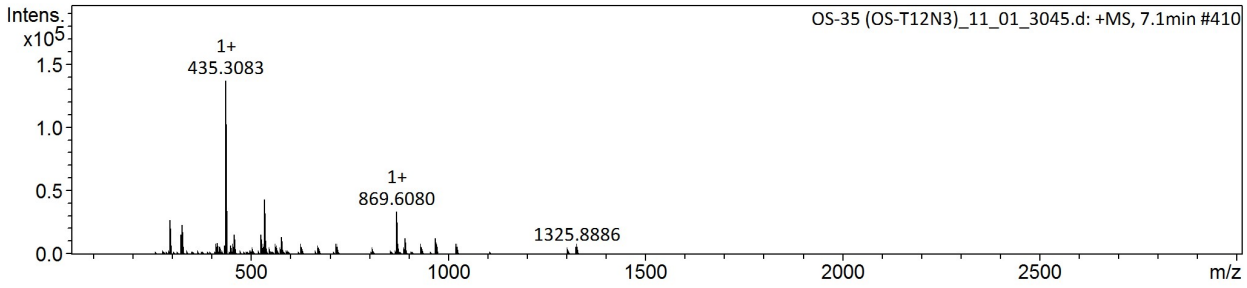
Analysis Info

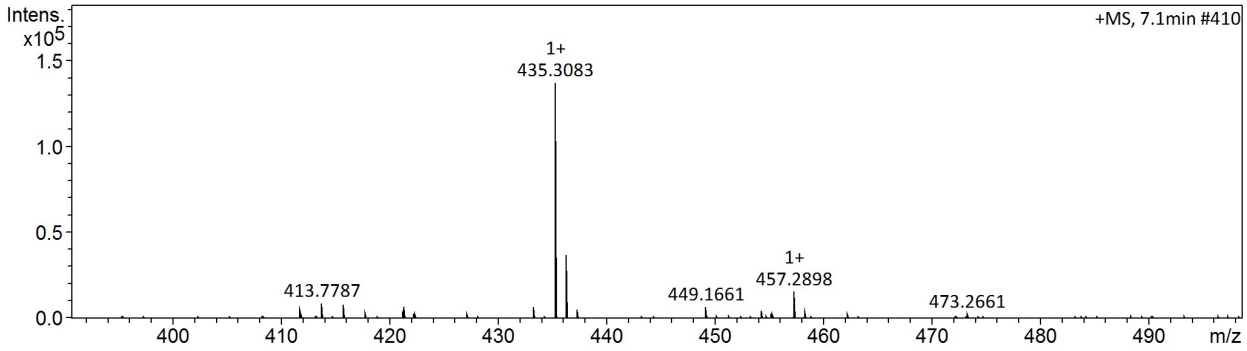
Analysis Name	D:\Data\OS-35 (OS-T12N3)_11_01_3045.d	Acquisition Date	11/22/2019 1:51:15 PM
Method	la_2.2.m	Operator	BDAL@DE
Sample Name	OS-35 (OS-T12N3)	Instrument	compact 8255754.20088
Comment			

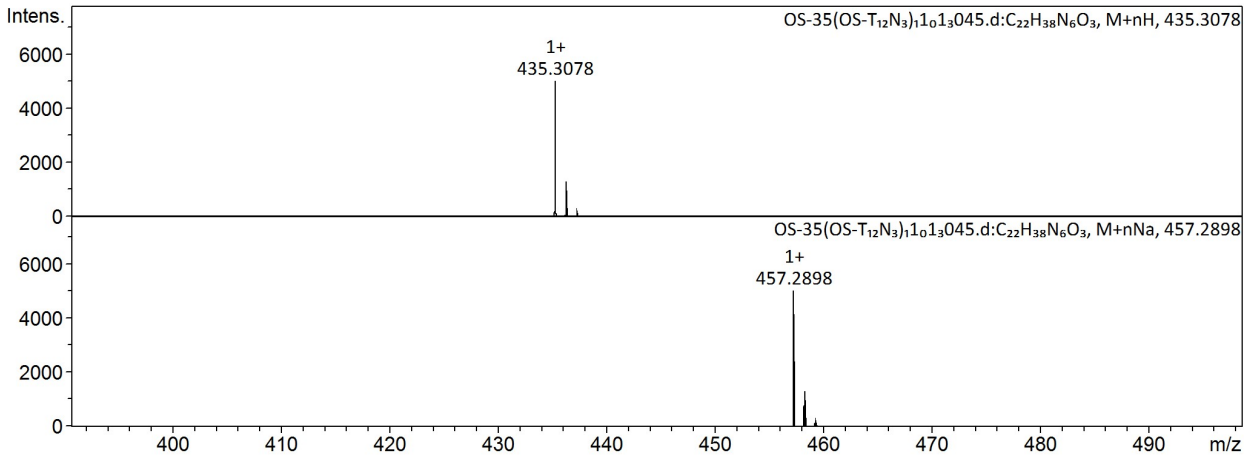
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 \C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 \C









HPLC-chromatogram and HRMS spectrum of **8a**

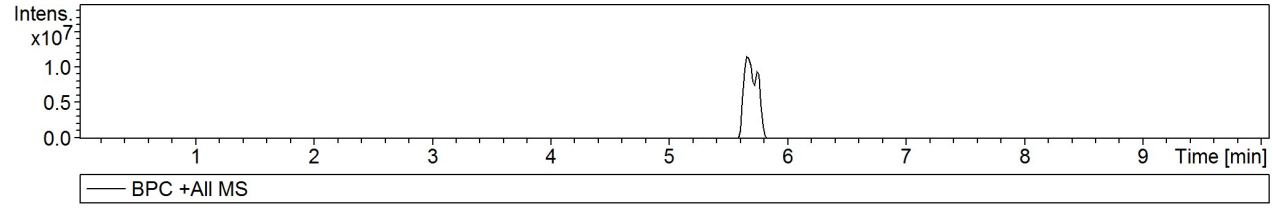
Display Report

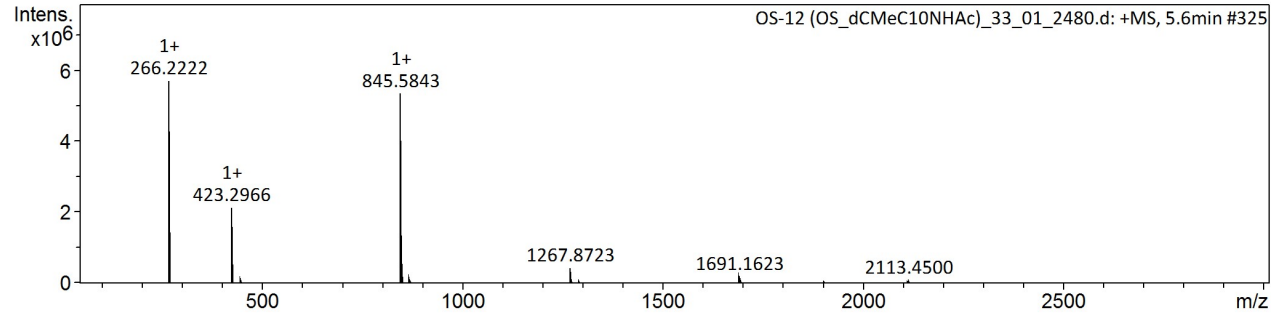
Analysis Info

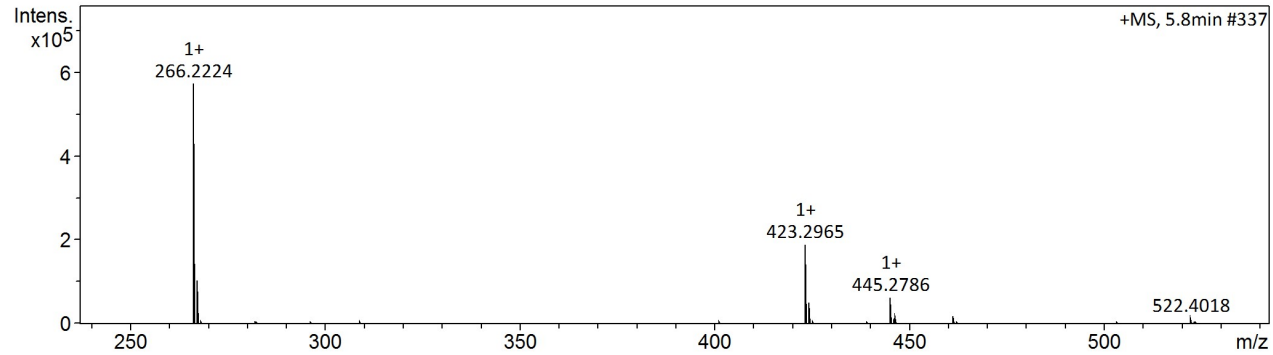
Analysis Name	D:\Data\OS-12 (OS_dCMeC10NHAc)_33_01_2480.d	Acquisition Date	3/19/2019 6:34:34 PM
Method	la_2.2.m	Operator	BDAL@DE
Sample Name	OS-12 (OS_dCMeC10NHAc)	Instrument	compact 8255754.20088
Comment			

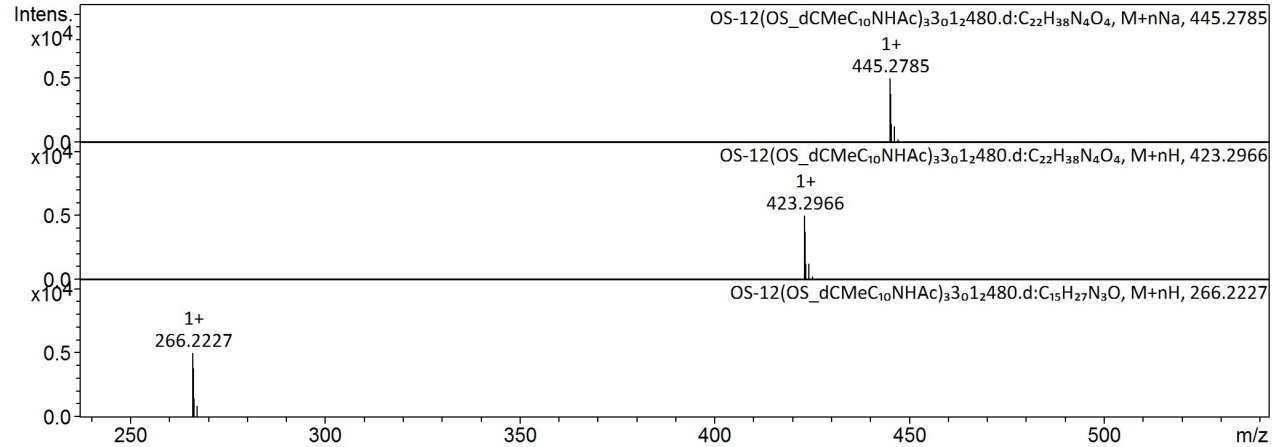
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 \C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 \C









HPLC-chromatogram and HRMS spectrum of **10a**

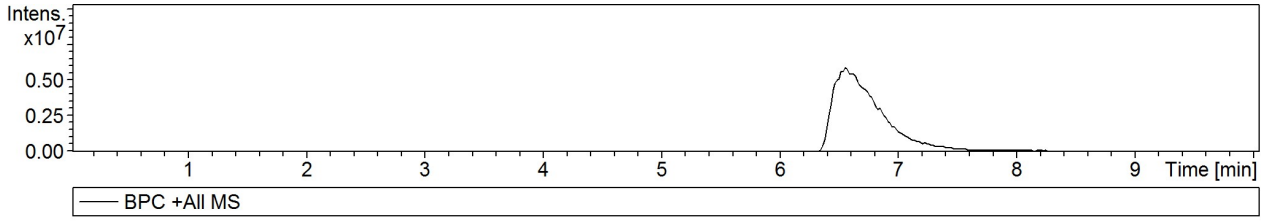
Display Report

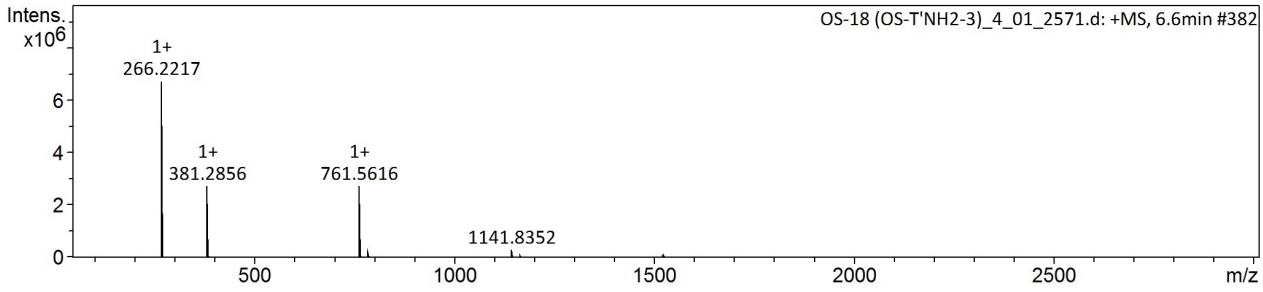
Analysis Info

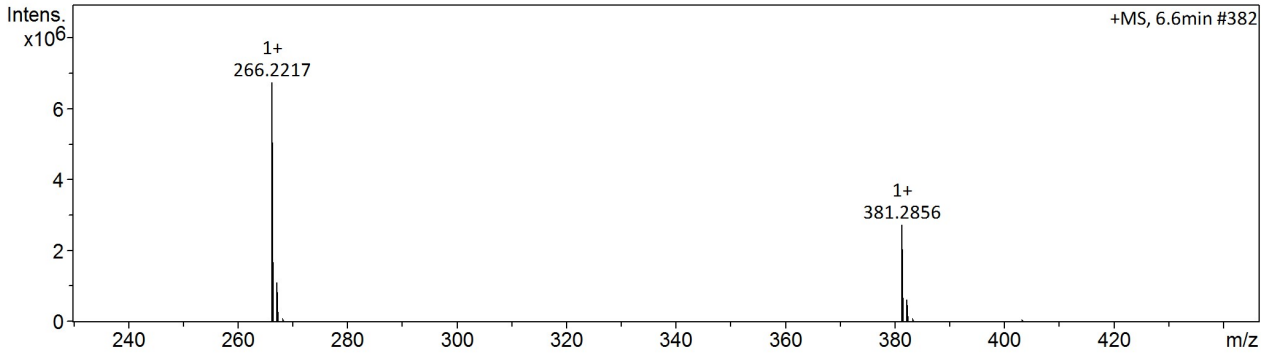
Analysis Name	D:\Data\OS-18 (OS-T'NH2-3)_4_01_2571.d	Acquisition Date	4/30/2019 5:27:14 PM
Method	la_2.2.m	Operator	BDAL@DE
Sample Name	OS-18 (OS-T'NH2-3)	Instrument	compact 8255754.20088
Comment			

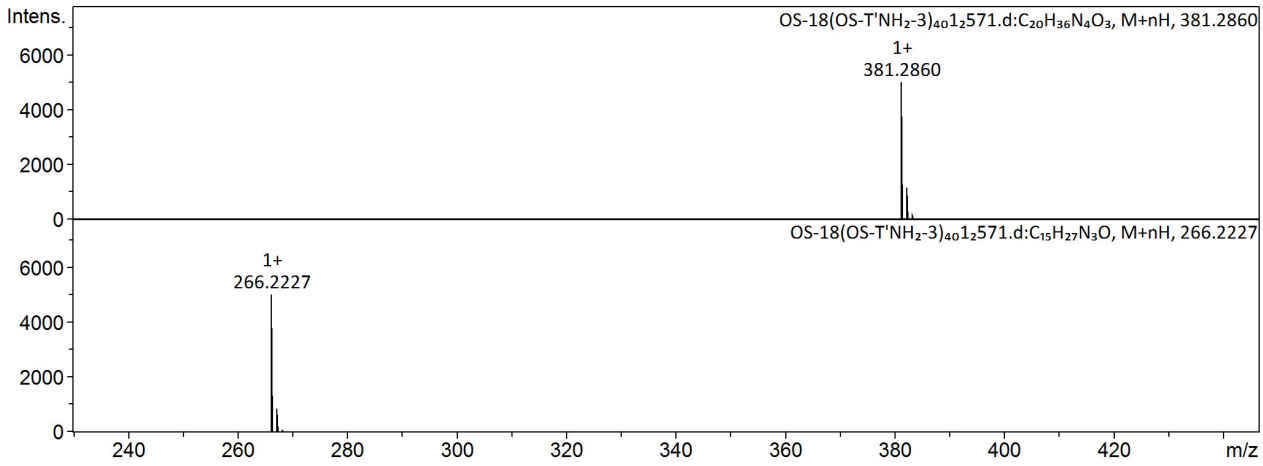
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 \C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 \C









HPLC-chromatogram and HRMS spectrum of **10b**

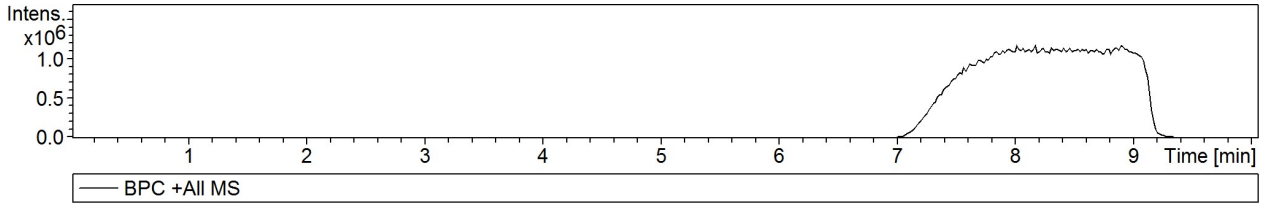
Display Report

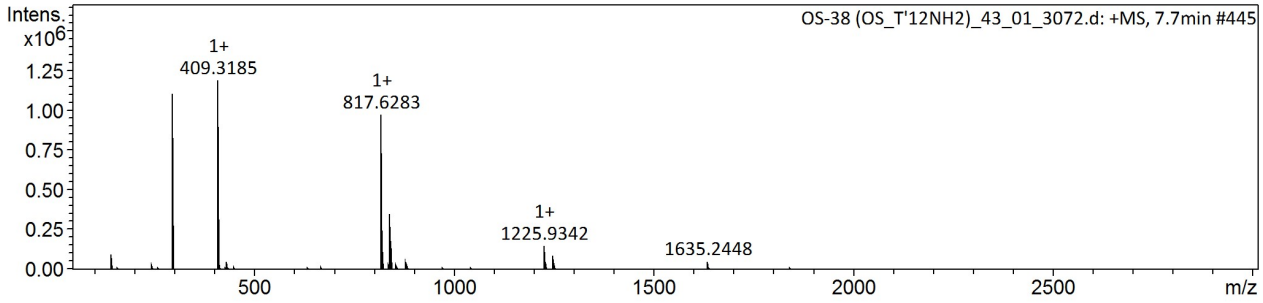
Analysis Info

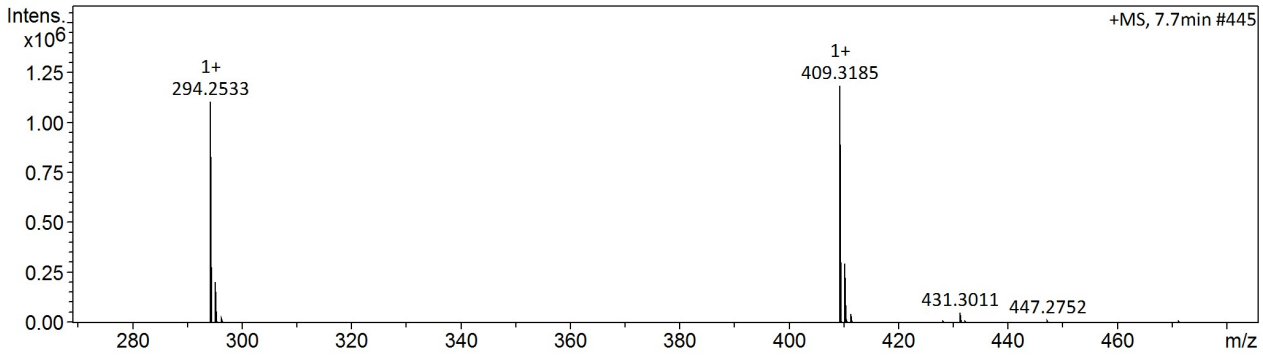
Analysis Name	D:\Data\OS-38 (OS_T'12NH2)_43_01_3072.d	Acquisition Date	11/28/2019 4:29:04 PM
Method	la_2.2_small.m	Operator	BDAL@DE
Sample Name	OS-38 (OS_T'12NH2)	Instrument	compact 8255754.20088
Comment			

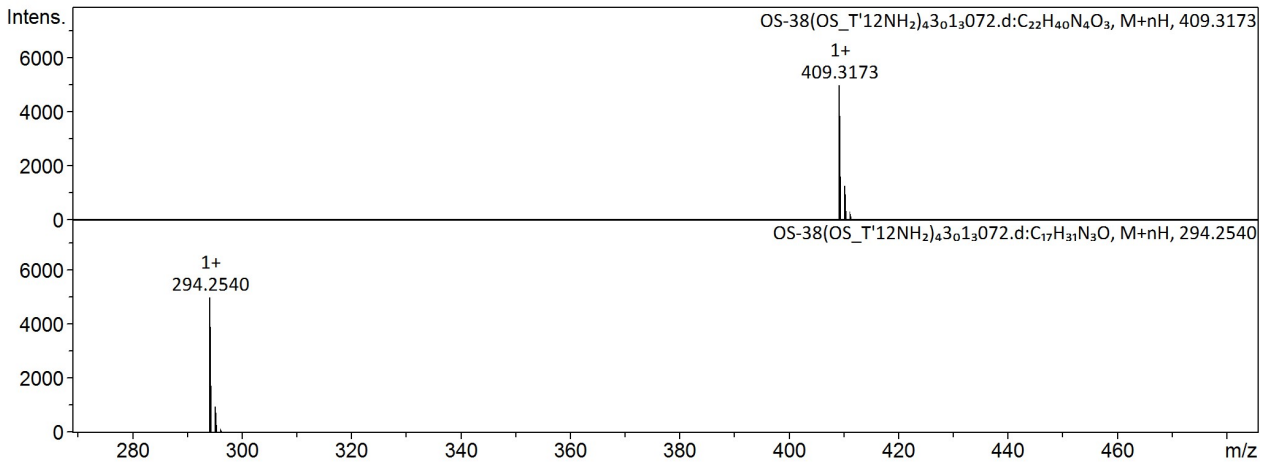
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 \C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 \C









HPLC-chromatogram and HRMS spectrum of **12b**

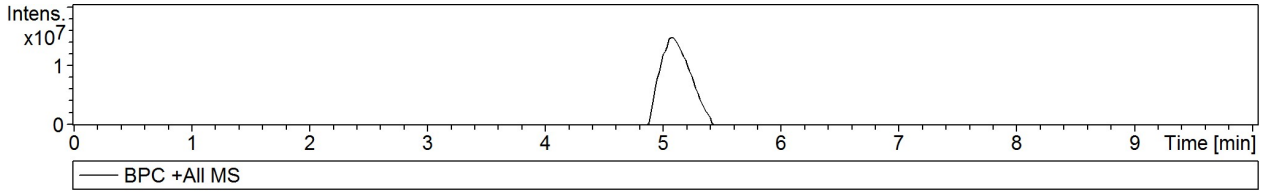
Display Report

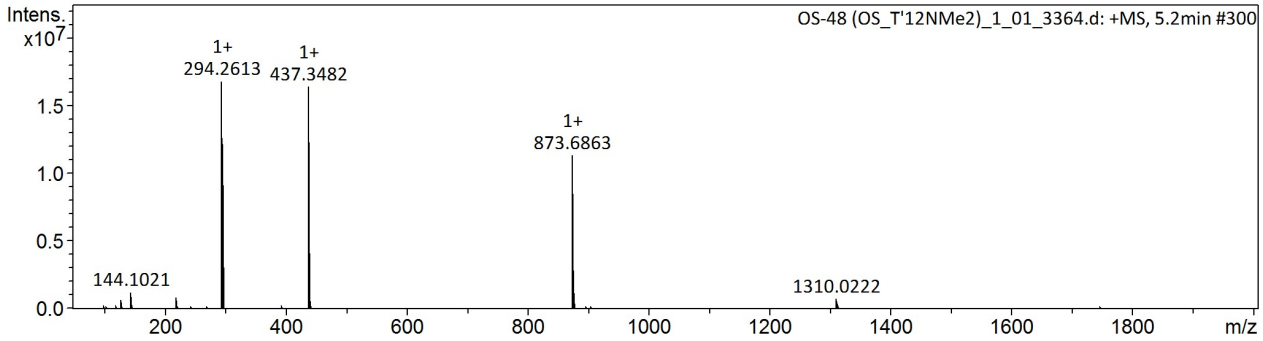
Analysis Info

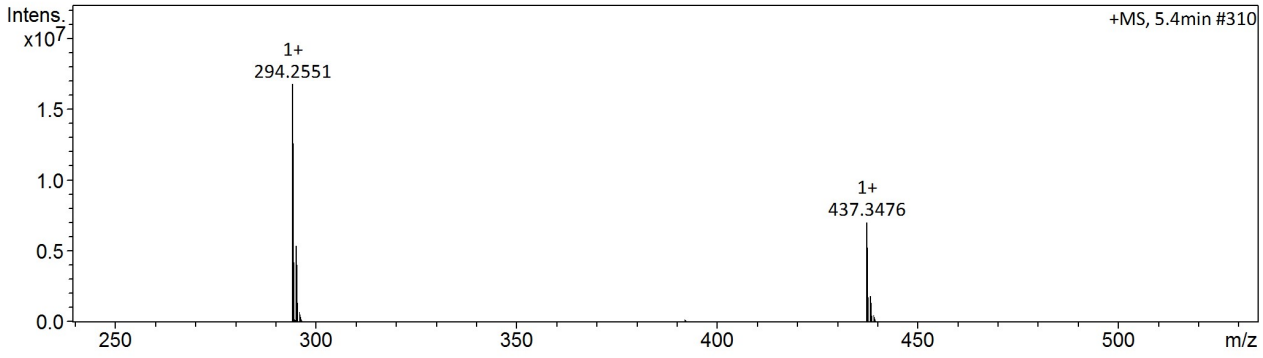
Analysis Name	D:\Data\OS-48 (OS_T'12NMe2)_1_01_3364.d	Acquisition Date	7/16/2020 4:03:36 PM
Method	la_2.2_small.m	Operator	BDAL@DE
Sample Name	OS-48 (OS_T'12NMe2)	Instrument	compact 8255754.20088
Comment			

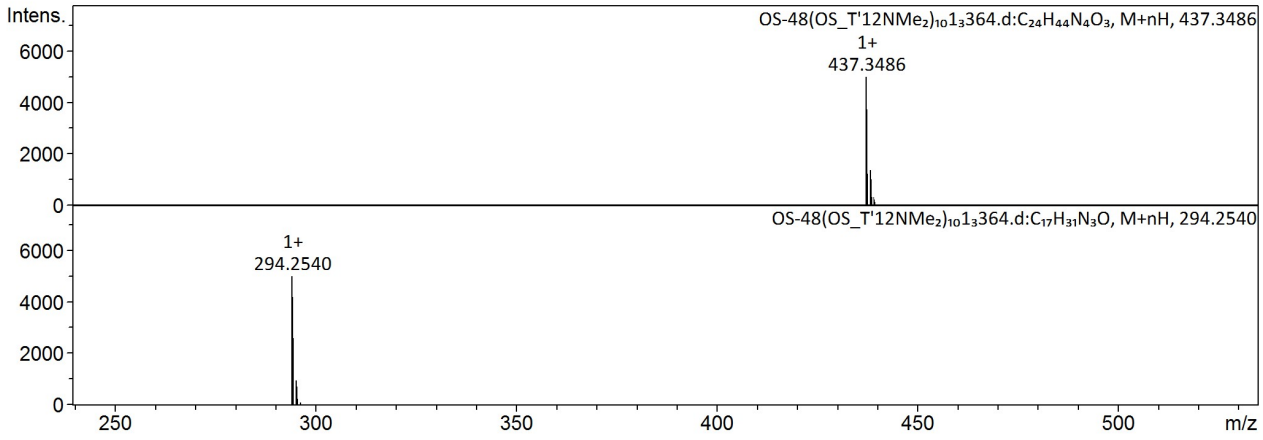
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 \C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 \C









HPLC-chromatogram and HRMS spectrum of **14a**

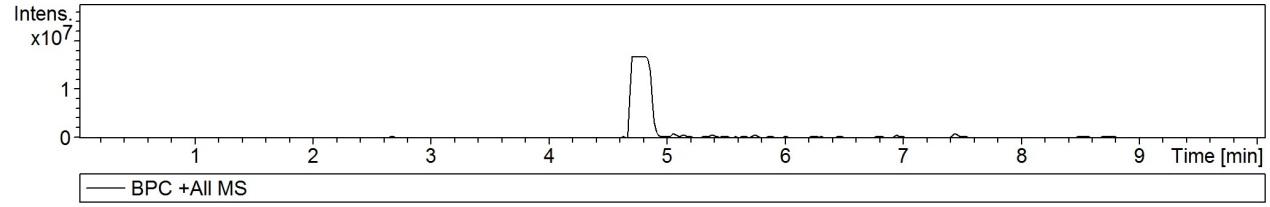
Display Report

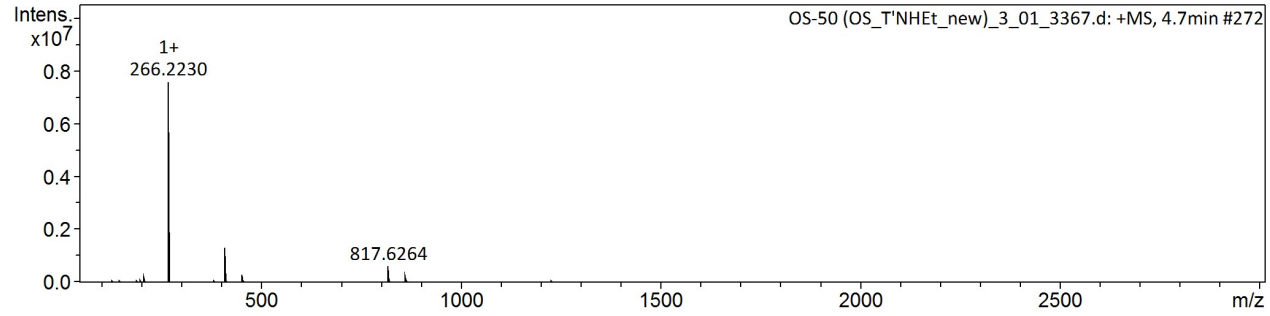
Analysis Info

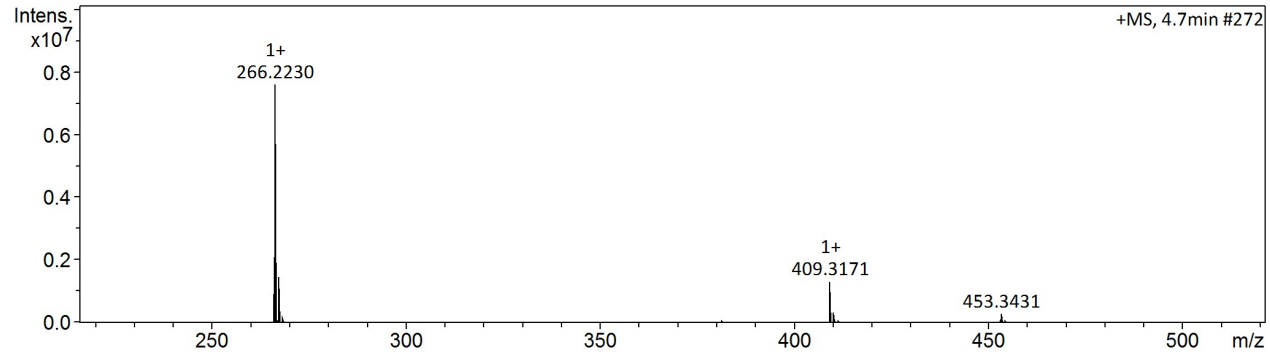
Analysis Name	D:\Data\OS-50 (OS_T'NHEt_new)_3_01_3367.d	Acquisition Date	7/16/2020 4:37:50 PM
Method	la_2.2_small.m	Operator	BDAL@DE
Sample Name	OS-50 (OS_T'NHEt_new)	Instrument	compact 8255754.20088
Comment			

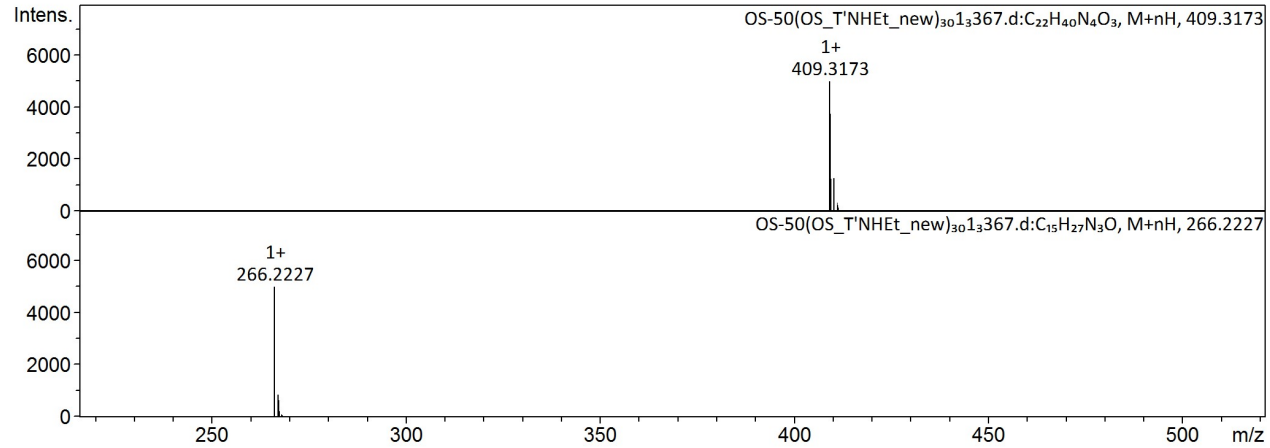
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 \C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 \C









HPLC-chromatogram and HRMS spectrum of **14b**

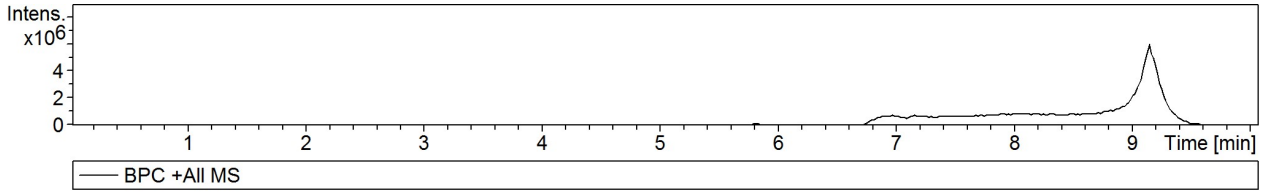
Display Report

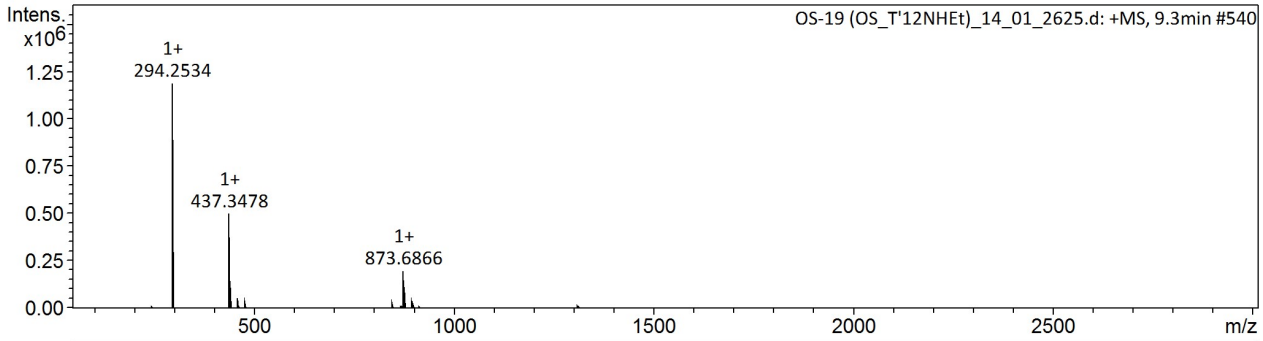
Analysis Info

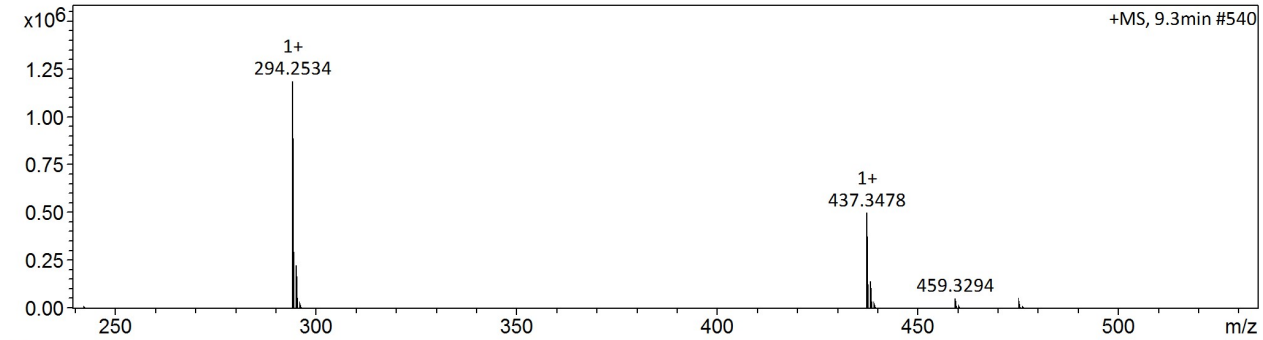
Analysis Name	D:\Data\OS-19 (OS_T'12NHEt)_14_01_2625.d	Acquisition Date	7/9/2019 8:15:15 PM
Method	la_2.2.m	Operator	BDAL@DE
Sample Name	OS-19 (OS_T'12NHEt)	Instrument	compact 8255754.20088
Comment			

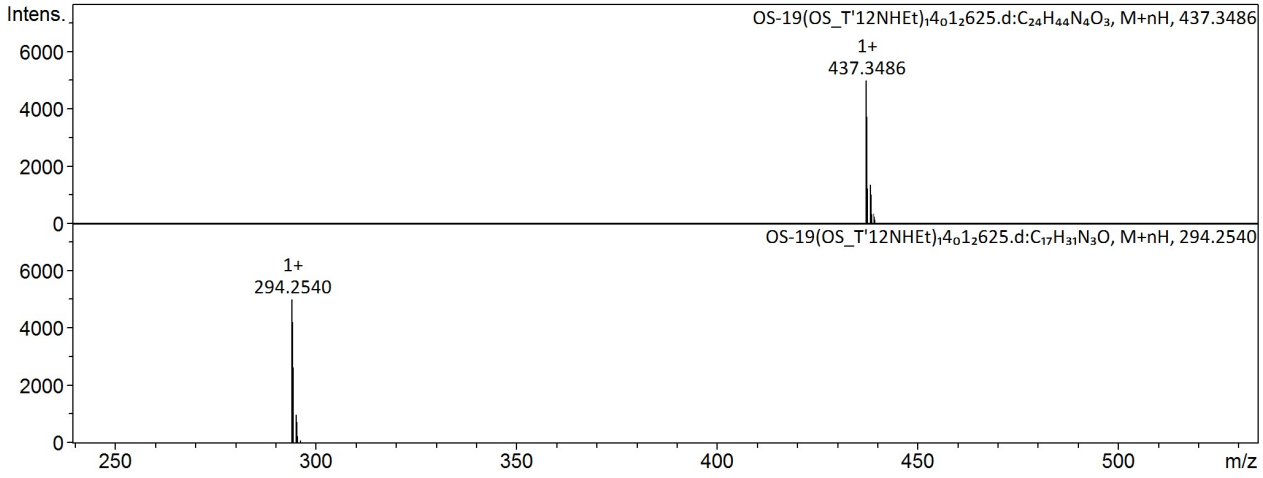
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 \C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 \C









HPLC-chromatogram and HRMS spectrum of **16a**

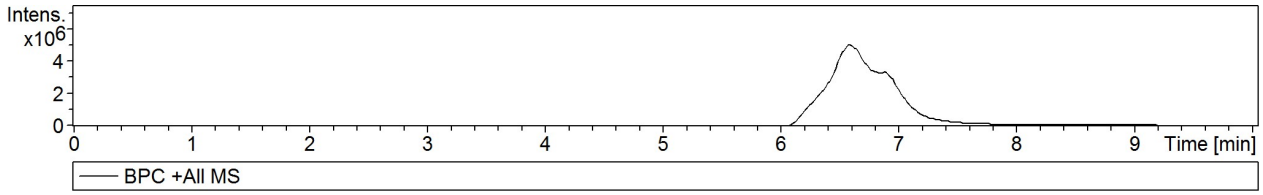
Display Report

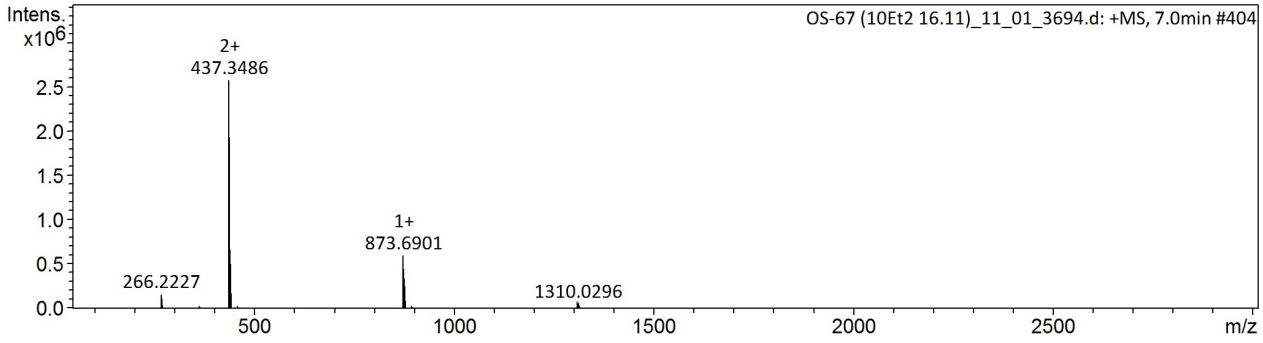
Analysis Info

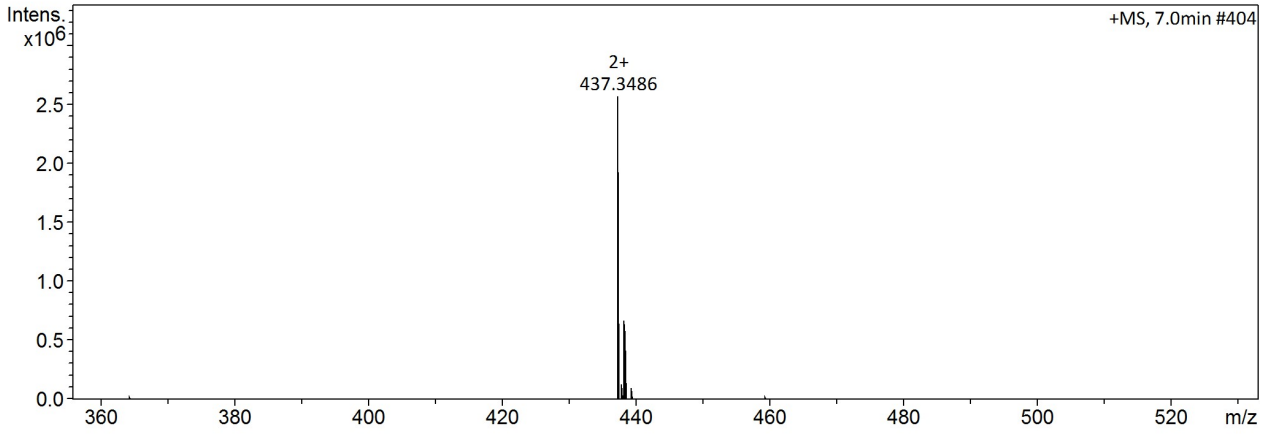
Analysis Name	D:\Data\OS-67 (10Et2 16.11)_11_01_3694.d	Acquisition Date	11/17/2020 6:20:50 PM
Method	la_2.2.m	Operator	BDAL@DE
Sample Name	OS-67 (10Et2 16.11)	Instrument	compact 8255754.20088
Comment			

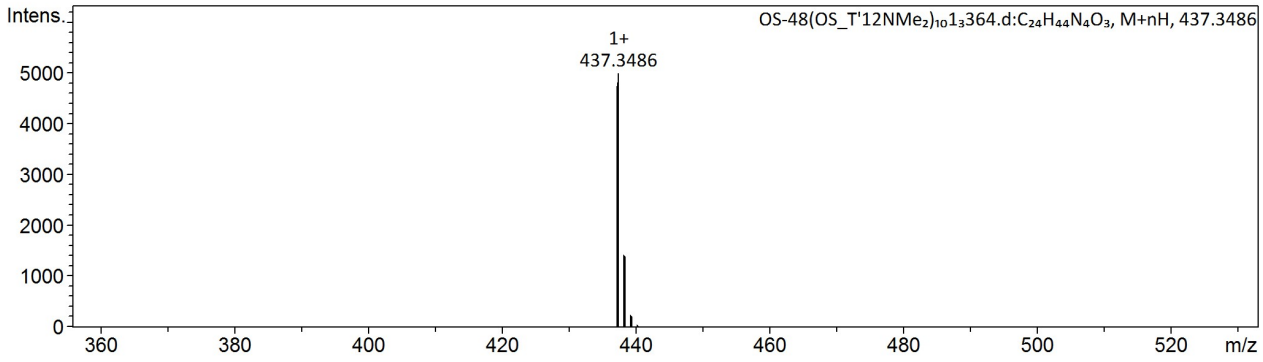
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 \C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 \C









HPLC-chromatogram and HRMS spectrum of **16b**

Display Report

Analysis Info

Analysis Name	D:\Data\OS-49 (OS_T'12NEt2)_2_01_3365.d	Acquisition Date	7/16/2020 4:15:12 PM
Method	la_2.2_small.m	Operator	BDAL@DE
Sample Name	OS-49 (OS_T'12NEt2)	Instrument	compact 8255754.20088
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 \C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 \C