Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Preparation and characterization of pyrene modified uridines as potential electron donors in RNA

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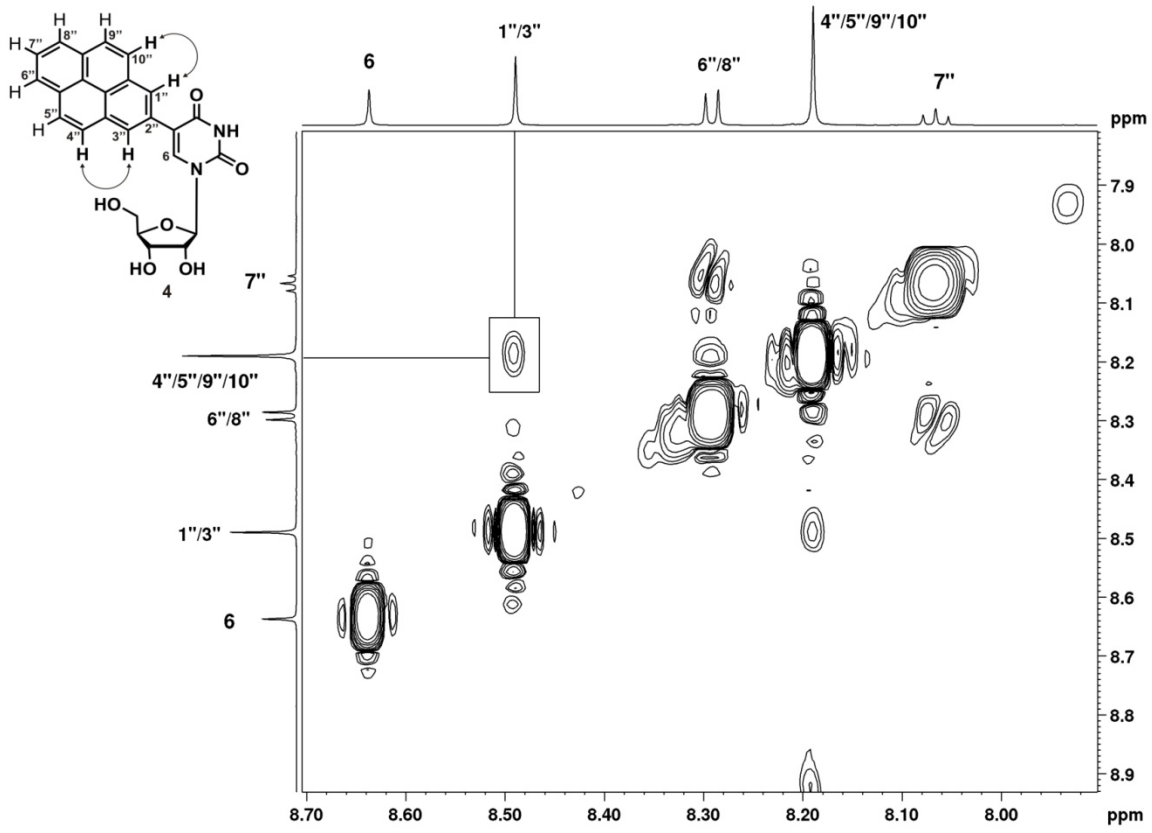


Figure S1 NOESY spectra showing the aromatic protons of the pyrene modified nucleoside **4**. The NOE contact between H1”/H10” and H3”/H4” verify the C2”-C5-linkage between pyrene and the pyrimidine base.

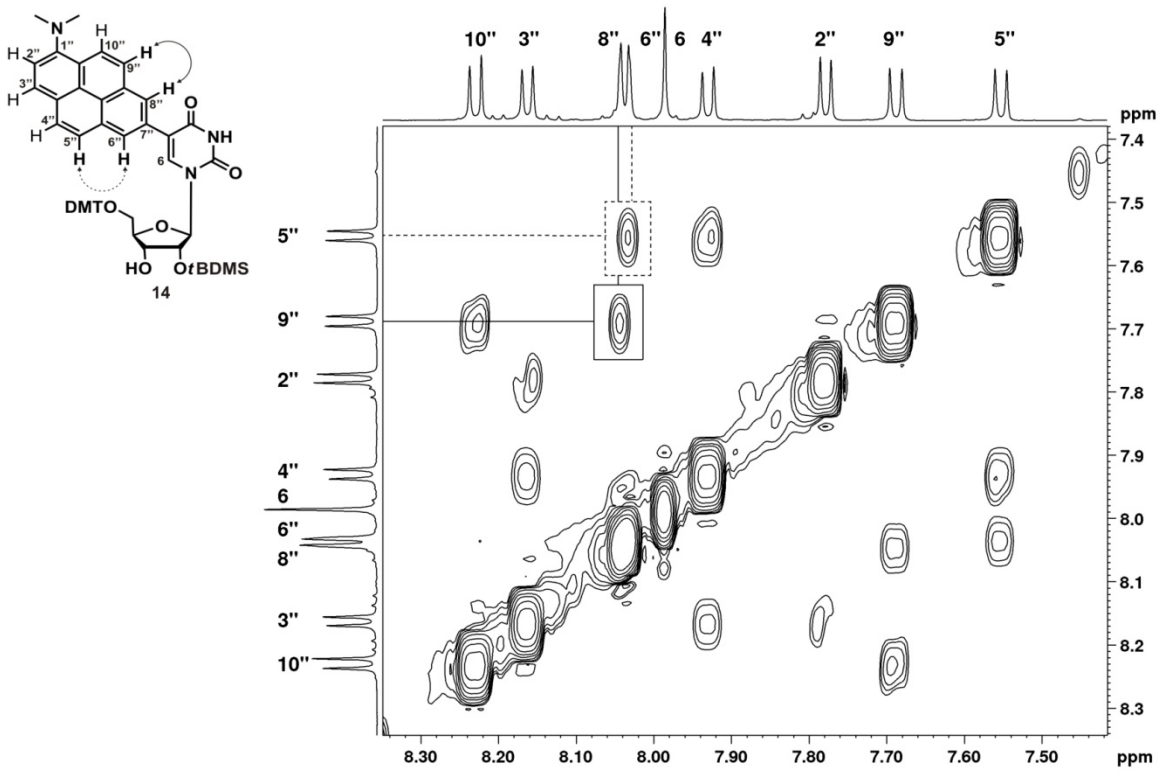


Figure S2 NOESY spectra showing the aromatic protons of the pyrene modified nucleoside **14**. The two NOE contacts between H6”/5” and H8”/H9” serve as evidence for the C7”-C5-linkage between the pyrene and the pyrimidine base of the nucleoside.

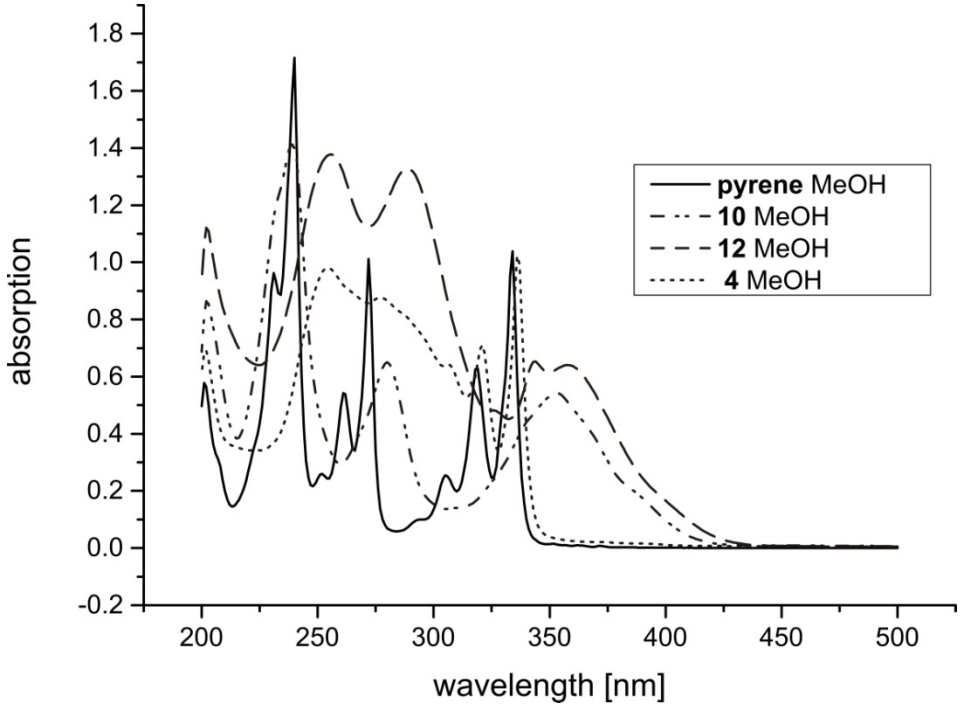


Figure S3 UV/Vis absorption spectra of pyrene, DMAPy **10**, DMAPyU **12** and PyU **4** in MeOH. All compounds were measured at a concentration of 25 µM.

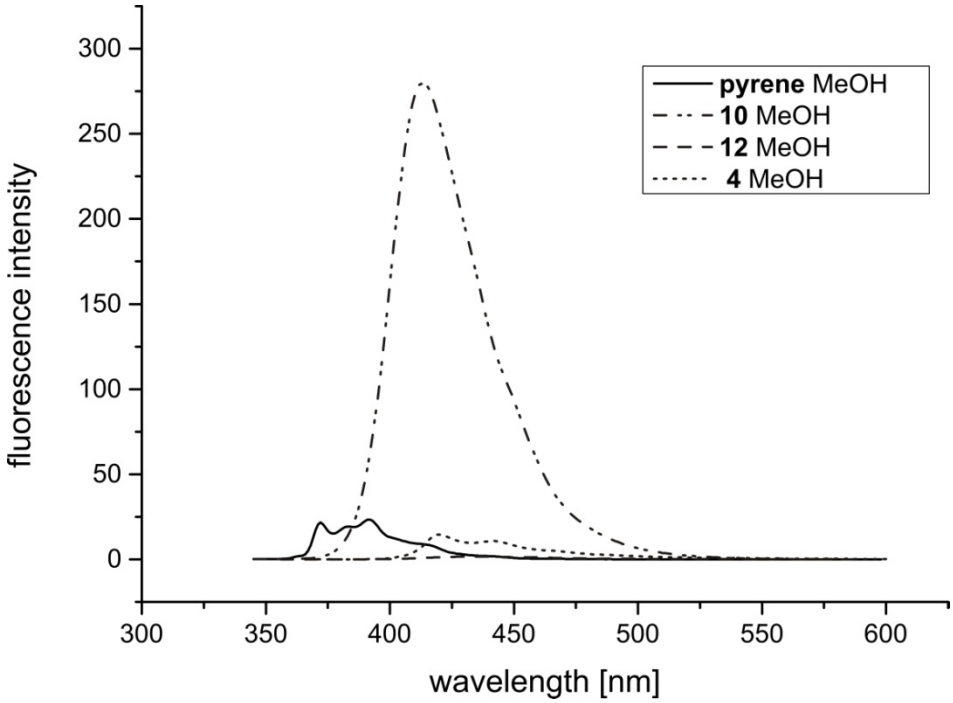
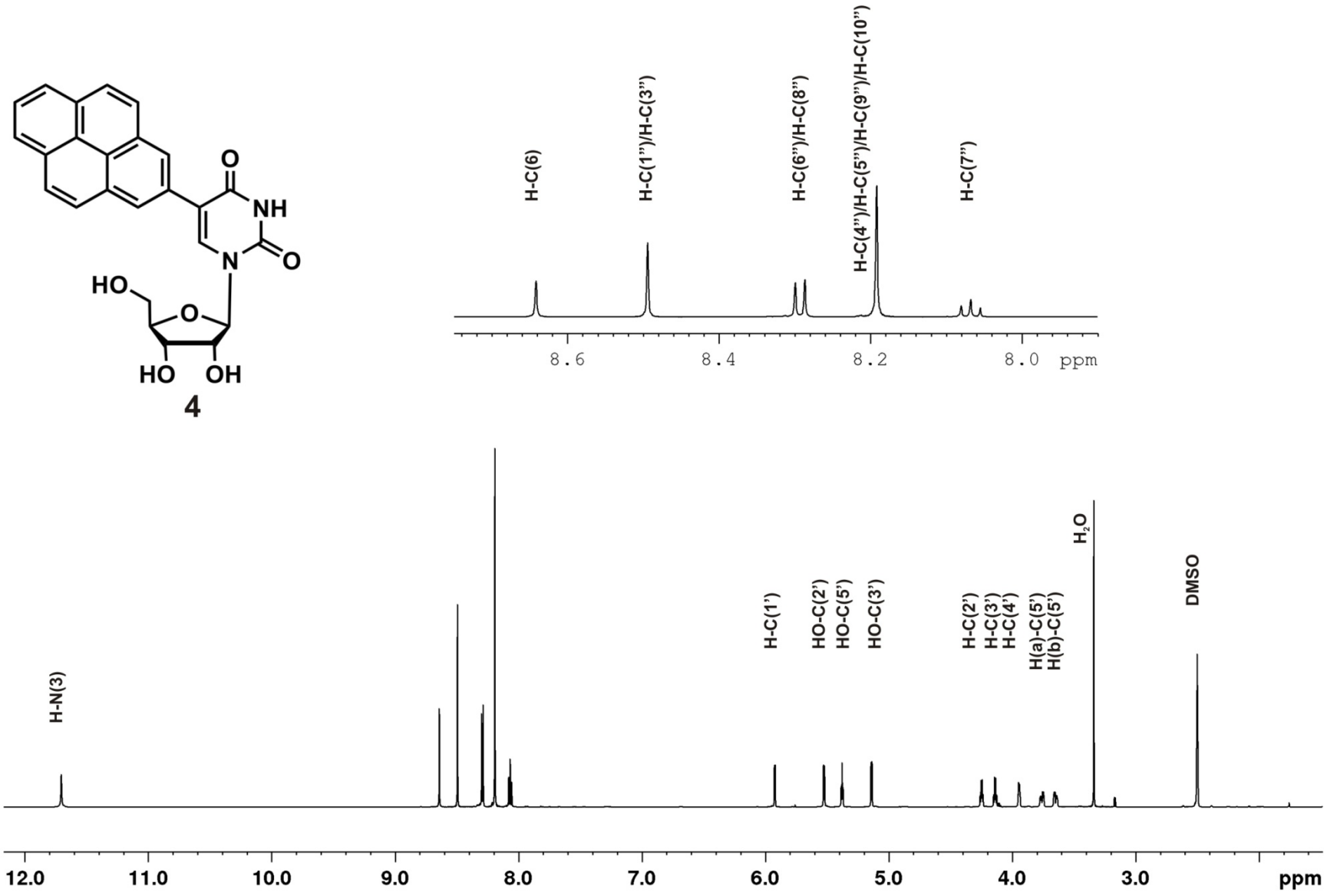


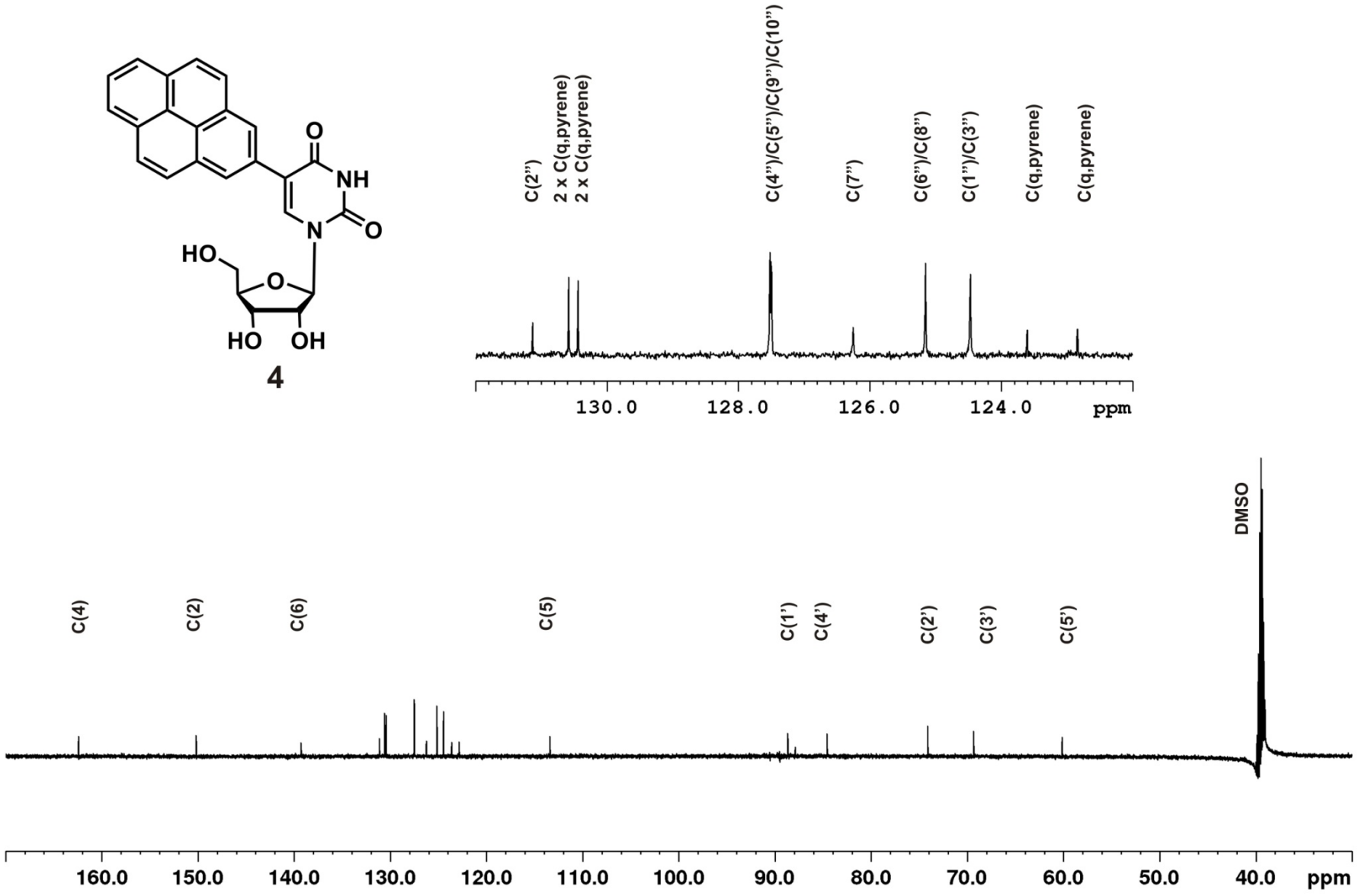
Figure S4 Fluorescence spectra of pyrene, DMAPy **10**, DMAPyU **12** and PyU **4** in MeOH. Concentration of all compounds was adjusted to uniform optical density at the characteristic excitation wavelength. In MeOH: pyrene (334 nm, 0.5 µM); **10** (350 nm, 1 µM); **12** (355 nm; 0.75 µM); **4** (337 nm, 1 µM).

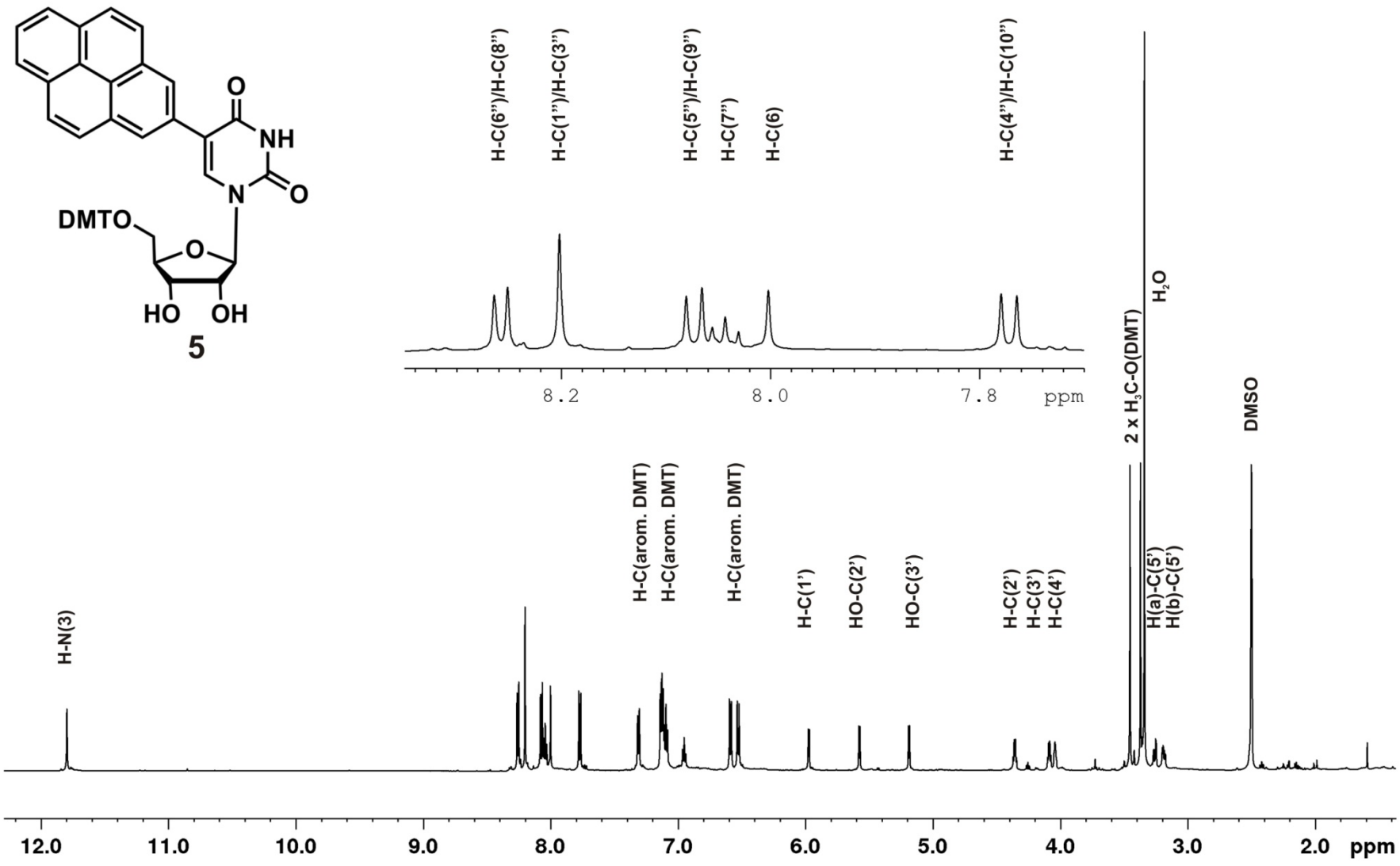
Table S1 Fluorescence quantum yields of pyrene, DMAPy **10**, DMAPyU **12** and PyU **4** in MeOH. Quantum yields were determined using quinine sulfate in 0.1 N H_2SO_4 as standard.

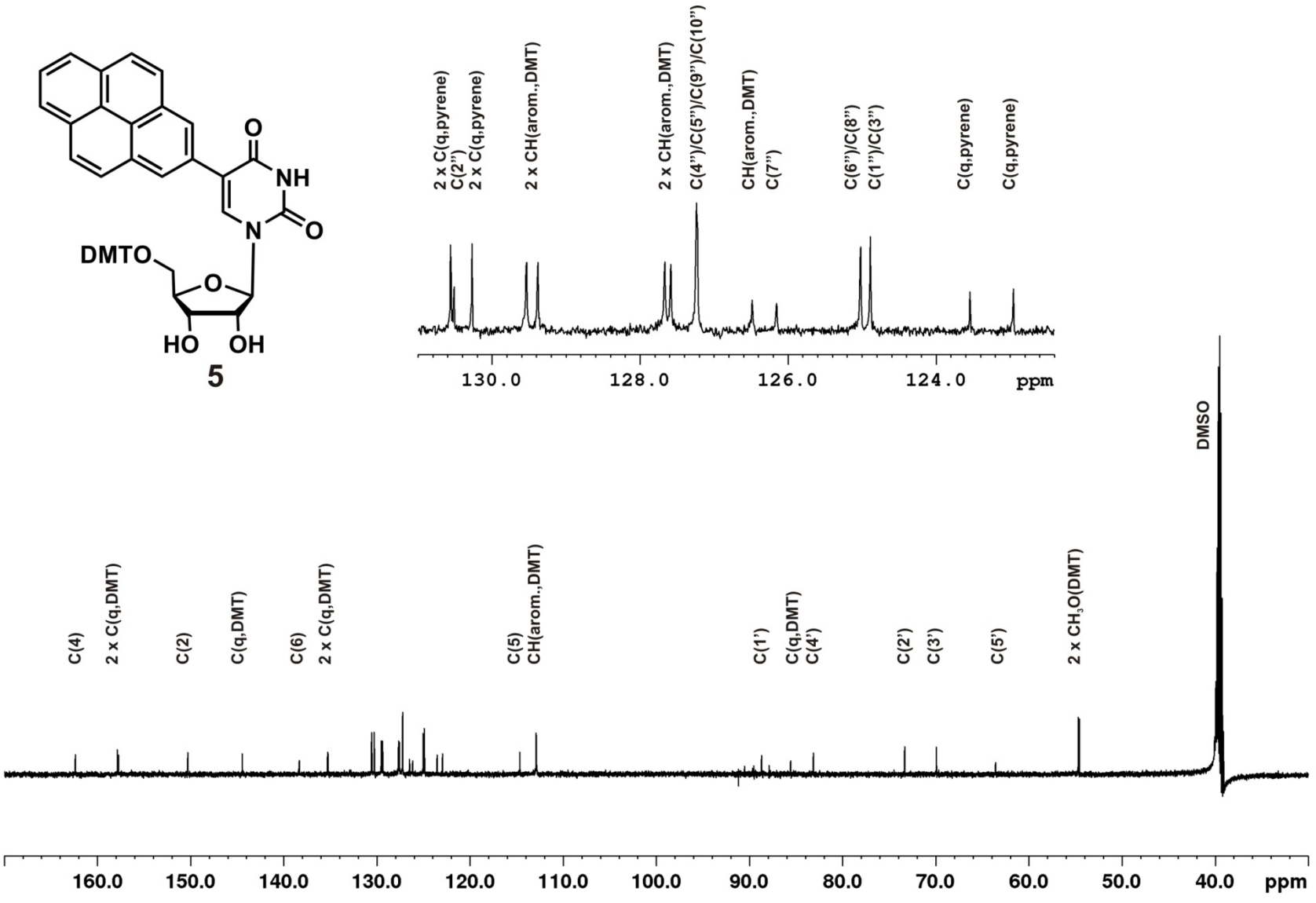
Compound	Φ (MeOH)
pyrene	0.023
10	0.385
12	0.003
4	0.018

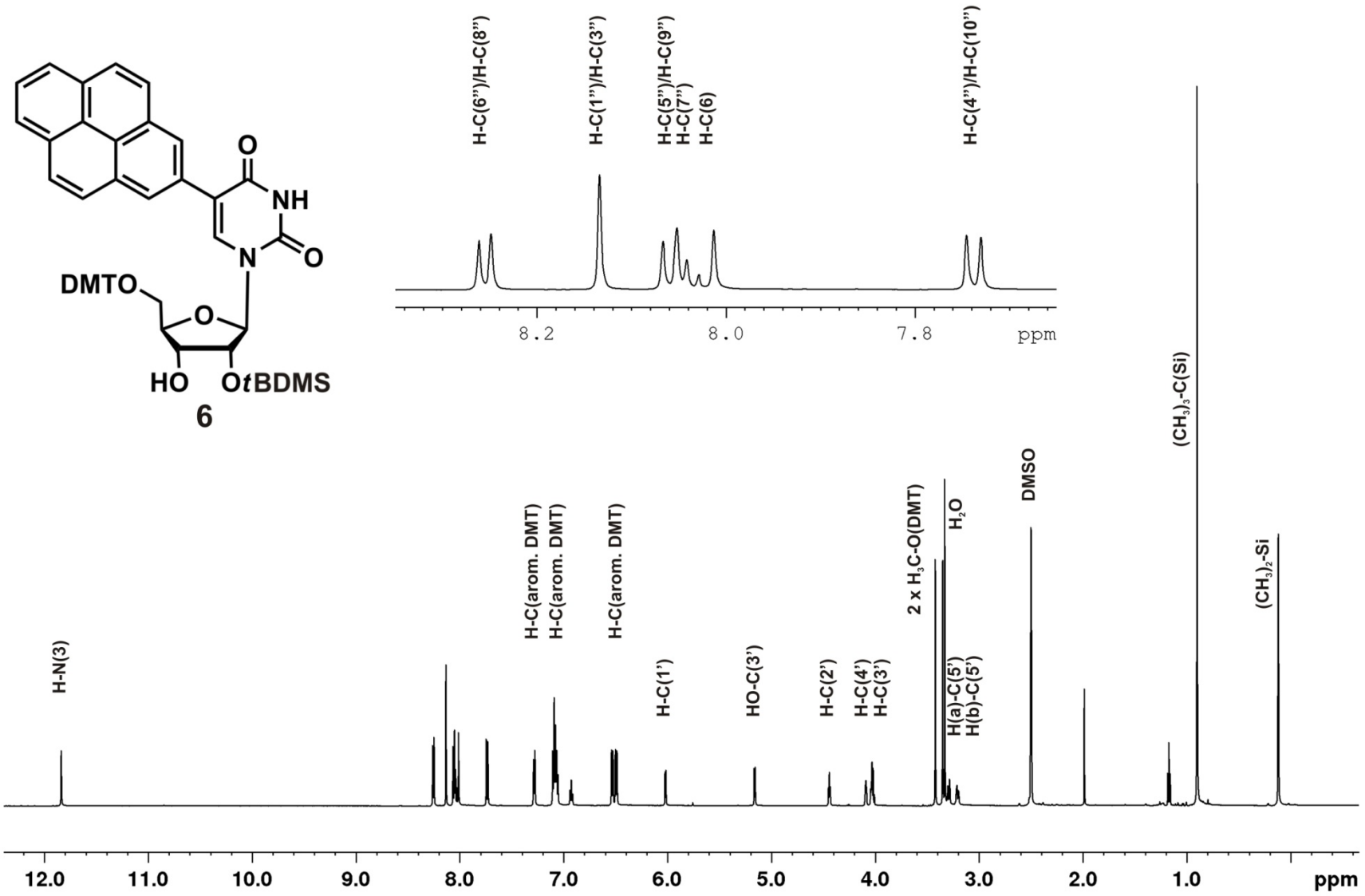
NMR spectra:

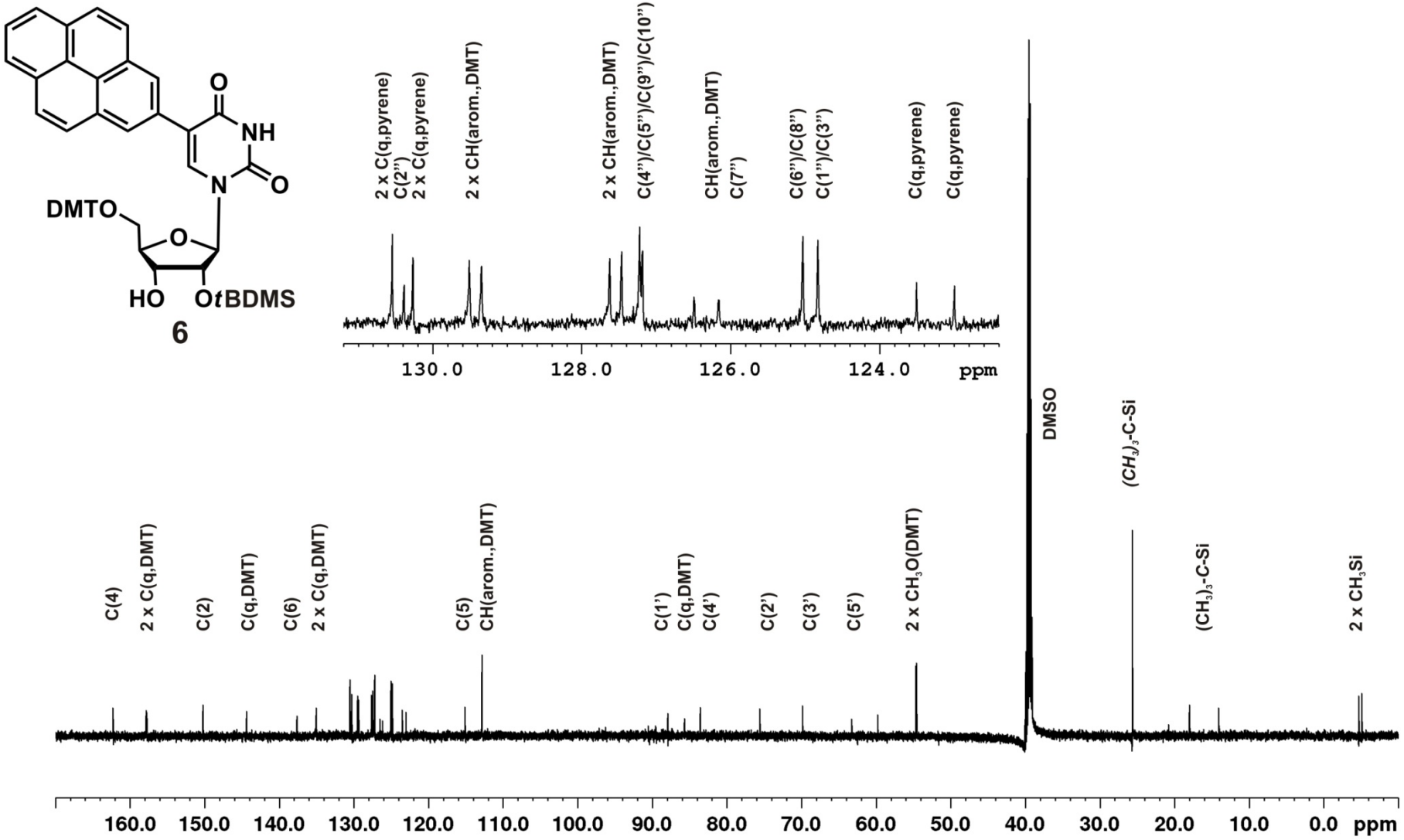

O
NH
N
O
HO
O
HO
OH
4
H-C(6)
H-C(1")/H-C(3")
H-C(6")/H-C(8")
H-C(4")/H-C(5")/H-C(9")/H-C(10")
H-C(7")
8.6
8.4
8.2
8.0
ppm
H-N(3)
H-C(1')
HO-C(2')
HO-C(5')
HO-C(3')
H-C(2')
H-C(3')
H-C(4')
H(a)-C(5')
H(b)-C(5')
H2O
DMSO
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
ppm

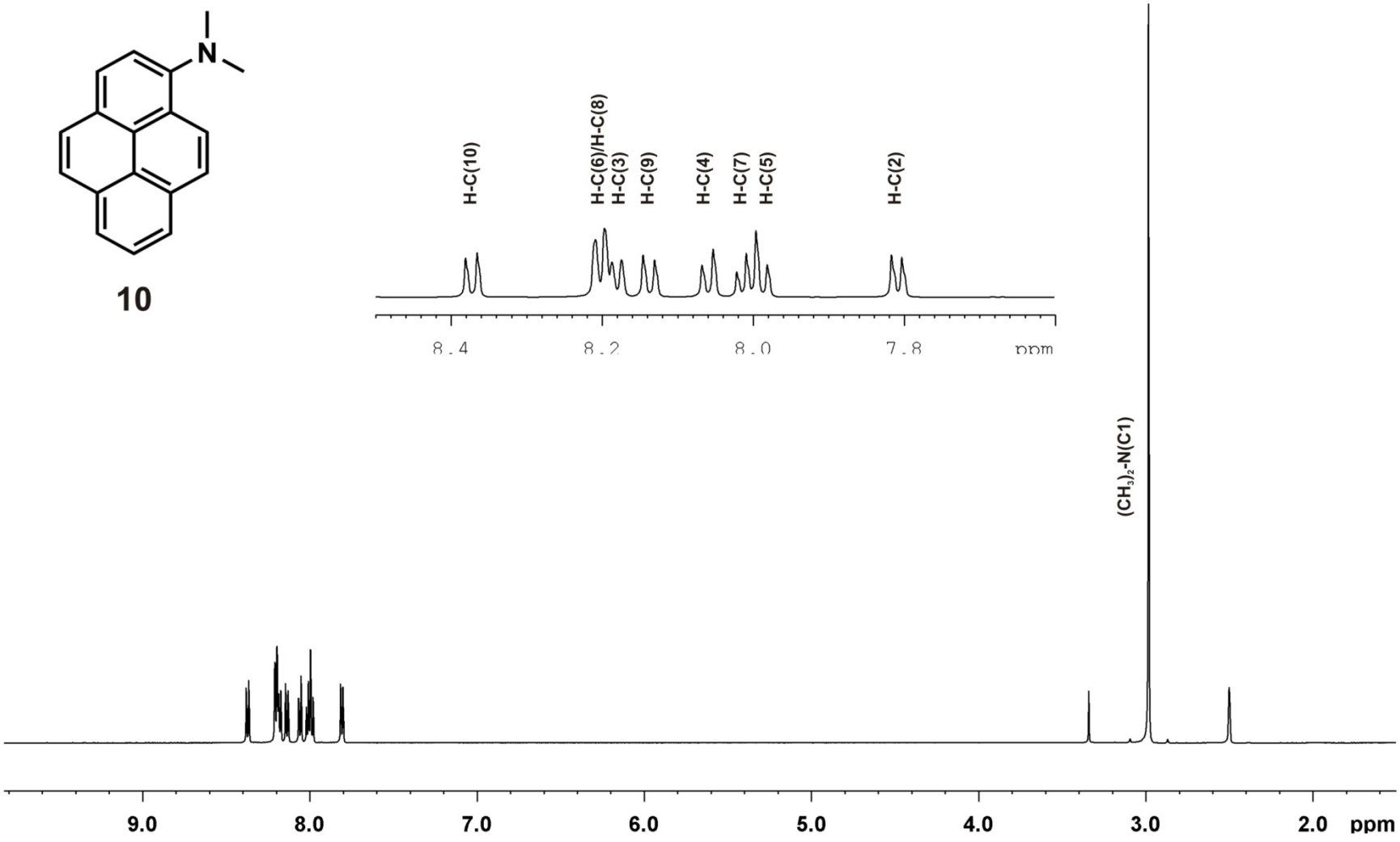

O
NH
N
O
HO
O
HO
OH
4
C(2'')
2 x C(q,pyrene)
2 x C(q,pyrene)
C(4'')/C(5'')/C(9'')/C(10'')
C(7'')
C(6'')/C(8'')
C(1'')/C(3'')
C(q,pyrene)
C(q,pyrene)
130.0
128.0
126.0
124.0
ppm
DMSO
C(4)
C(2)
C(6)
C(5)
C(1')
C(4')
C(2')
C(3')
C(5')
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
ppm

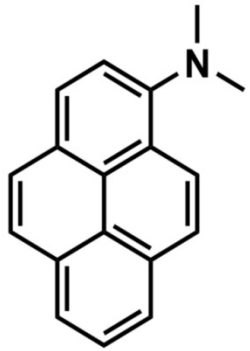

O
NH
N
O
DMTO
O
HO
OH
5
H-C(6'')/H-C(8'')
H-C(1'')/H-C(3'')
H-C(5'')/H-C(9'')
H-C(7'')
H-C(6)
H-C(4'')/H-C(10'')
8.2
8.0
7.8
ppm
2 x H3C-O(DMT)
H2O
DMSO
H-N(3)
H-C(arom. DMT)
H-C(arom. DMT)
H-C(arom. DMT)
H-C(1')
HO-C(2')
HO-C(3')
H-C(2')
H-C(3')
H-C(4')
H(a)-C(5')
H(b)-C(5')
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm


O
NH
N
O
DMTO
O
HO
OH
5
2 x C(q,pyrene)
C(2")
2 x C(q,pyrene)
2 x CH(arom.,DMT)
2 x CH(arom.,DMT)
C(4")/C(5")/C(9")/C(10")
CH(arom.,DMT)
C(7")
C(6")/C(8")
C(1")/C(3")
C(q,pyrene)
C(q,pyrene)
130.0
128.0
126.0
124.0
ppm
DMSO
C(4)
2 x C(q,DMT)
C(2)
C(q,DMT)
C(6)
2 x C(q,DMT)
C(5)
CH(arom.,DMT)
C(1')
C(q,DMT)
C(4')
C(2')
C(3')
C(5')
2 x CH3O(DMT)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
ppm

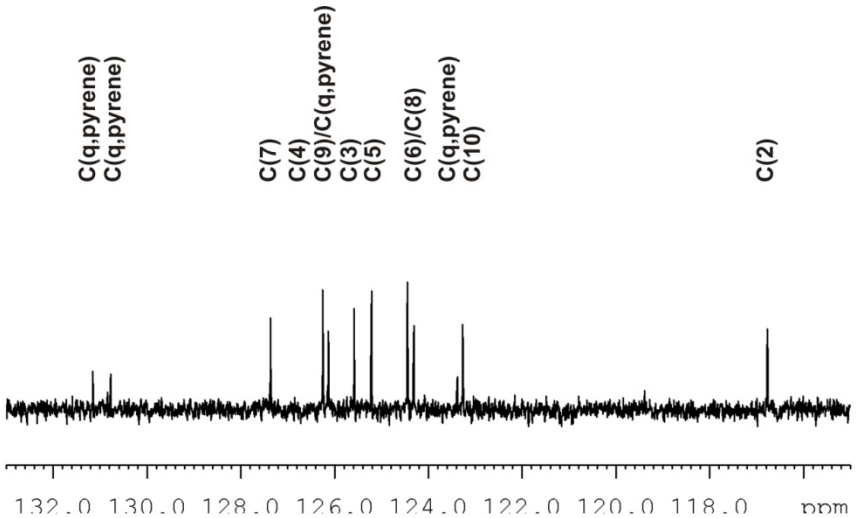

O
NH
N
O
DMTO
O
HO
OtBDMS
6
H-C(6")/H-C(8")
H-C(1")/H-C(3")
H-C(5")/H-C(9")
H-C(7")
H-C(6)
H-C(4")/H-C(10")
8.2
8.0
7.8
ppm
H-N(3)
H-C(arom. DMT)
H-C(arom. DMT)
H-C(arom. DMT)
H-C(1')
HO-C(3')
H-C(2')
H-C(4')
H-C(3')
2 x H3C-O(DMT)
H2O
H(a)-C(5')
H(b)-C(5')
DMSO
(CH3)3-C(Si)
(CH3)2-Si
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm

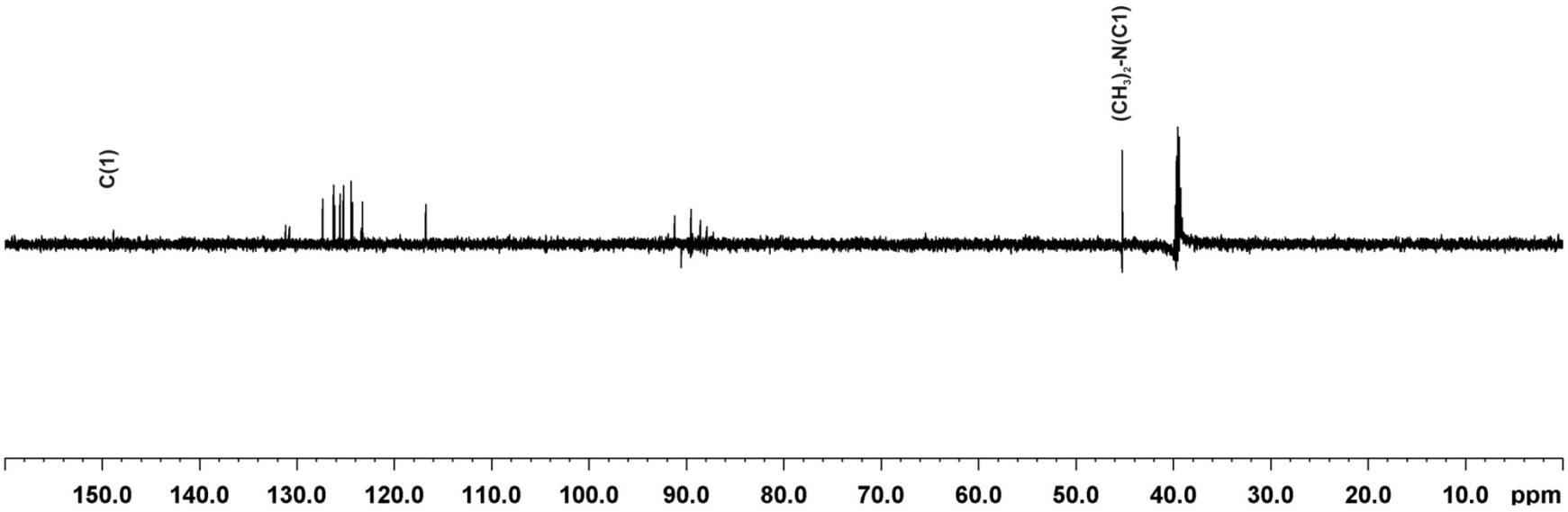

O
NH
N
O
DMTO
O
HO
OtBDMS
6
2 x C(q,pyrene)
C(2'')
2 x C(q,pyrene)
2 x CH(arom.,DMT)
2 x CH(arom.,DMT)
C(4'')/C(5'')/C(9'')/C(10'')
CH(arom.,DMT)
C(7'')
C(6'')/C(8'')
C(1'')/C(3'')
C(q,pyrene)
C(q,pyrene)
130.0
128.0
126.0
124.0
ppm
C(4)
2 x C(q,DMT)
C(2)
C(q,DMT)
C(6)
2 x C(q,DMT)
C(5)
CH(arom.,DMT)
C(1')
C(q,DMT)
C(4')
C(2')
C(3')
C(5')
2 x CH3O(DMT)
DMSO
(CH3)3-C-Si
(CH3)3-C-Si
2 x CH3Si
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
ppm

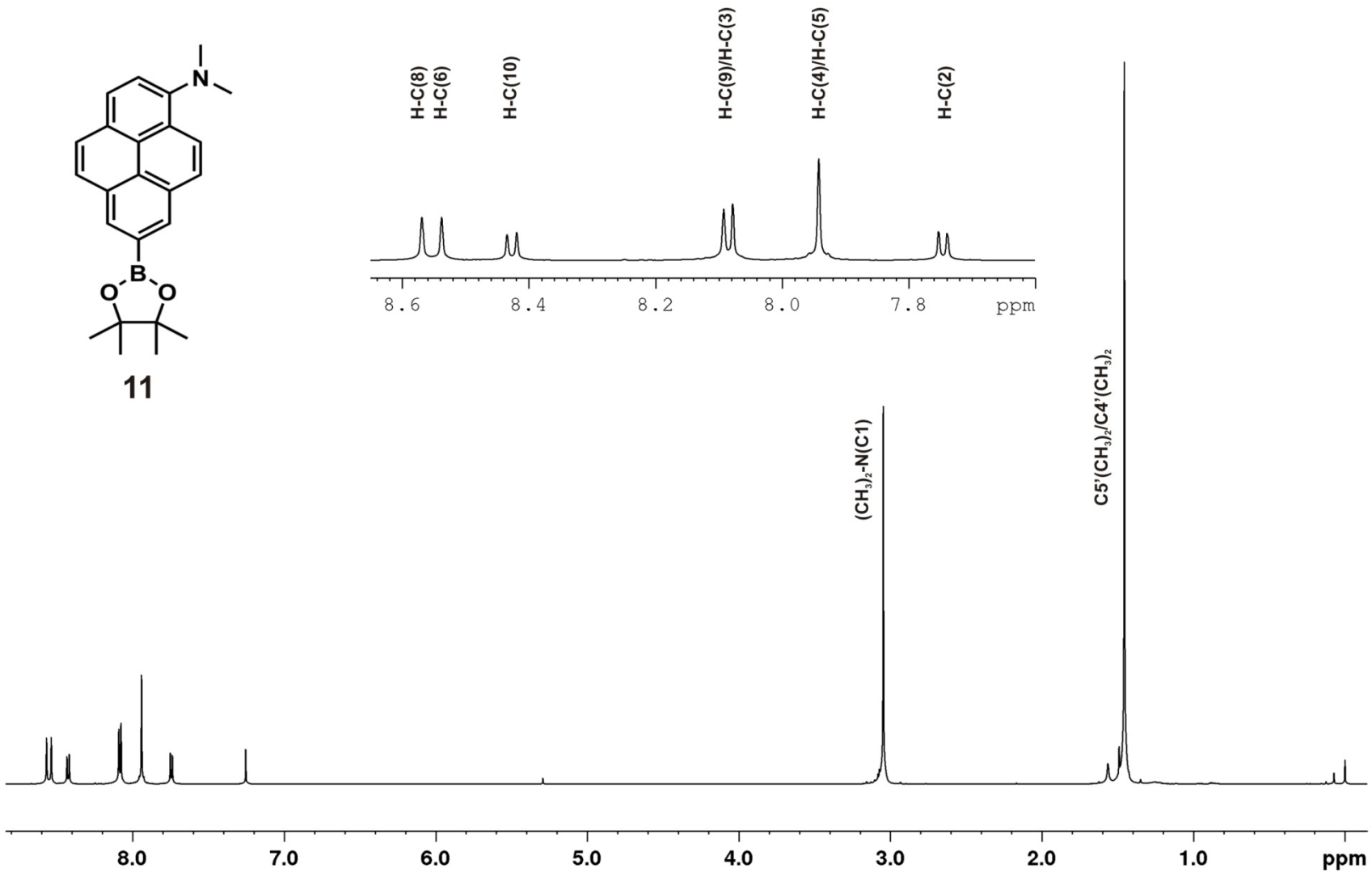

N
10
H-C(10)
H-C(6)/H-C(8)
H-C(3)
H-C(9)
H-C(4)
H-C(7)
H-C(5)
H-C(2)
8.4
8.2
8.0
7.8
ppm
(CH3)2-N(C1)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm

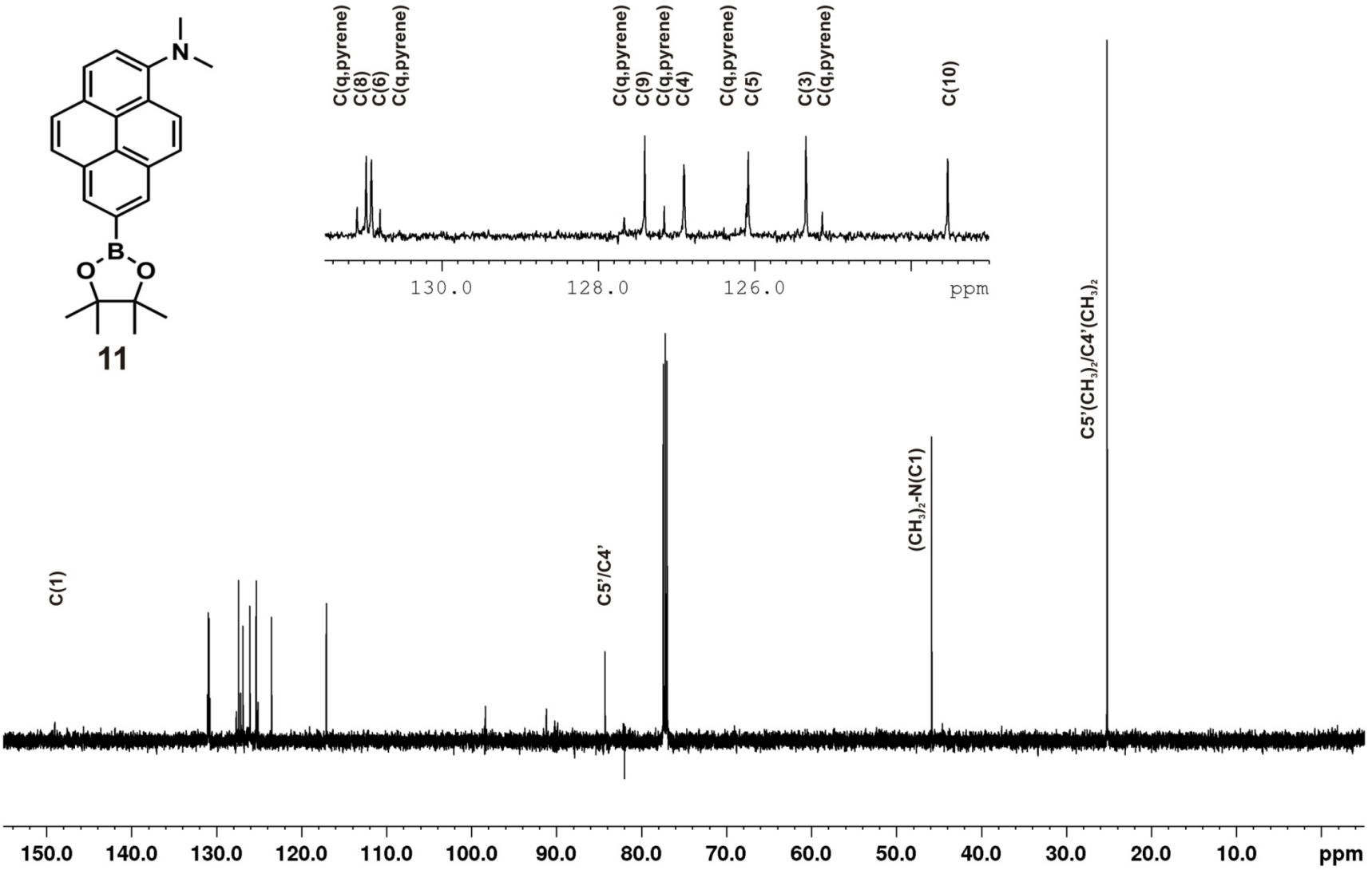


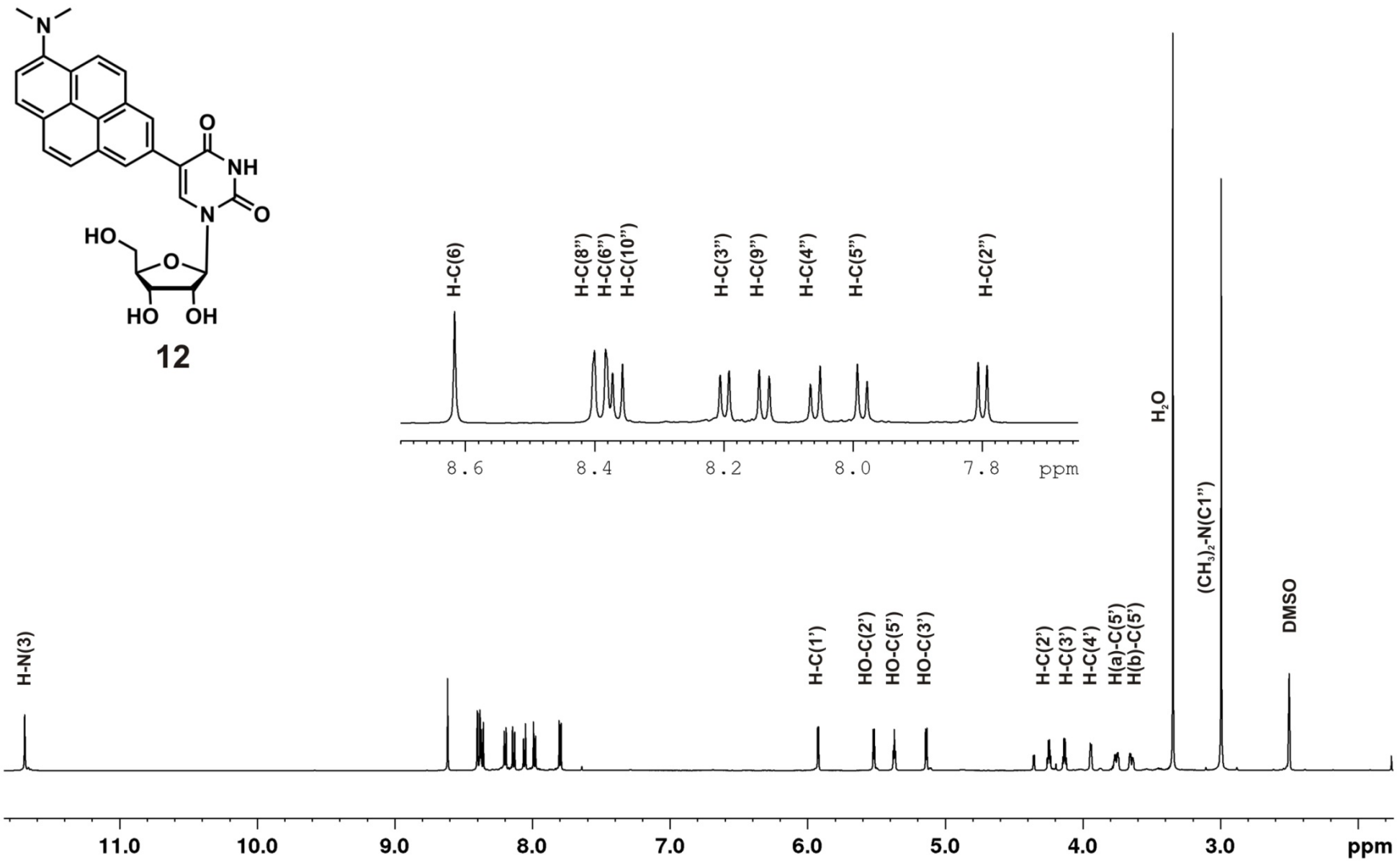
10

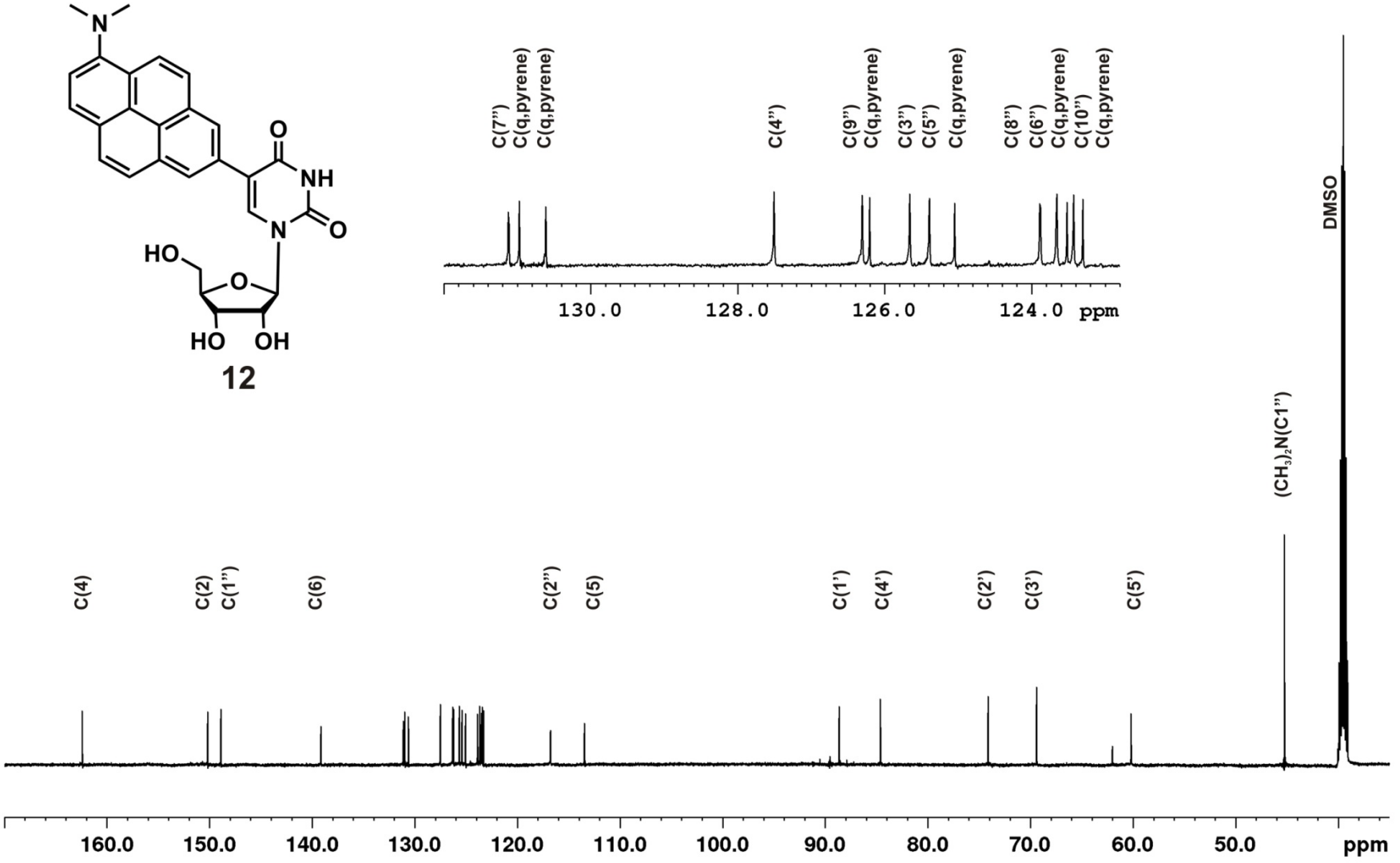

C(q,pyrene)
C(q,pyrene)
C(7)
C(4)
C(9)/C(q,pyrene)
C(3)
C(5)
C(6)/C(8)
C(q,pyrene)
C(10)
C(2)
132.0 130.0 128.0 126.0 124.0 122.0 120.0 118.0 ppm

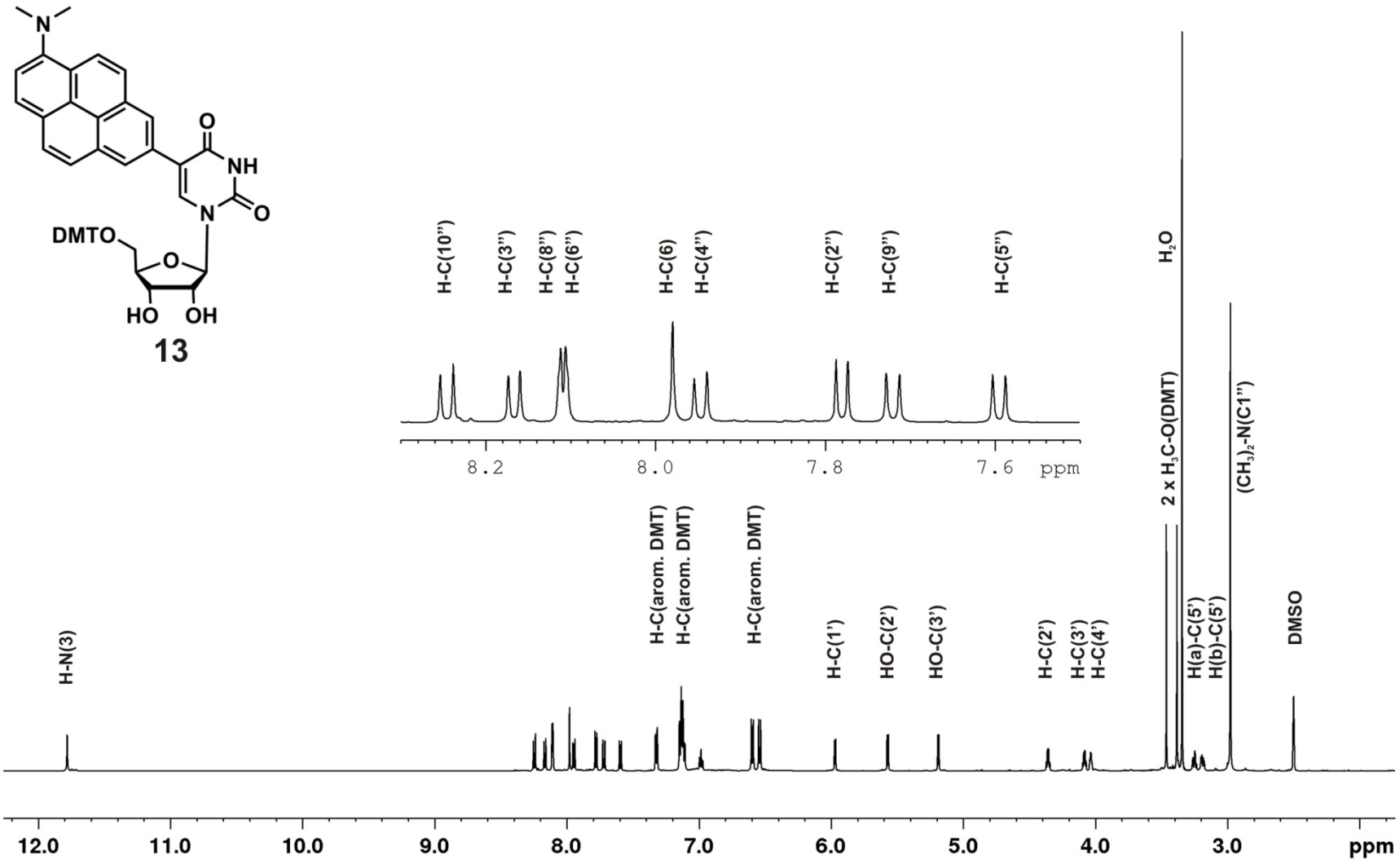

C(1)
$(CH_3)_2$-N(C1)
150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 ppm

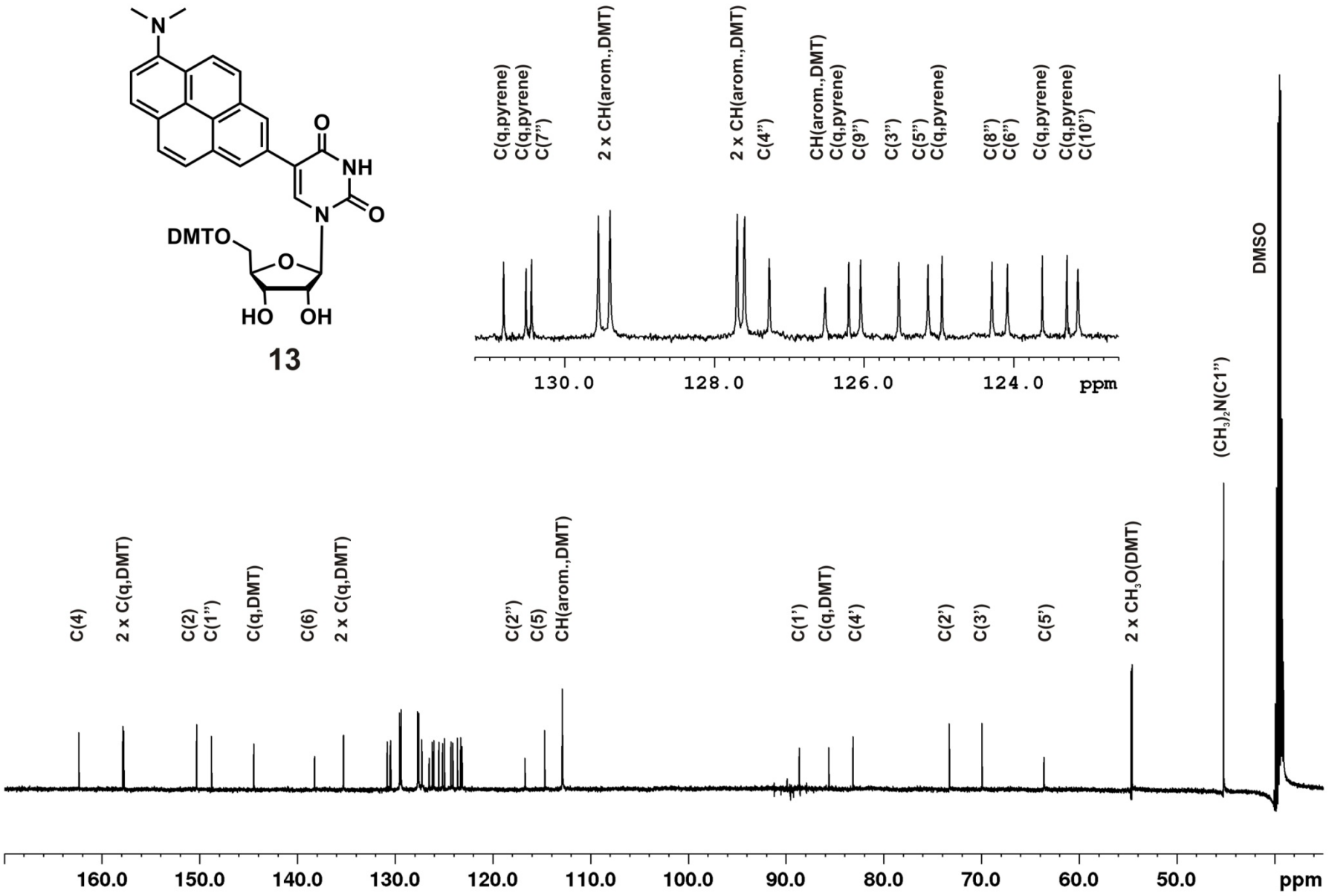

11
H-C(8)
H-C(6)
H-C(10)
H-C(9)/H-C(3)
H-C(4)/H-C(5)
H-C(2)
8.6
8.4
8.2
8.0
7.8
ppm
(CH3)2-N(C1)
C5'(CH3)2/C4'(CH3)2
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm

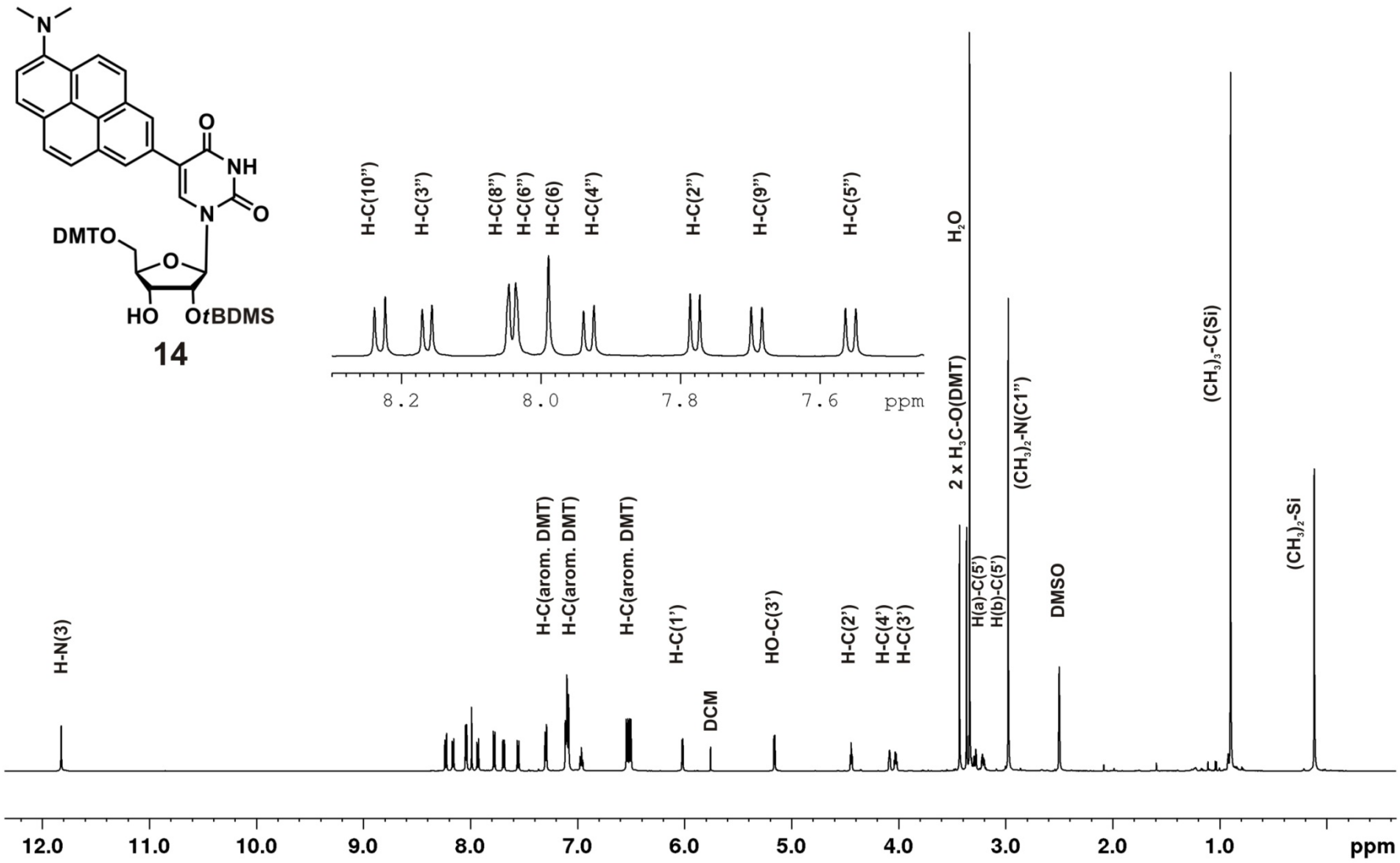

N
B
O
O
11
C(q,pyrene)
C(8)
C(6)
C(q,pyrene)
C(q,pyrene)
C(9)
C(q,pyrene)
C(4)
C(q,pyrene)
C(5)
C(3)
C(q,pyrene)
C(10)
130.0
128.0
126.0
ppm
C(1)
C5'/C4'
(CH3)2-N(C1)
C5'(CH3)2/C4'(CH3)2
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
ppm

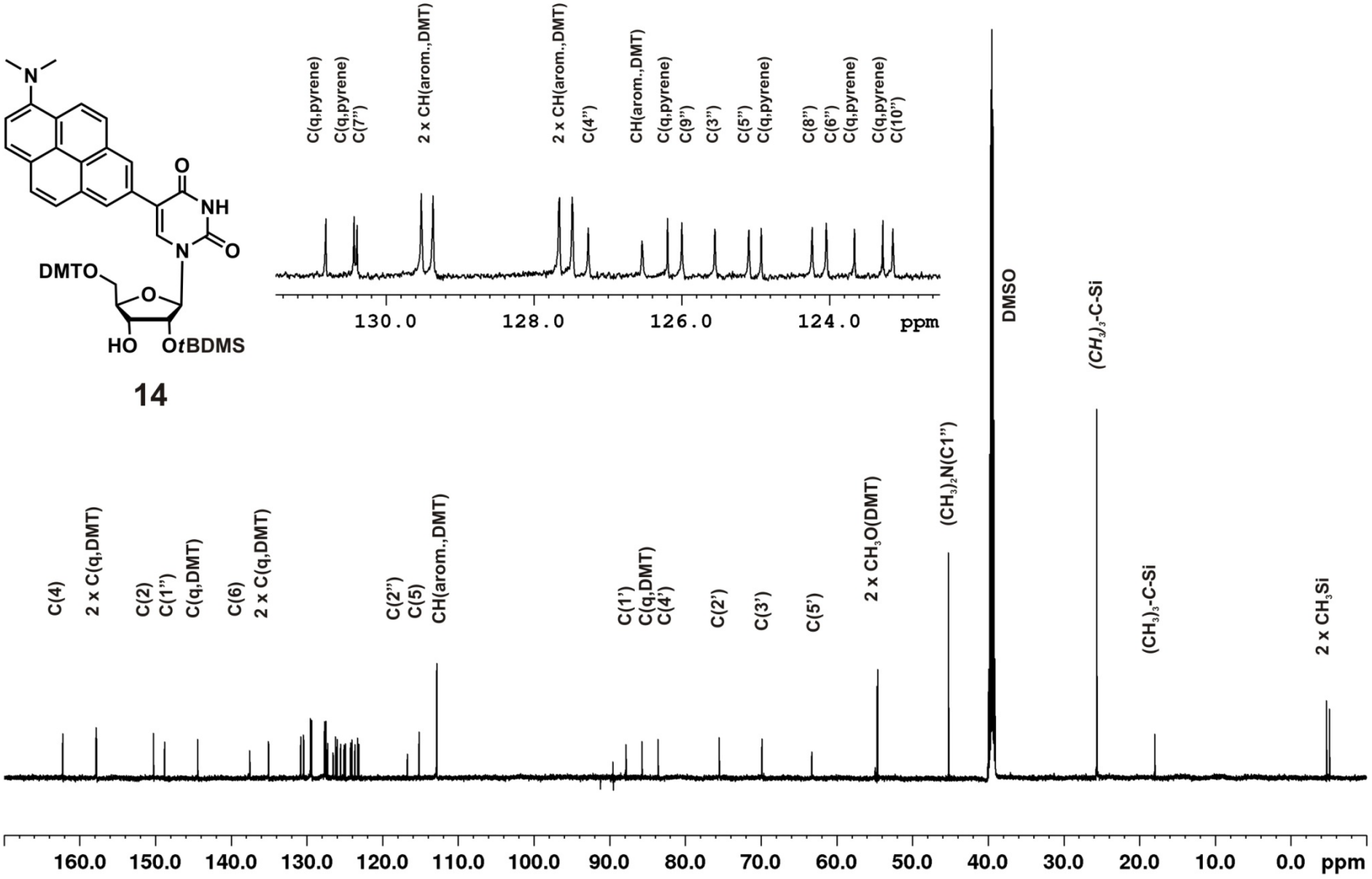

N
O
NH
N
O
HO
O
HO
OH
12
H-C(6)
H-C(8")
H-C(6")
H-C(10")
H-C(3")
H-C(9")
H-C(4")
H-C(5")
H-C(2")
8.6
8.4
8.2
8.0
7.8
ppm
H-N(3)
H-C(1')
HO-C(2')
HO-C(5')
HO-C(3')
H-C(2')
H-C(3')
H-C(4')
H(a)-C(5')
H(b)-C(5')
H2O
(CH3)2-N(C1")
DMSO
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
ppm


N
O
NH
N
O
HO
O
HO
OH
12
C(7'')
C(q,pyrene)
C(q,pyrene)
C(4'')
C(9'')
C(q,pyrene)
C(3'')
C(5'')
C(q,pyrene)
C(8'')
C(6'')
C(q,pyrene)
C(10'')
C(q,pyrene)
130.0
128.0
126.0
124.0
ppm
DMSO
(CH3)2N(C1'')
C(4)
C(2)
C(1'')
C(6)
C(2'')
C(5)
C(1')
C(4')
C(2')
C(3')
C(5')
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
ppm


N
O
NH
O
N
DMTO
O
HO
OH
13
H-C(10'')
H-C(3'')
H-C(8'')
H-C(6'')
H-C(6)
H-C(4'')
H-C(2'')
H-C(9'')
H-C(5'')
8.2
8.0
7.8
7.6
ppm
H2O
2 x H3C-O(DMT)
(CH3)2-N(C1'')
H-N(3)
H-C(arom. DMT)
H-C(arom. DMT)
H-C(arom. DMT)
H-C(1')
HO-C(2')
HO-C(3')
H-C(2')
H-C(3')
H-C(4')
H(a)-C(5')
H(b)-C(5')
DMSO
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
ppm


N
O
NH
N
O
DMTO
O
HO
OH
13
C(q,pyrene)
C(q,pyrene)
C(7'')
2 x CH(arom.,DMT)
2 x CH(arom.,DMT)
C(4'')
CH(arom.,DMT)
C(q,pyrene)
C(9'')
C(3'')
C(5'')
C(q,pyrene)
C(8'')
C(6'')
C(q,pyrene)
C(q,pyrene)
C(10'')
130.0
128.0
126.0
124.0
ppm
DMSO
(CH3)2N(C1'')
C(4)
2 x C(q,DMT)
C(2)
C(1'')
C(q,DMT)
C(6)
2 x C(q,DMT)
C(2'')
C(5)
CH(arom.,DMT)
C(1')
C(q,DMT)
C(4')
C(2')
C(3')
C(5')
2 x CH3O(DMT)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
ppm


N
O
NH
N
O
DMTO
O
HO
OtBDMS
14
H-C(10'')
H-C(3'')
H-C(8'')
H-C(6'')
H-C(6)
H-C(4'')
H-C(2'')
H-C(9'')
H-C(5'')
8.2
8.0
7.8
7.6
ppm
H-N(3)
H-C(arom. DMT)
H-C(arom. DMT)
H-C(arom. DMT)
H-C(1')
DCM
HO-C(3')
H-C(2')
H-C(4')
H-C(3')
H2O
2 x H3C-O(DMT)
H(a)-C(5')
H(b)-C(5')
(CH3)2-N(C1'')
DMSO
(CH3)3-C(Si)
(CH3)2-Si
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm


N
O
NH
N
O
DMTO
O
HO
OtBDMS
14
C(q,pyrene)
C(q,pyrene)
C(7'')
2 x CH(arom.,DMT)
2 x CH(arom.,DMT)
C(4'')
CH(arom.,DMT)
C(q,pyrene)
C(9'')
C(3'')
C(5'')
C(q,pyrene)
C(8'')
C(6'')
C(q,pyrene)
C(q,pyrene)
C(10'')
130.0
128.0
126.0
124.0
ppm
DMSO
(CH3)3-C-Si
C(4)
2 x C(q,DMT)
C(2)
C(1'')
C(q,DMT)
C(6)
2 x C(q,DMT)
C(2'')
C(5)
CH(arom.,DMT)
C(1')
C(q,DMT)
C(4')
C(2')
C(3')
C(5')
2 x CH3O(DMT)
(CH3)2N(C1'')
(CH3)3-C-Si
2 x CH3Si
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
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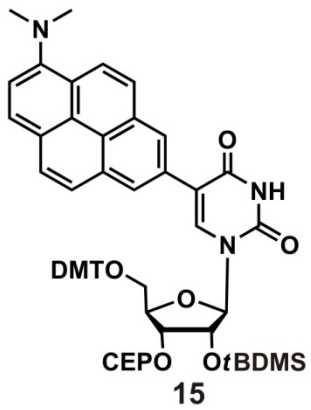
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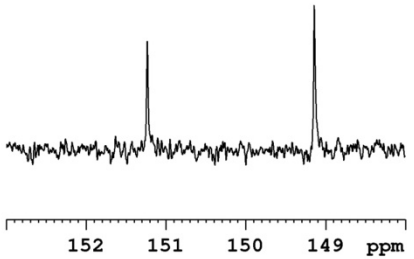
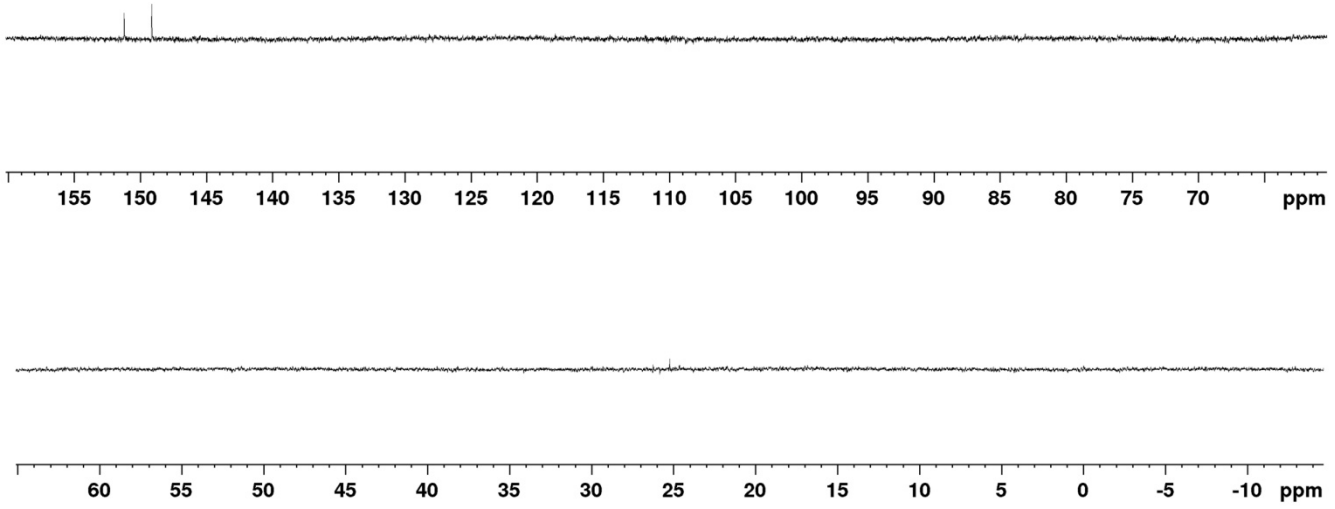
NH
N
O
DMTO
O
CEPO
OtBDMS

15


152
151
150
149
ppm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95
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ppm
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45
40
35
30
25
20
15
10
5
0
-5
-10
ppm