Locked Nucleic Acid (LNA) induced effect on hybridization and fluorescence properties of oligodeoxyribonucleotides modified with nucleobase-functionalized DNA monomers

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ELECTRONIC SUPPLEMENTARY INFORMATION

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Table S1. MALDI-ToF MS of modified 9-mer ONs.[a]

		(M+H)				(M+H)	
ON	**Sequence**	**CALC**	**OBS**	**ON**	**Sequence**	**CALC**	**OBS**
T2	5′-GTG **a**T**a** TGC	2809.5	2810.7	**A5**	5′-GCA **t**A**t** CAC	2739.5	2738.2
T3	5′-GT**g** ATA **t**GC	2809.5	2810.6	**A6**	5′-GC**a** TAT **c**AC	2752.5	2751.2
W1	5′-GTG A**W**A TGC	2762.5	2763.6	**L4**	5′-GCA T**L**T CAC	2706.5	2706.3
W2	5′-GTG **aWa** TGC	2818.5	2819.6	**L5**	5′-GCA **tLt** CAC	2775.0	2776.0
W3	5′-GT**g** A**W**A **t**GC	2818.5	2819.6	**L6**	5′-GC**a** T**L**T **c**AC	2761.5	2762.3
X1	5′-GTG A**X**A TGC	2791.5	2793.0	**M4**	5′-GCA T**M**T CAC	2907.7	2906.7
X2	5′-GTG **aXa** TGC	2847.5	2848.0	**M5**	5′-GCA **tMt** CAC	2977.0	2977.0
X3	5′-GT**g** A**X**A **t**GC	2847.5	2848.7	**M6**	5′-GC**a** T**M**T **c**AC	2964.7	2964.0
Y1	5′-GTG A**Y**A TGC	2964.7	2962.1	**N4**	5′-GCA T**N**T CAC	2962.6	2963.3
Y2	5′-GTG **aYa** TGC	3020.7	3019.6	**N5**	5′-GCA **tNt** CAC	3033.6	3033.3
Y3	5′-GT**g** A**Y**A **t**GC	3020.7	3020.0	**N6**	5′-GC**a** T**N**T **c**AC	3018.6	3021.0
Z1	5′-GTG A**Z**A TGC	3019.6	3020.7				
Z2	5′-GTG **aZa** TGC	3075.5	3076.6				
Z3	5′-GT**g** A**Z**A **t**GC	3075.5	3076.6				

[a] A/C/G/T = adenin-9-yl/cytosin-1-yl/guanin-9-yl/thymin-1-yl DNA monomers. For structures of monomers **W/X/Y/Z** and **L**/**M/N**, see Figure 1 in main manuscript. LNA modifications are shown in lower case ("c" = 5-methylcytosine LNA monomer). Modified ONs were obtained in a purity of at least 75%.

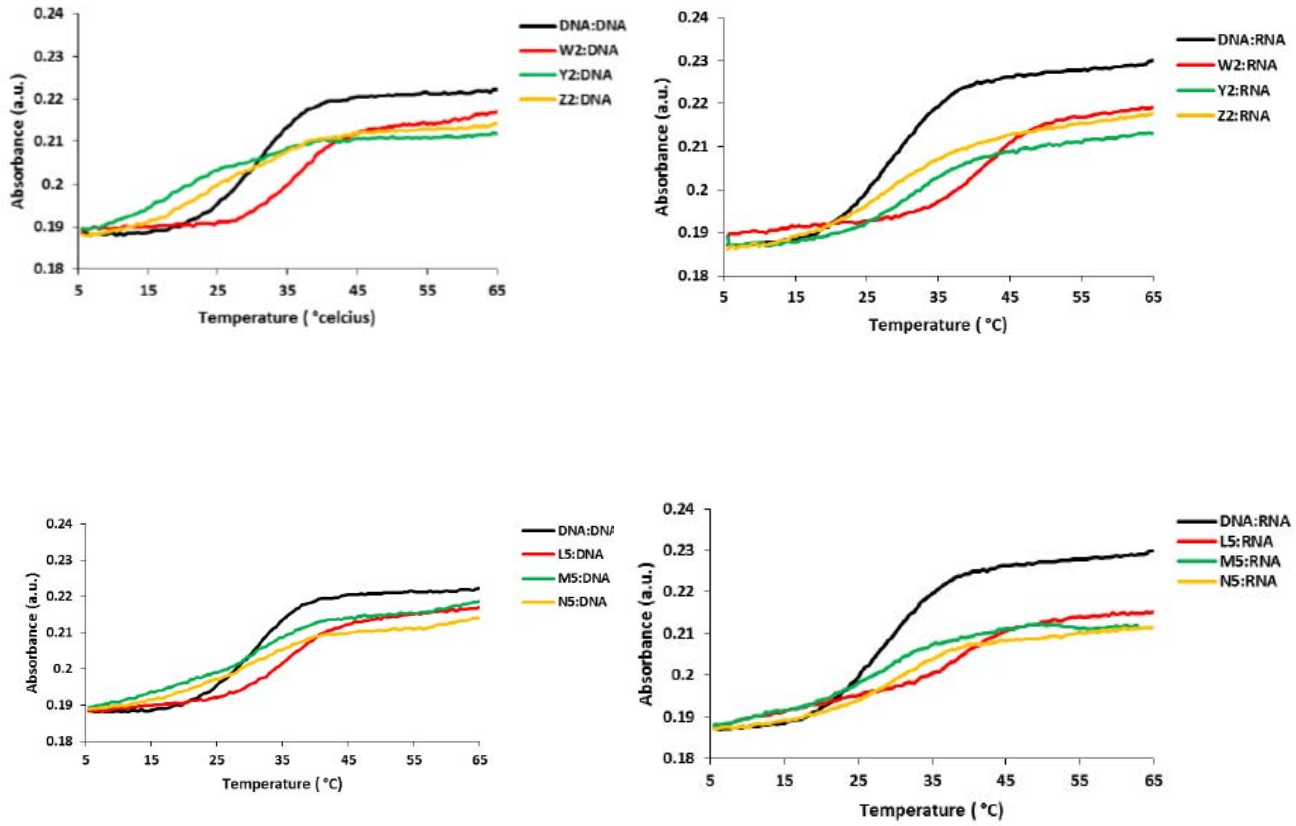


Figure S1. Representative thermal denaturation curves of duplexes between **W2**/**Y2**/**Z2**/**L5**/**M5**/**N5** and complementary DNA or RNA targets. For experimental conditions, see Table 1.

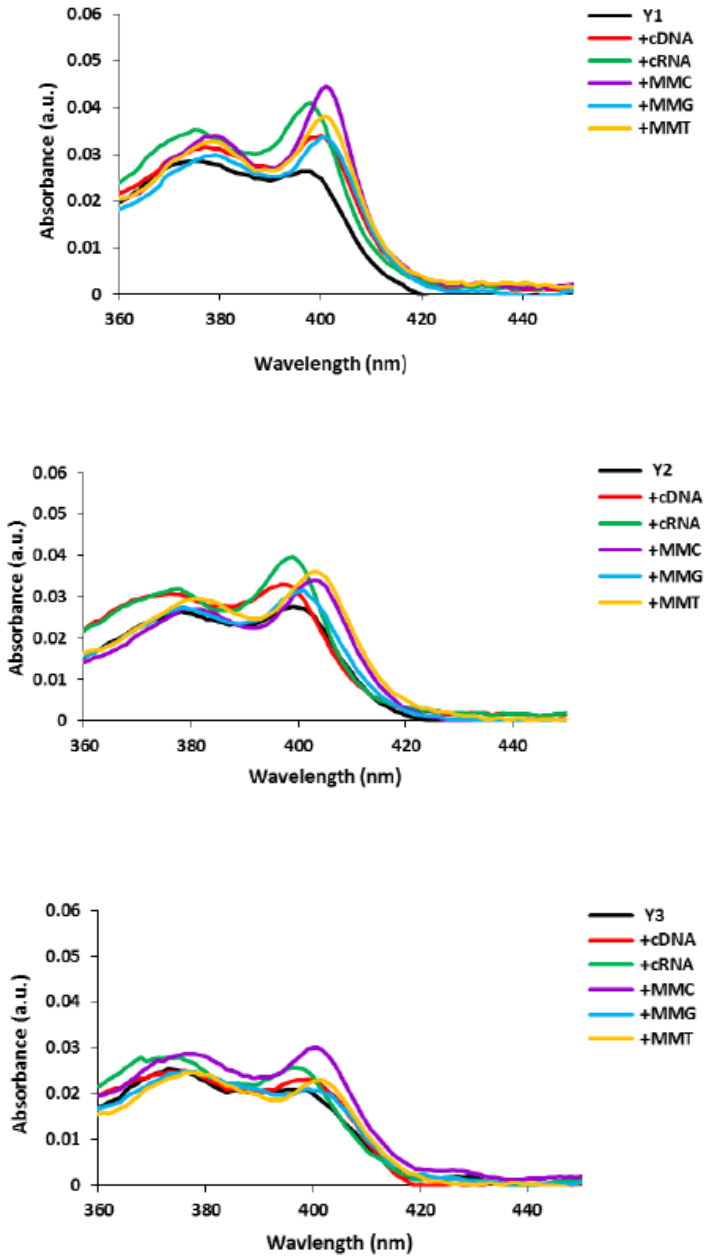


Figure S2. Absorption spectra of single-stranded **Y1**-**Y3** and the corresponding duplexes with complementary DNA/RNA (cDNA/cRNA) or centrally mismatched DNA targets (mismatched nucleoside is specified) - for sequences of matched/mismatched targets, see footnote of Table 5. Spectra were recorded in T_m buffer at T = 5 °C using each strand at 1 μM concentration.

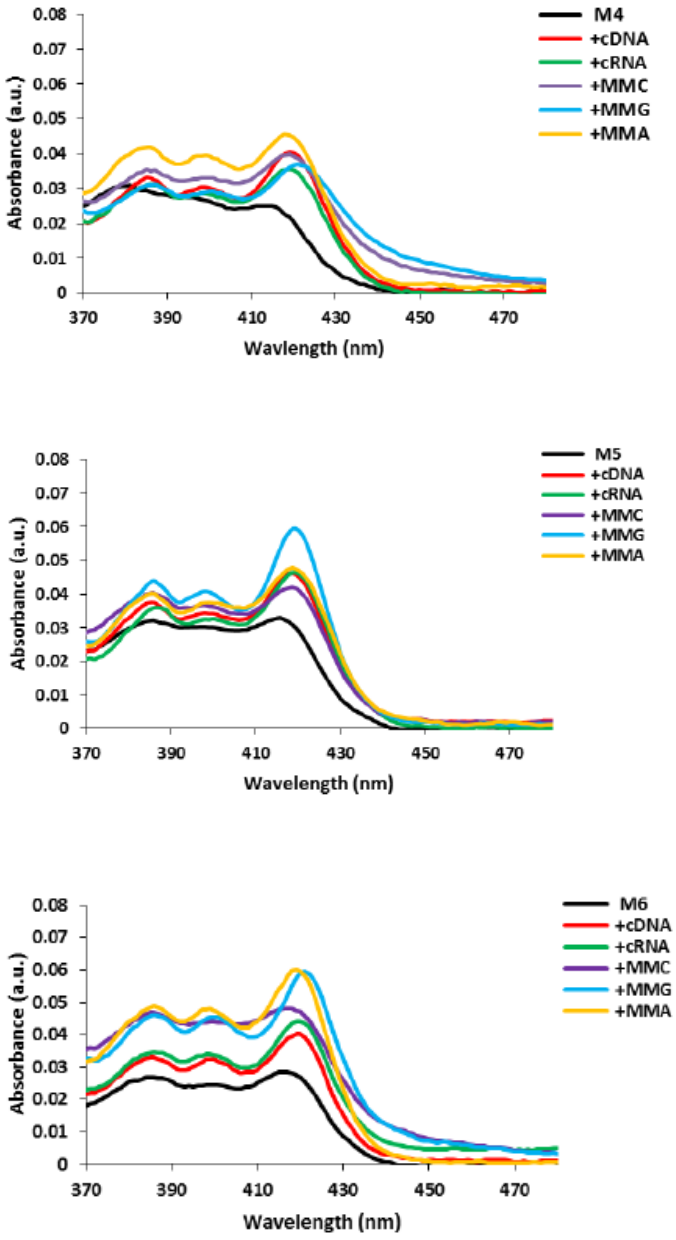


Figure S3. Absorption spectra of single-stranded **M4-M6** and the corresponding duplexes with complementary DNA/RNA or centrally mismatched DNA targets (mismatched nucleoside is specified) - for sequences of matched/mismatched targets, see footnote of Table 5. For experimental conditions, see Figure S2.

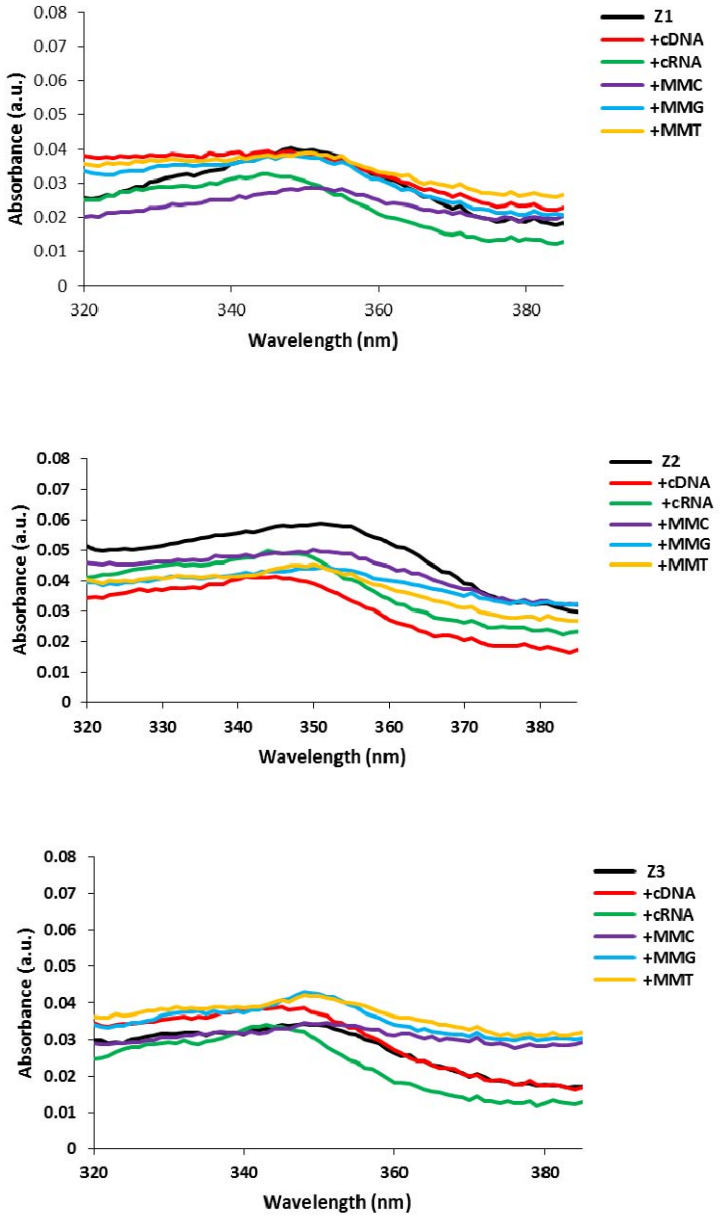


Figure S4. Absorption spectra of single-stranded **Z1**-**Z3** and the corresponding duplexes with complementary DNA/RNA or centrally mismatched DNA targets (mismatched nucleoside is specified) - for sequences of matched/mismatched targets, see footnote of Table 5. For experimental conditions, see Figure S2.

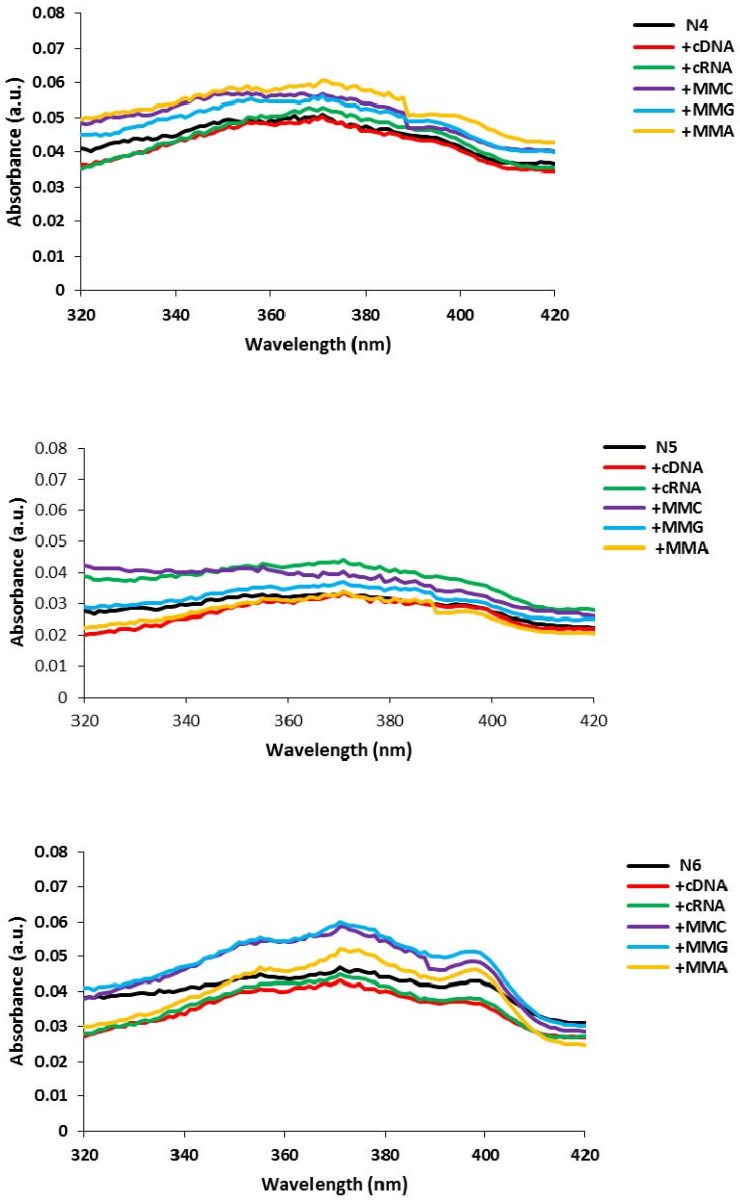


Figure S5. Absorption spectra of single-stranded **N4**-**N6** and the corresponding duplexes with complementary DNA/RNA or centrally mismatched DNA targets (mismatched nucleoside is specified) - for sequences of matched/mismatched targets, see footnote of Table 5. For experimental conditions, see Figure S2.

Biophysical characterization of 13-mer Y/M-modified ONs. Systematic studies of 13-mer ONs, in which the C5- or C8-ethynylpyrene functionalized monomers **Y** or **M** are directly flanked by LNA nucleotides, were performed (Table S2). The observed trends mirror those for the 9-mer ONs (see main manuscript), with the following exceptions: i) **M11**-**M14** exhibit lower-than-anticipated cDNA (Table S4), ii) **Y10** displays minimal blue-shifts in pyrene absorption maxima upon cDNA hybridization (Table S5), iii) **M13** displays blue-shifts in pyrene absorption maxima upon hybridization with matched/mismatched DNA targets; this may be due to a structured state of the single-stranded probe (note the high absolute λ_{max} value for **M13**, Table S5), and iv) hybridization of **M11**-**M14** to cDNA targets does not result in increased emission.

Table S2. MALDI-ToF MS of modified 13-mer ONs.[a]

		(M+H)	
ON	**Sequence**	**CALC**	**OBS**
Y7	5′-CG CAA **aYa** AAC GC	4185.0	4184.0
Y8	5′-CG CAA **cYc** AAC GC	4232.7	4233.0
Y9	5′-CG CAA **gYg** AAC GC	4180.7	4182.0
Y10	5′-CG CAA **tYt** AAC GC	4200.0	4202.0
M11	3′-GCGTT **aMa** TTGCG	4249.7	4250.6
M12	3′-GCGTT **cMc** TTGCG	4299.7	4300.0
M13	3′-GCGTT **gMg** TTGCG	4247.7	4248.0
M14	3′-GCGTT **tMt** TTGCG	4267.8	4268.5

[a] A/C/G/T = adenin-9-yl/cytosin-1-yl/guanin-9-yl/thymin-1-yl DNA monomers. LNA modifications are shown in lower case (**c** = 5-methylcytosine LNA). For structures of monomers **Y** and **M**, see Figure 1 in main manuscript.

Table S3. Thermal denaturation data for duplexes between **Y**-modified ONs and complementary or singly mismatched DNA targets.

			T_m/°C	ΔT_m/°C		
ON	Sequence	**B** =	A	C	G	T
Y7	5′-CG CAA **aYa** AAC GC 3′-GC GTT T**B**T TTG CG		45.0	0.0	+1.0	+1.0
Y8	5′-CG CAA **cYc** AAC GC 3′-GC GTT G**B**G TTG CG		57.0	-5.0	-2.0	-6.0
Y9	5′-CG CAA **gYg** AAC GC 3′-GC GTT C**B**C TTG CG		49.0	0.0	-8.0	-3.0
Y10	5′-CG CAA **tYt** AAC GC 3′-GC GTT A**B**A TTG CG		45.5	-1.0	-1.0	-3.0

[a]For experimental conditions, see Table 1 in main manuscript. T_m's of the duplexes between cDNA and the unmodified control ONs for **Y7**-**Y10** are 48.5 °C, 55.5 °C, 55.0 °C and 48.5 °C, respectively. ΔT_m = change in T_m's relative to fully matched duplex (**B** = A).

Table S4. Thermal denaturation data for duplexes between **M**-modified ONs and complementary or singly mismatched DNA targets.

			T_m/°C	ΔT_m/°C		
ON	Sequence	**B** =	T	A	C	G
M11	5′-CGCAA T**B**T AACGC 3′-GCGTT **aMa** TTGCG		41.0	-0.5	+2.5	-0.5
M12	5′-CGCAA G**B**G AACGC 3′-GCGTT **cMc** TTGCG		54.0	-1.5	-2.5	-1.5
M13	5′-CGCAA C**B**C AACGC 3′-GCGTT **gMg** TTGCG		47.0	+1.5	+2.5	-3.5
M14	5′-CGCAA A**B**A AACGC 3′-GCGTT **tMt** TTGCG		42.0	-1.5	-0.5	+1.5

[a]For experimental conditions, see Table 1 in main manuscript. T_m's of the duplexes between cDNA and the unmodified control ONs for **M11**-**M14** are 48.5 °C, 55.0 °C, 55.5 °C and 48.5 °C, respectively. ΔT_m = change in T_m's relative to fully matched duplex (**B** = T).

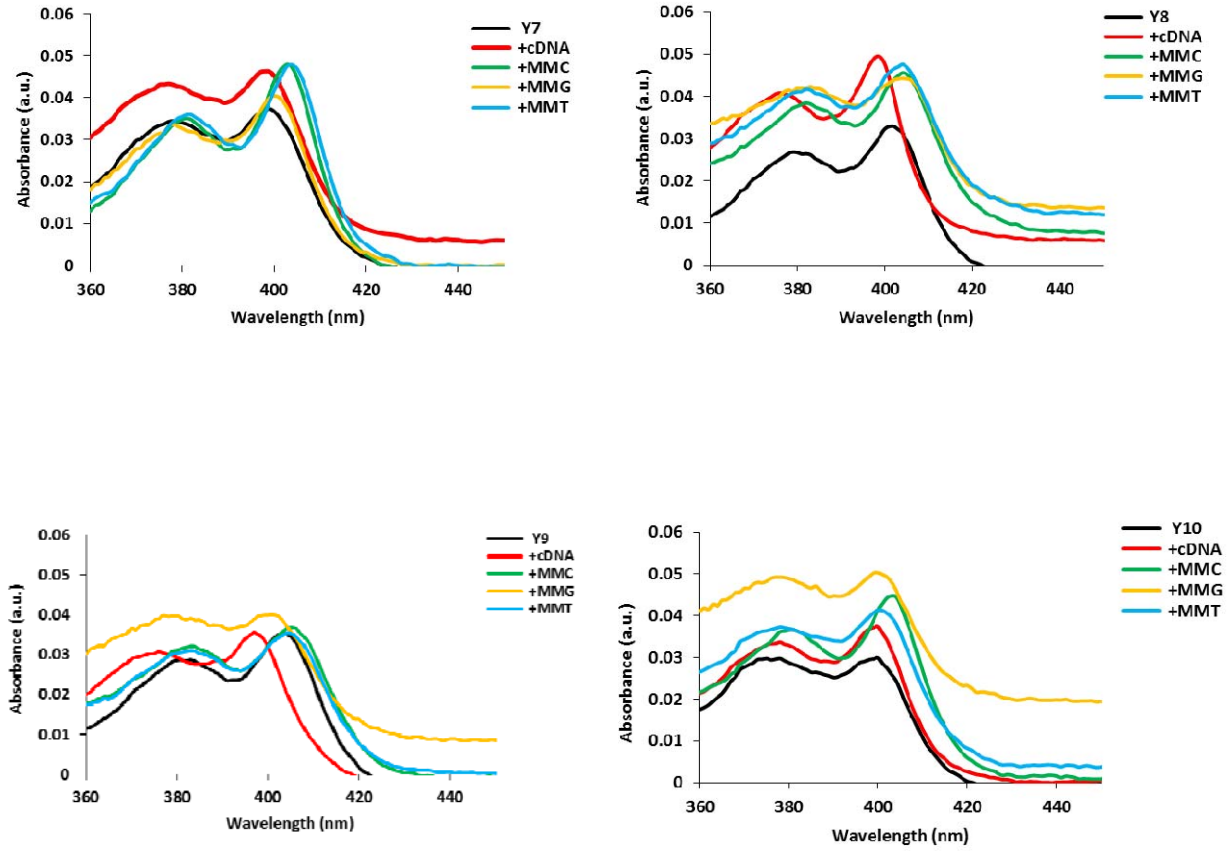


Figure S6. Absorption spectra of 13-mer **Y**-modified ONs and the corresponding duplexes with complementary or centrally mismatched DNA targets (nucleoside opposite of monomer **Y** is specified) – for sequences see Table S3. Spectra were recorded in T_m buffer at T = 5 °C using each strand at 1 μM concentration.

Table S5. Absorption maxima of 13-mer **Y**-modified ONs in the presence or absence of complementary or singly mismatched DNA targets (nucleoside opposite of monomer **Y** is specified).

		λ_{max}/nm ($\Delta\lambda_{max}$)				
ON	**Sequence**	**SSP**	**B** = A	**B** = C	**B** = G	**B** = T
Y7	5′-CG CAA **aYa** AAC GC 3′-GC GTT T**B**T TTG CG	399	-1	+4	+1	+5
Y8	5′-CG CAA **cYc** AAC GC 3′-GC GTT G**B**G TTG CG	402	-4	+2	+2	+2
Y9	5′-CG CAA **gYg** AAC GC 3′-GC GTT C**B**C TTG CG	403	-6	+2	-1	+1
Y10	5′-CG CAA **tYt** AAC GC 3′-GC GTT A**B**A TTG CG	400	+0	+4	±0	±0

[a] Recorded in T_m buffer at T = 5 °C using 1.0 μM of each strand. SSP = single-stranded probe.

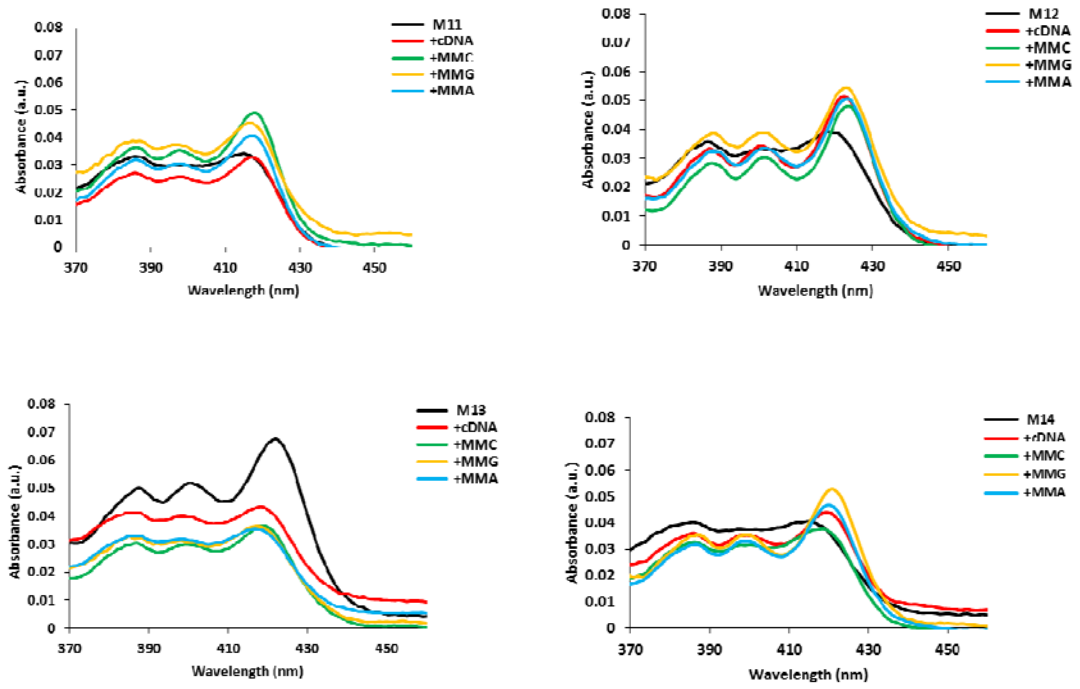


Figure S7. Absorption spectra of 13-mer **M**-modified ONs and the corresponding duplexes with complementary or centrally mismatched DNA targets (nucleoside opposite of monomer **M** is specified) – for sequences see Table S4. Spectra were recorded in T_m buffer at T = 5 °C using each strand at 1 μM concentration.

Table S6. Absorption maxima of 13-mer **M**-modified ONs in the absence (SSP) or presence of complementary or singly mismatched DNA targets (nucleoside opposite of monomer **M** is specified).[a]

		λ_{max}/nm ($\Delta\lambda_{max}$)				
ON	**Sequence**	**SSP**	**B** = T	**B** = C	**B** = G	**B** = A
M11	3′-GCGTT **aMa** TTGCG 5′-CGCAA T**B**T AACGC	415	+2	+3	+2	+2
M12	3′-GCGTT **cMc** TTGCG 5′-CGCAA G**B**G AACGC	418	+4	+5	+5	+5
M13	3′-GCGTT **gMg** TTGCG 5′-CGCAA C**B**C AACGC	422	-4	-3	-5	-5
M14	3′-GCGTT **tMt** TTGCG 5′-CGCAA A**B**A AACGC	415	+4	+3	+3	+5

[a] Recorded in T_m buffer at T = 5 °C using 1.0 μM of each strand. SSP = single-stranded probe.

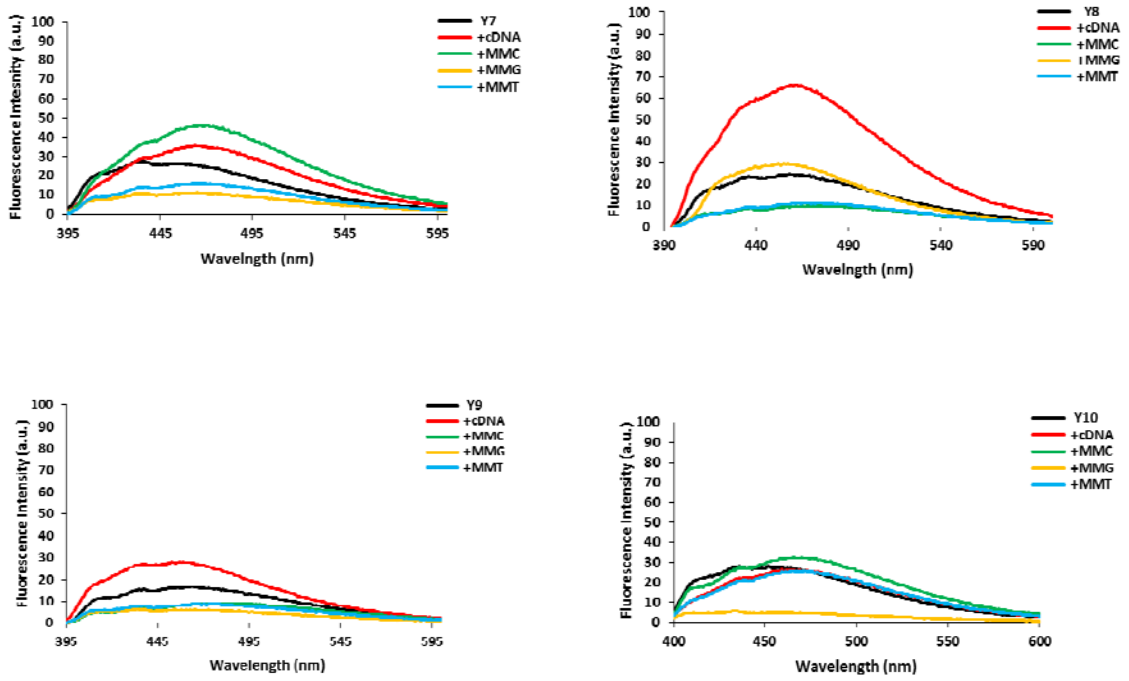


Figure S8. Steady-state fluorescence emission spectra of 13-mer **Y**-modified ONs in the presence or absence of complementary or centrally mismatched DNA targets (mismatched nucleoside opposite of monomer **Y** is specified) – for sequences see Table S3. Spectra were recorded in T_m buffer at T = 5 °C using each strand at 1 μM concentration and λ_{ex} = 380 nm.

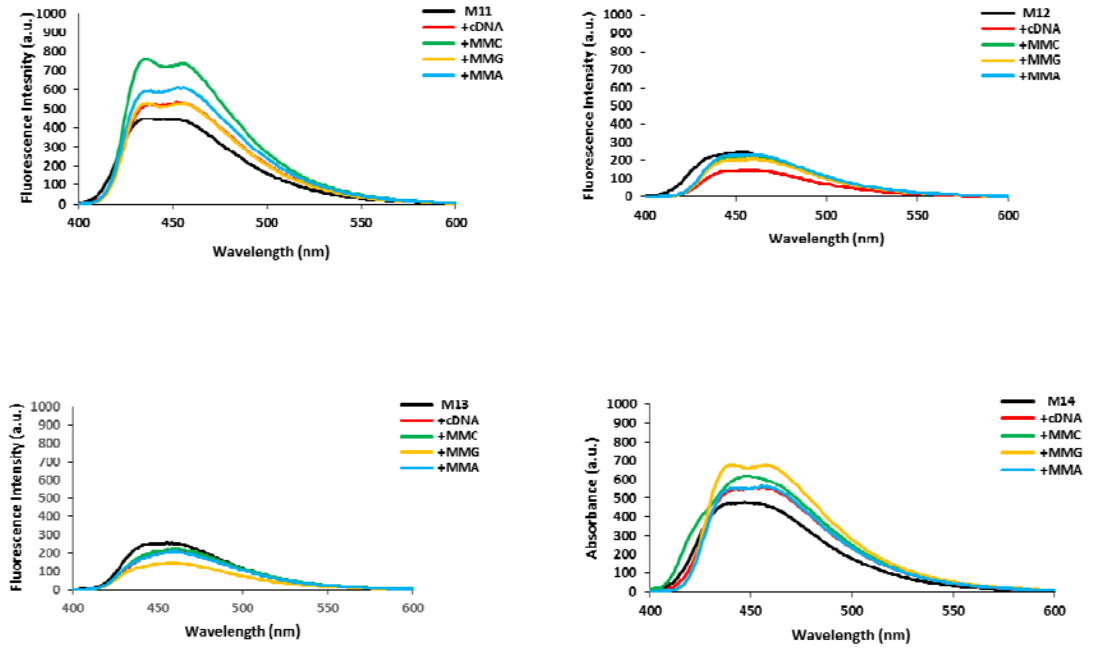
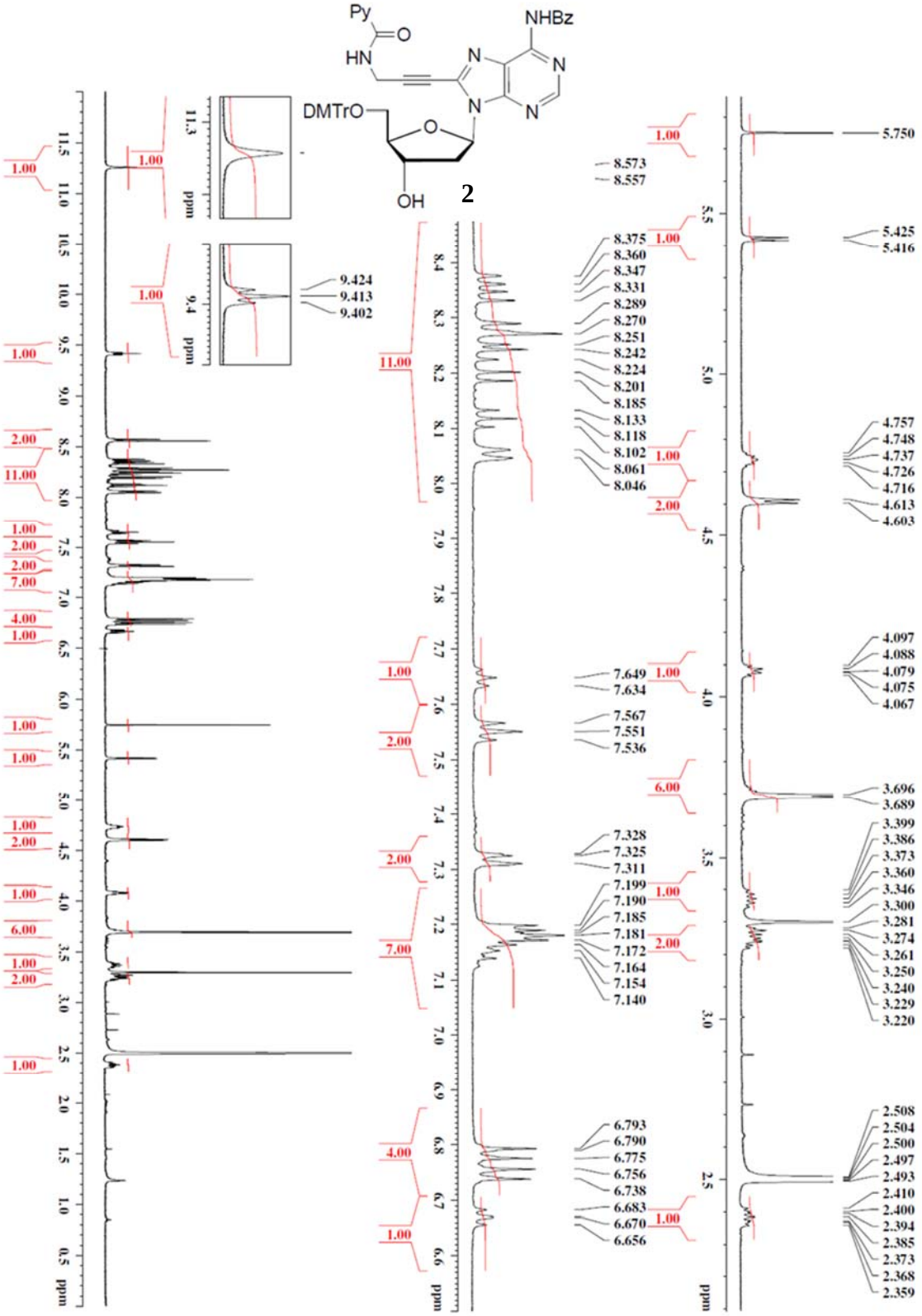


Figure S9. Steady-state fluorescence emission spectra of 13-mer **M**-modified ONs in the presence or absence of complementary or centrally mismatched DNA targets (mismatched nucleoside opposite of monomer **M** is specified) – for sequences see Table S4. Spectra were recorded in T_m buffer at T = 5 °C using each strand at 1 μM concentration, λ_{ex} = 385 nm.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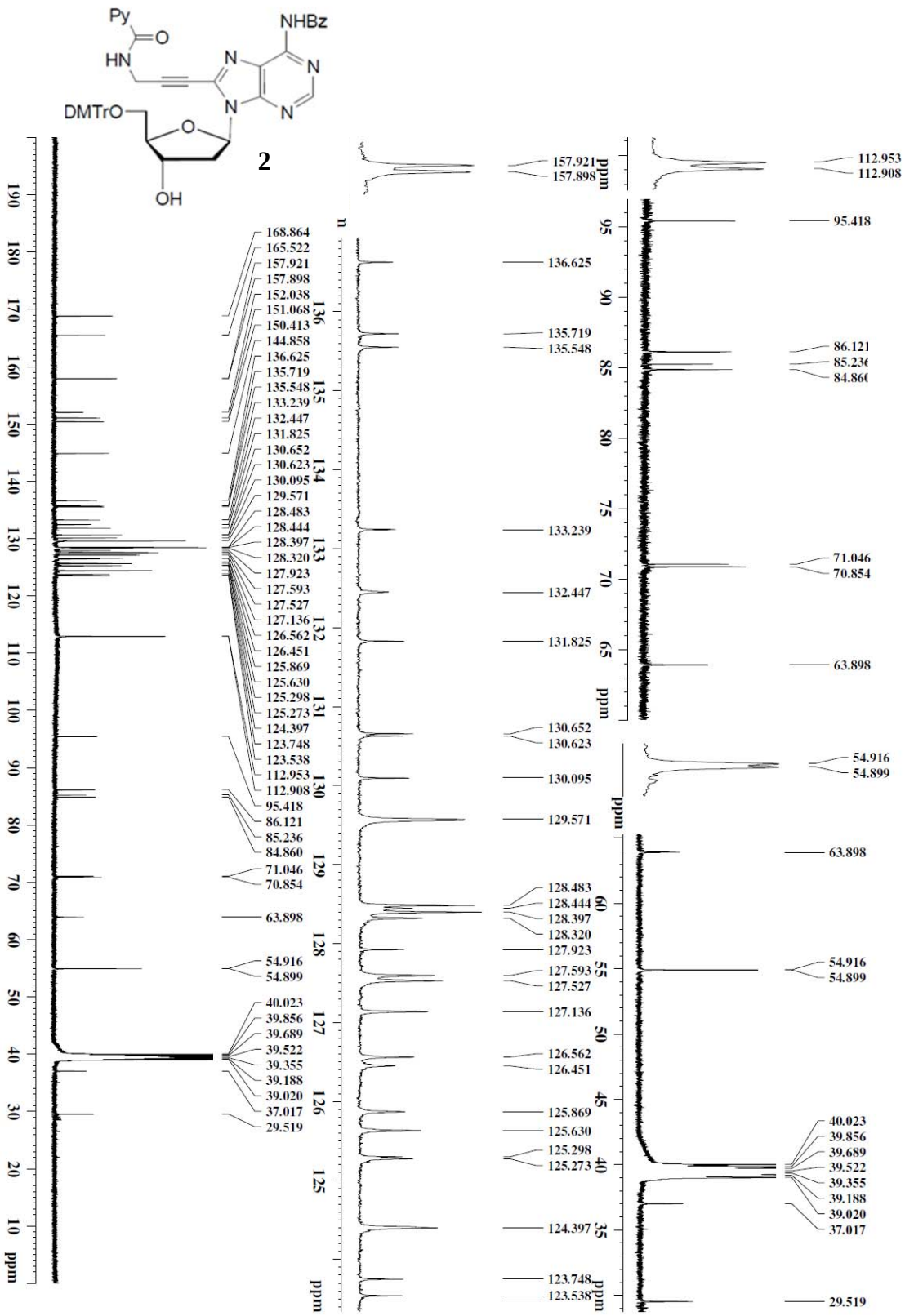
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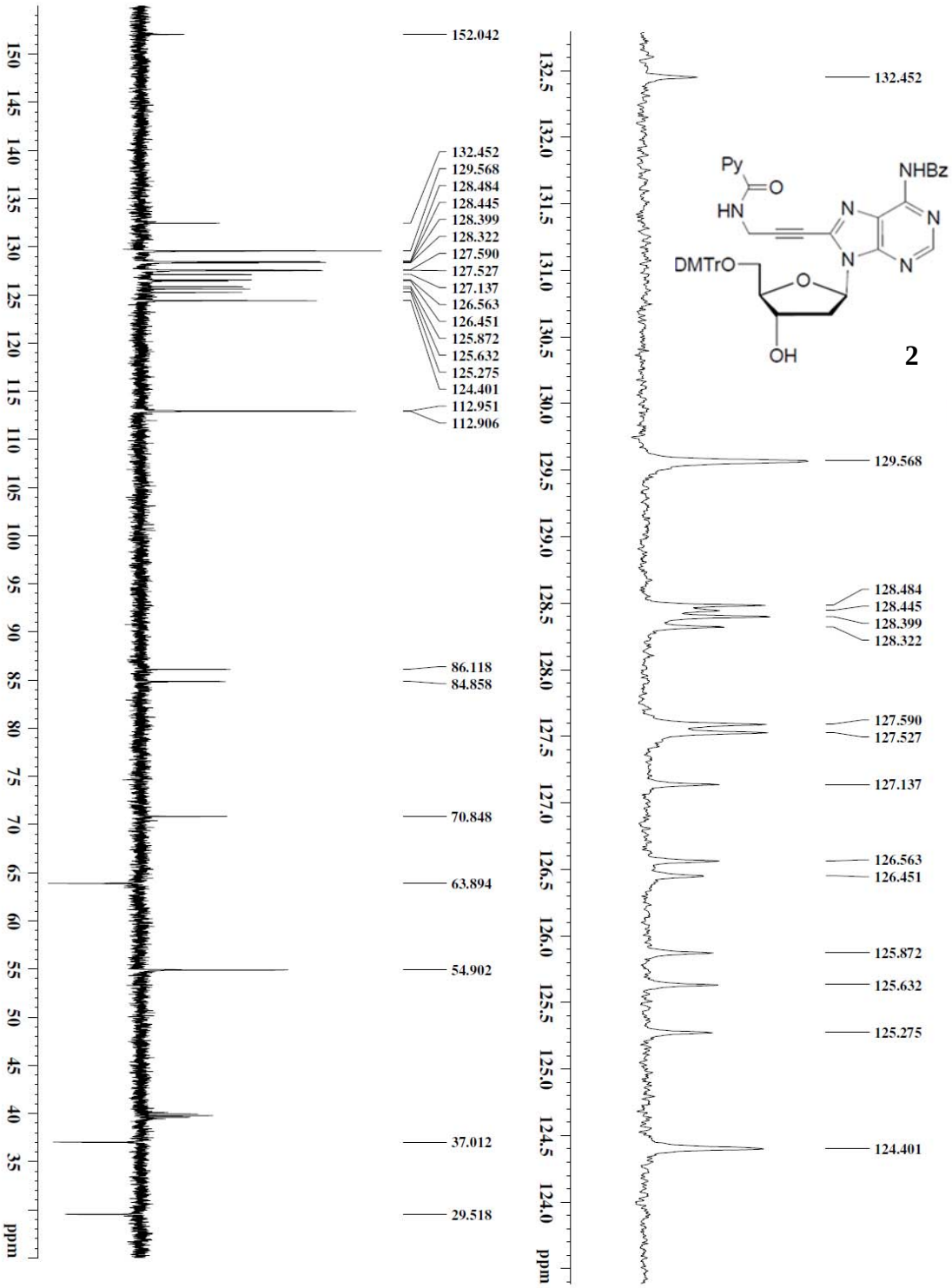
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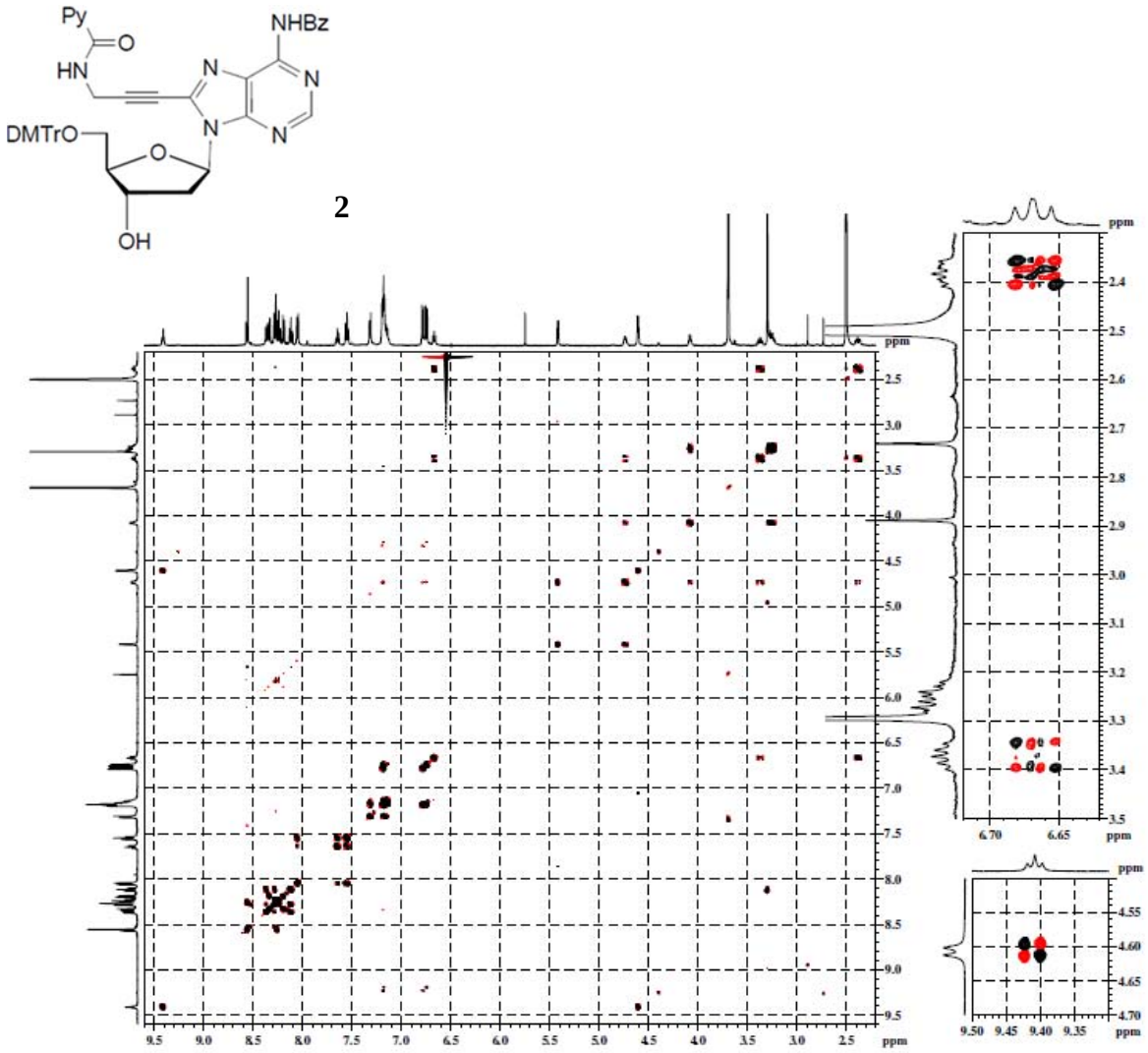
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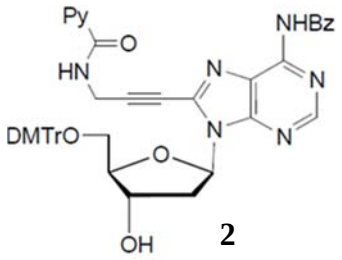
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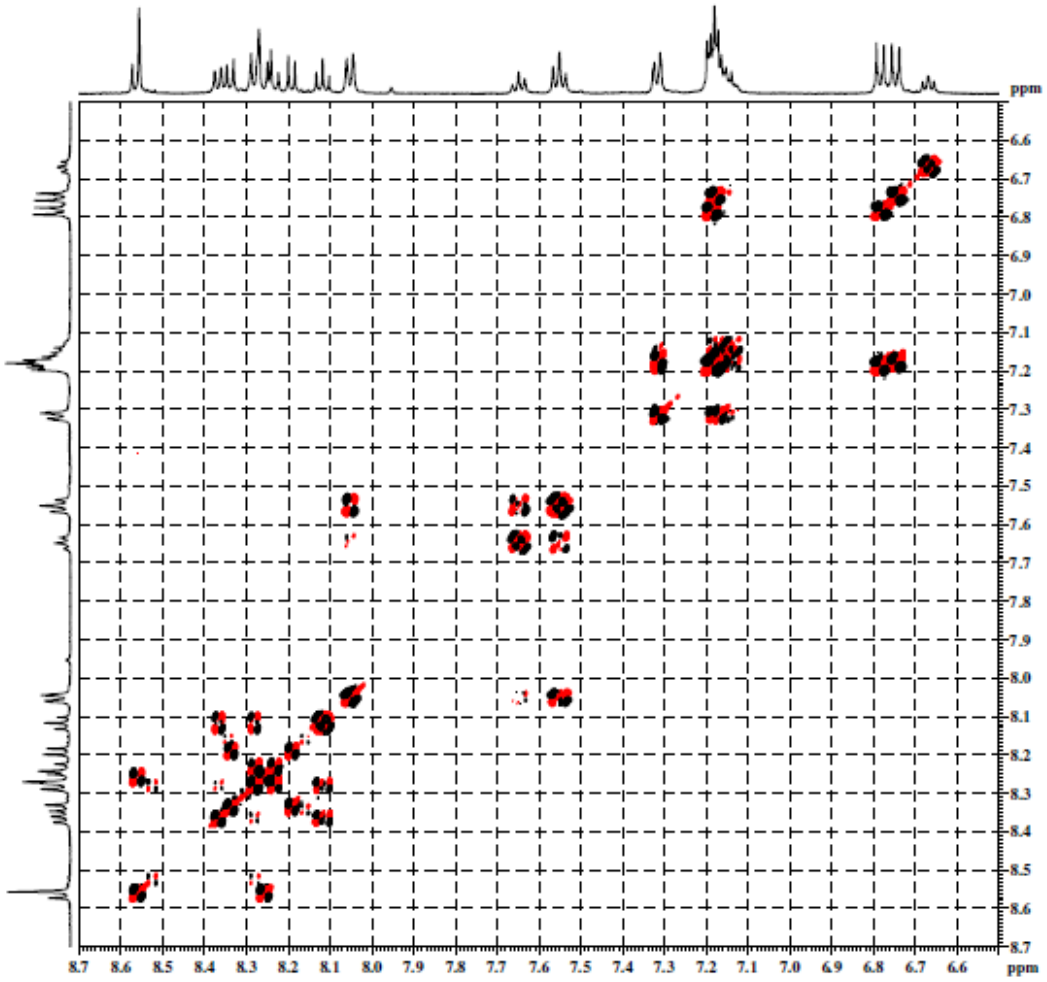
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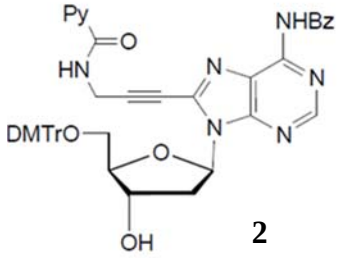
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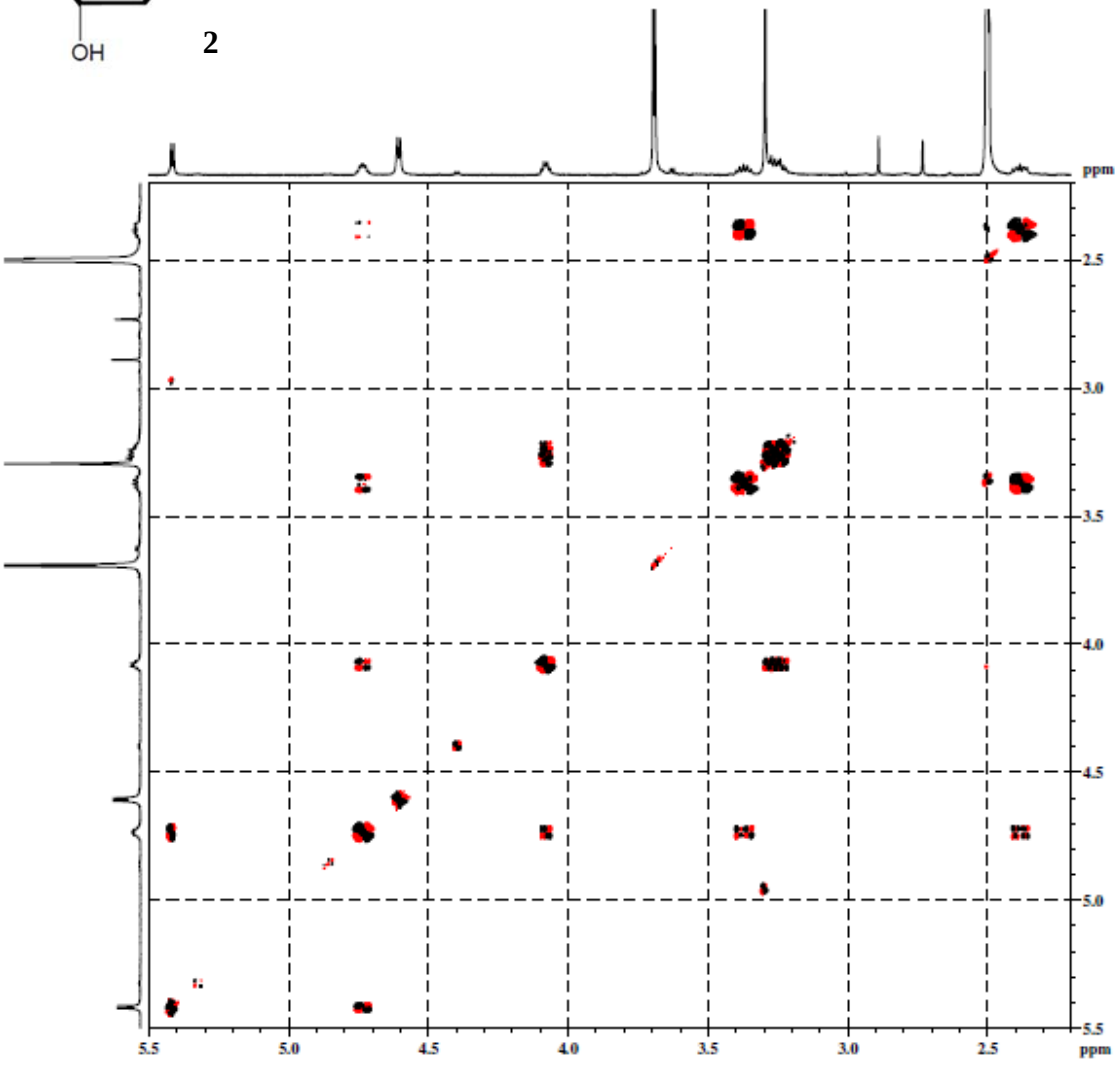
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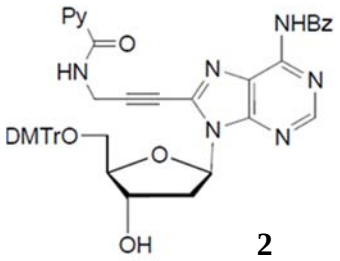
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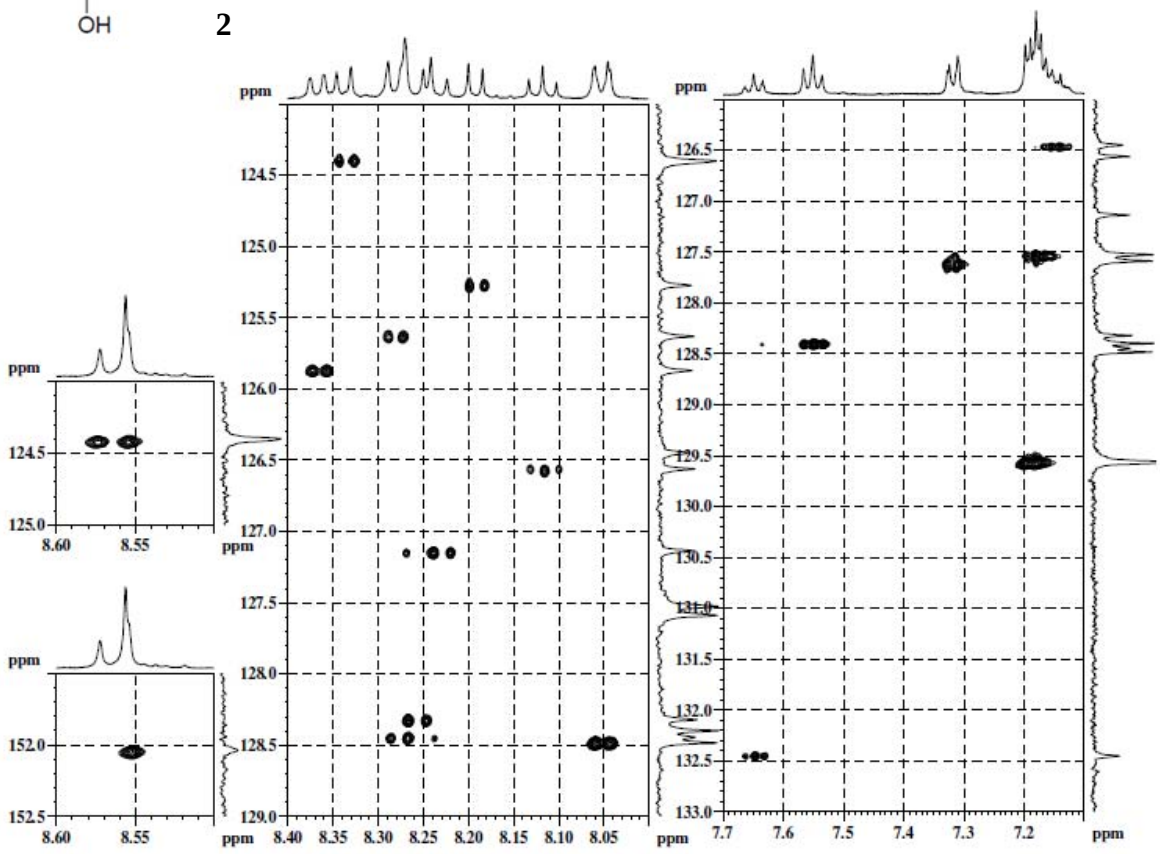
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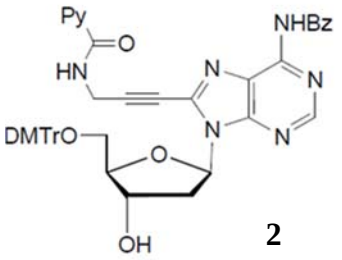
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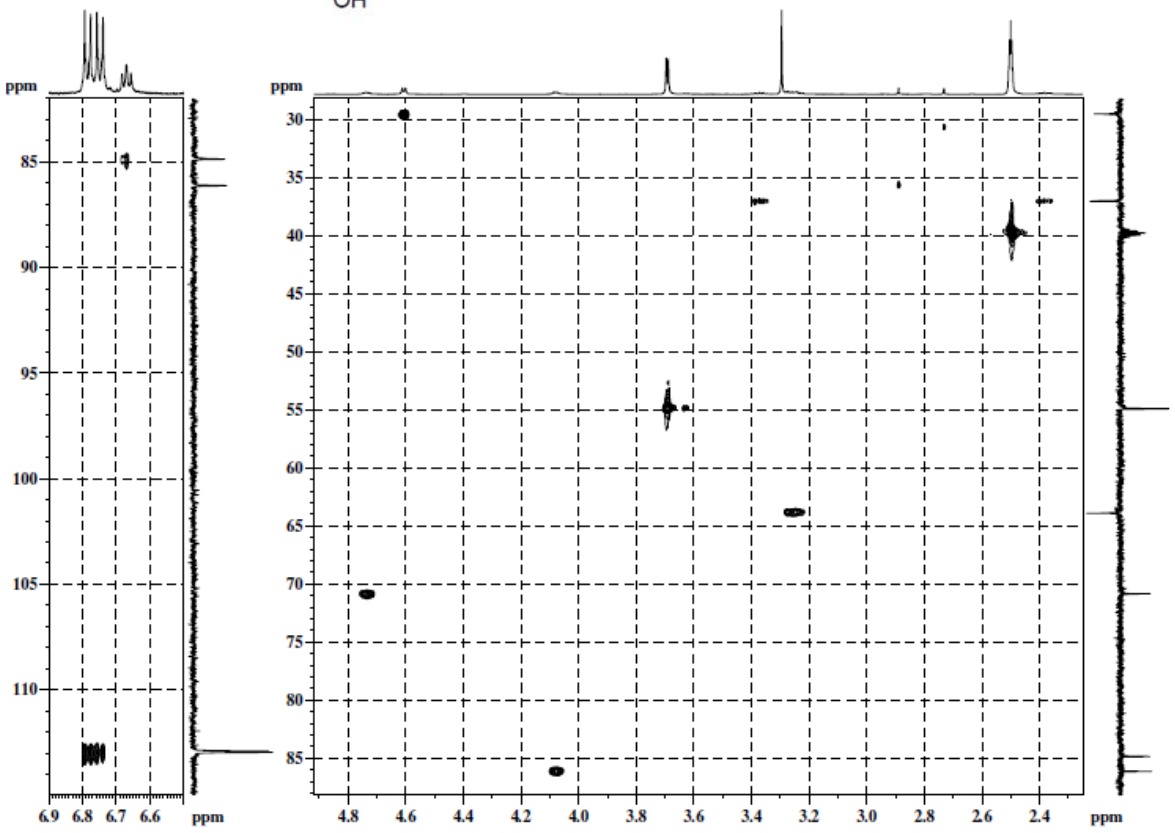
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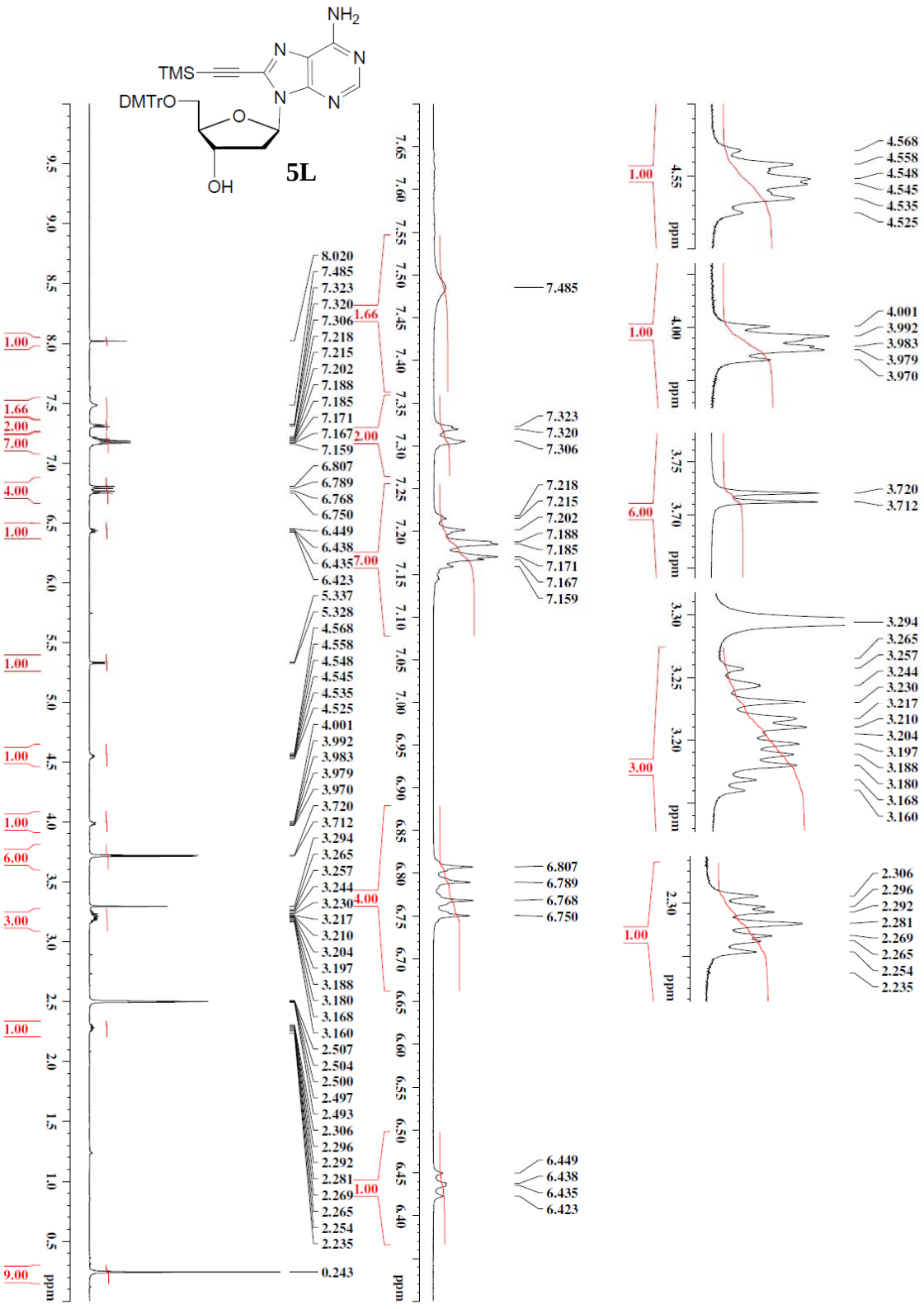
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3.294
3.265
3.257
3.244
3.230
3.217
3.210
3.204
3.197
3.188
3.180
3.168
3.160
2.507
2.504
2.500
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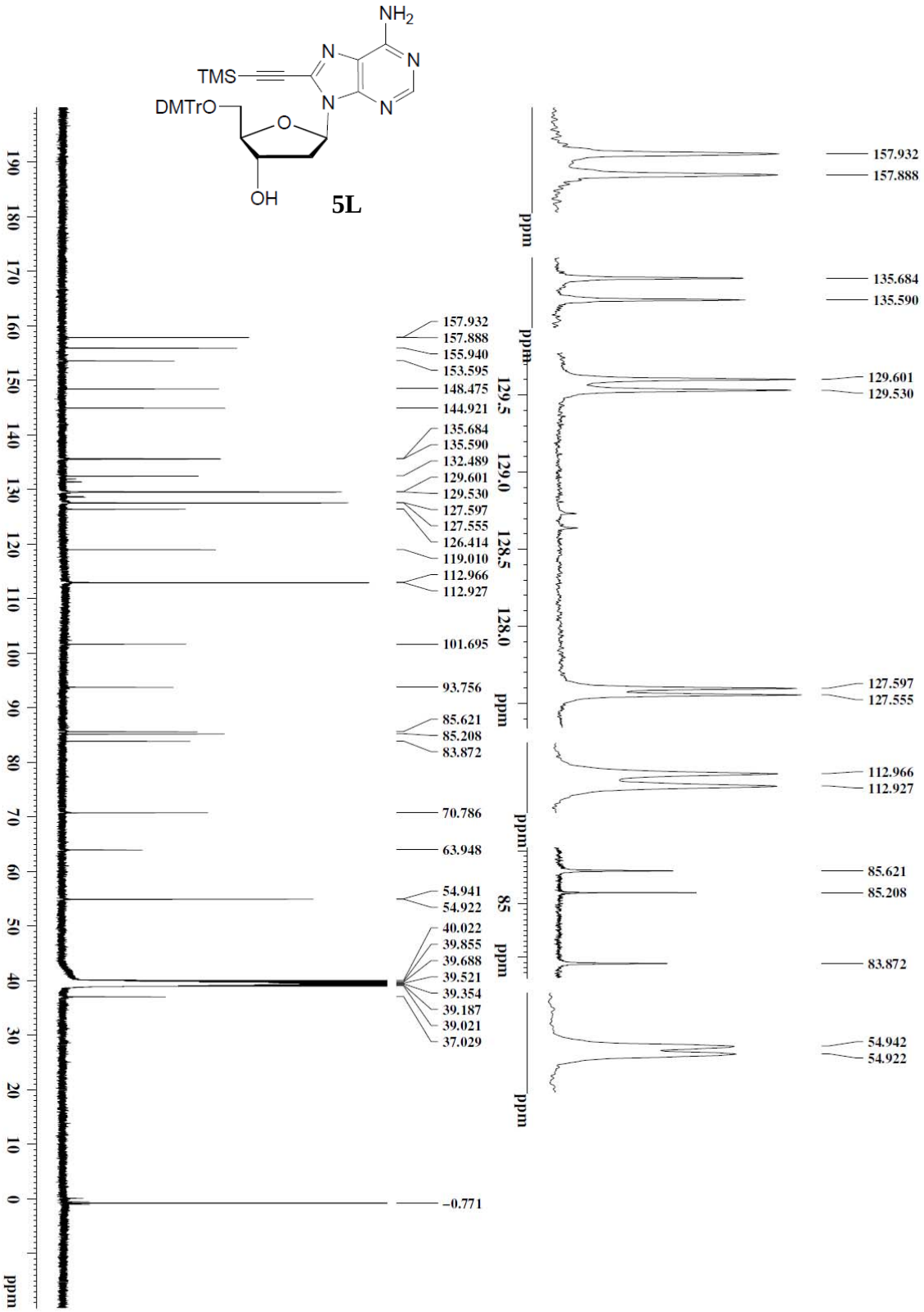
2.493
2.306
2.296
2.292
2.281
2.269
2.265
2.254
2.235
0.243
ppm


NH2
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N
N
N
TMS
DMTrO
O
OH
5L
ppm
157.932
157.888
155.940
153.595
148.475
144.921
135.684
135.590
132.489
129.601
129.530
127.597
127.555
126.414
119.010
112.966
112.927
101.695
93.756
85.621
85.208
83.872
70.786
63.948
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39.855
39.688
39.521
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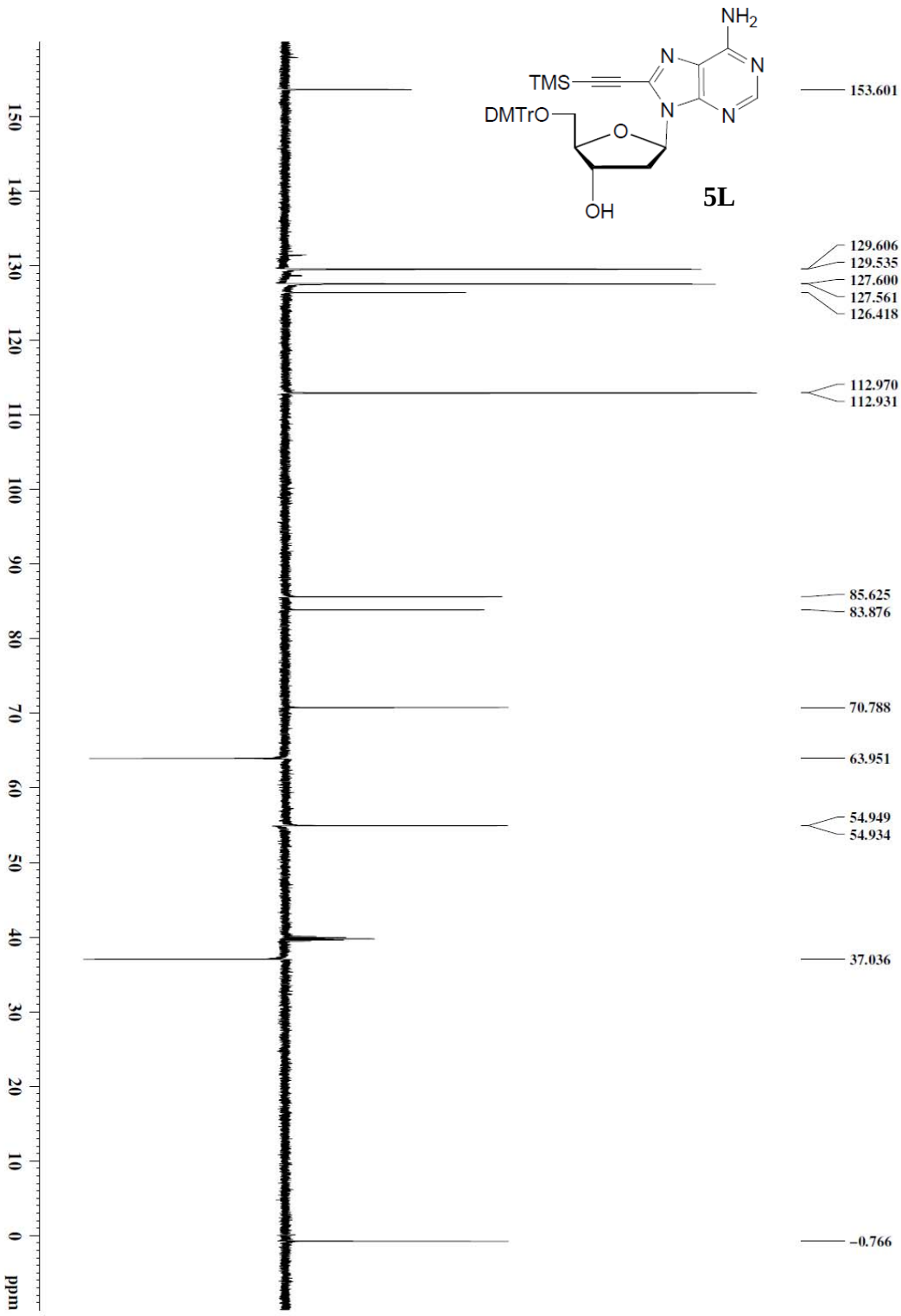
37.029
-0.771


NH2
N
N
TMS
N
N
DMTrO
O
OH
5L
153.601
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129.535
127.600
127.561
126.418
112.970
112.931
85.625
83.876
70.788
63.951
54.949
54.934
37.036
−0.766
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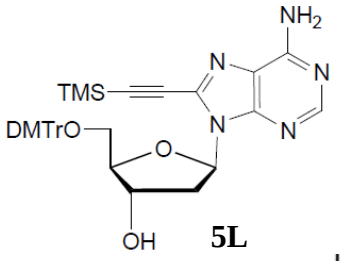
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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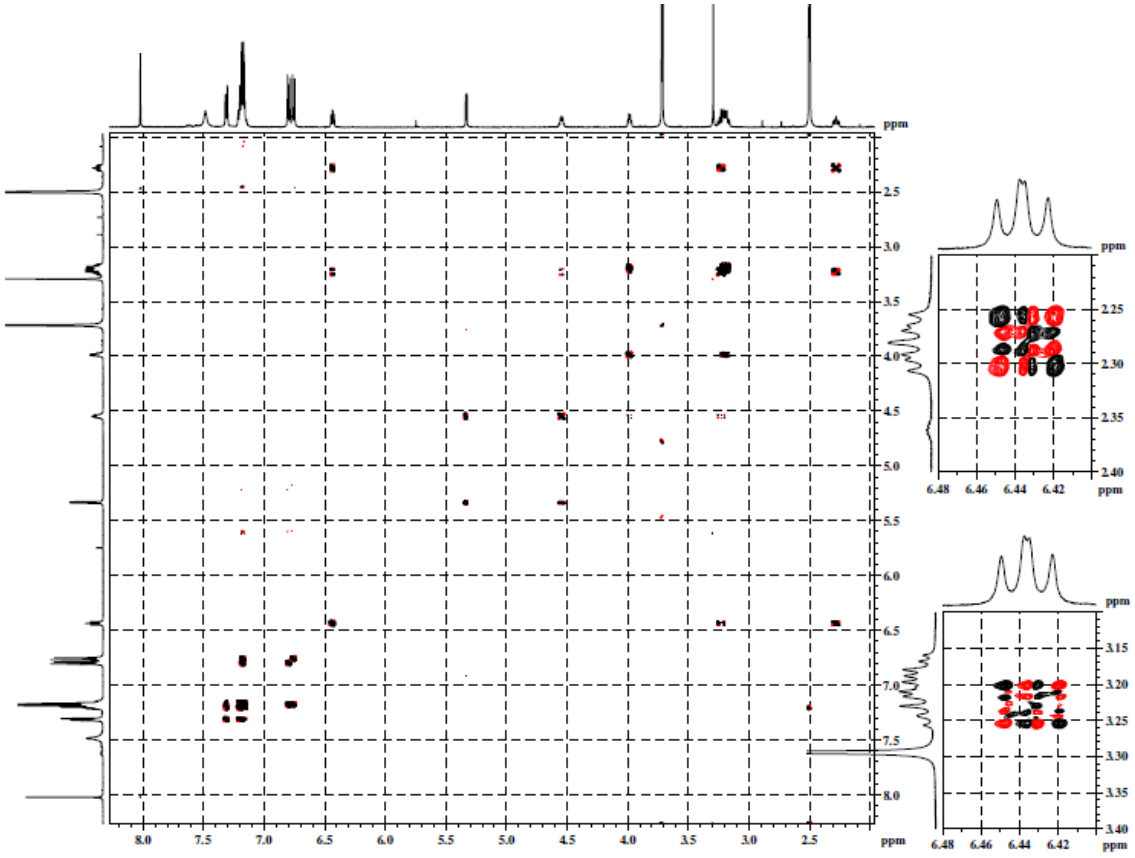
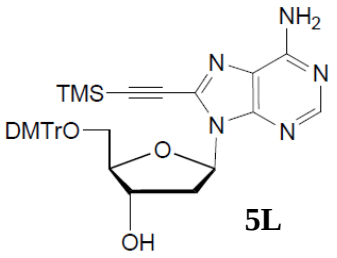
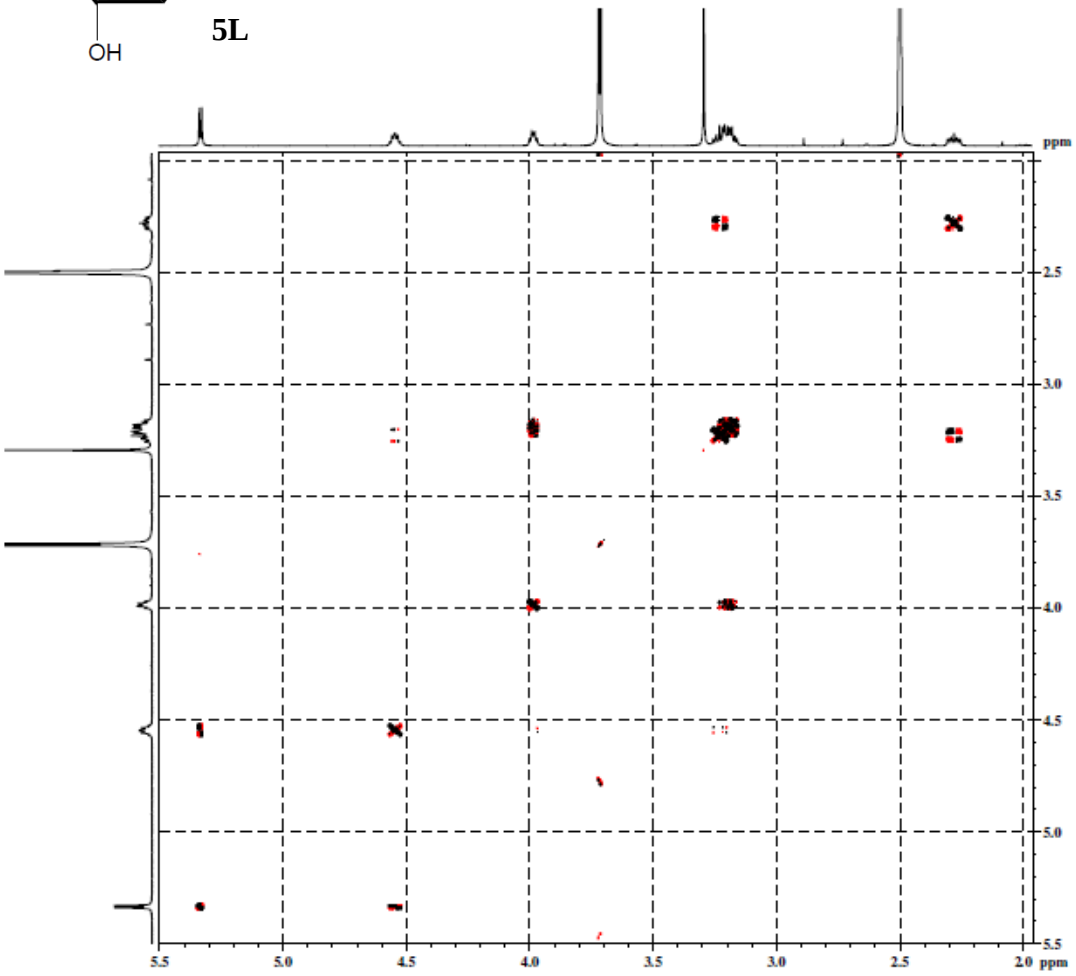
N
TMS
N
N
DMTrO
O
OH

5L


ppm
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
6.48
6.46
6.44
6.42
2.25
2.30
2.35
2.40
3.15
3.20
3.25
3.30
3.35
3.40


NH2
N
N
N
N
TMS
DMTrO
O
OH

5L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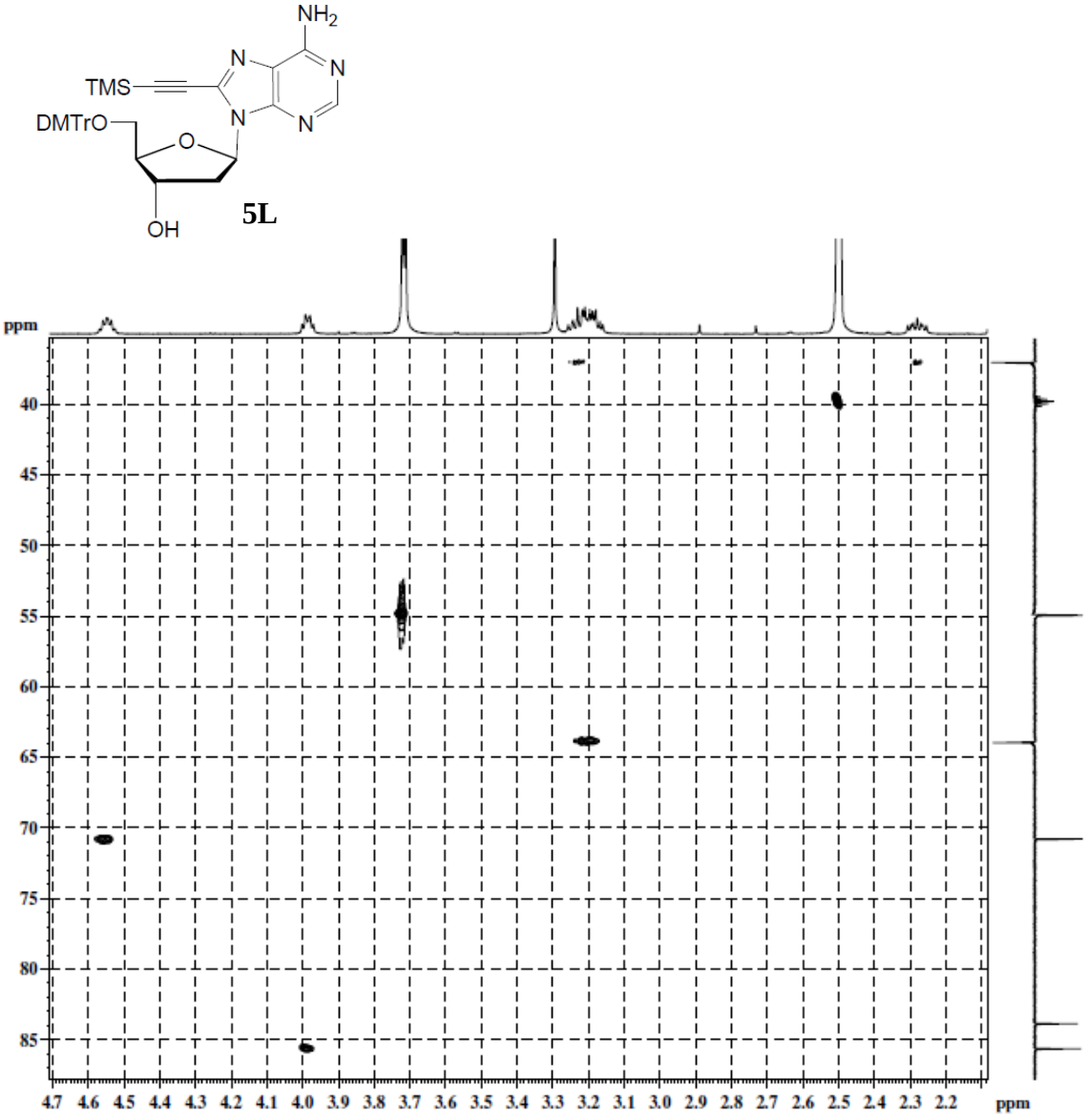
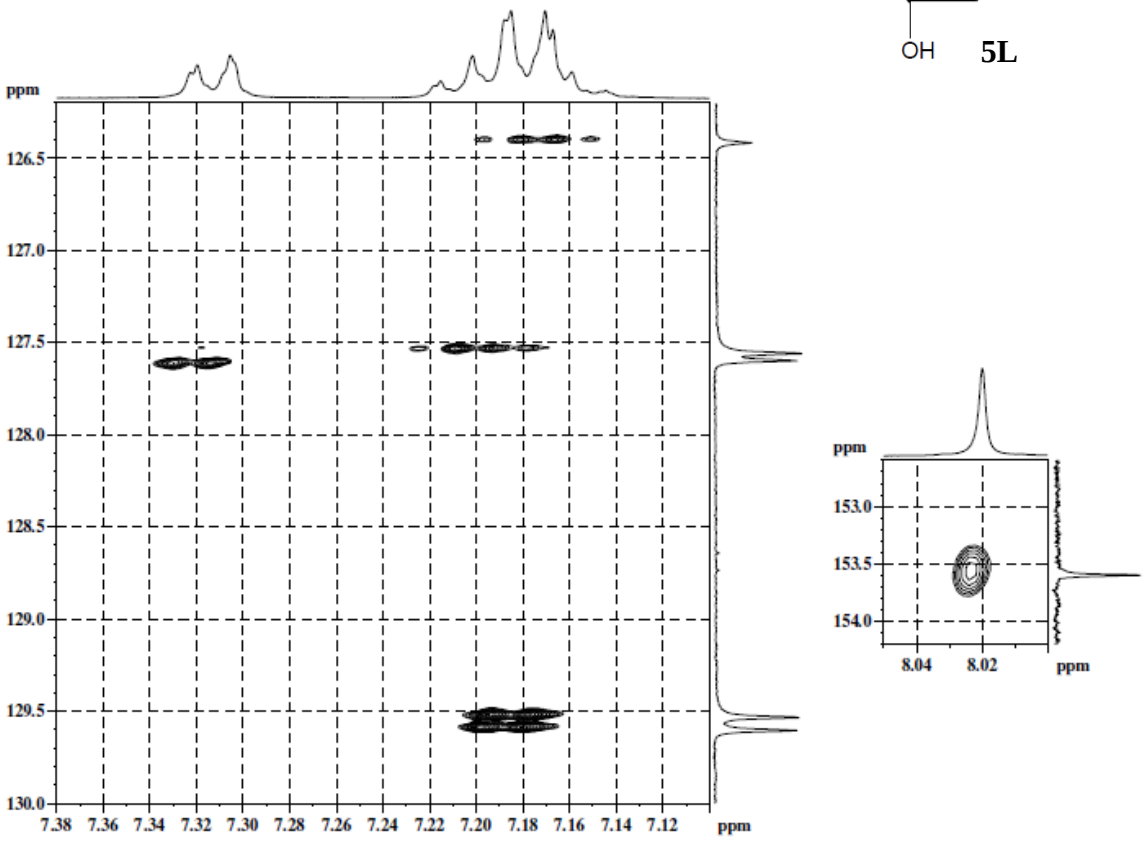
3.5
4.0
4.5
5.0
5.5
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm


NH2
N
N
TMS
N
N
DMTrO
O
OH
5L
ppm
40
45
50
55
60
65
70
75
80
85
4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2
ppm


ppm
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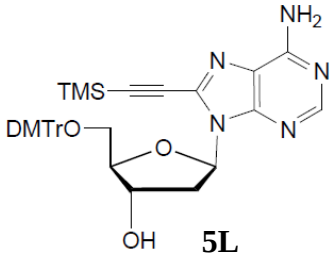
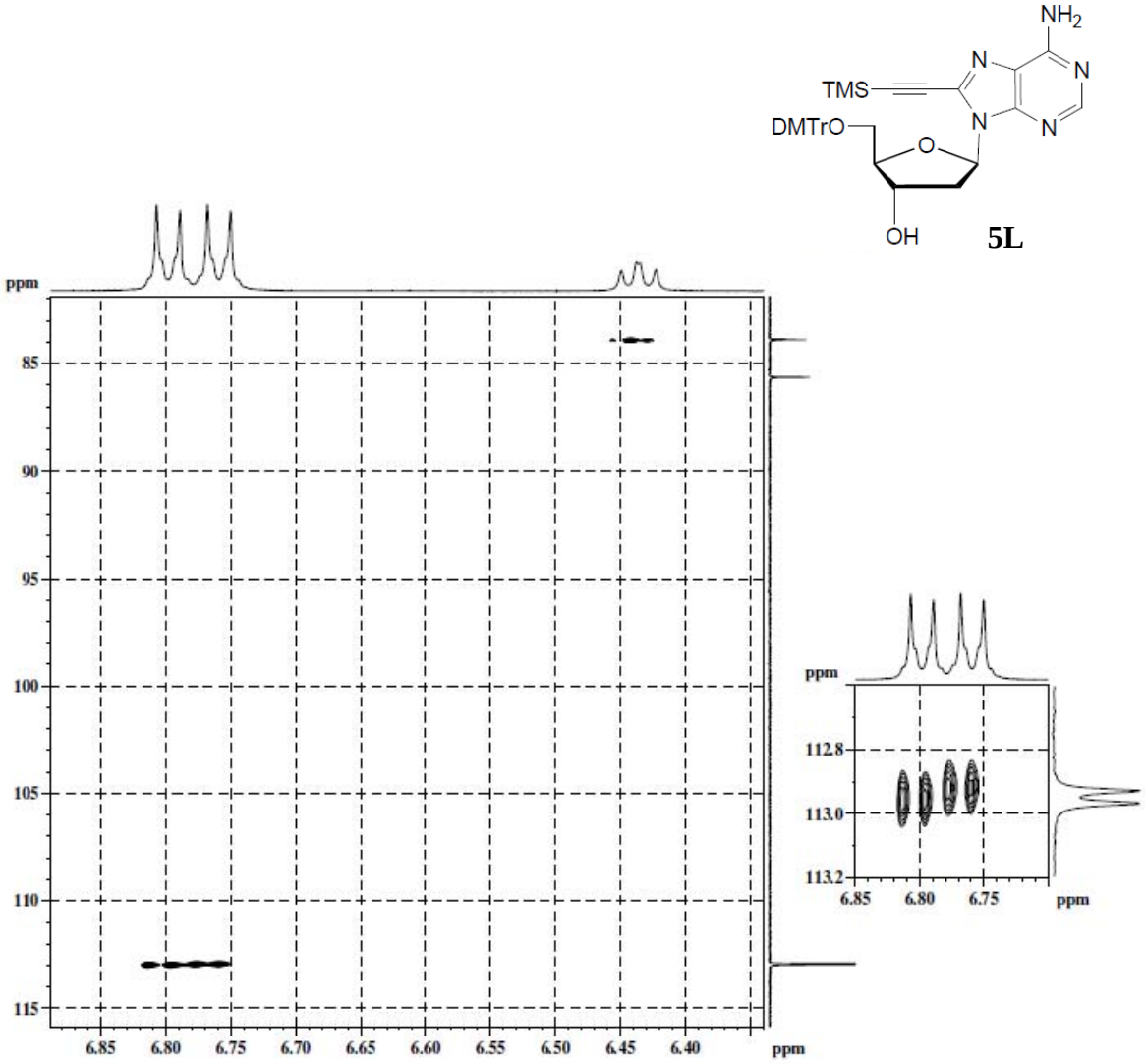
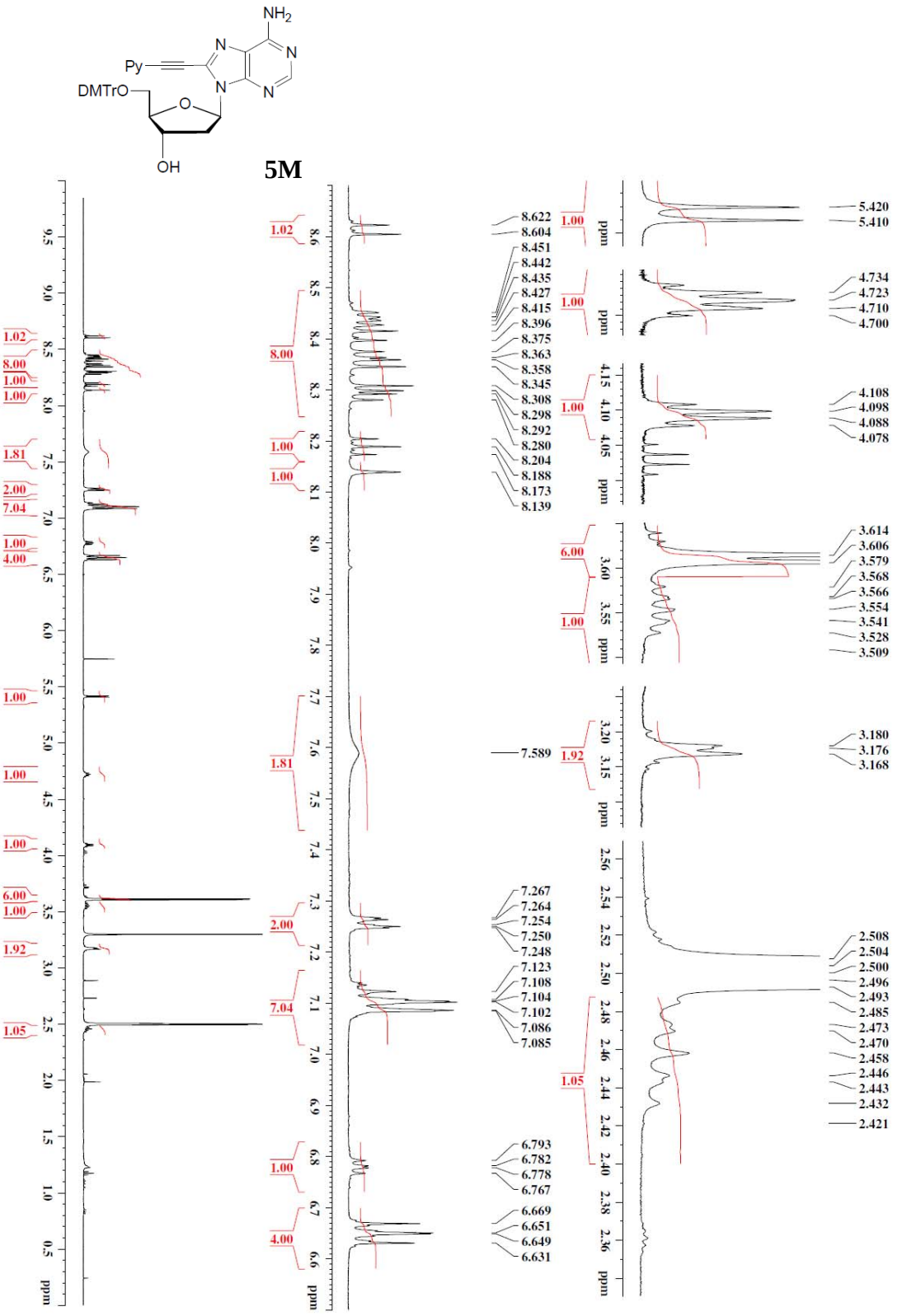
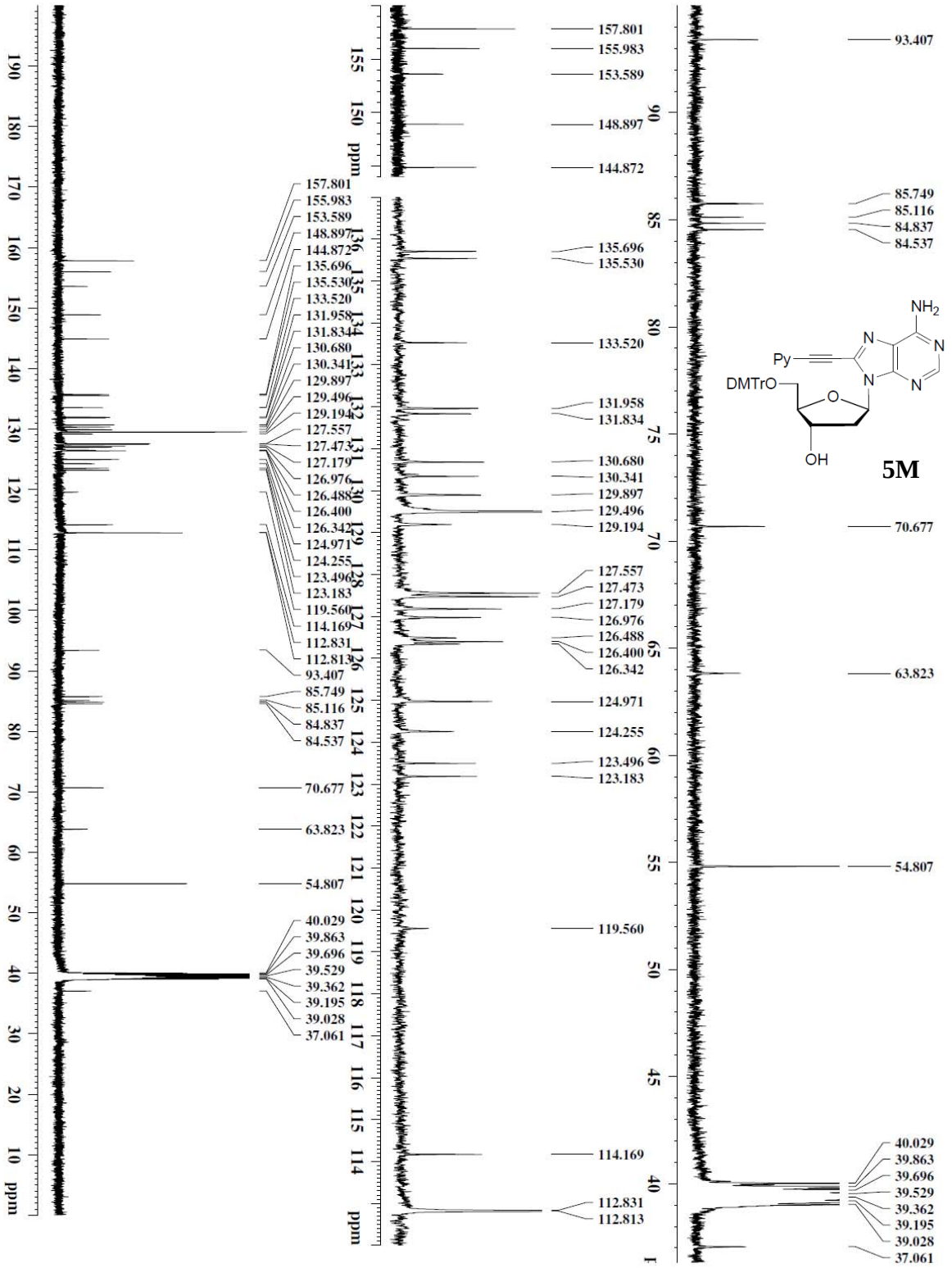
127.0
127.5
128.0
128.5
129.0
129.5
130.0
7.38 7.36 7.34 7.32 7.30 7.28 7.26 7.24 7.22 7.20 7.18 7.16 7.14 7.12
ppm
ppm
153.0
153.5
154.0
8.04 8.02
ppm


NH2
N
N
TMS
N
N
DMTrO
O
OH

5L


NH2
N
N
TMS
N
DMTrO
N
O
OH
5L
ppm
85
90
95
100
105
110
115
6.85
6.80
6.75
6.70
6.65
6.60
6.55
6.50
6.45
6.40
ppm
ppm
112.8
113.0
113.2
6.85
6.80
6.75
ppm


NH2
N
N
N
N
Py
DMTrO
O
OH
5M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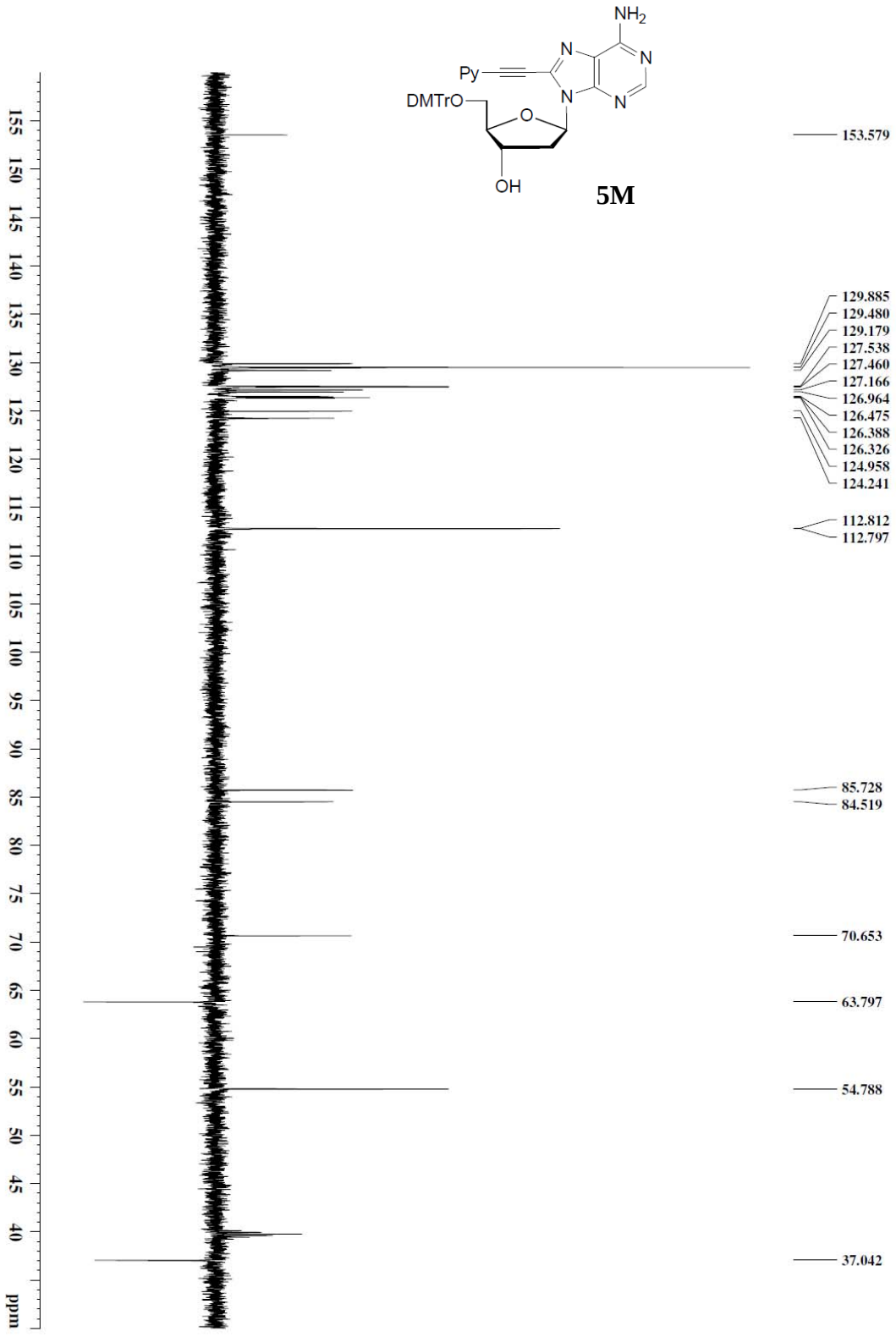
148.897
144.872
135.696
135.530
133.520
131.958
131.834
130.680
130.341
129.897
129.496
129.194
127.557
127.473
127.179
126.976
126.488
126.400
126.342
124.971
124.255
123.496
123.183
119.560
114.169
112.831
112.813
93.407
85.749
85.116
84.837
84.537
70.677
63.823
54.807
40.029
39.863
39.696
39.529
39.362
39.195
39.028
37.061
NH2
N
N
N
N
Py
DMTrO
O
OH
5M


NH2
N
N
Py
N
N
DMTrO
O
OH
5M
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129.480
129.179
127.538
127.460
127.166
126.964
126.475
126.388
126.326
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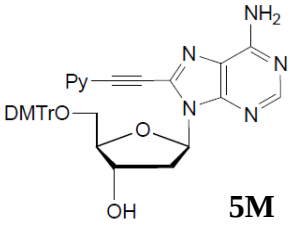
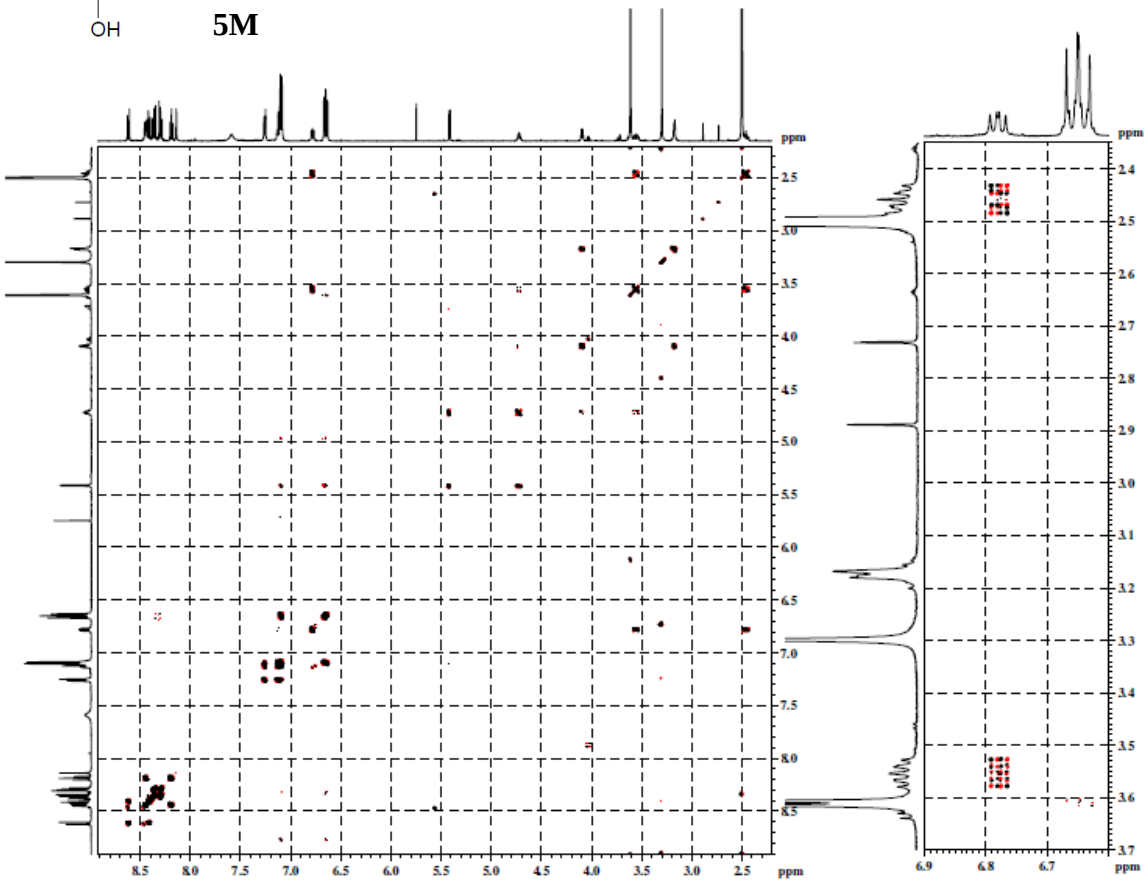
124.241
112.812
112.797
85.728
84.519
70.653
63.797
54.788
37.042
ppm


NH2
N
N
Py
N
N
DMTrO
O
OH

5M


ppm
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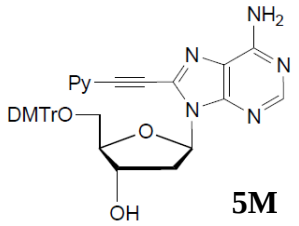
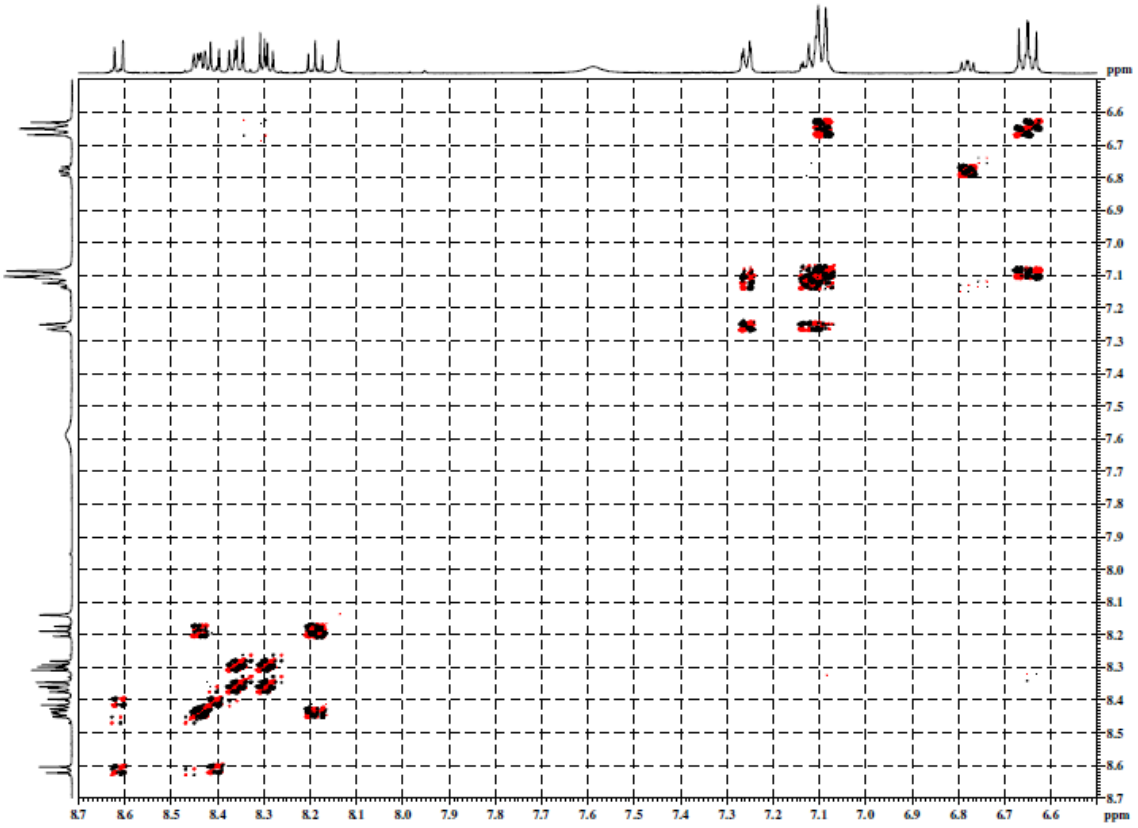
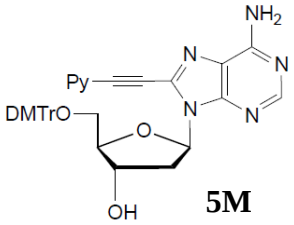
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
8.5
ppm
2.4
2.5
2.6
2.7
2.8
2.9
3.0
3.1
3.2
3.3
3.4
3.5
3.6
3.7
6.9
6.8
6.7
ppm


NH2
N
N
N
N
Py
DMTrO
O
OH

5M


ppm
6.6
6.7
6.8
6.9
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
8.4
8.5
8.6
8.7
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 ppm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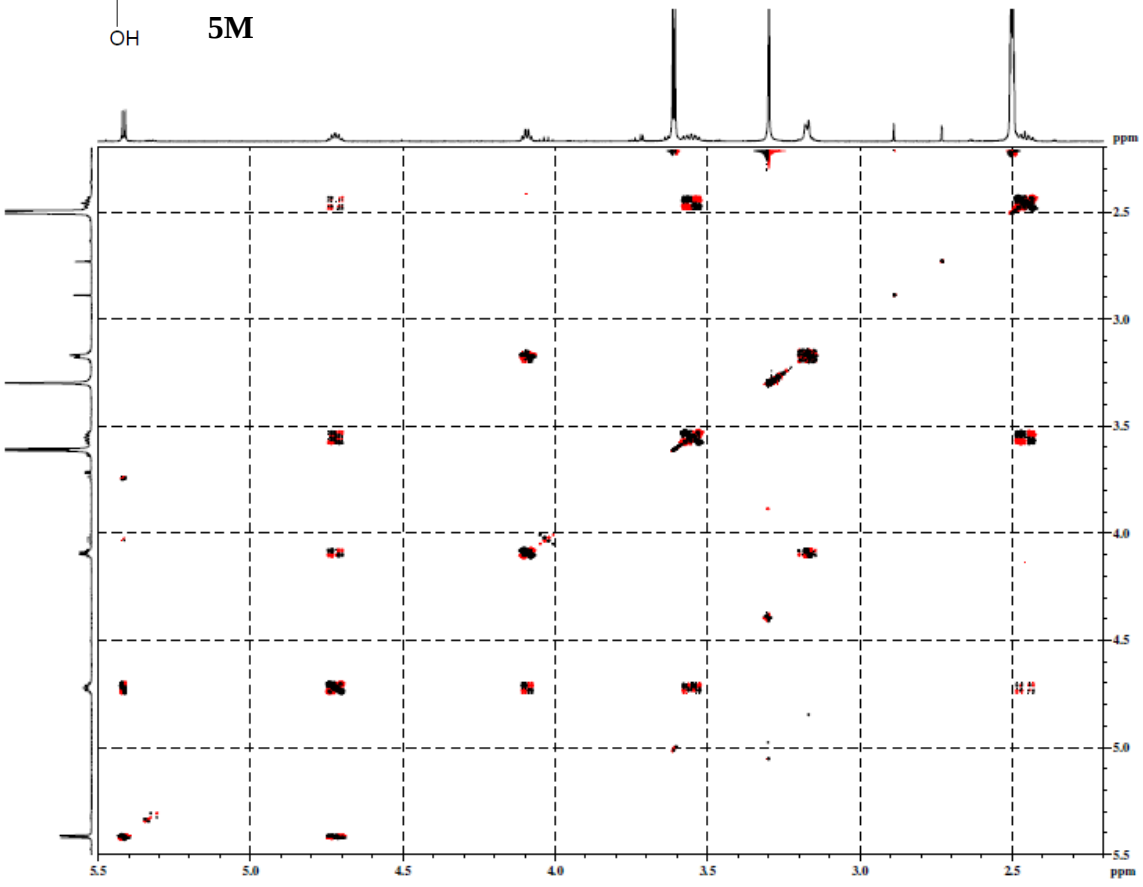
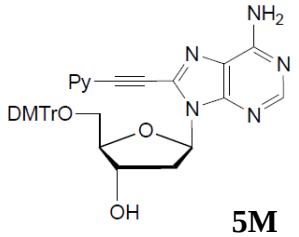
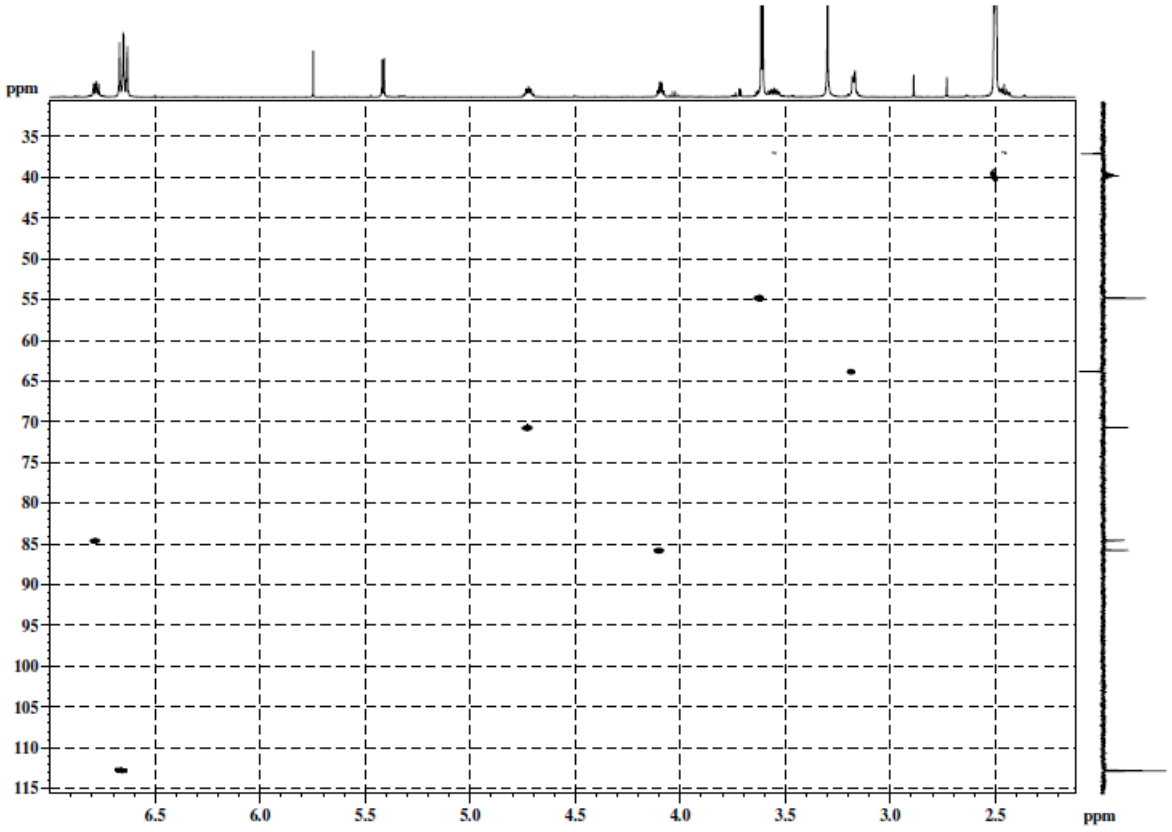
N
N
Py
N
N
DMTrO
O
OH

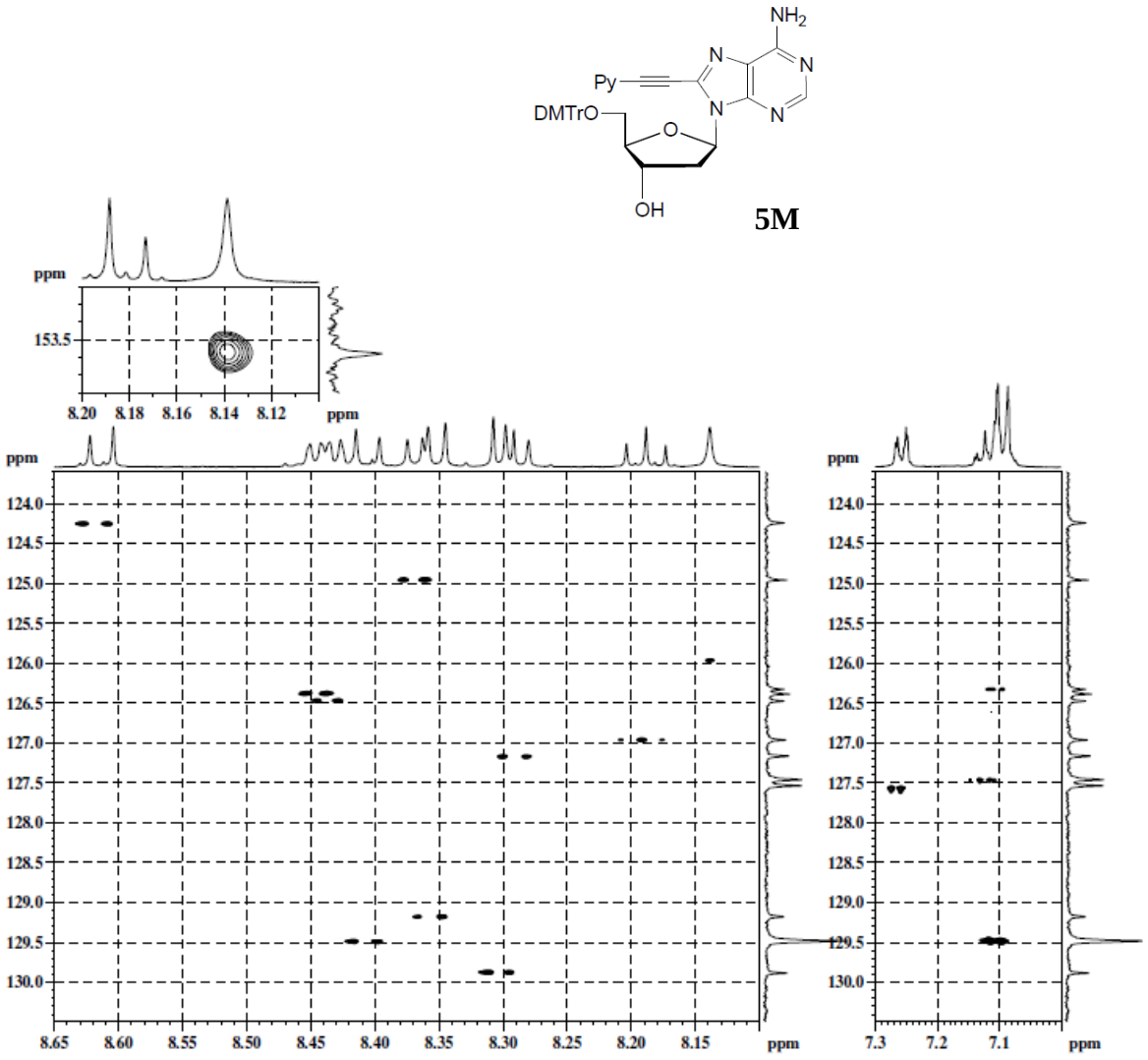
5M

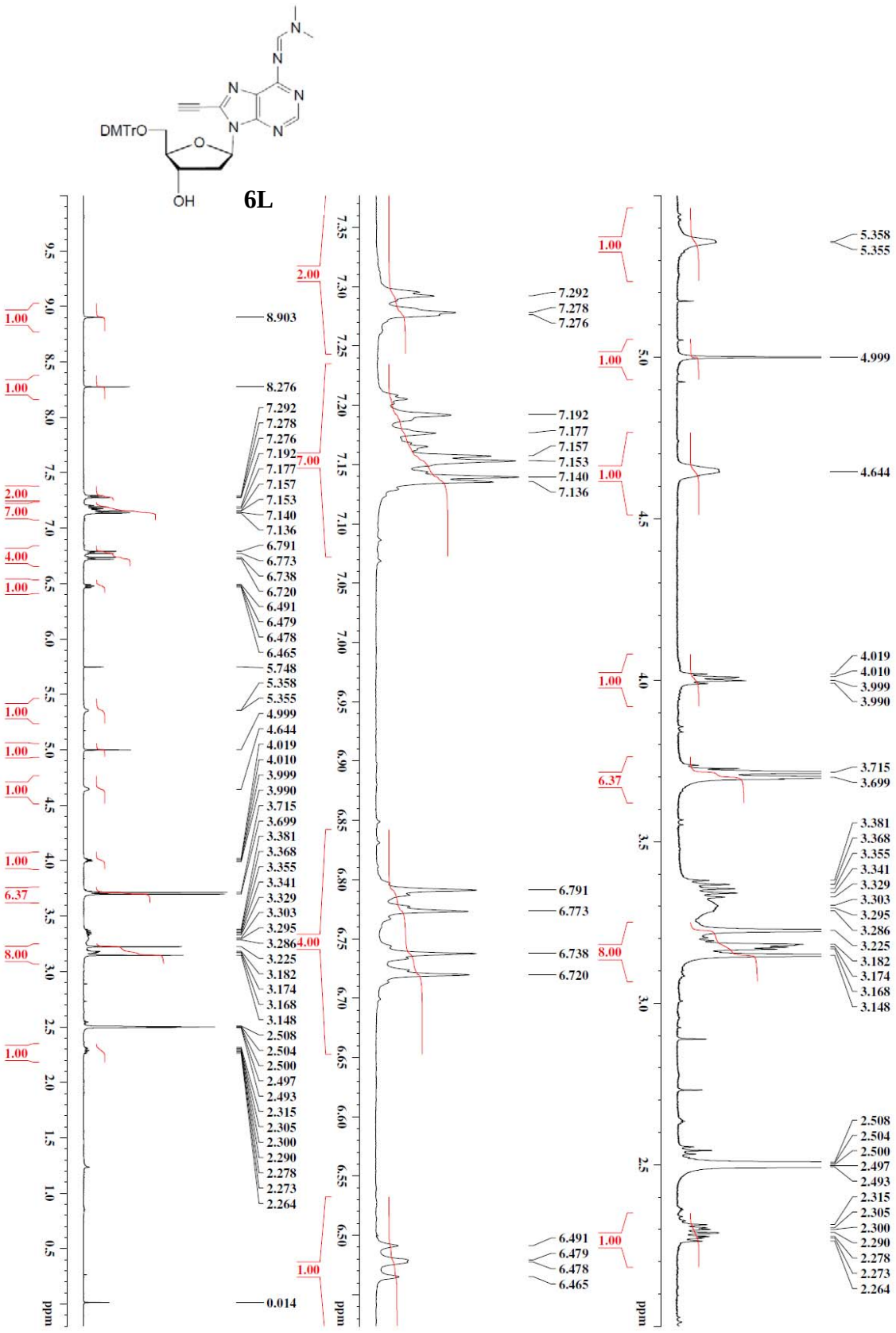

ppm
2.5
3.0
3.5
4.0
4.5
5.0
5.5
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm

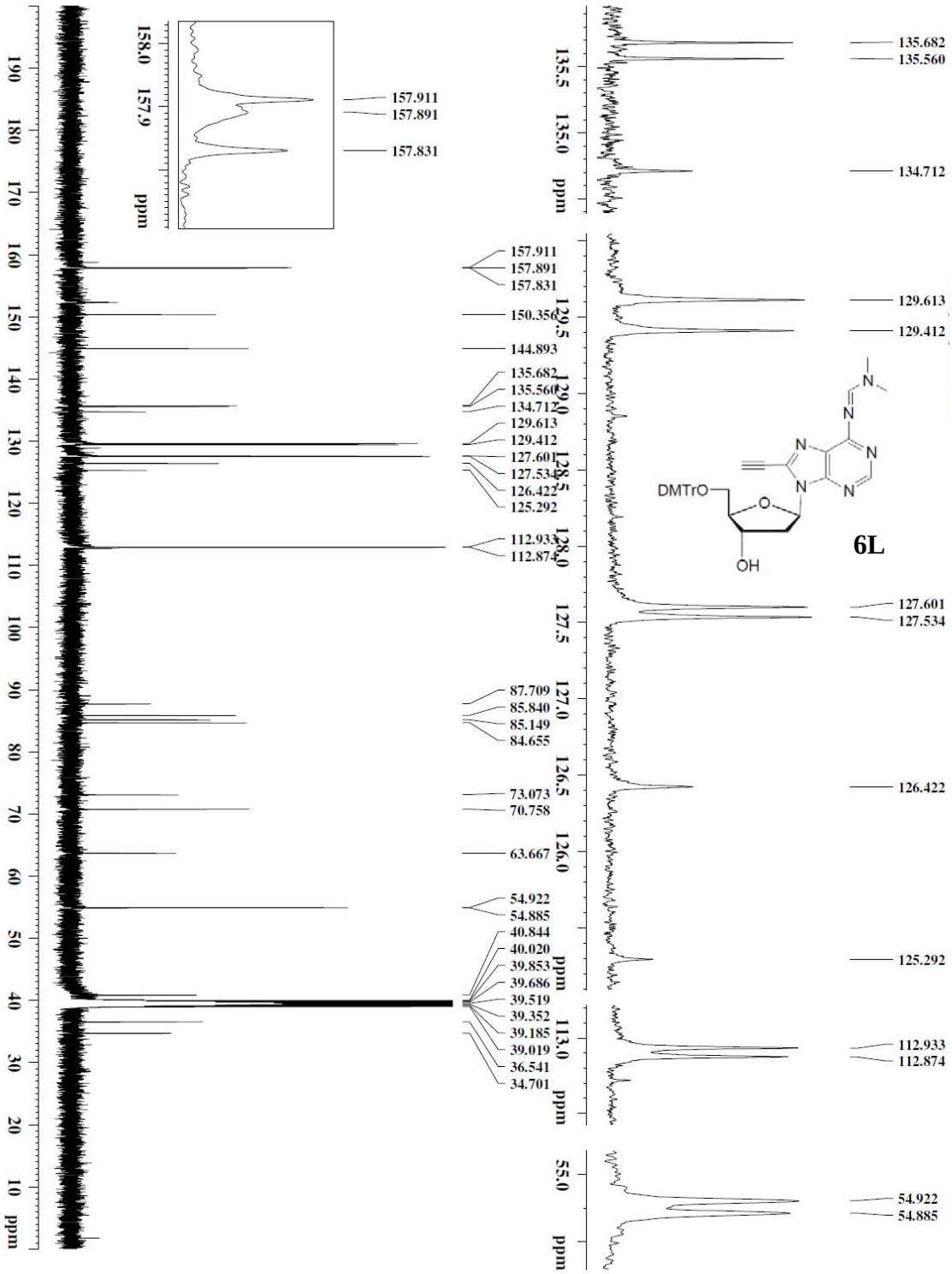

NH2
N
N
Py
N
DMTrO
O
N
OH

5M


ppm
35
40
45
50
55
60
65
70
75
80
85
90
95
100
105
110
115
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm


NH2
N
N
N
N
Py
DMTrO
O
OH
5M
ppm
153.5
8.20 8.18 8.16 8.14 8.12
ppm
ppm
124.0 124.5 125.0 125.5 126.0 126.5 127.0 127.5 128.0 128.5 129.0 129.5 130.0
8.65 8.60 8.55 8.50 8.45 8.40 8.35 8.30 8.25 8.20 8.15
ppm
ppm
124.0 124.5 125.0 125.5 126.0 126.5 127.0 127.5 128.0 128.5 129.0 129.5 130.0
7.3 7.2 7.1
ppm


DMTrO
OH
6L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135.682
135.560
134.712
129.613
129.412
127.601
127.534
126.422
125.292
112.933
112.874
87.709
85.840
85.149
84.655
73.073
70.758
63.667
54.922
54.885
40.844
40.020
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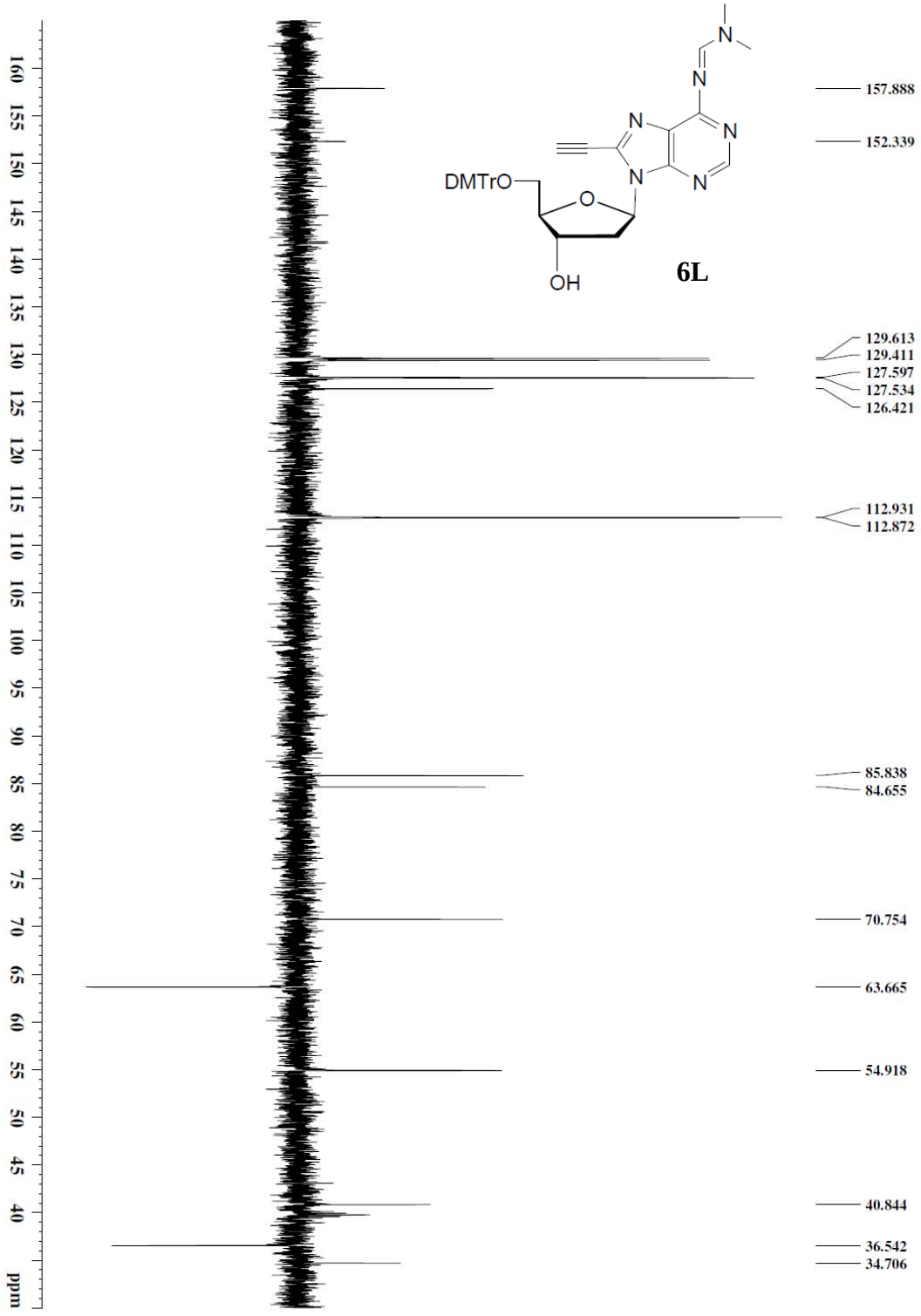
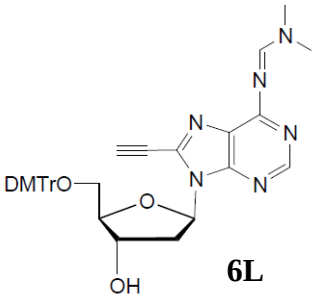
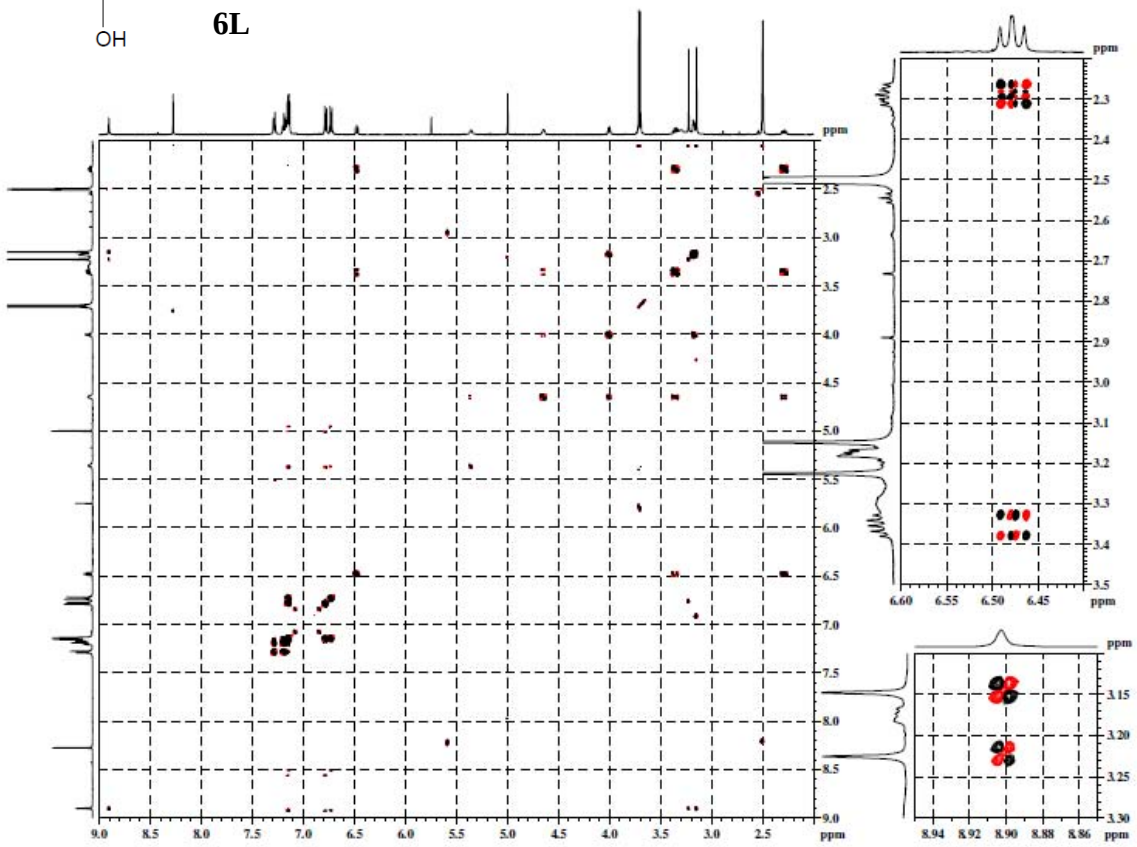
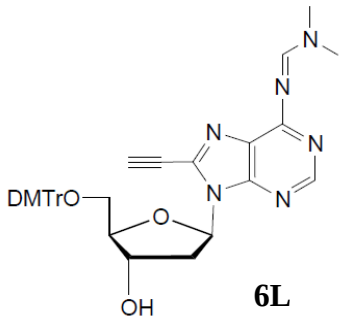
39.686
39.519
39.352
39.185
39.019
36.541
34.701
DMTrO
OH
6L


157.888
152.339
129.613
129.411
127.597
127.534
126.421
112.931
112.872
85.838
84.655
70.754
63.665
54.918
40.844
36.542
34.706
DMTrO
O
OH
N
N
N
N
N
6L
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
ppm

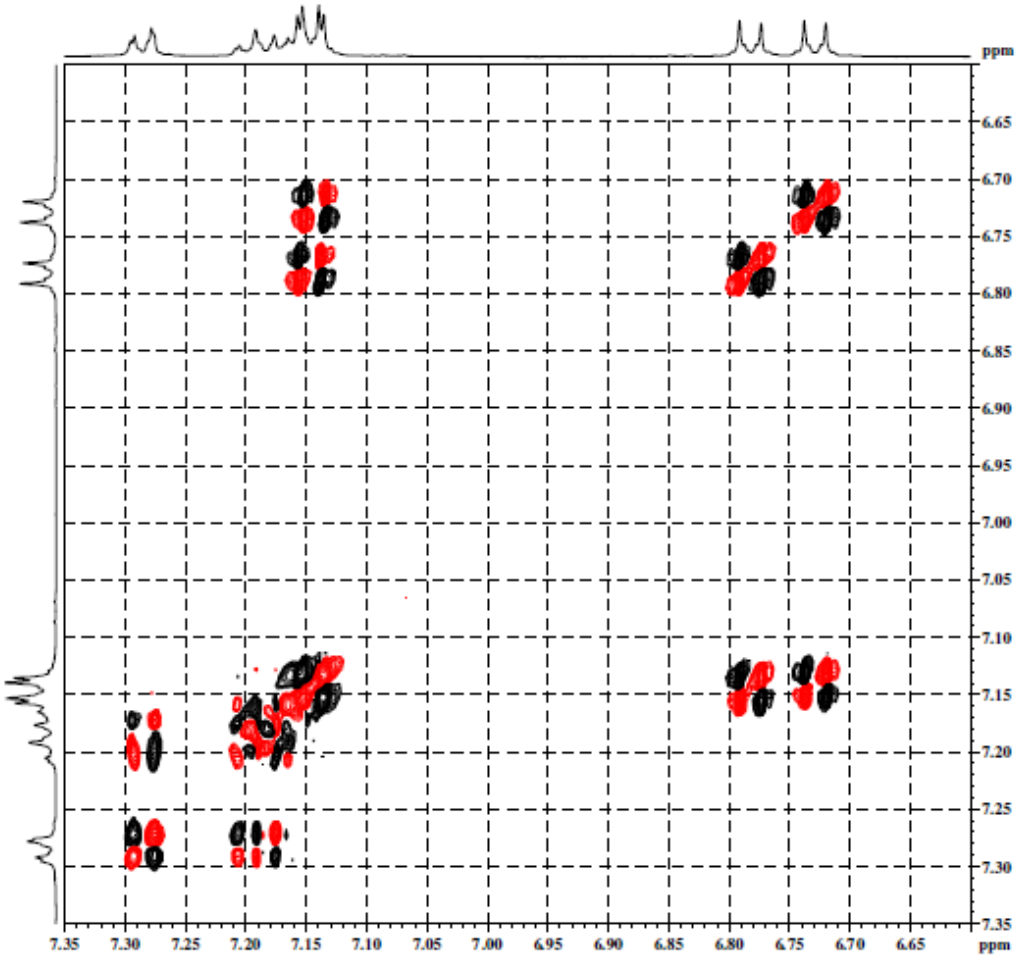

DMTrO
O
OH
N
N
N
N
N
N

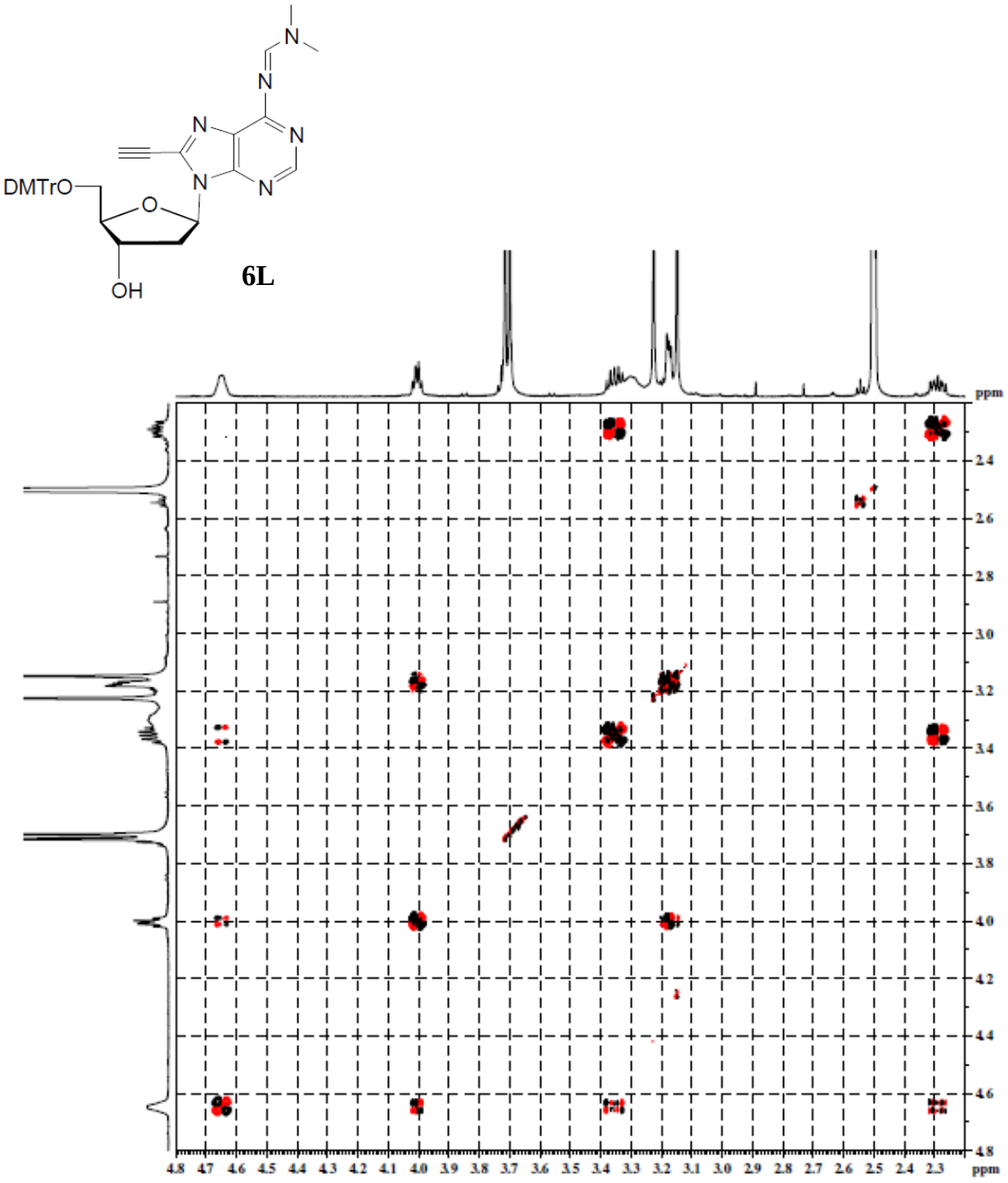
6L

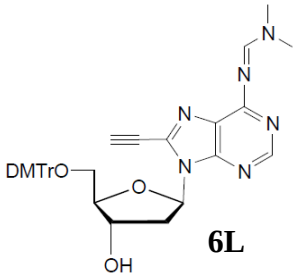

ppm
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5
2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0 8.5 9.0
6.60 6.55 6.50 6.45
2.3 2.4 2.5 2.6 2.7 2.8 2.9 3.0 3.1 3.2 3.3 3.4 3.5
8.94 8.92 8.90 8.88 8.86
3.15 3.20 3.25 3.30


DMTrO
O
N
N
N
N
N
N
OH

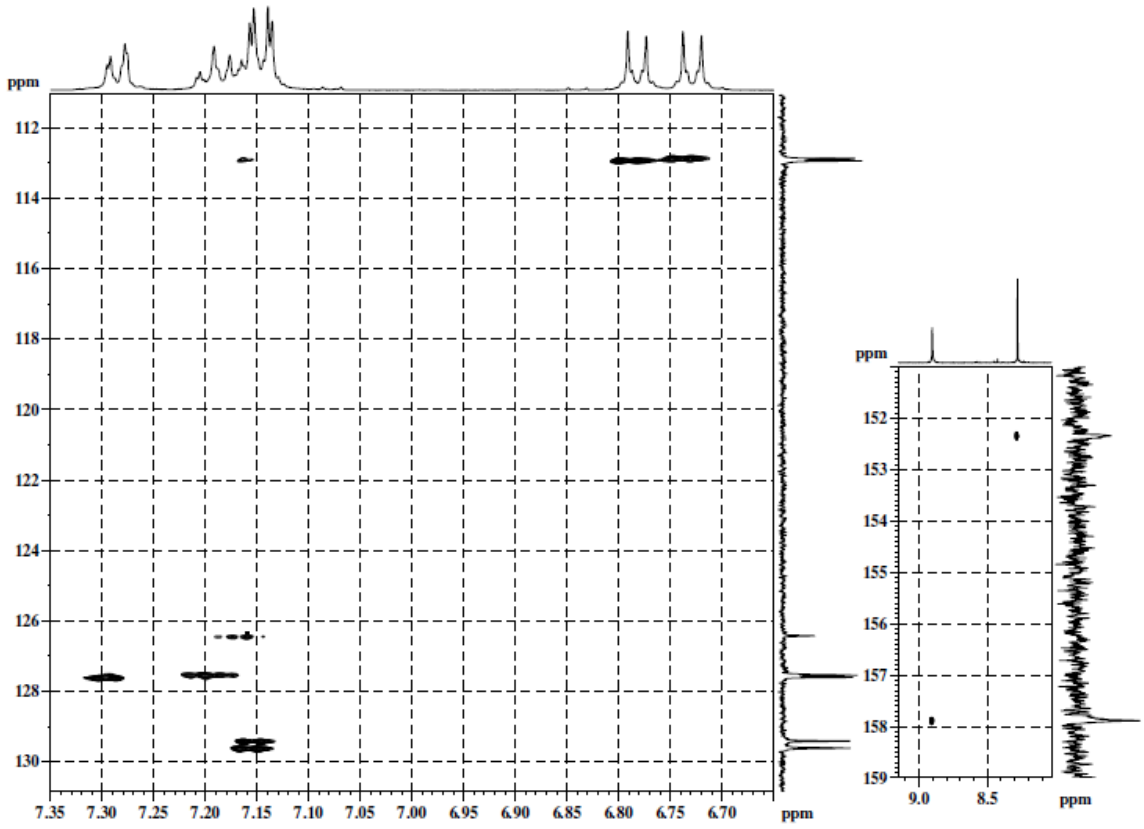
6L

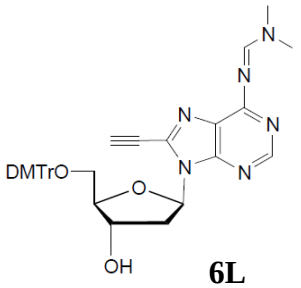

ppm
6.65
6.70
6.75
6.80
6.85
6.90
6.95
7.00
7.05
7.10
7.15
7.20
7.25
7.30
7.35
7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 6.75 6.70 6.65 ppm


DMTrO
O
OH
N
N
N
N
N
N
N
6L
ppm
2.4
2.6
2.8
3.0
3.2
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3
ppm

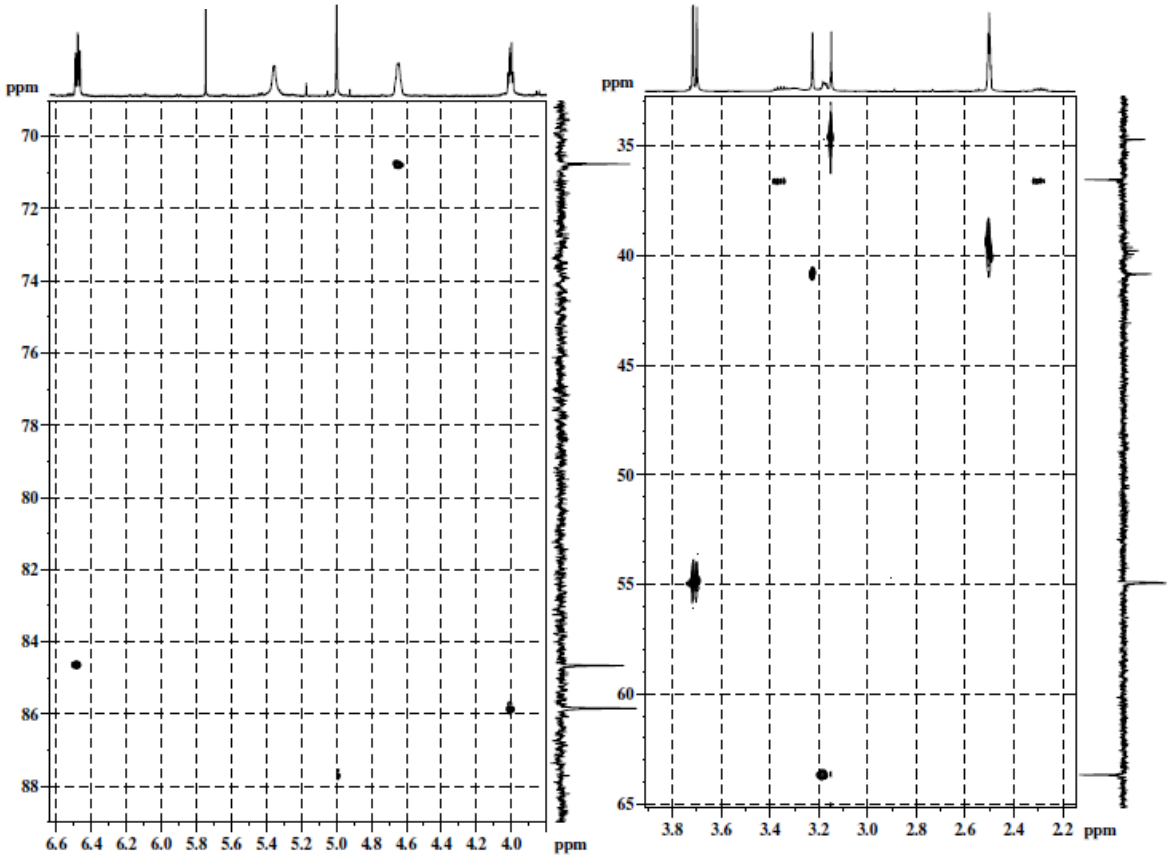

DMTrO
O
N
N
N
N
N
OH

6L


ppm
112
114
116
118
120
122
124
126
128
130
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
6.70
ppm
ppm
152
153
154
155
156
157
158
159
9.0
8.5
ppm


N
N
N
N
N
N
DMTrO
O
OH

6L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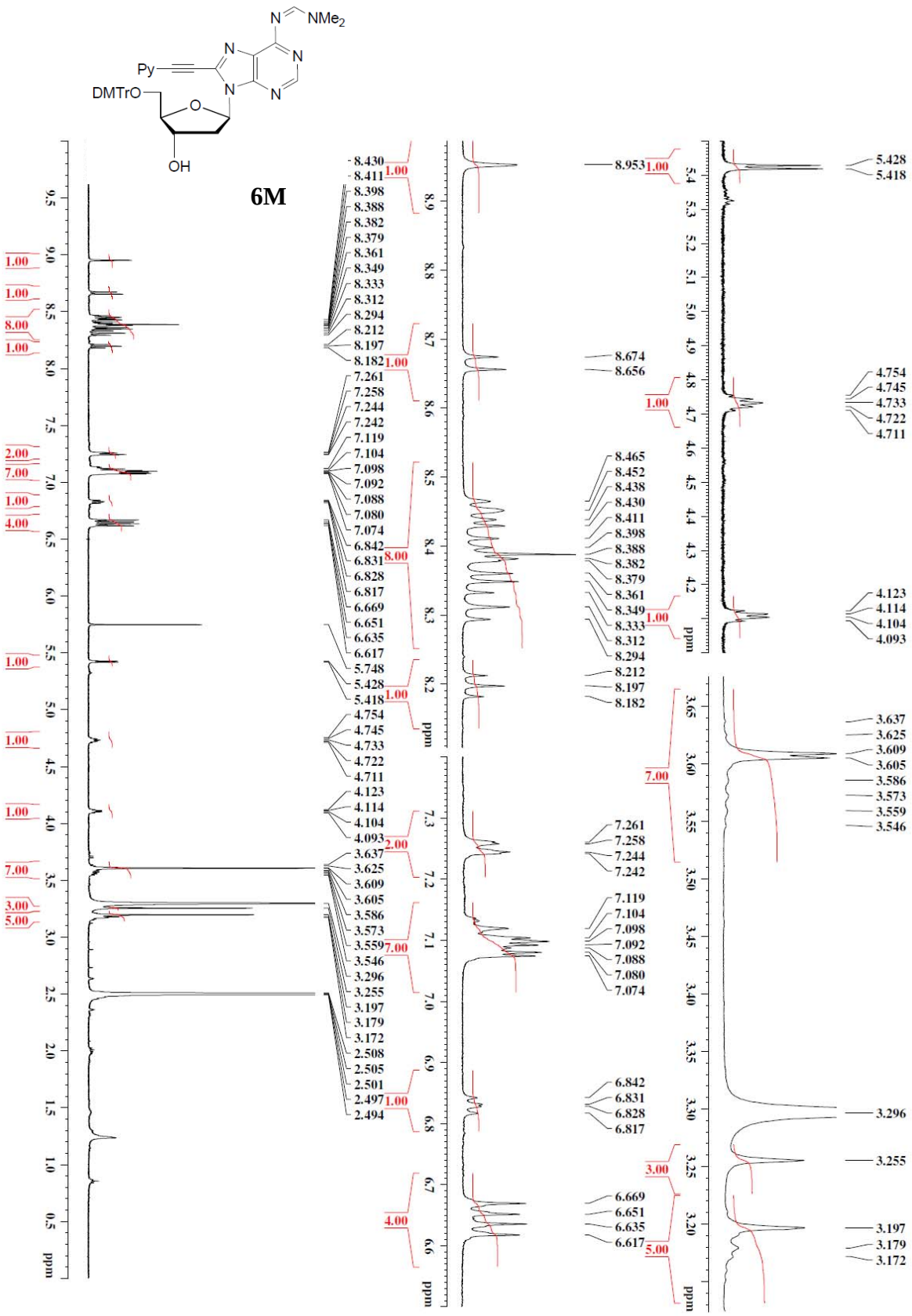
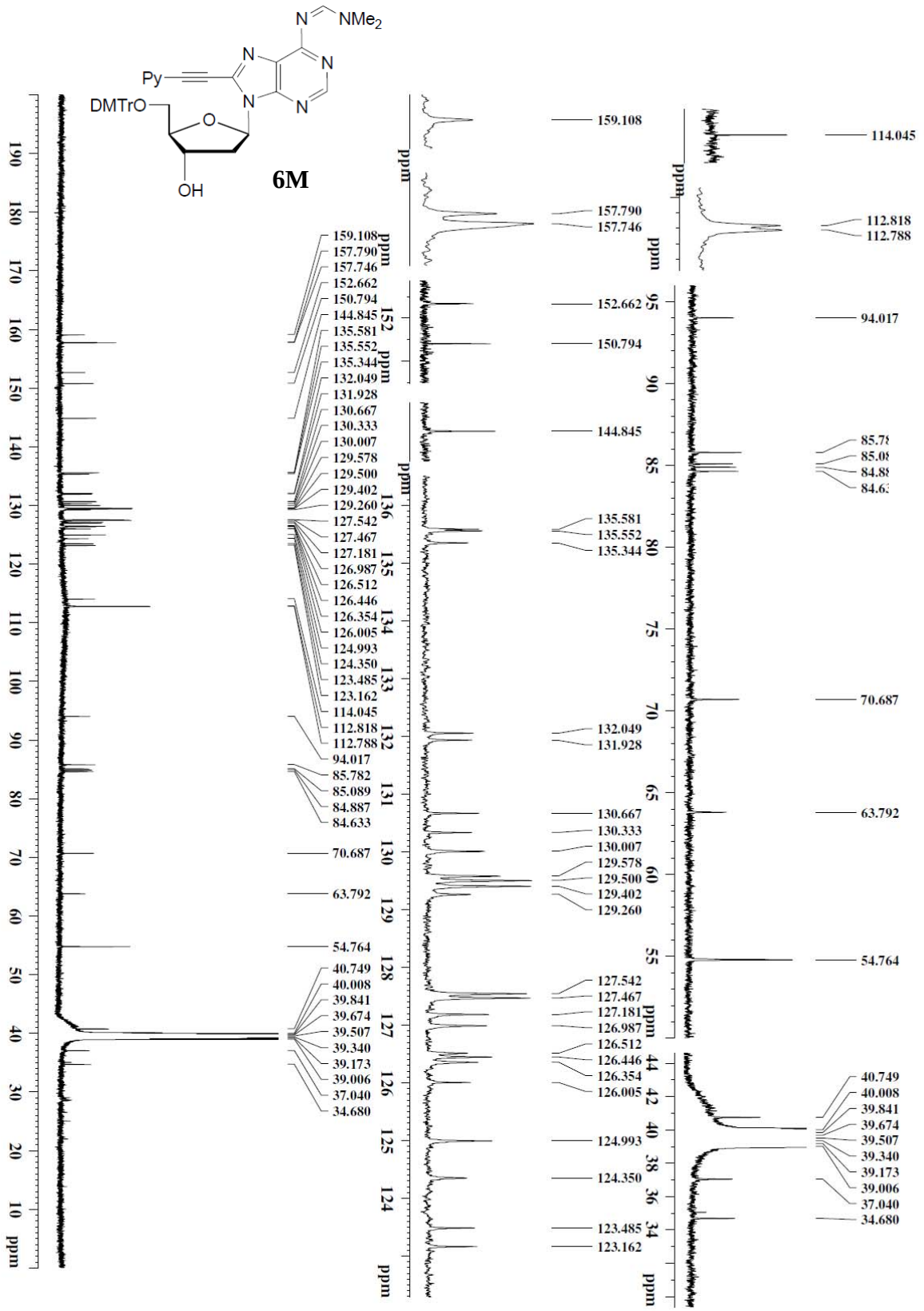
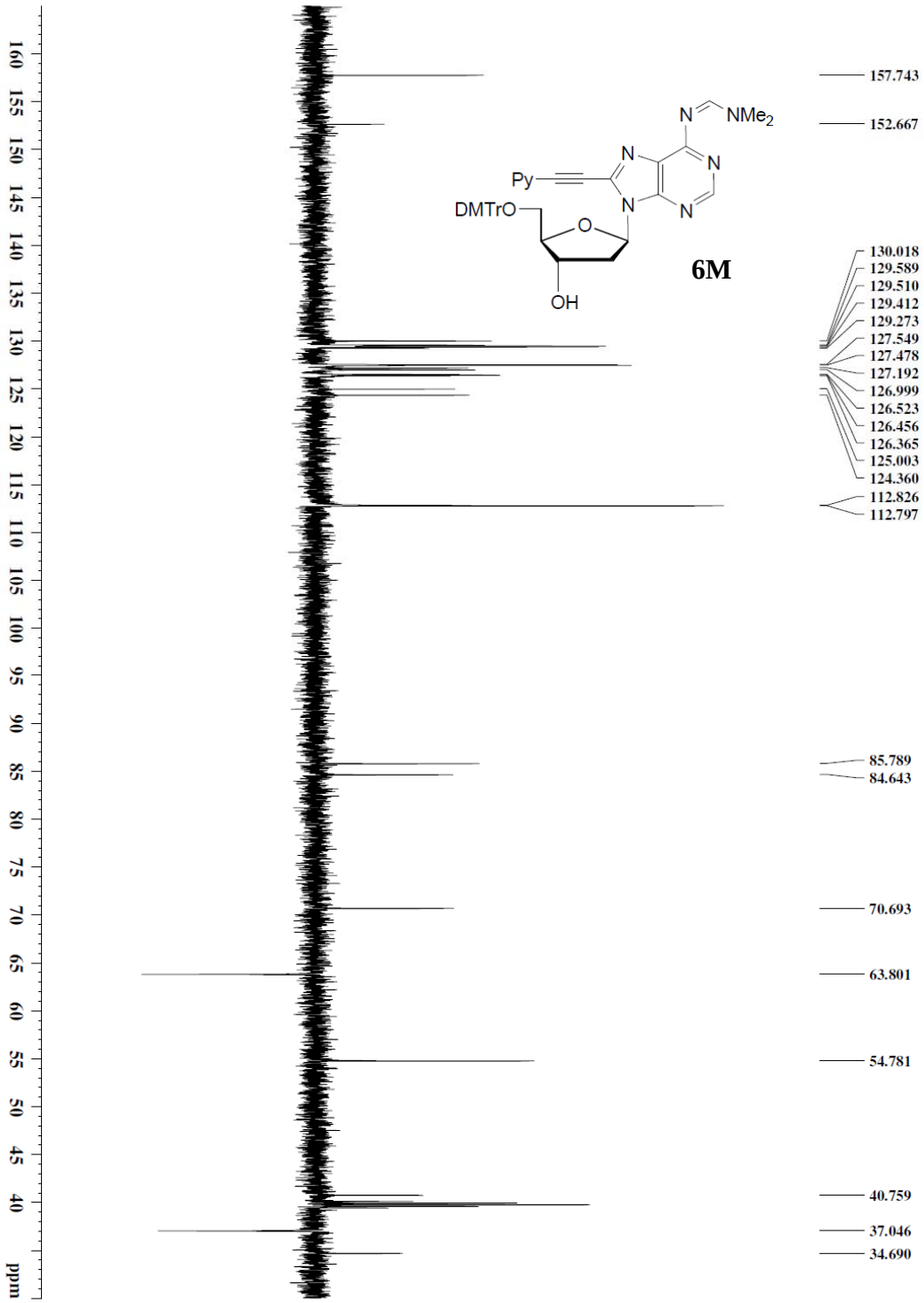
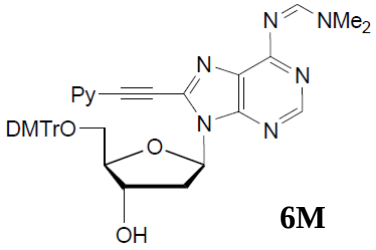
70
72
74
76
78
80
82
84
86
88
6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0
ppm
ppm
35
40
45
50
55
60
65
3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2
ppm

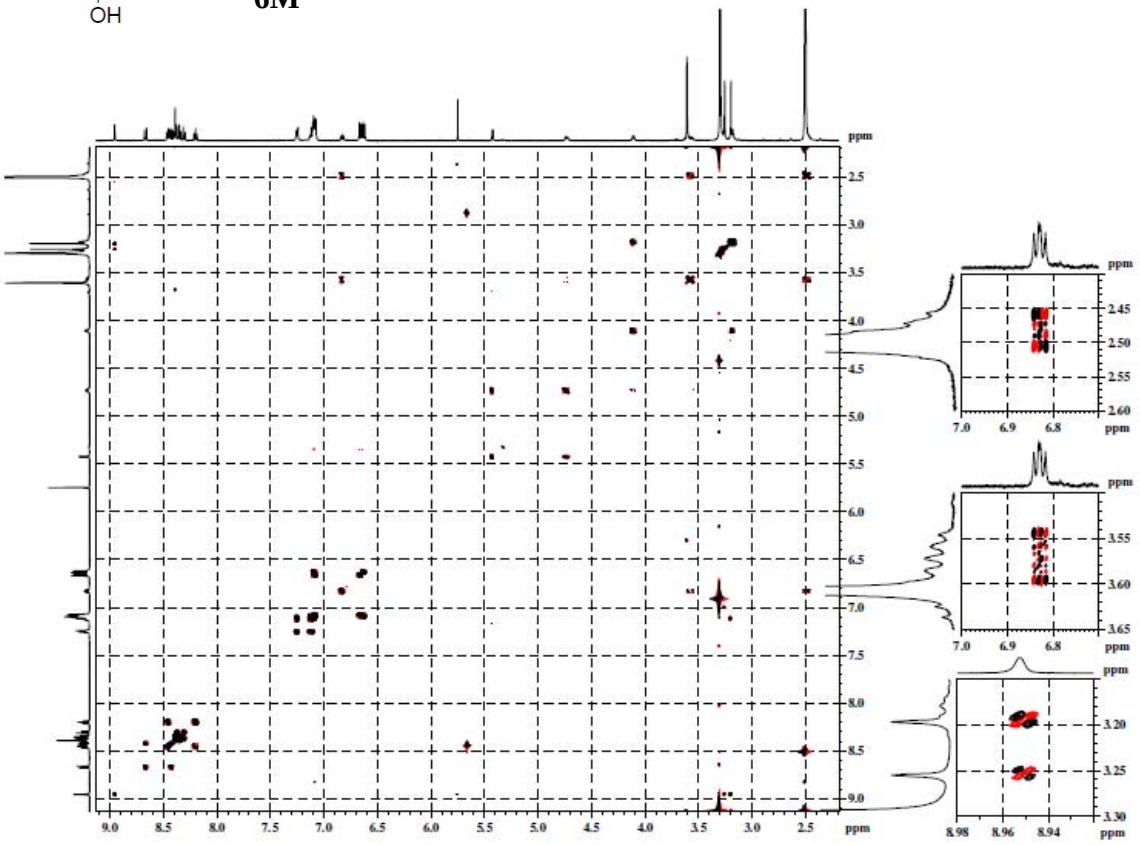

N
NMe2
N
N
Py
N
N
DMTrO
O
OH
6M
8.430
8.411
8.398
8.388
8.382
8.379
8.361
8.349
8.333
8.312
8.294
8.212
8.197
8.182
7.261
7.258
7.244
7.242
7.119
7.104
7.098
7.092
7.088
7.080
7.074
6.842
6.831
6.828
6.817
6.669
6.651
6.635
6.617
5.748
5.428
5.418
4.754
4.745
4.733
4.722
4.711
4.123
4.114
4.104
4.093
3.637
3.625
3.609
3.605
3.586
3.573
3.559
3.546
3.296
3.255
3.197
3.179
3.172
2.508
2.505
2.501
2.497
2.494
8.953
8.674
8.656
8.465
8.452
8.438
8.430
8.411
8.398
8.388
8.382
8.379
8.361
8.349
8.333
8.312
8.294
8.212
8.197
8.182
7.261
7.258
7.244
7.242
7.119
7.104
7.098
7.092
7.088
7.080
7.074
6.842
6.831
6.828
6.817
6.669
6.651
6.635
6.617
5.428
5.418
4.754
4.745
4.733
4.722
4.711
4.123
4.114
4.104
4.093
3.637
3.625
3.609
3.605
3.586
3.573
3.559
3.546
3.296
3.255
3.197
3.179
3.172
ppm

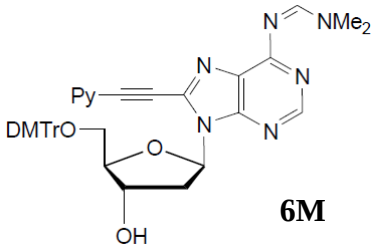

N
NMe2
N
N
Py
N
N
DMTrO
O
OH
6M
159.108
157.790
157.746
152.662
150.794
144.845
135.581
135.552
135.344
132.049
131.928
130.667
130.333
130.007
129.578
129.500
129.402
129.260
127.542
127.467
127.181
126.987
126.512
126.446
126.354
126.005
124.993
124.350
123.485
123.162
114.045
112.818
112.788
94.017
85.782
85.089
84.887
84.633
70.687
63.792
54.764
40.749
40.008
39.841
39.674
39.507
39.340
39.173
39.006
37.040
34.680
ppm


157.743
152.667
130.018
129.589
129.510
129.412
129.273
127.549
127.478
127.192
126.999
126.523
126.456
126.365
125.003
124.360
112.826
112.797
85.789
84.643
70.693
63.801
54.781
40.759
37.046
34.690
ppm
Py
DMTrO
OH
NMe2
6M

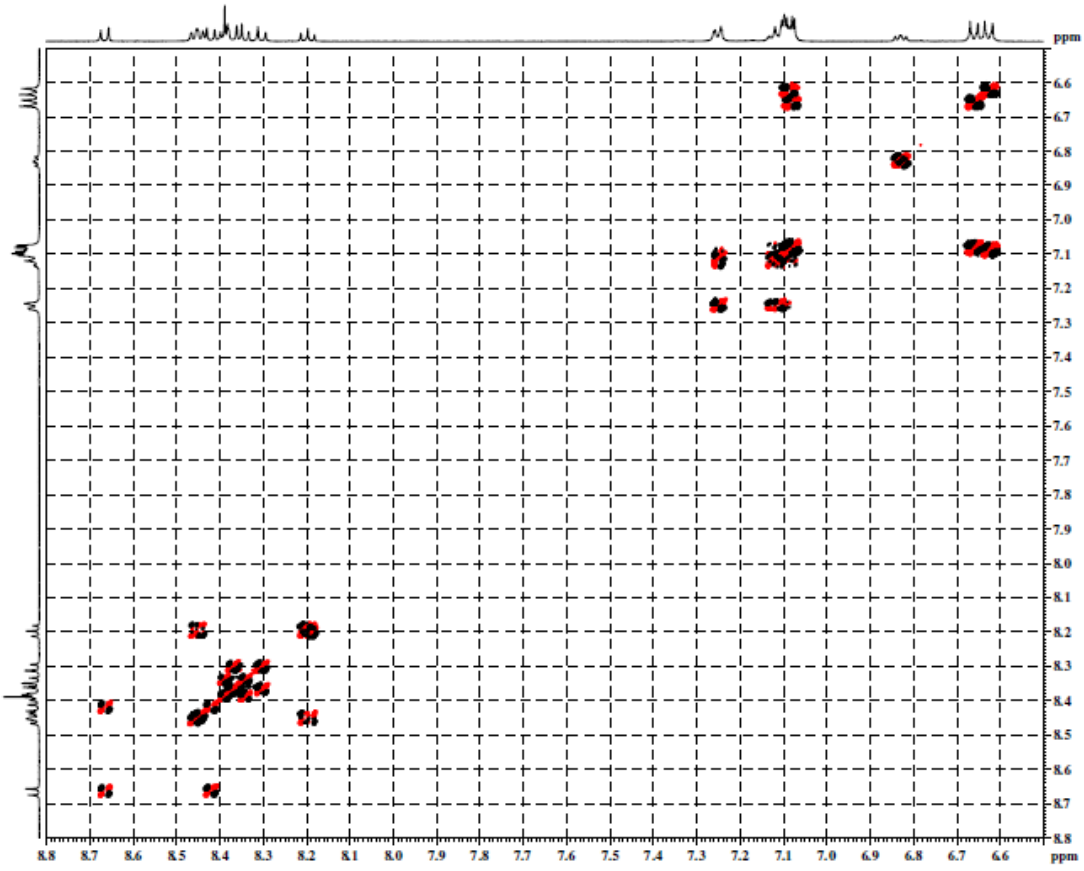

N
NMe2
N
N
Py
N
N
DMTrO
O
OH

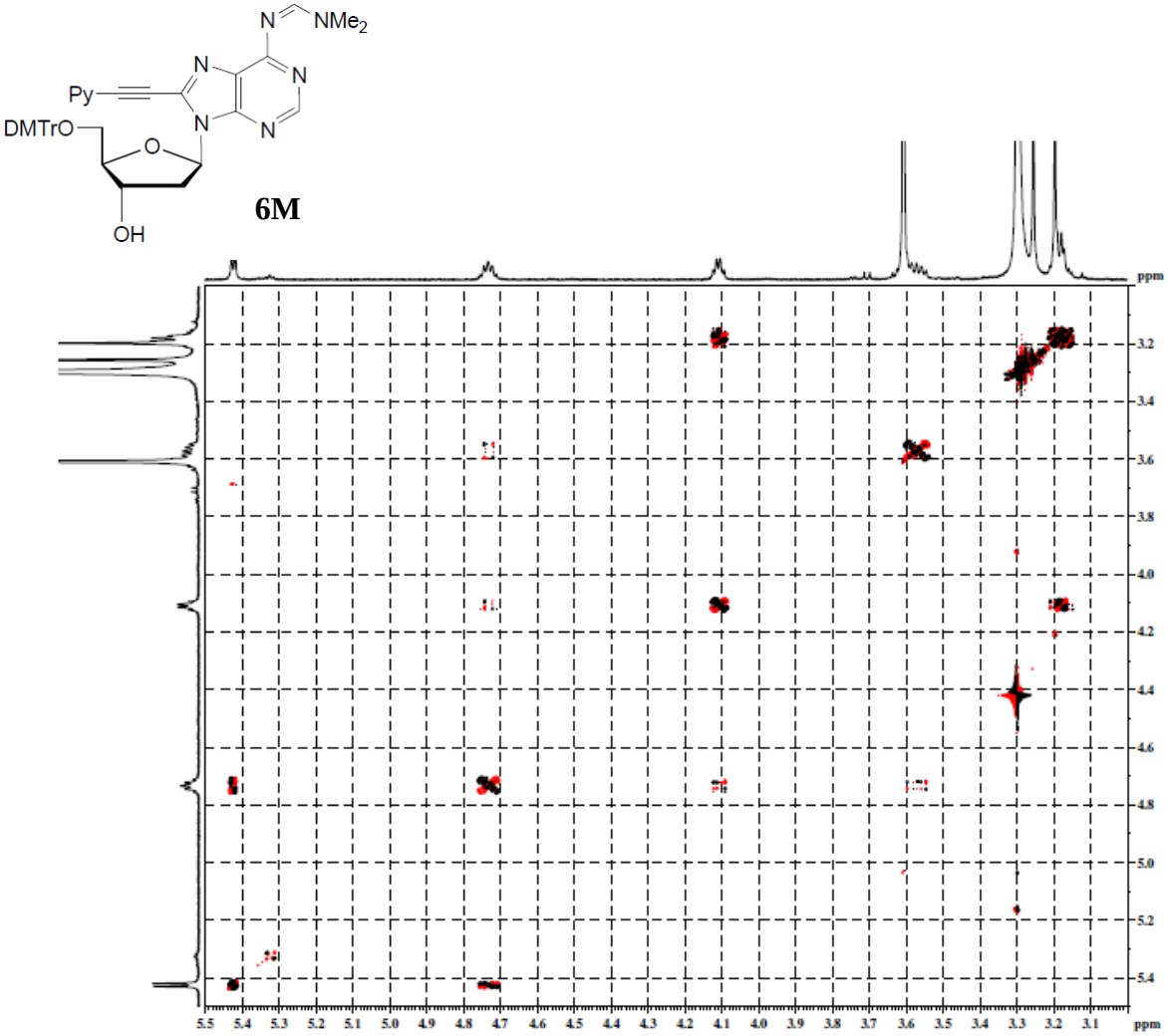
6M


ppm
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
7.0
6.9
6.8
2.45
2.50
2.55
2.60
3.55
3.60
3.65
8.98
8.96
8.94
3.20
3.25
3.30

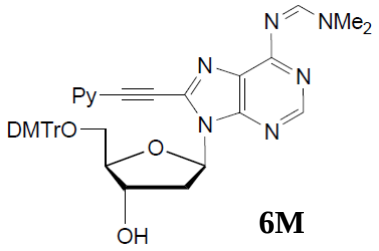

N
NMe2
N
N
Py
N
N
DMTrO
O
OH

6M

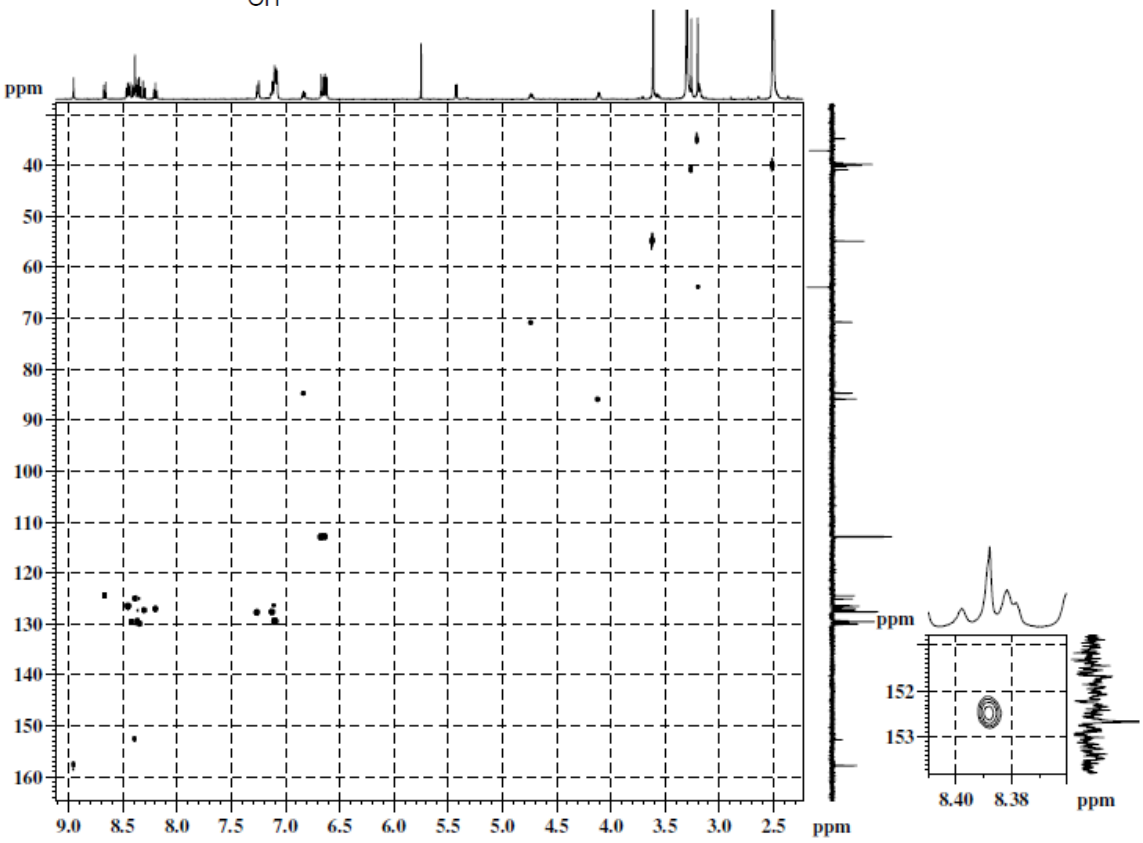

ppm
6.6
6.7
6.8
6.9
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
8.4
8.5
8.6
8.7
8.8
8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6
ppm

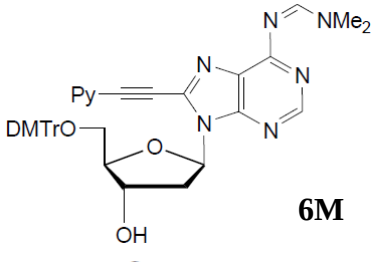

N
NMe2
N
N
Py
N
N
DMTrO
O
OH
ppm
3.2
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
5.0
5.2
5.4
5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1
ppm

6M

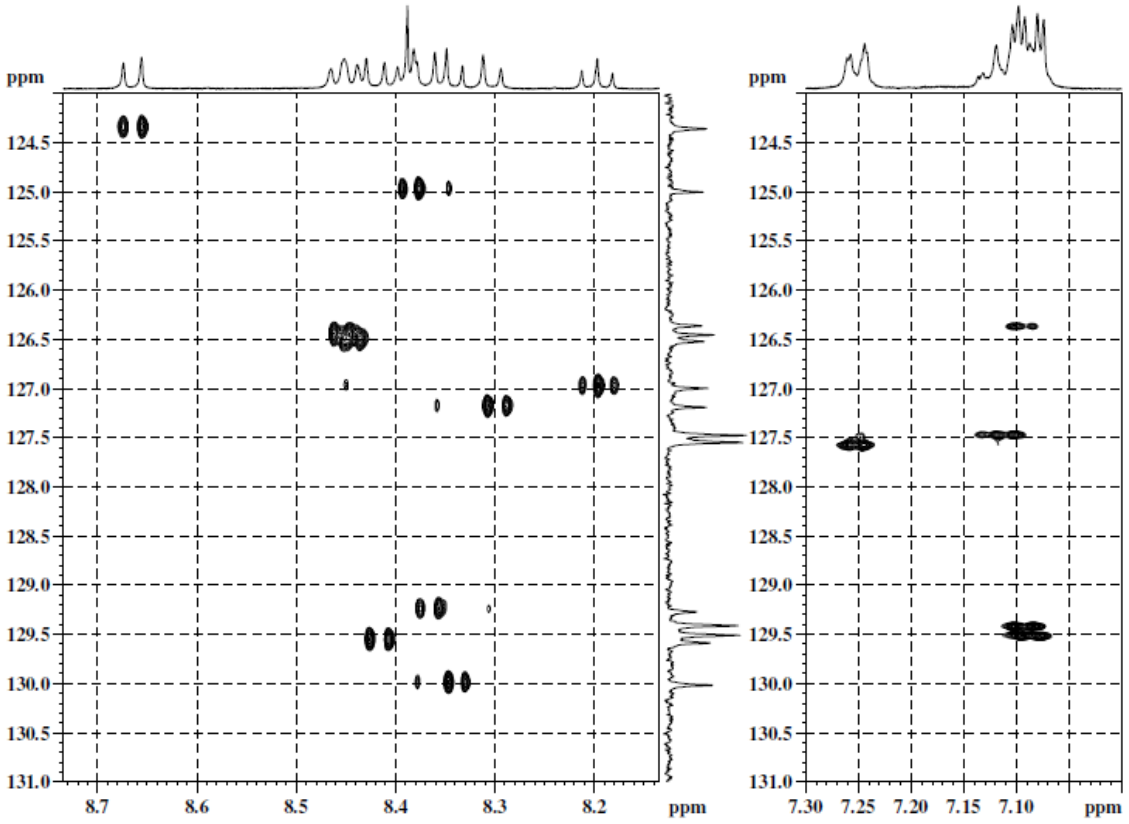

N
NMe2
N
N
Py
N
N
DMTrO
O
OH

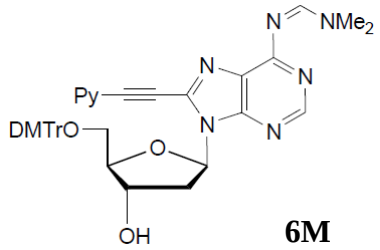
6M


ppm
40
50
60
70
80
90
100
110
120
130
140
150
160
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
ppm
ppm
152
153
8.40
8.38
ppm

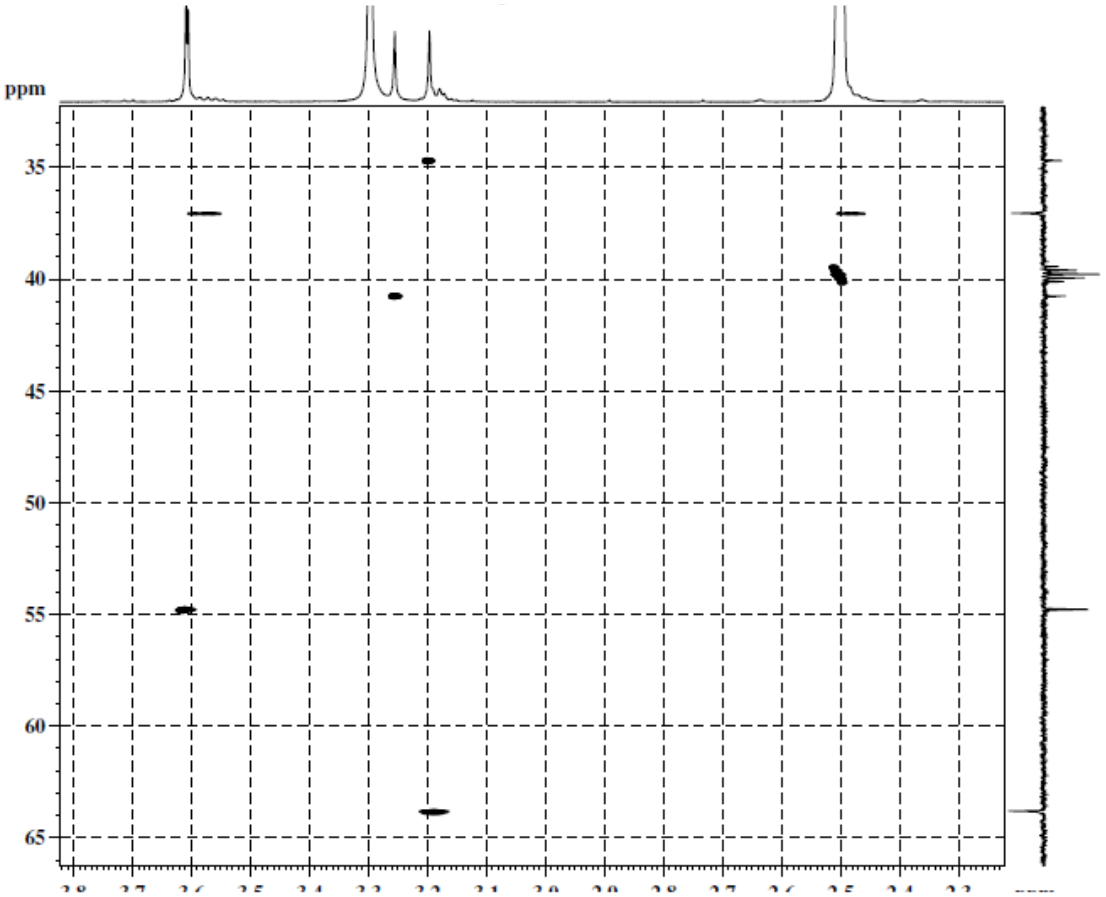

N
NMe2
N
N
Py
N
N
DMTrO
O
OH

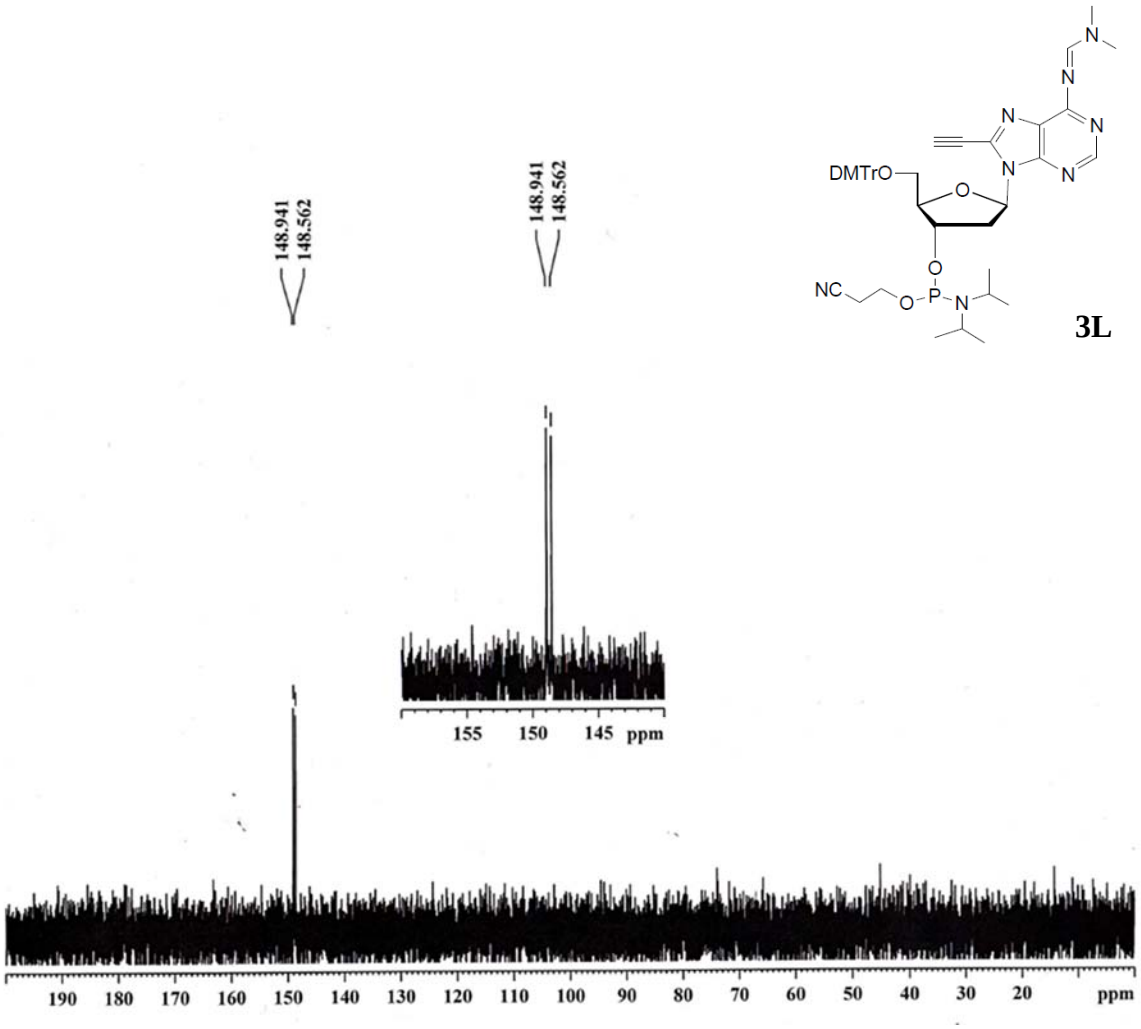
6M


ppm
124.5
125.0
125.5
126.0
126.5
127.0
127.5
128.0
128.5
129.0
129.5
130.0
130.5
131.0
8.7
8.6
8.5
8.4
8.3
8.2
ppm
ppm
7.30
7.25
7.20
7.15
7.10
ppm

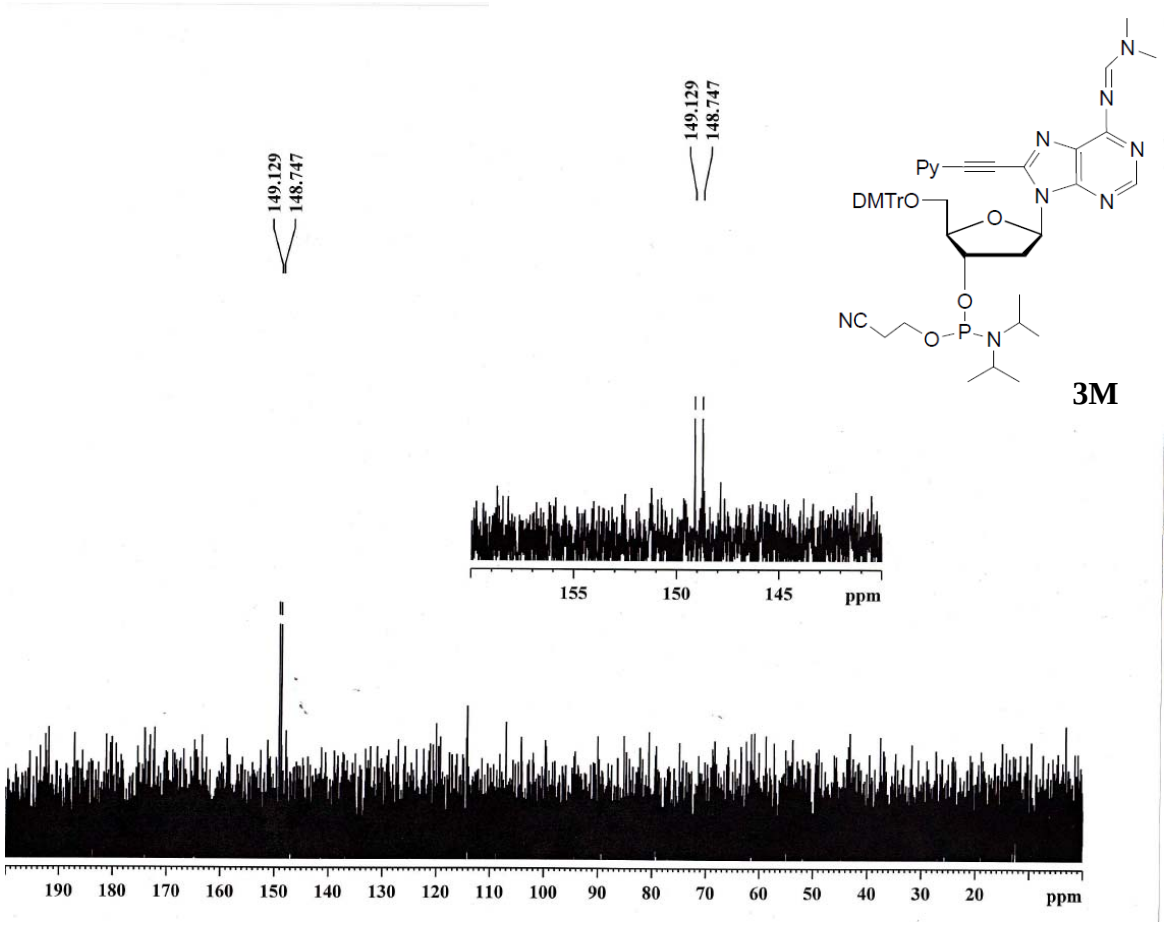


6M

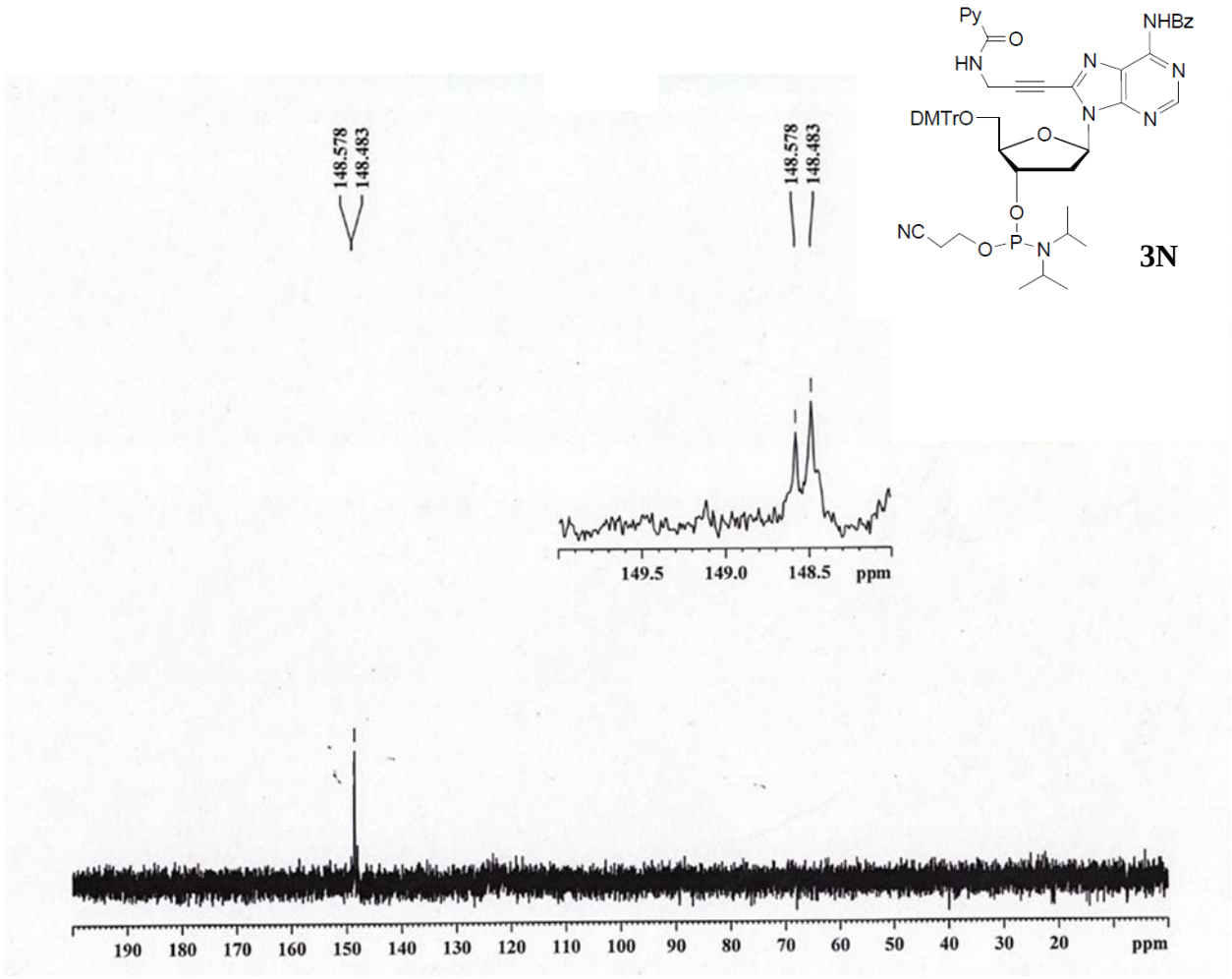



148.941
148.562
148.941
148.562
DMTrO
O
NC
O
P
N
N
N
N
N
155
150
145
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

3L


149.129
148.747
149.129
148.747
Py
DMTrO
NC
O
P
N
155
150
145
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

3M


Py
O
HN
NHBz
N
N
N
N
DMTrO
O
O
NC
O
P
N
3N
148.578
148.483
148.578
148.483
149.5
149.0
148.5
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm