Supporting Information

Synthesis of the Terminally Modified Oligonucleotides and Their Hybridization Dependent on the Size of the Target RNAs

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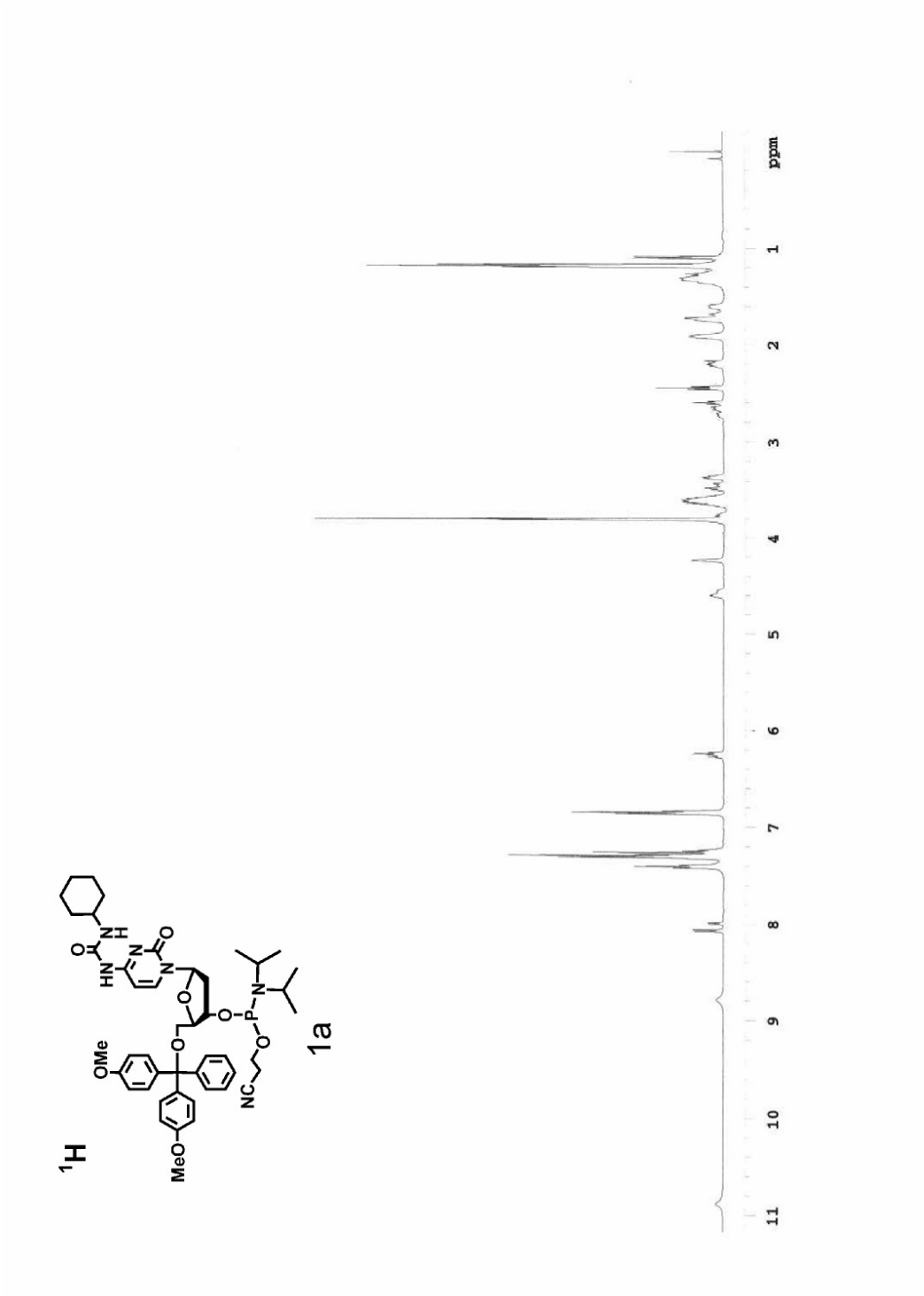
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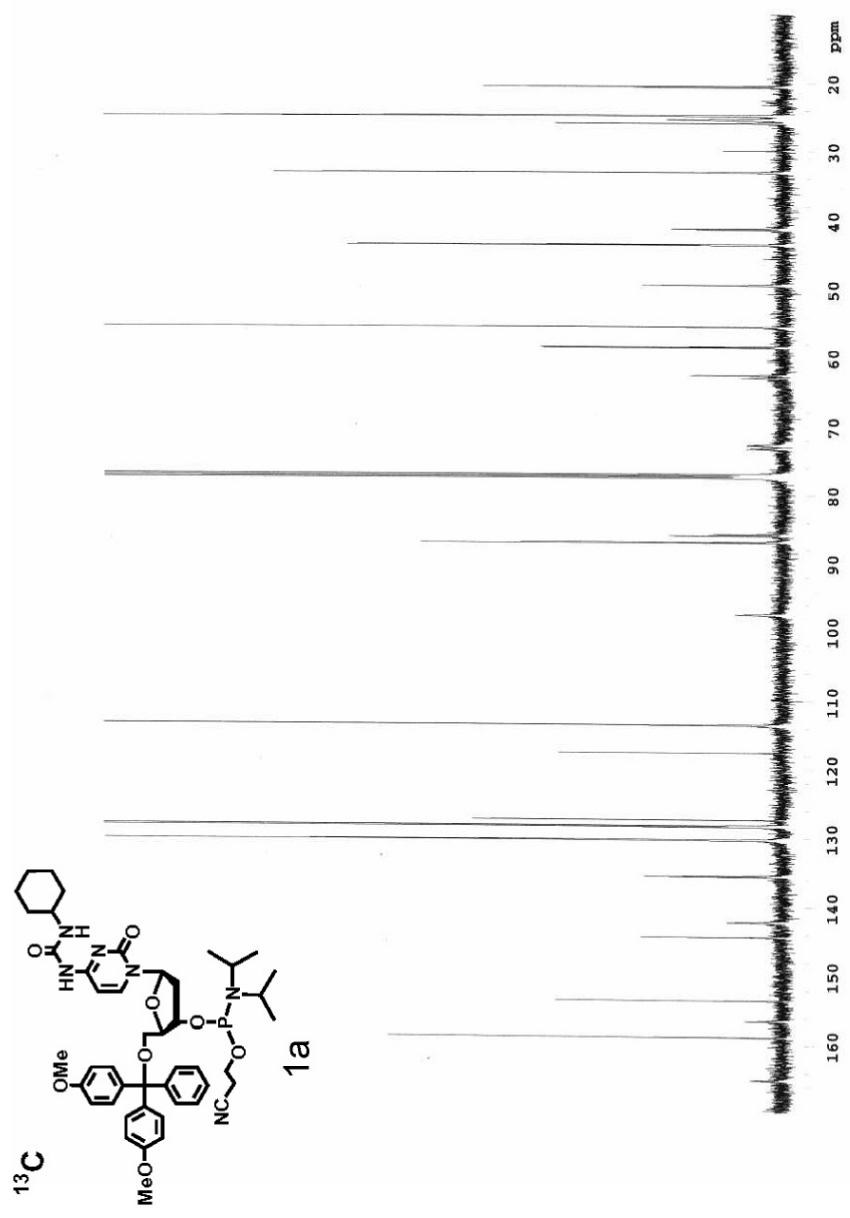
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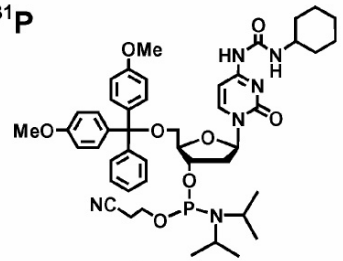

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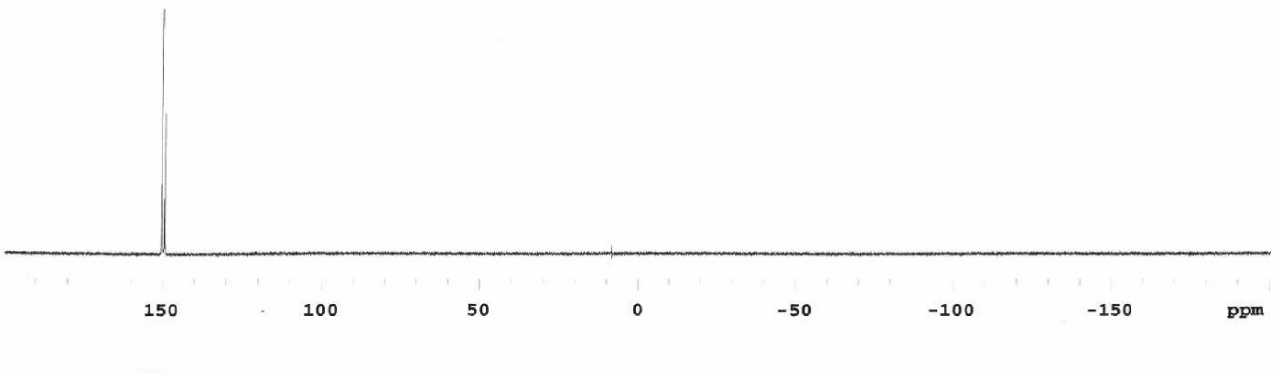

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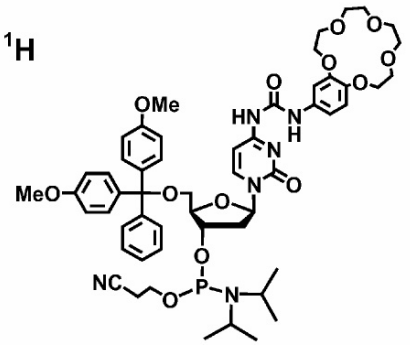

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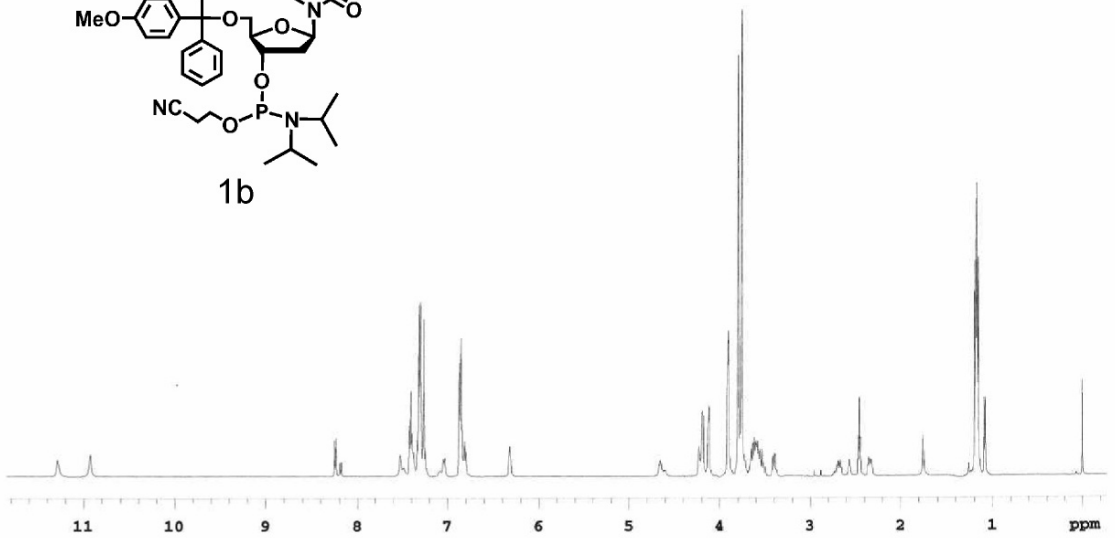

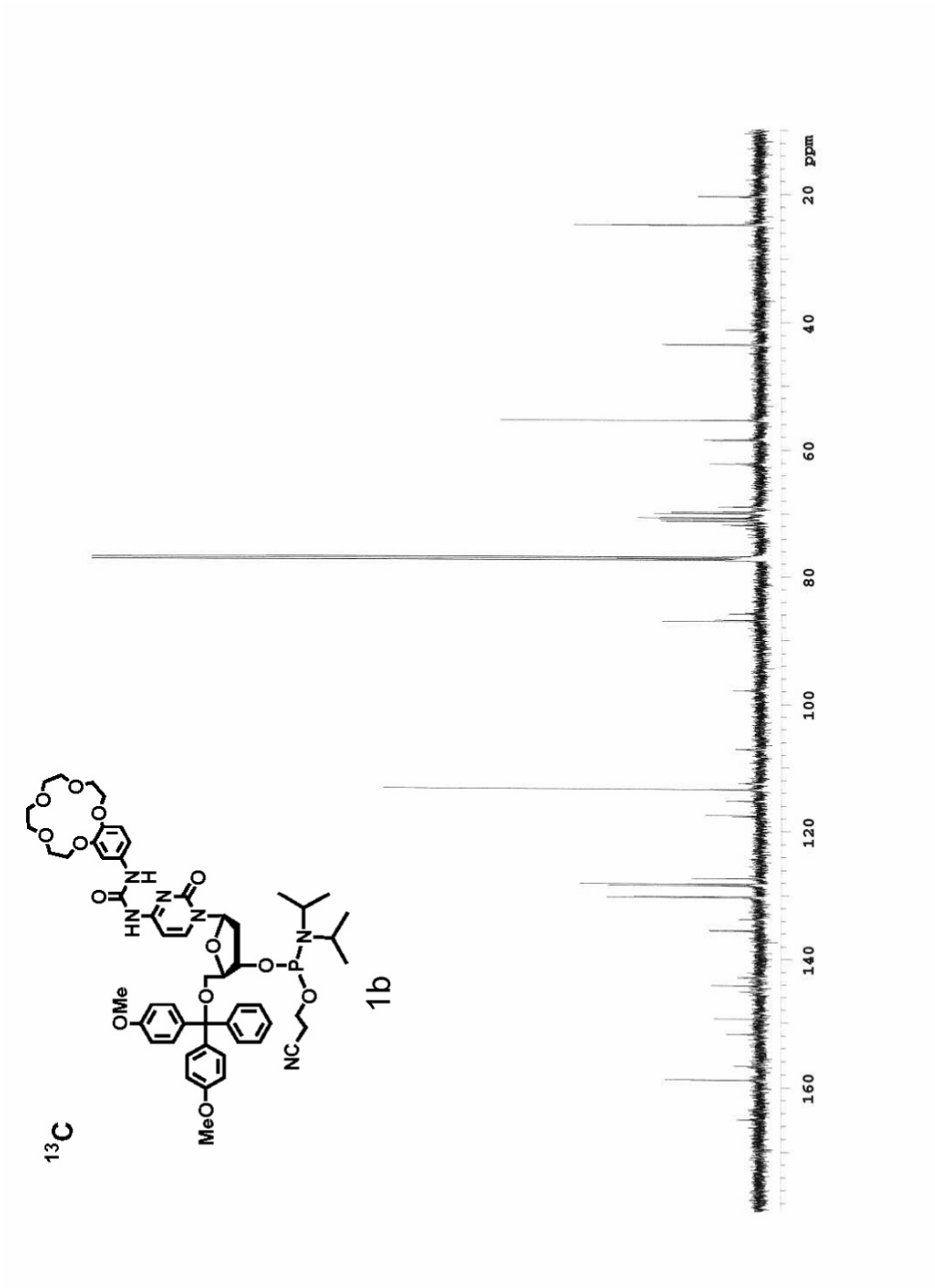

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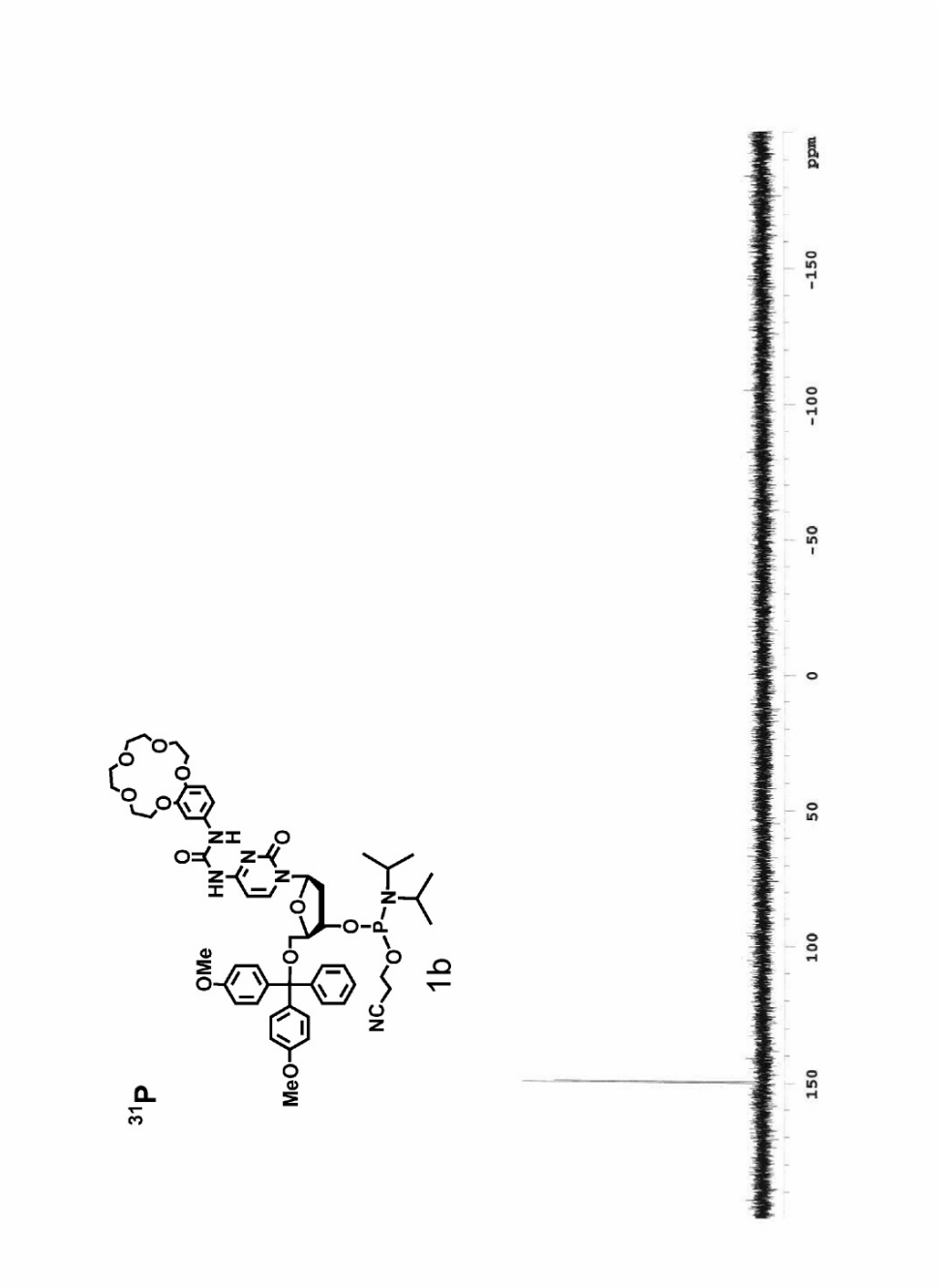
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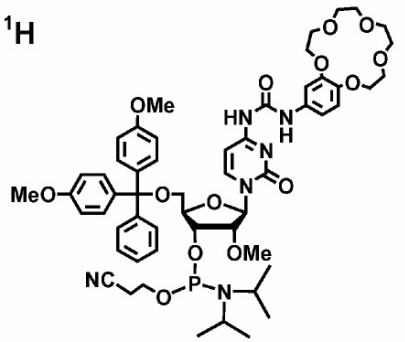
^{1}H



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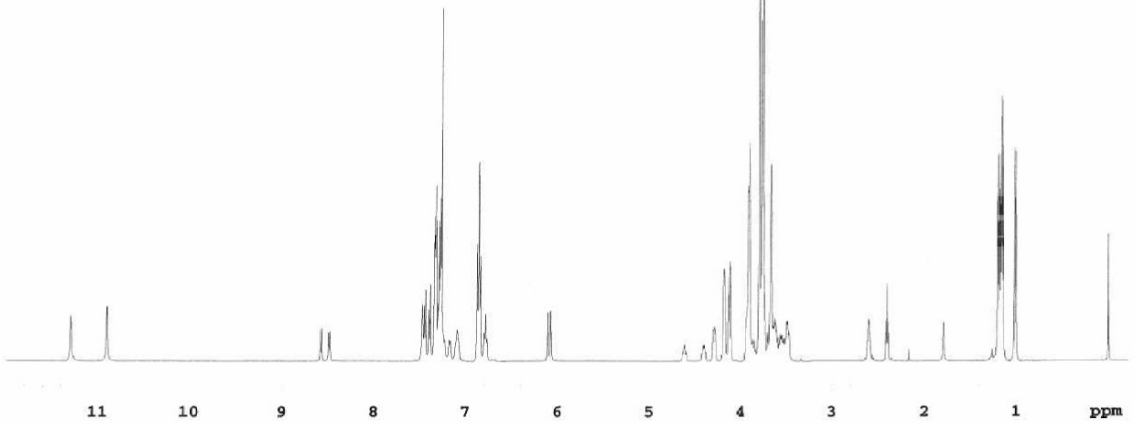

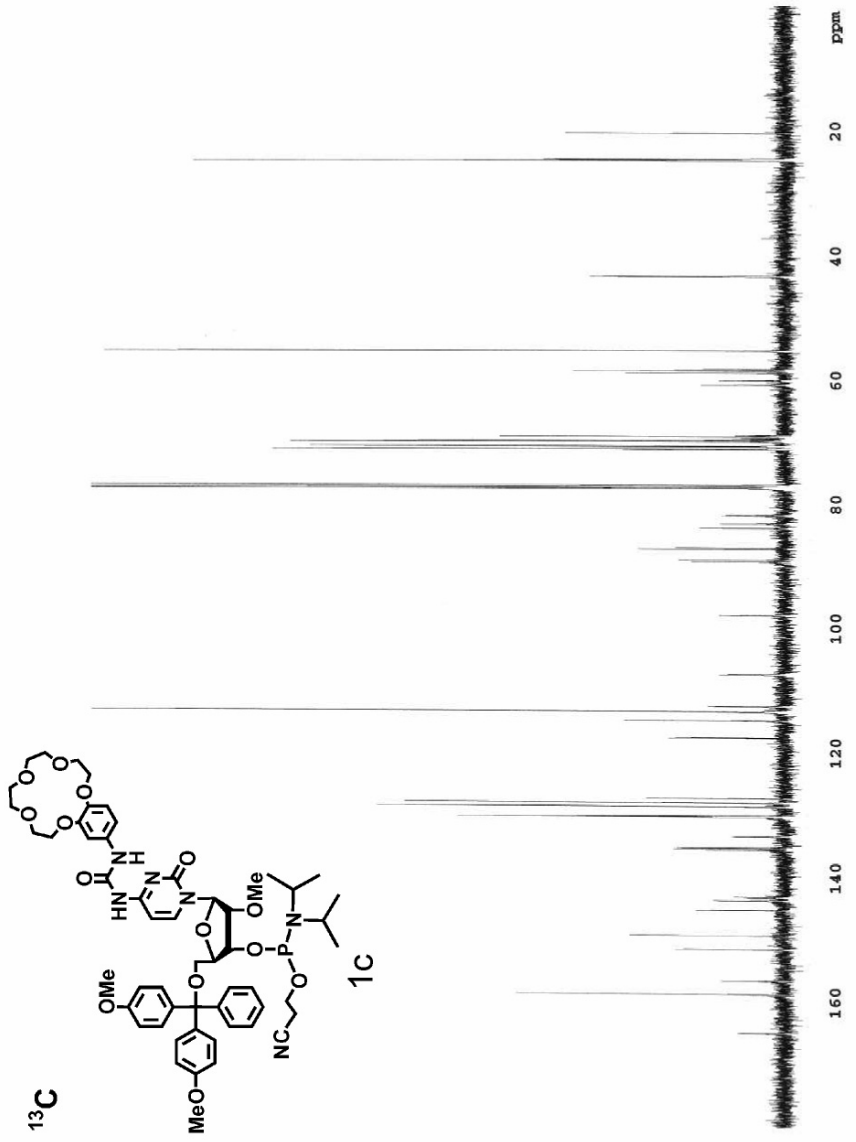
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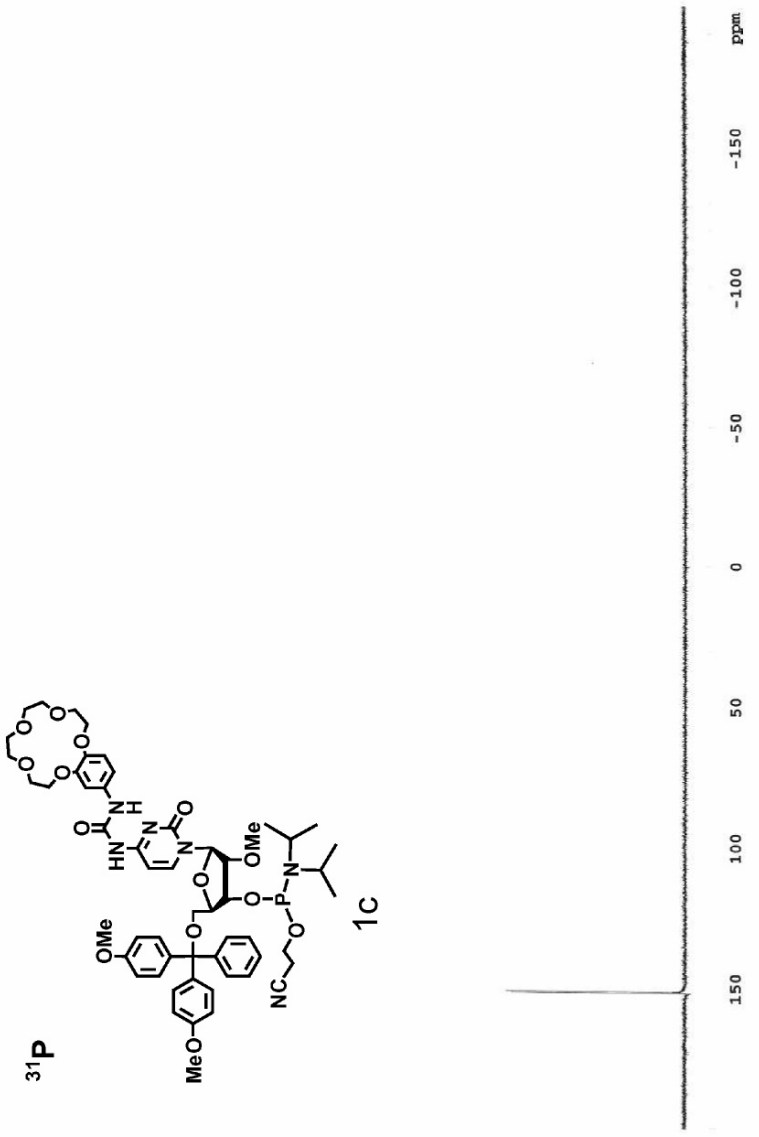
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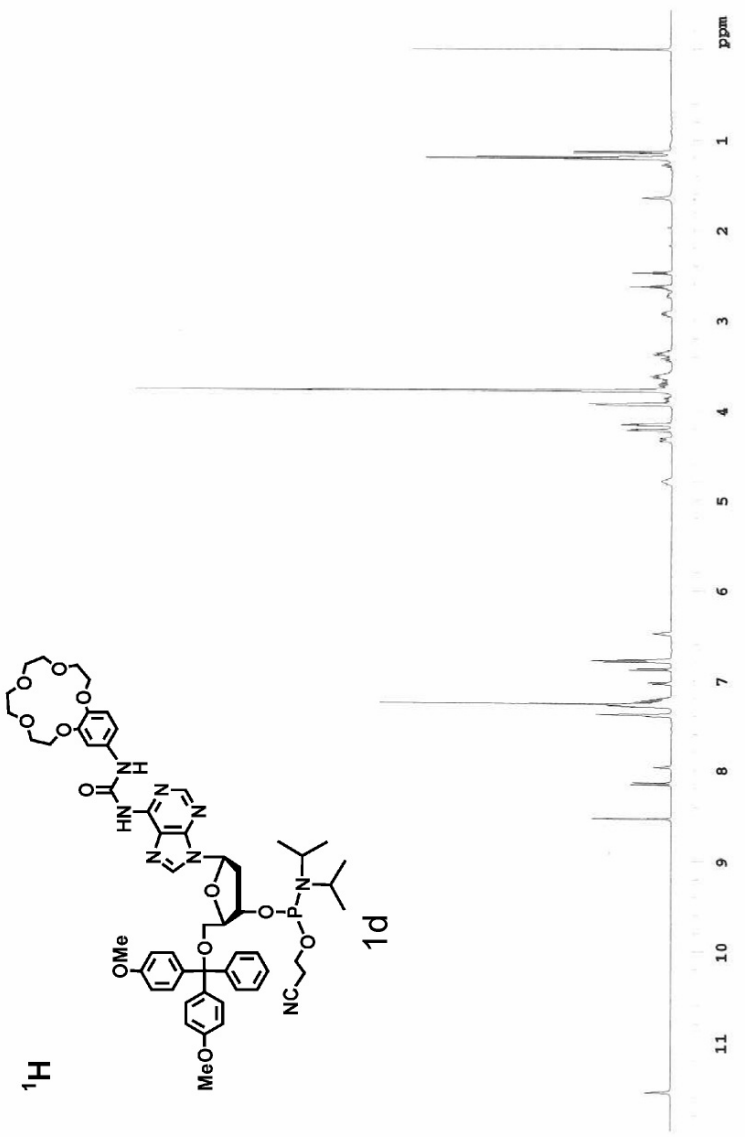
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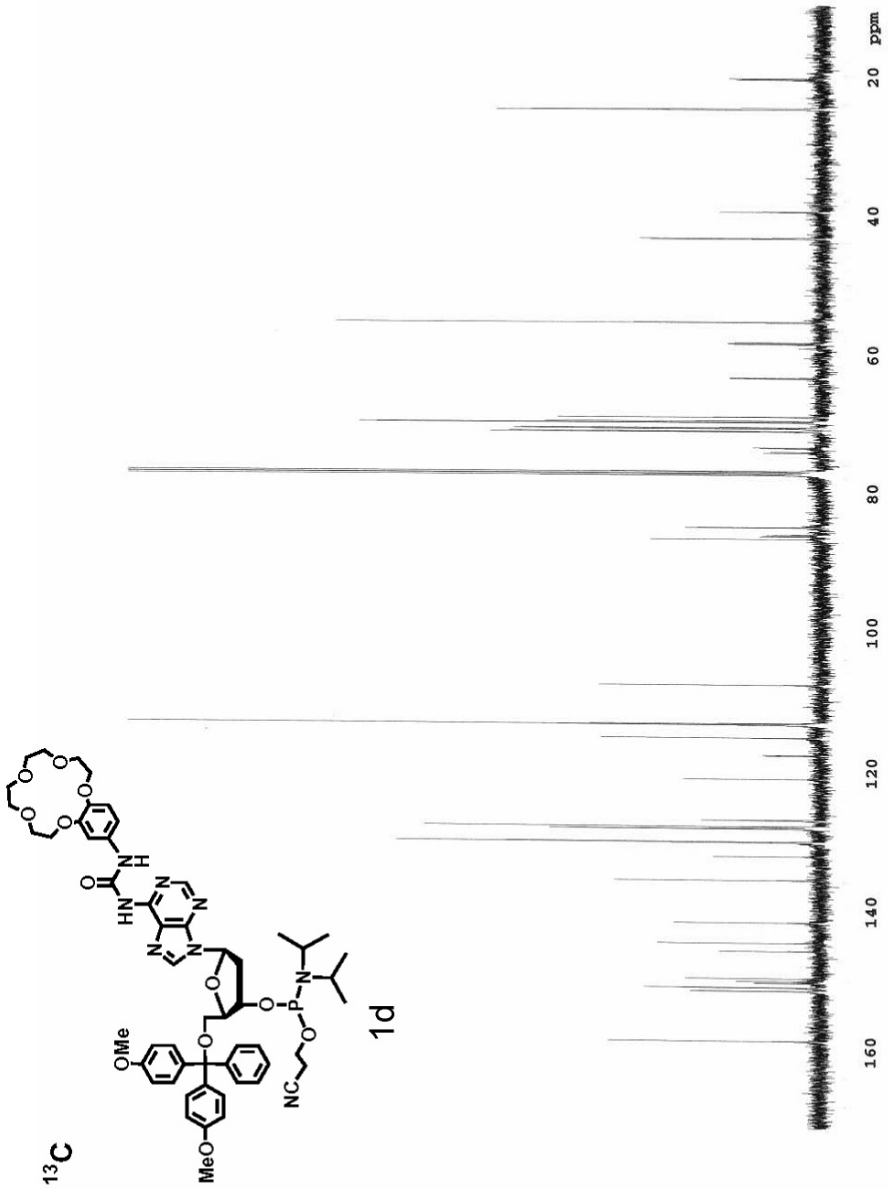

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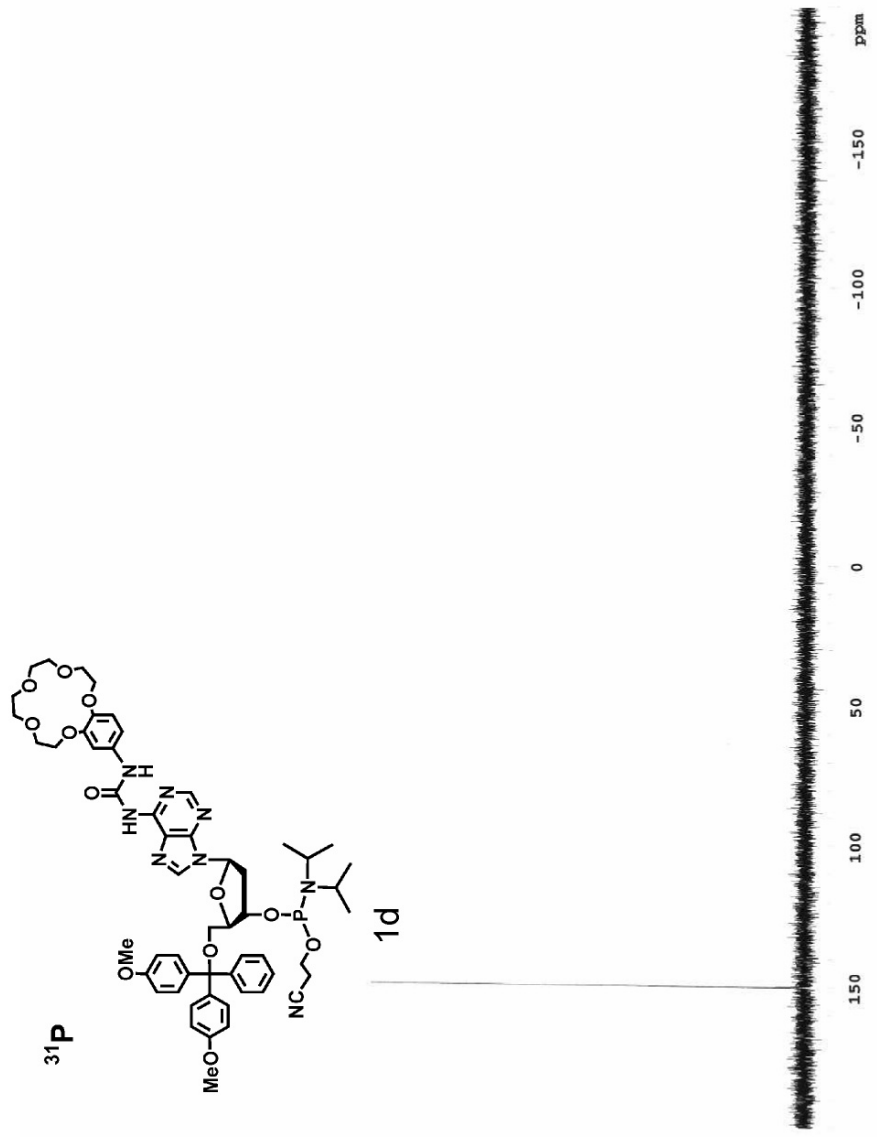
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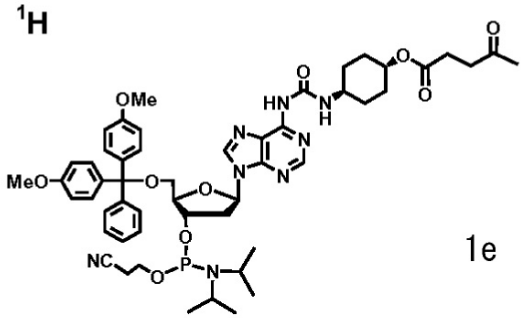

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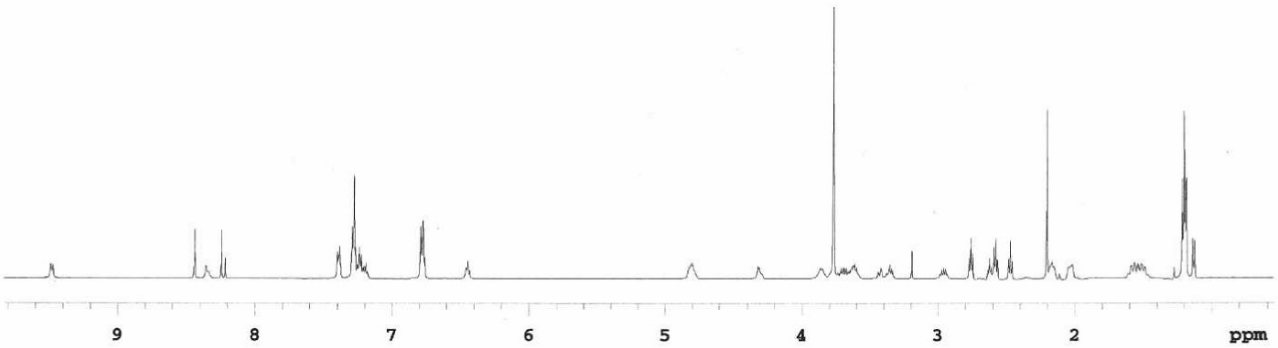

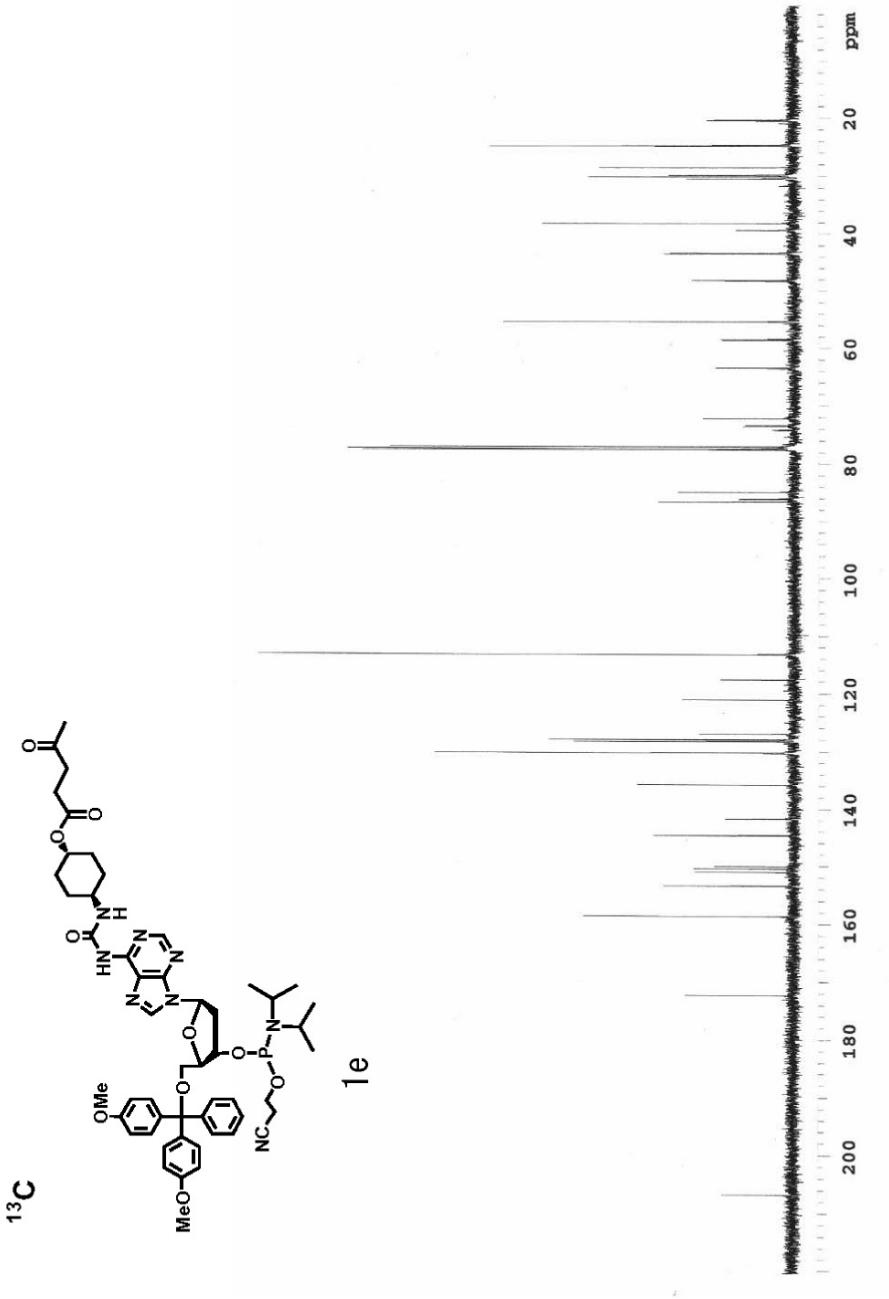
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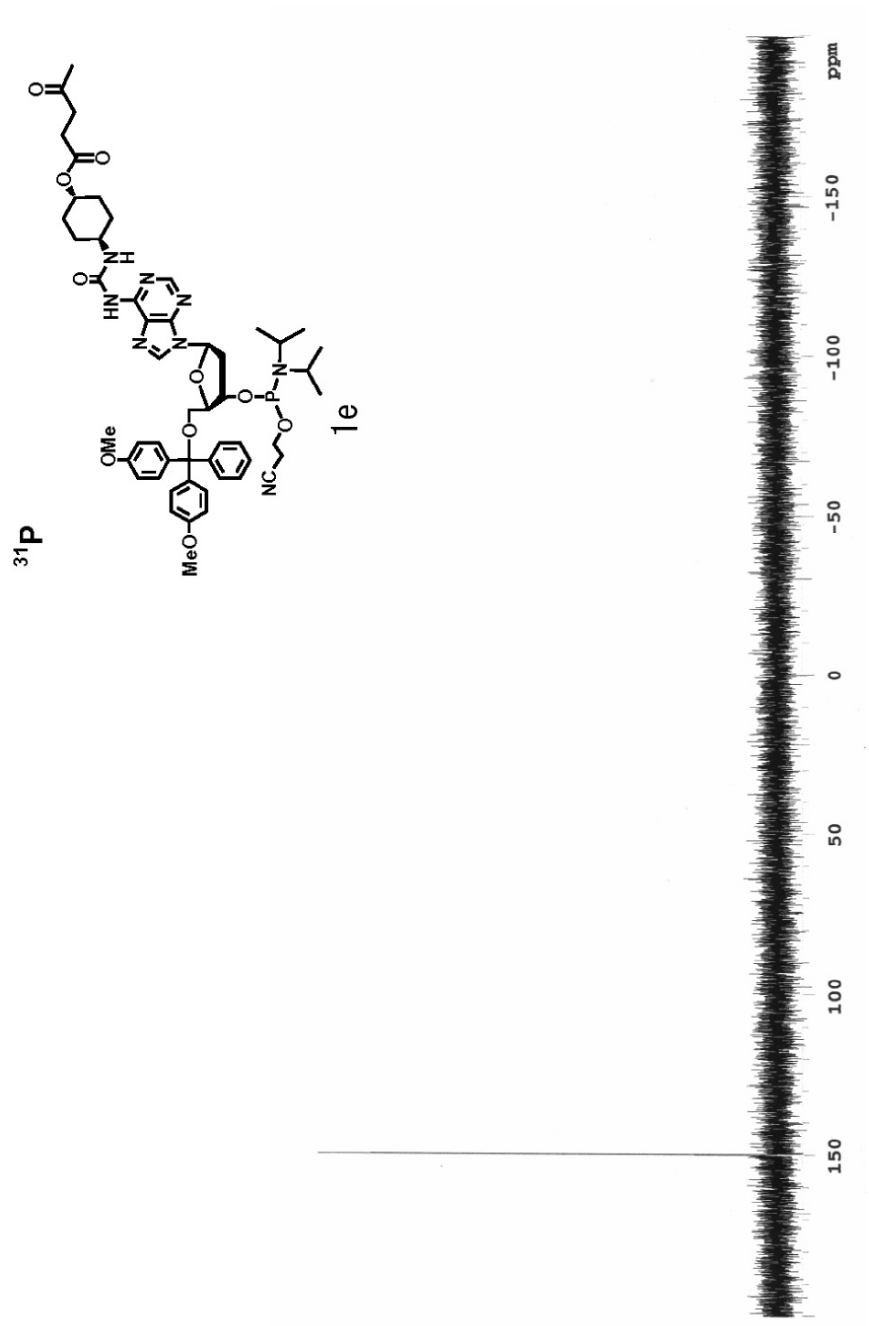
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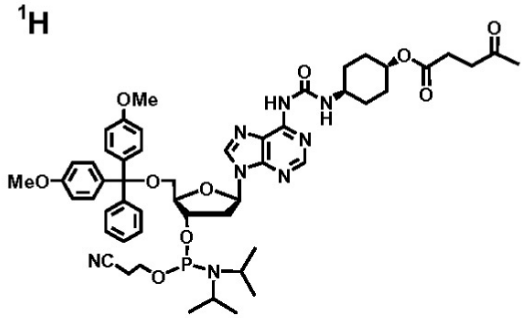

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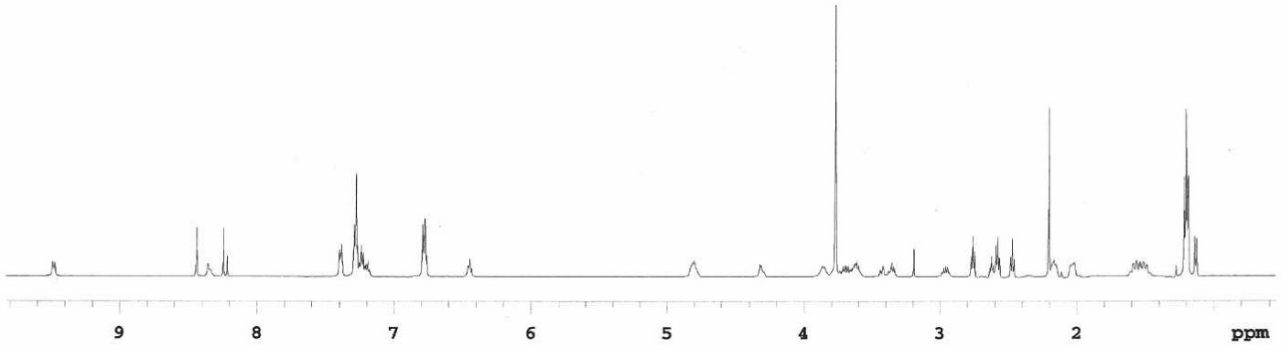

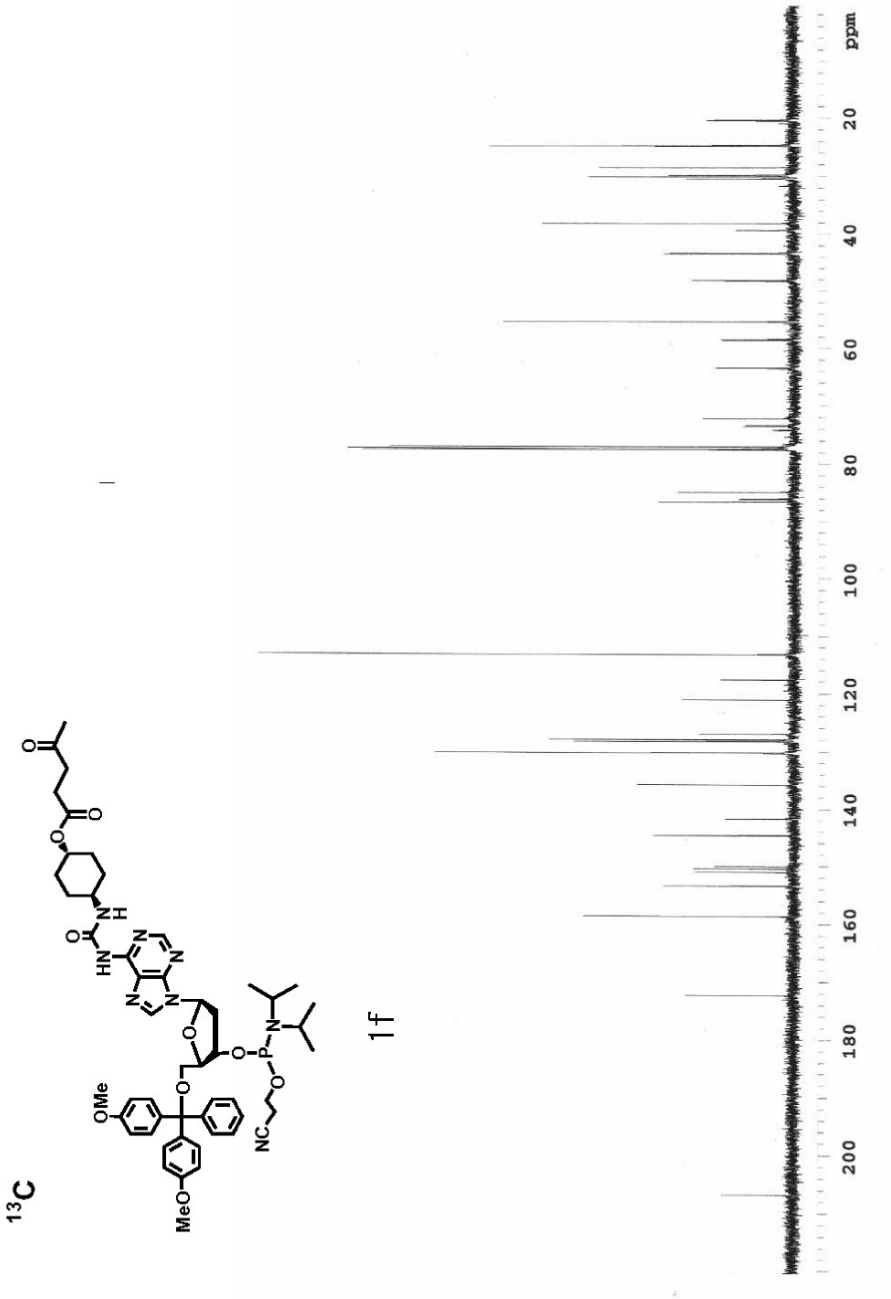
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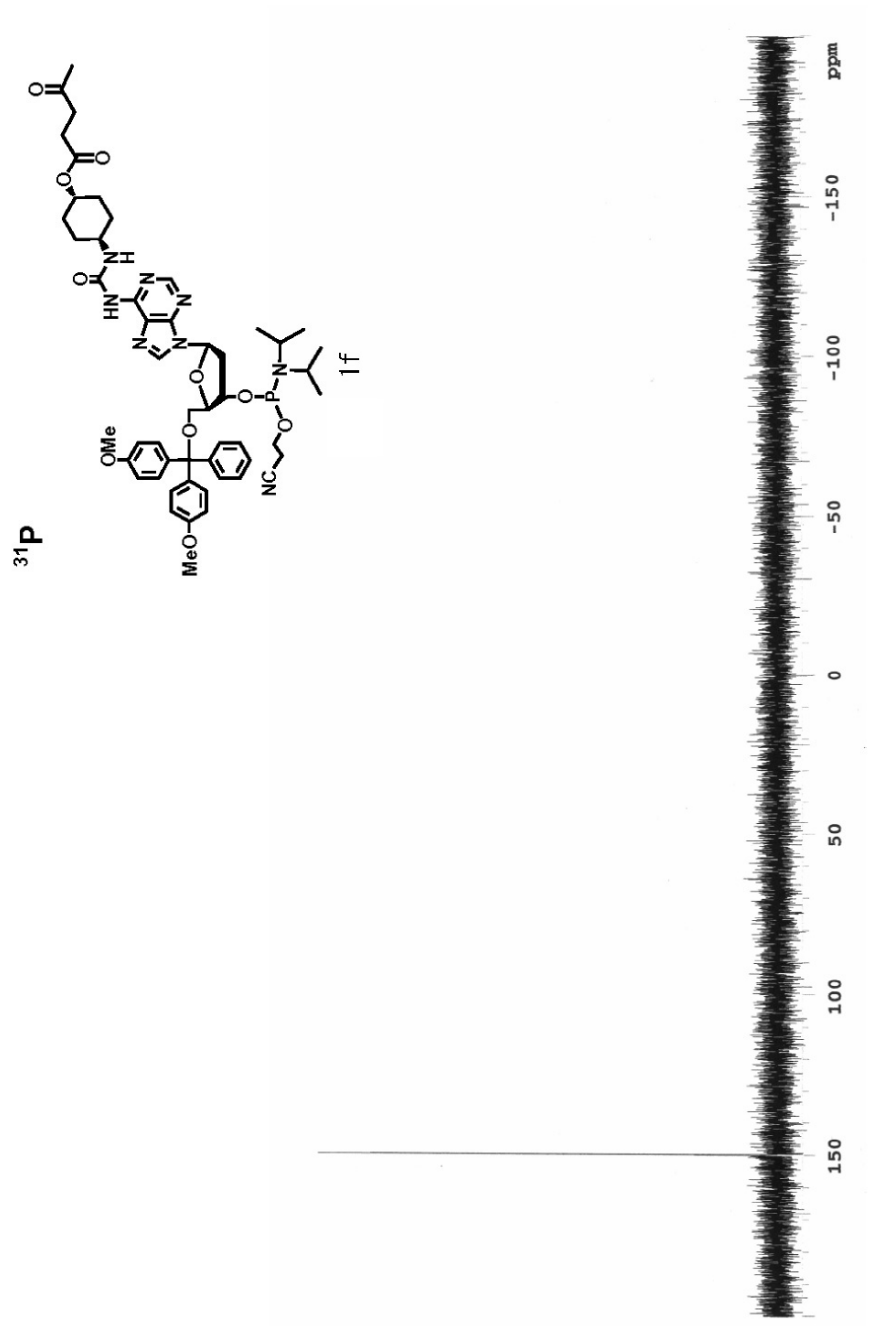
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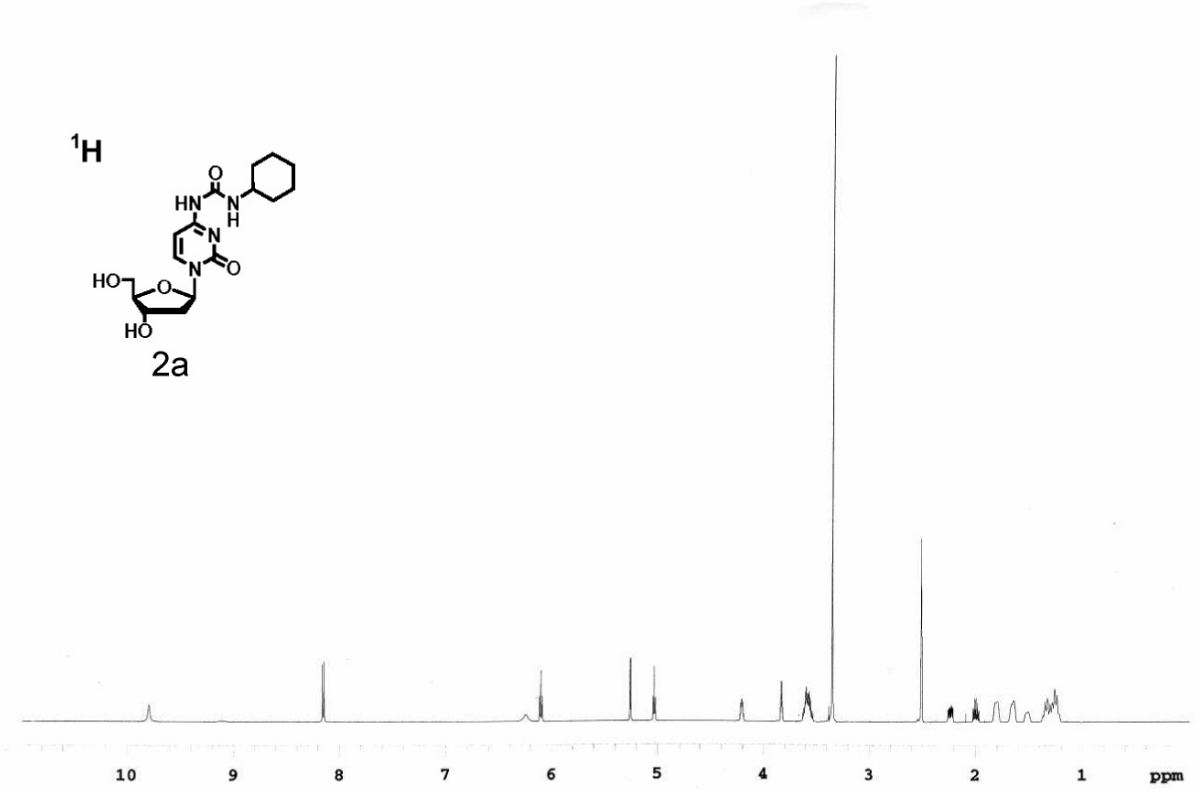
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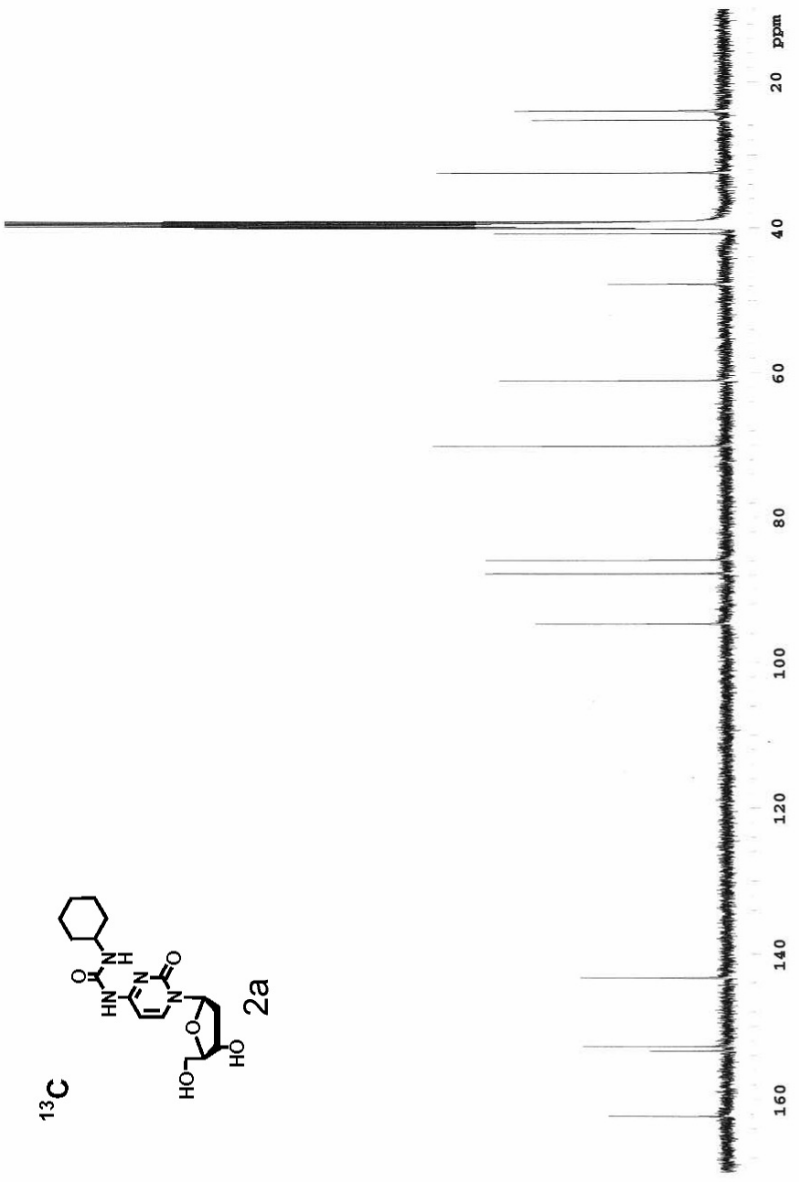
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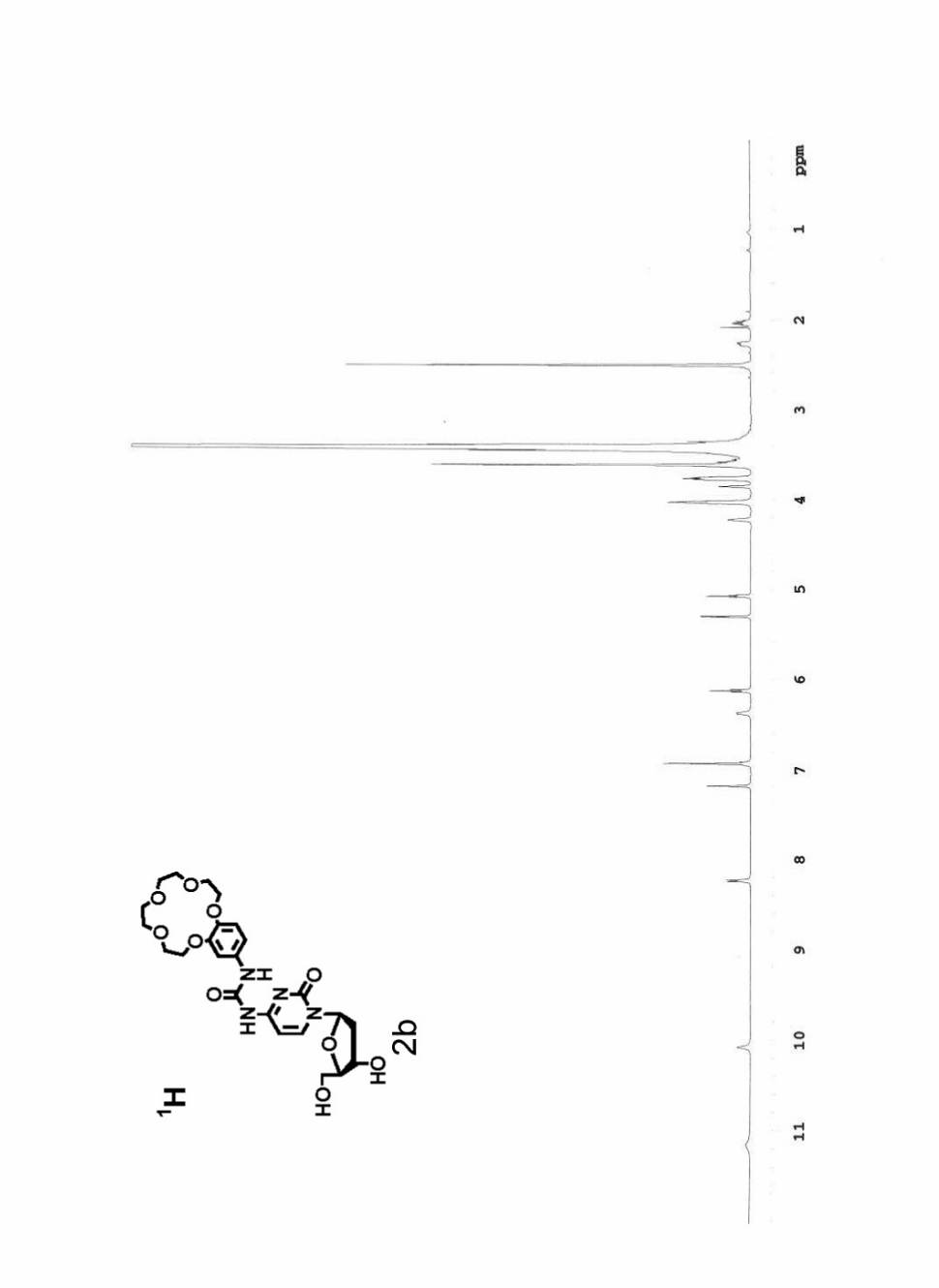

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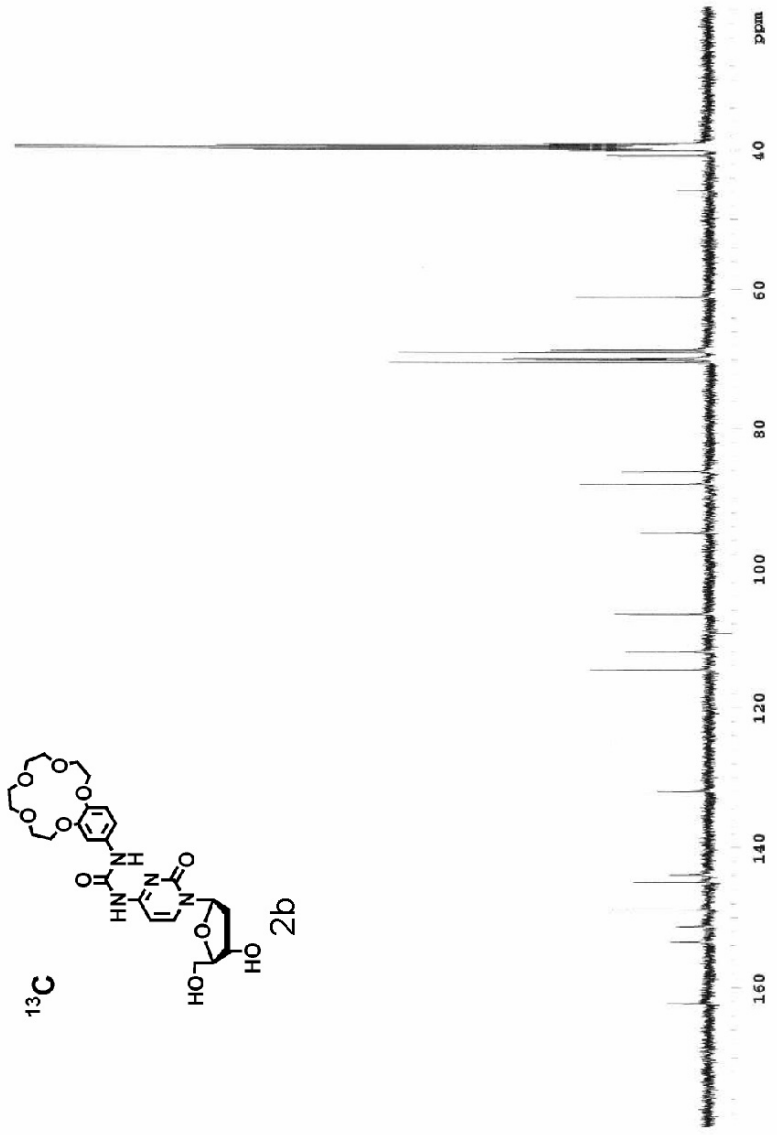
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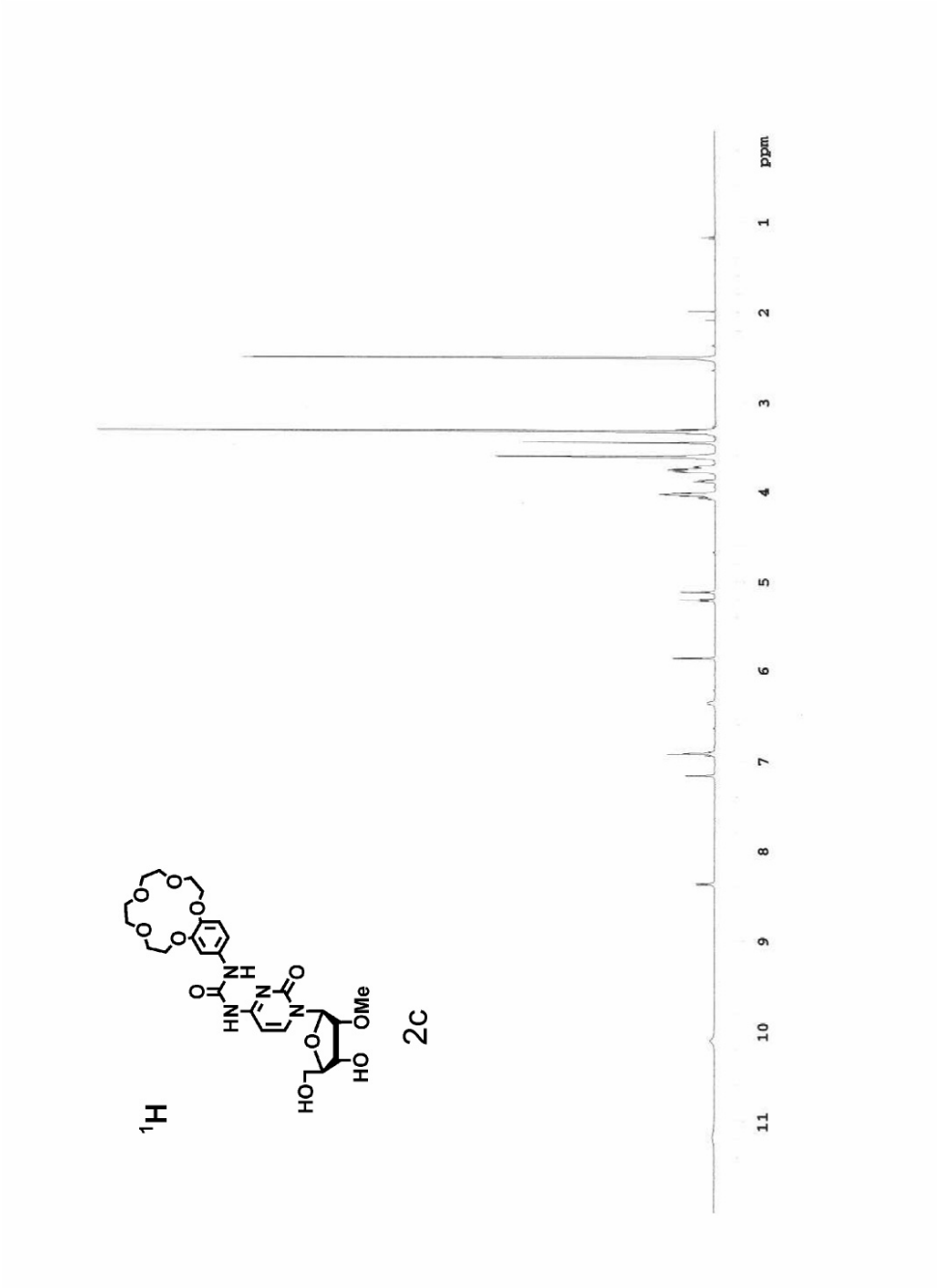

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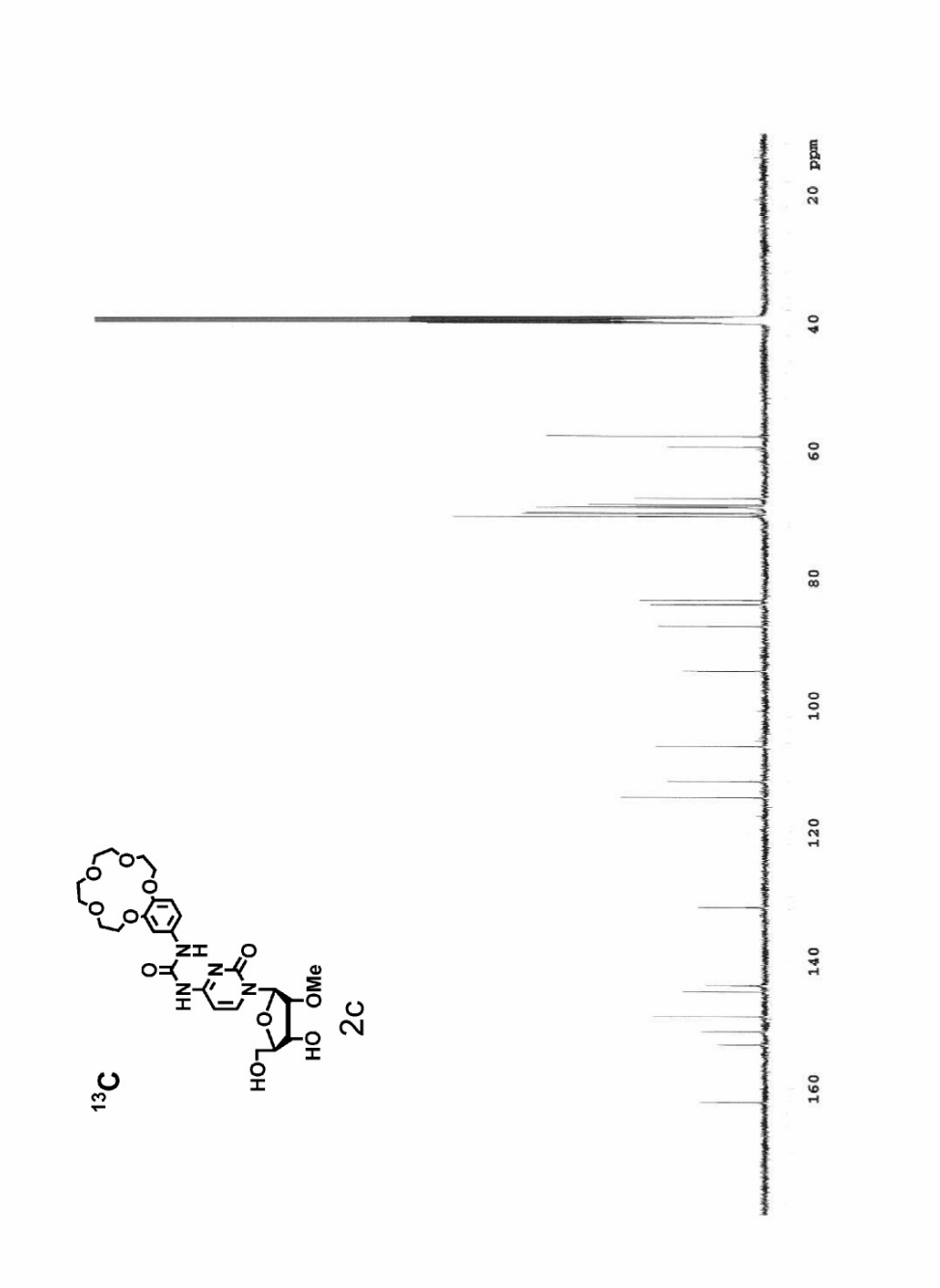

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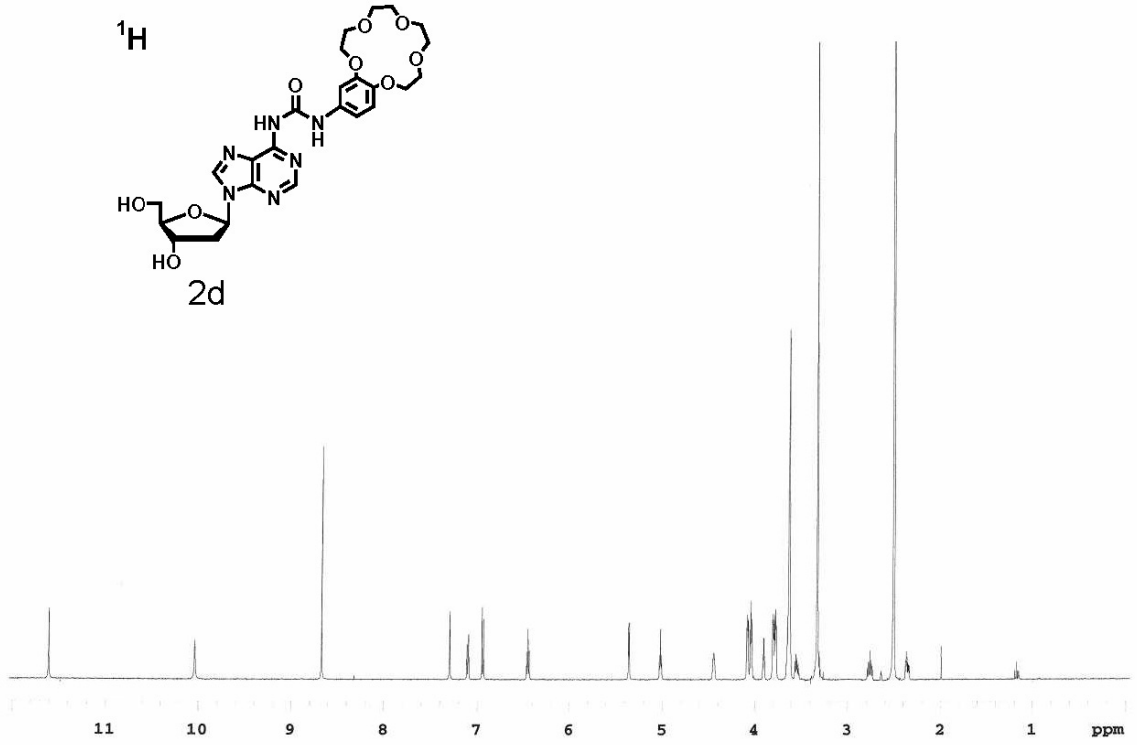
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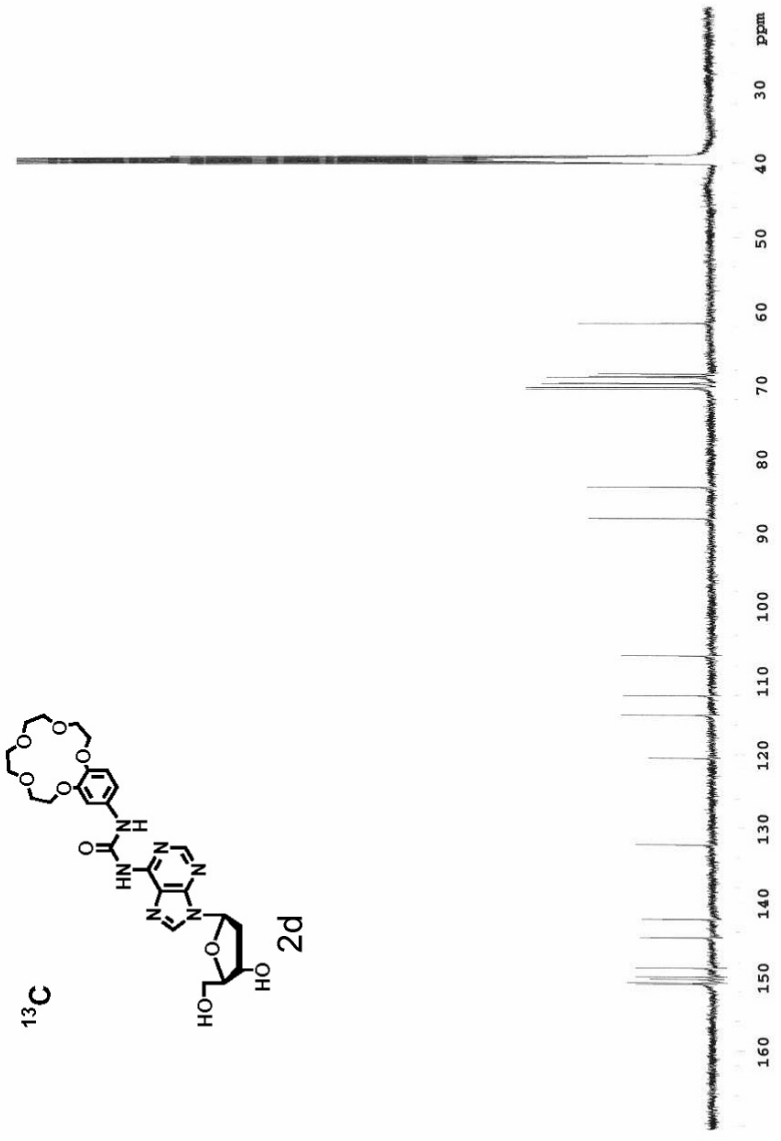
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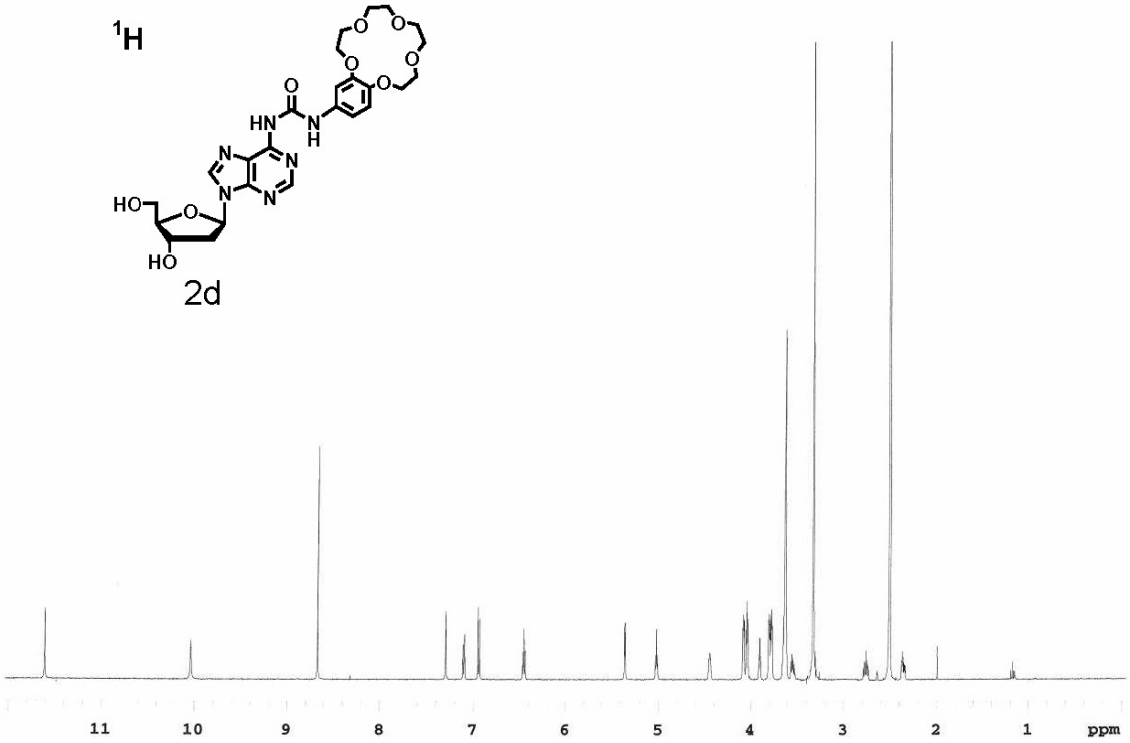
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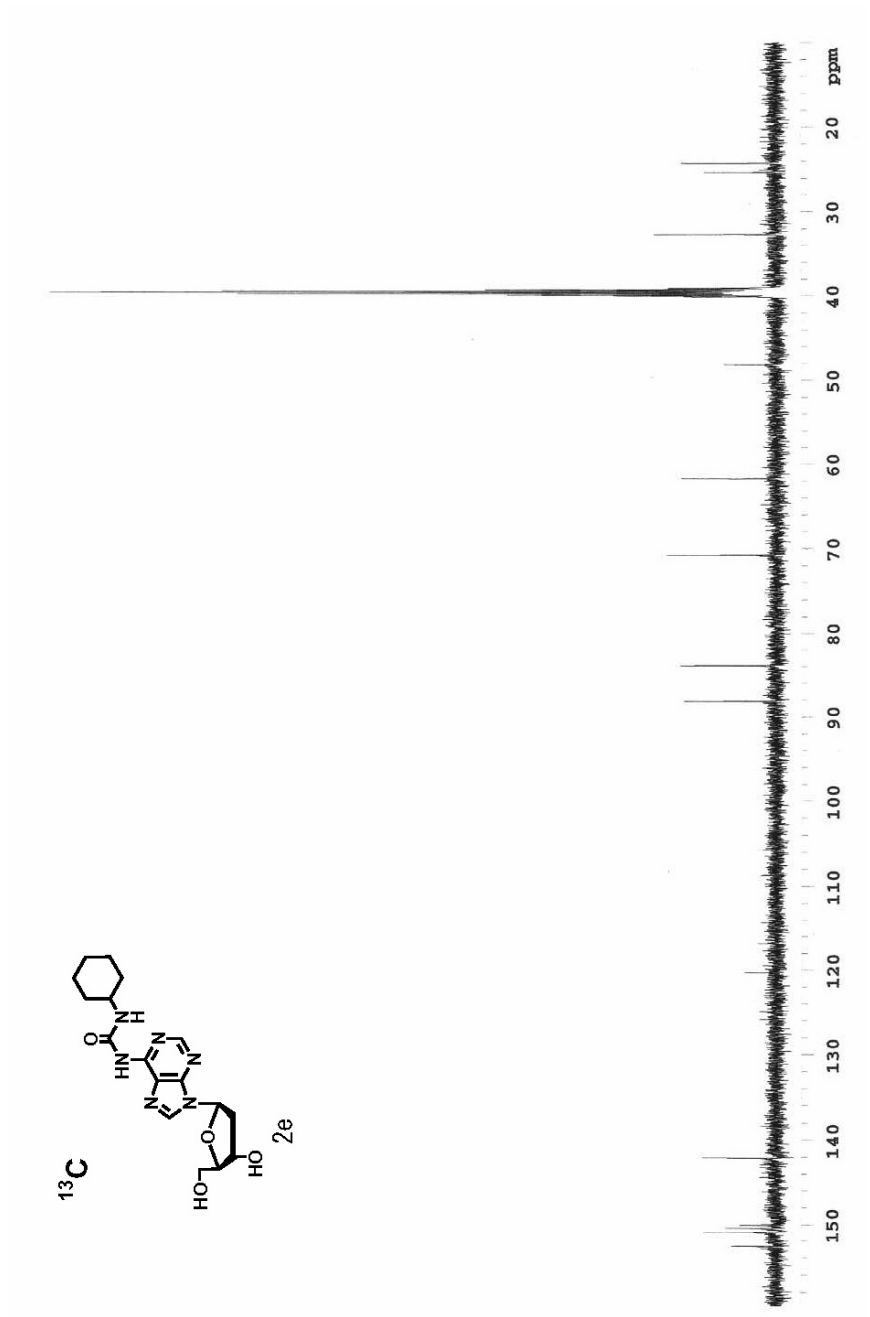
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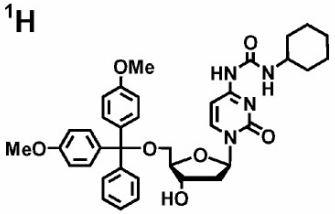

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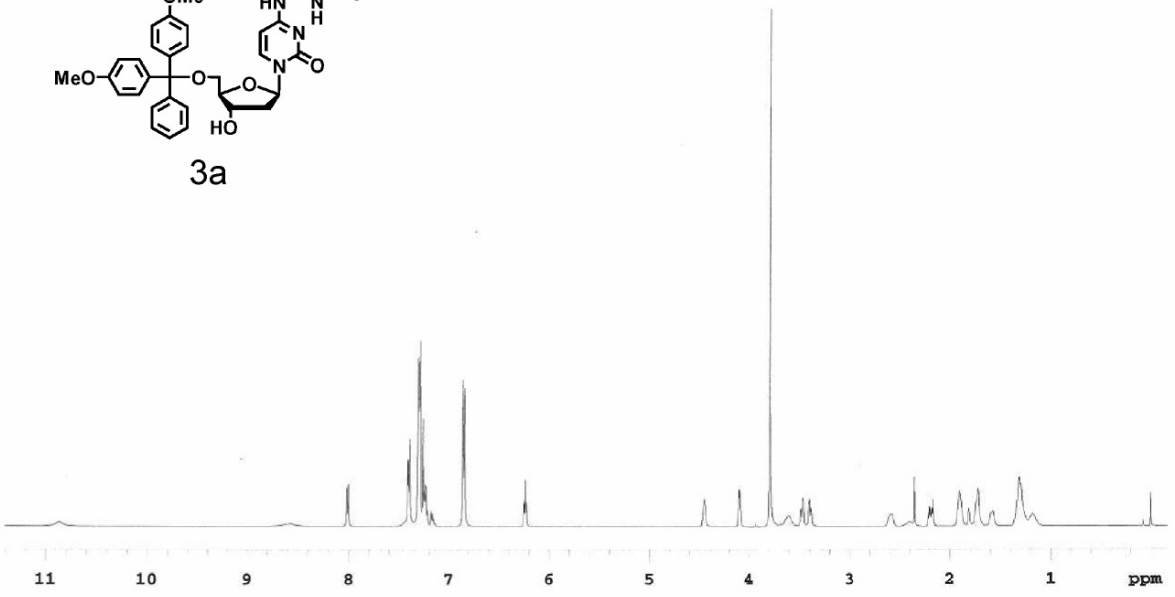

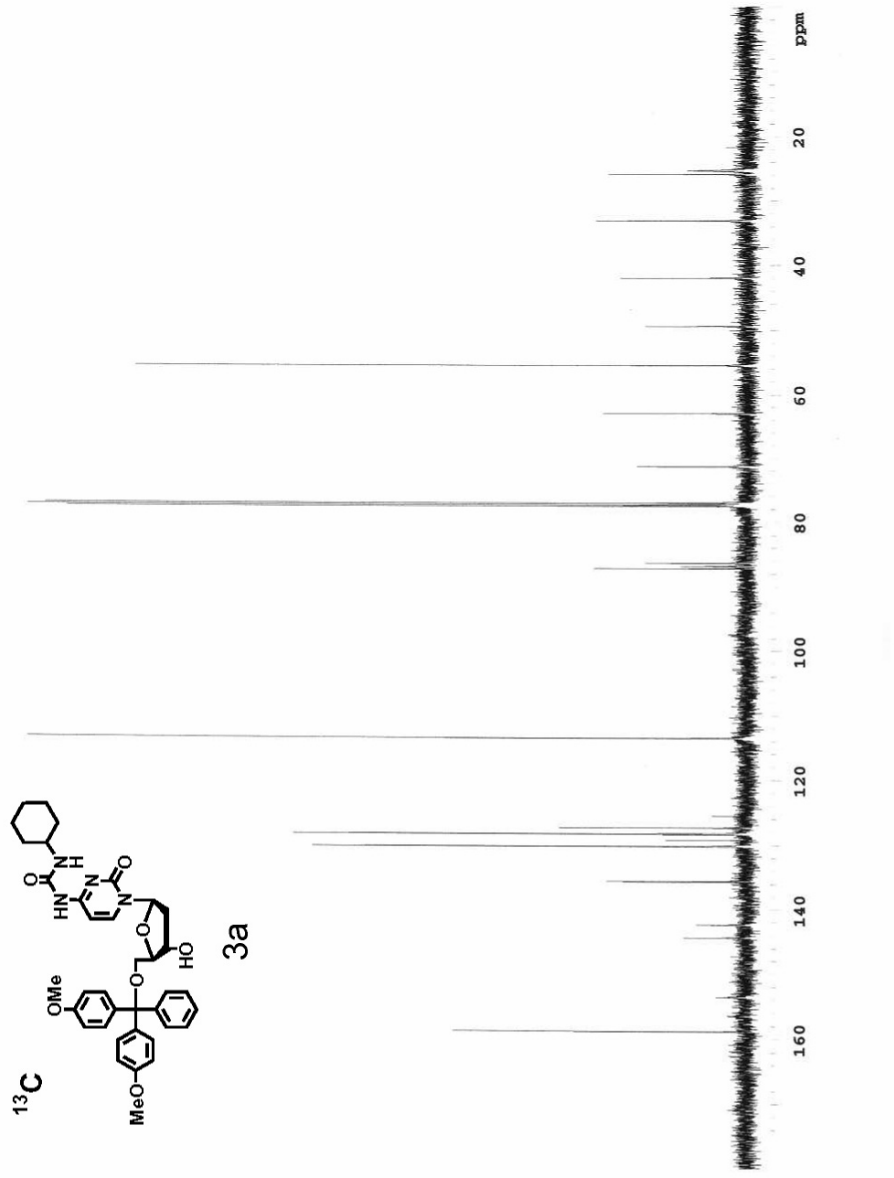
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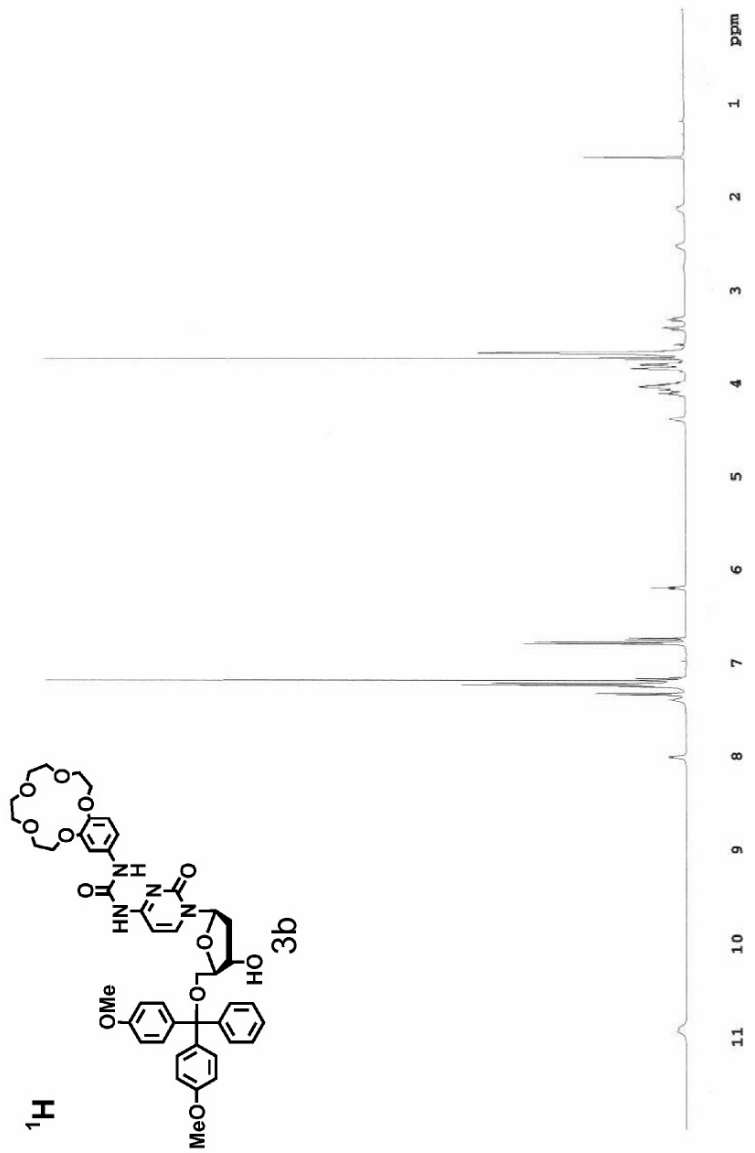
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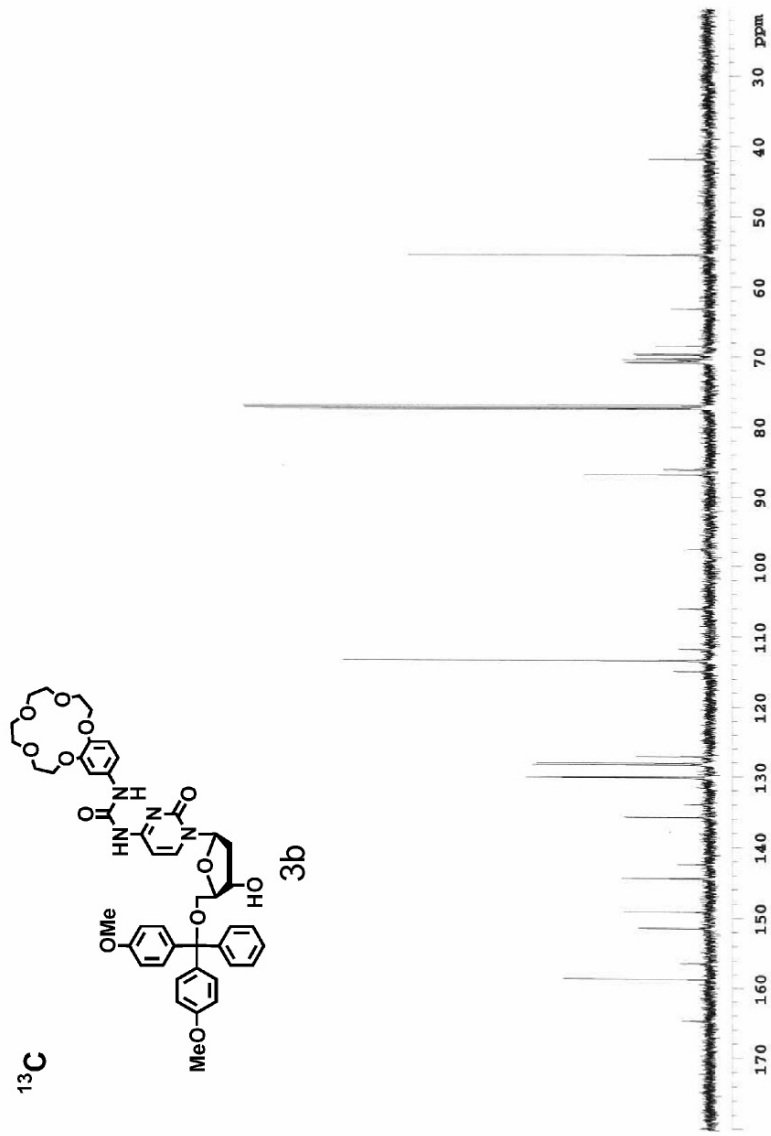
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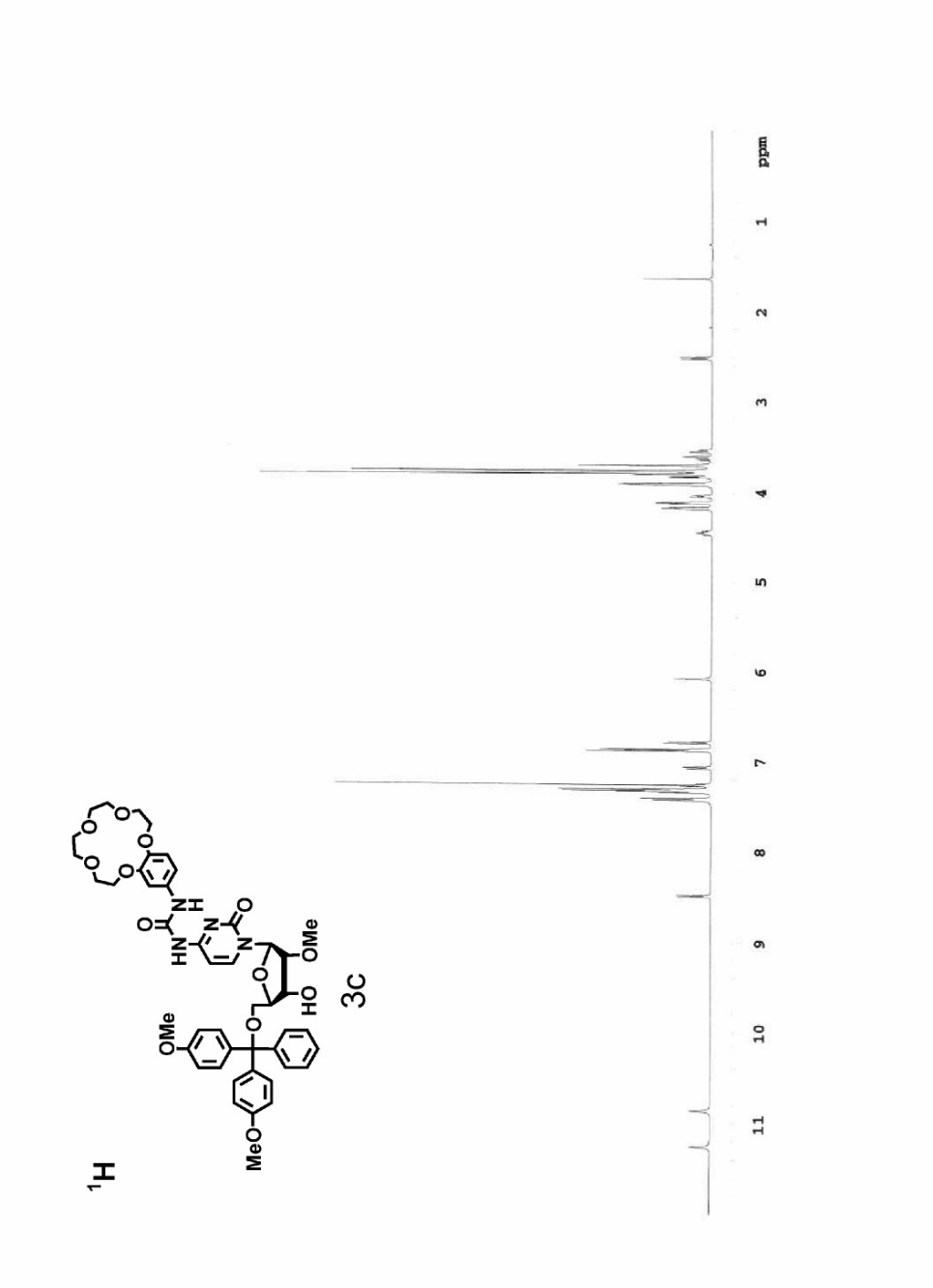

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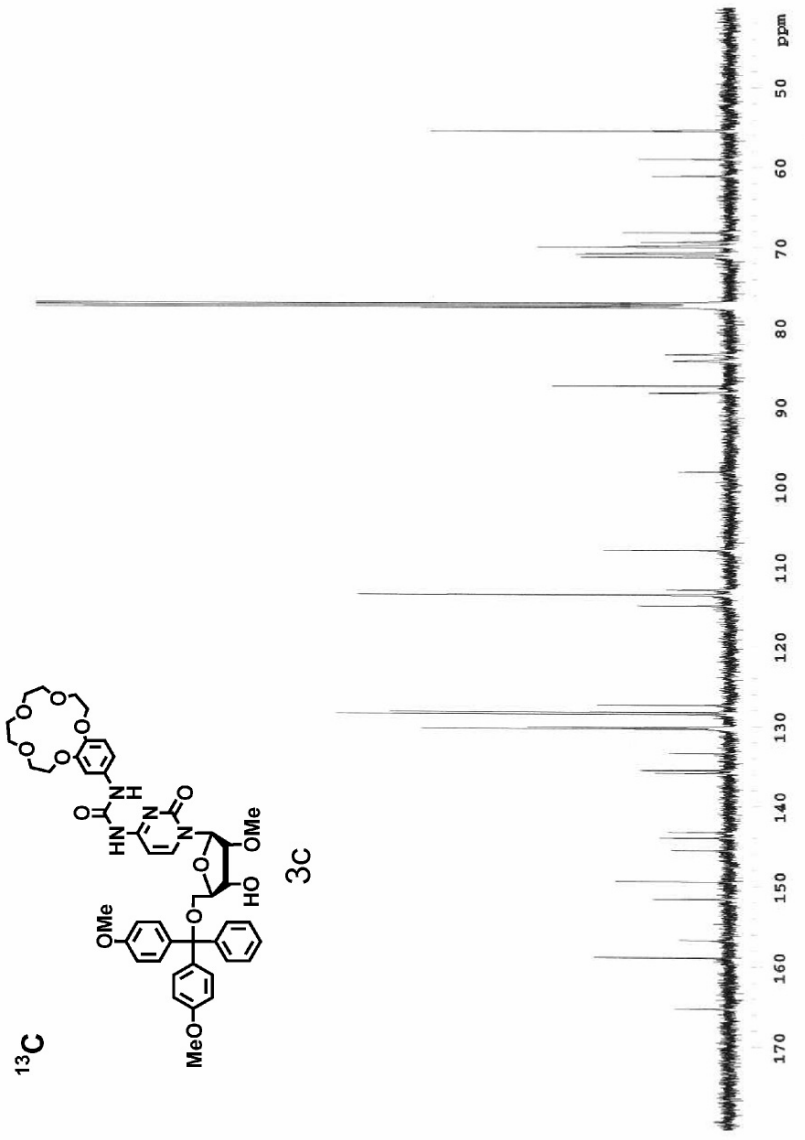
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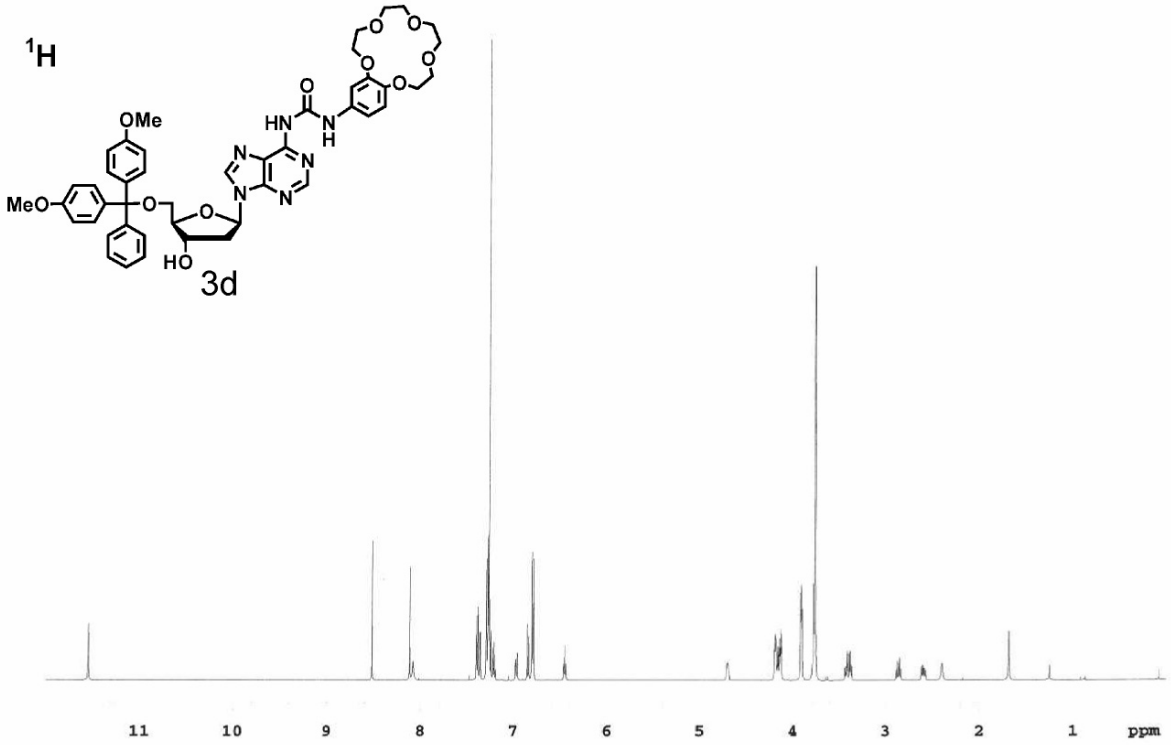
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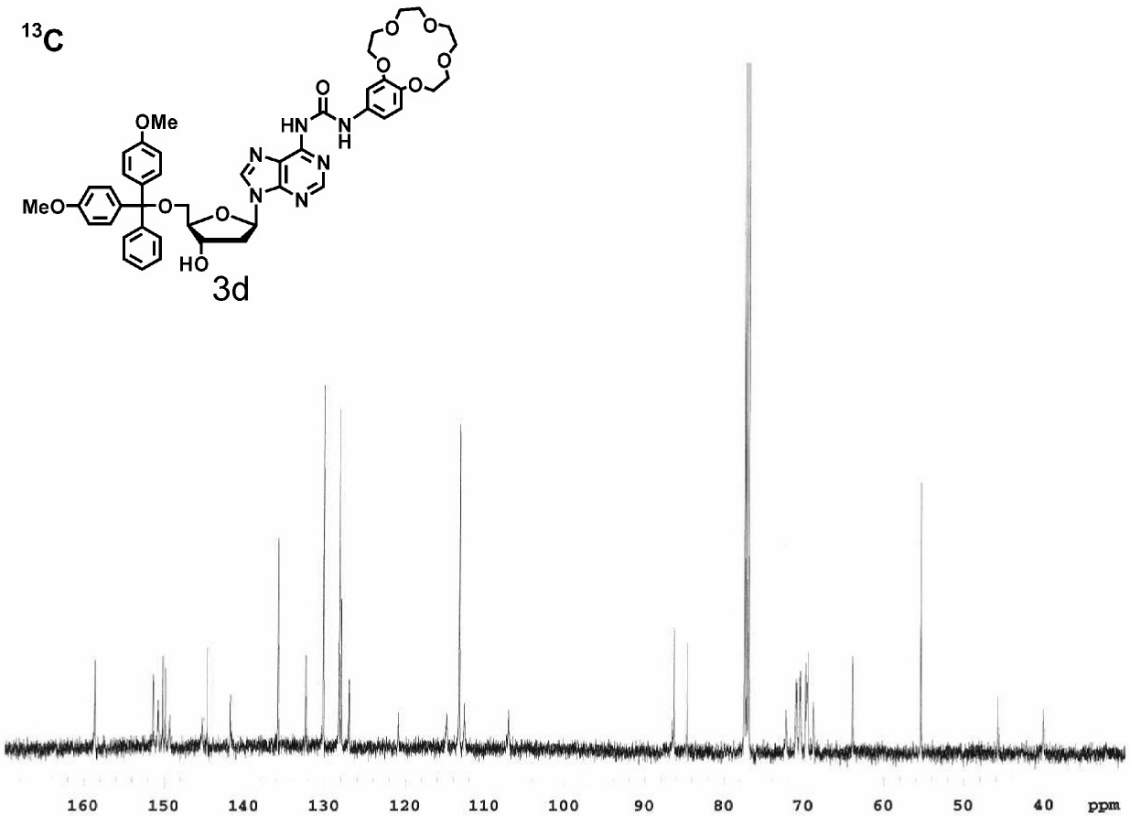
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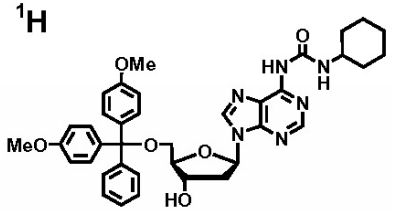

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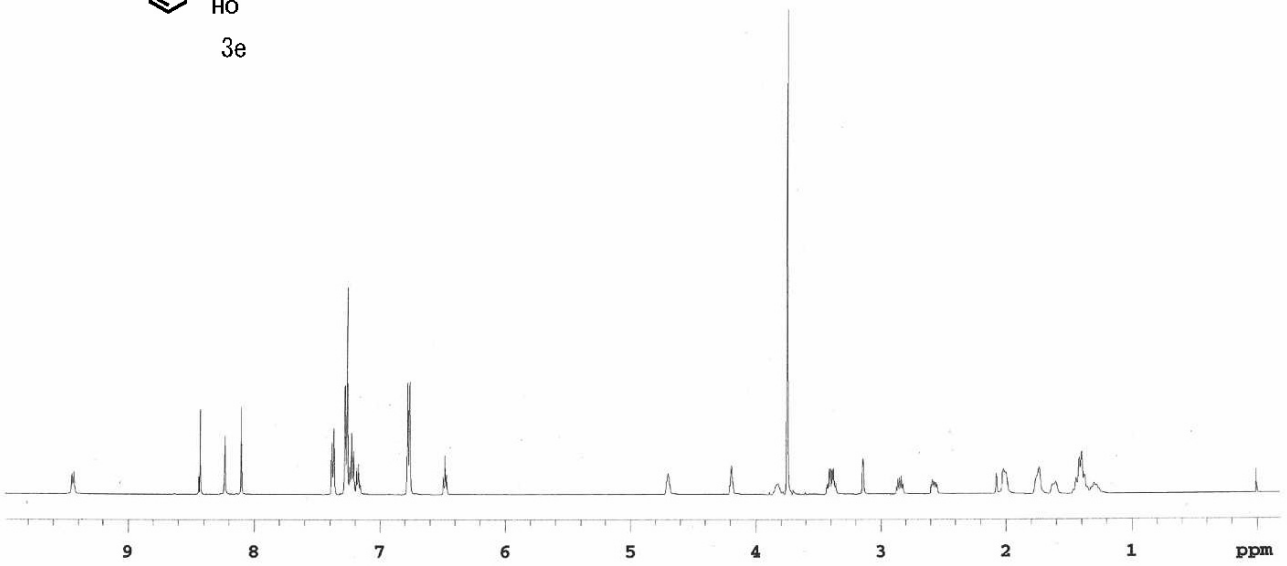
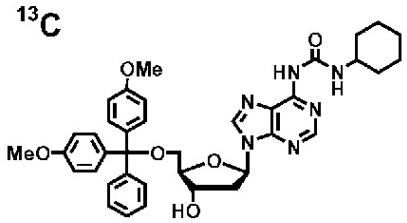
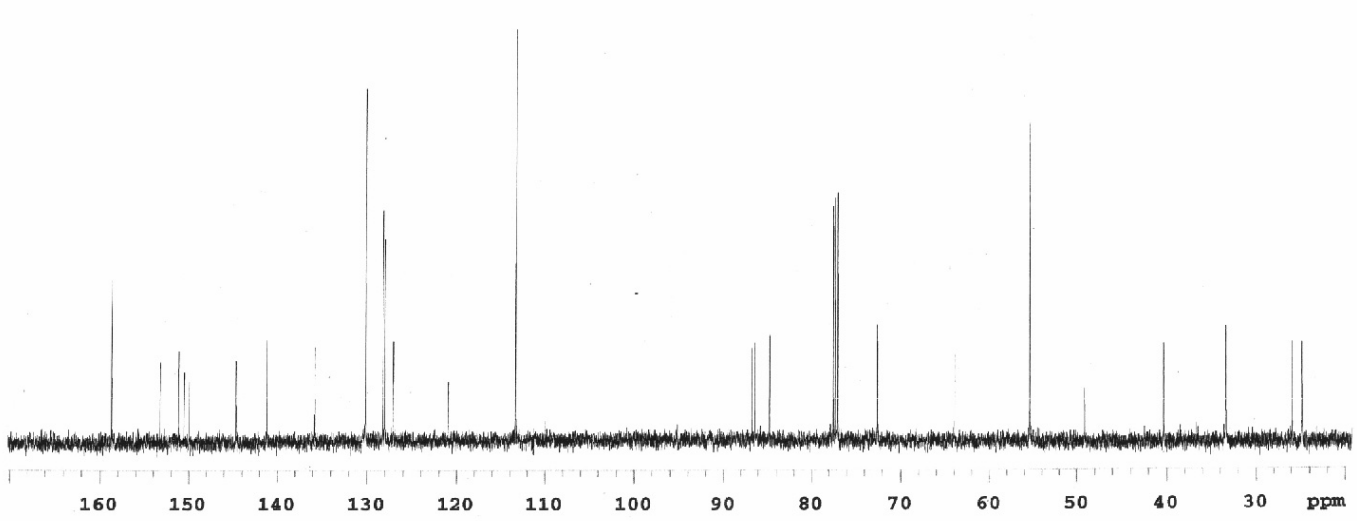


^{13}C


OMe
MeO
O
HO
HN
O
N
H
N
N
N
N

3e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150
140
130
120
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90
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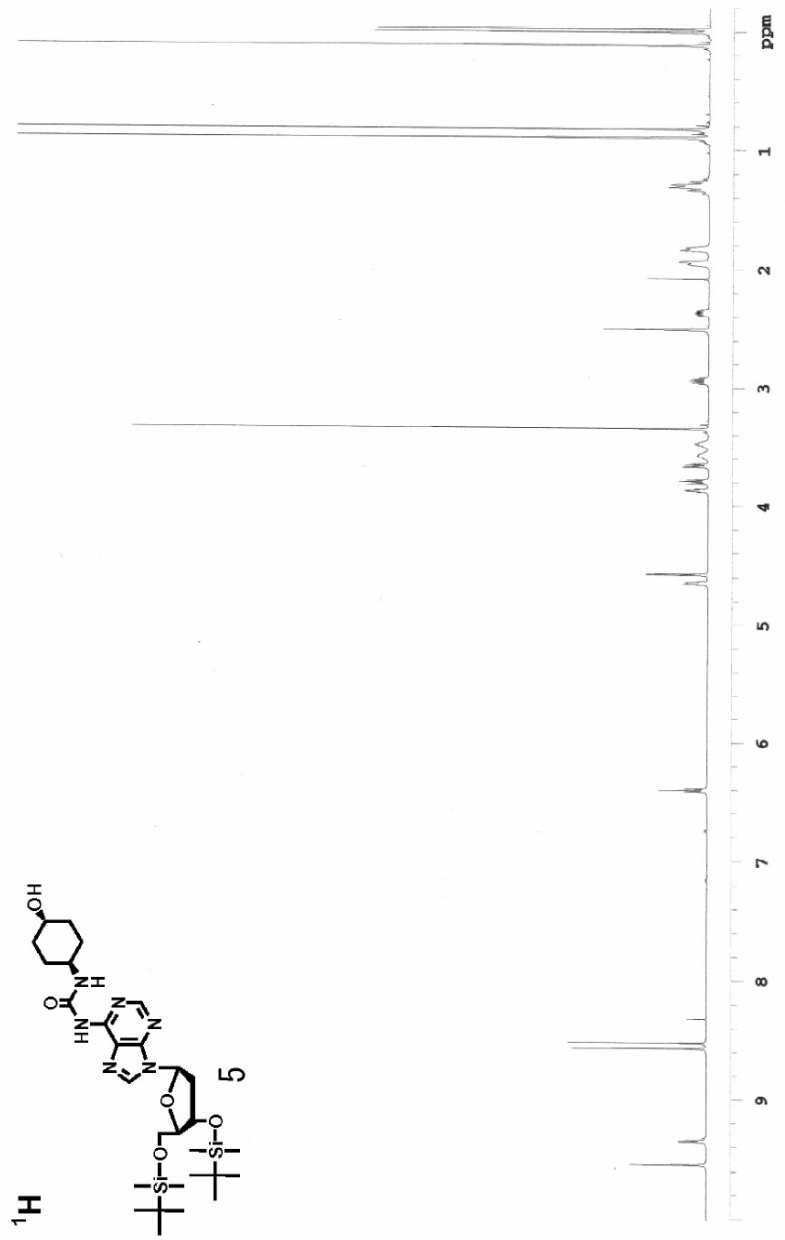
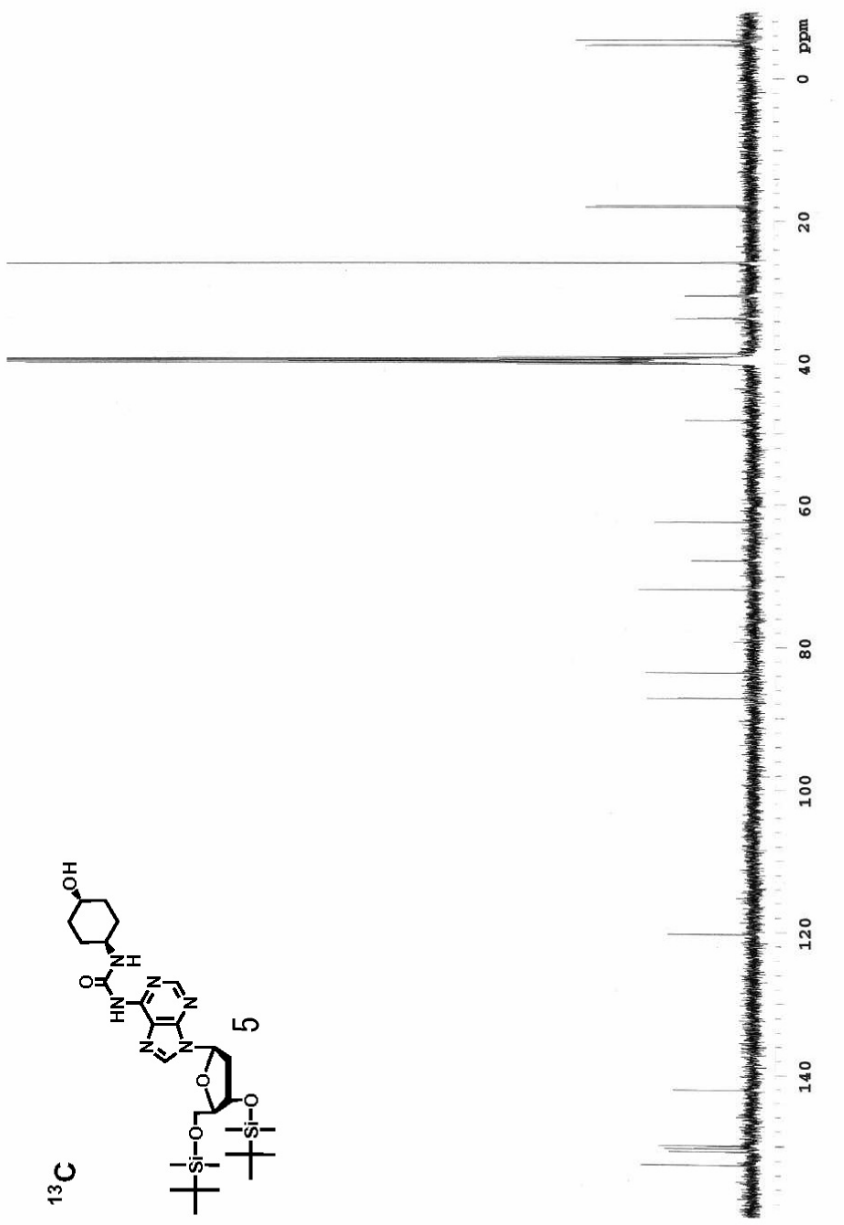
70
60
50
40
30
ppm


^{1}H
5
ppm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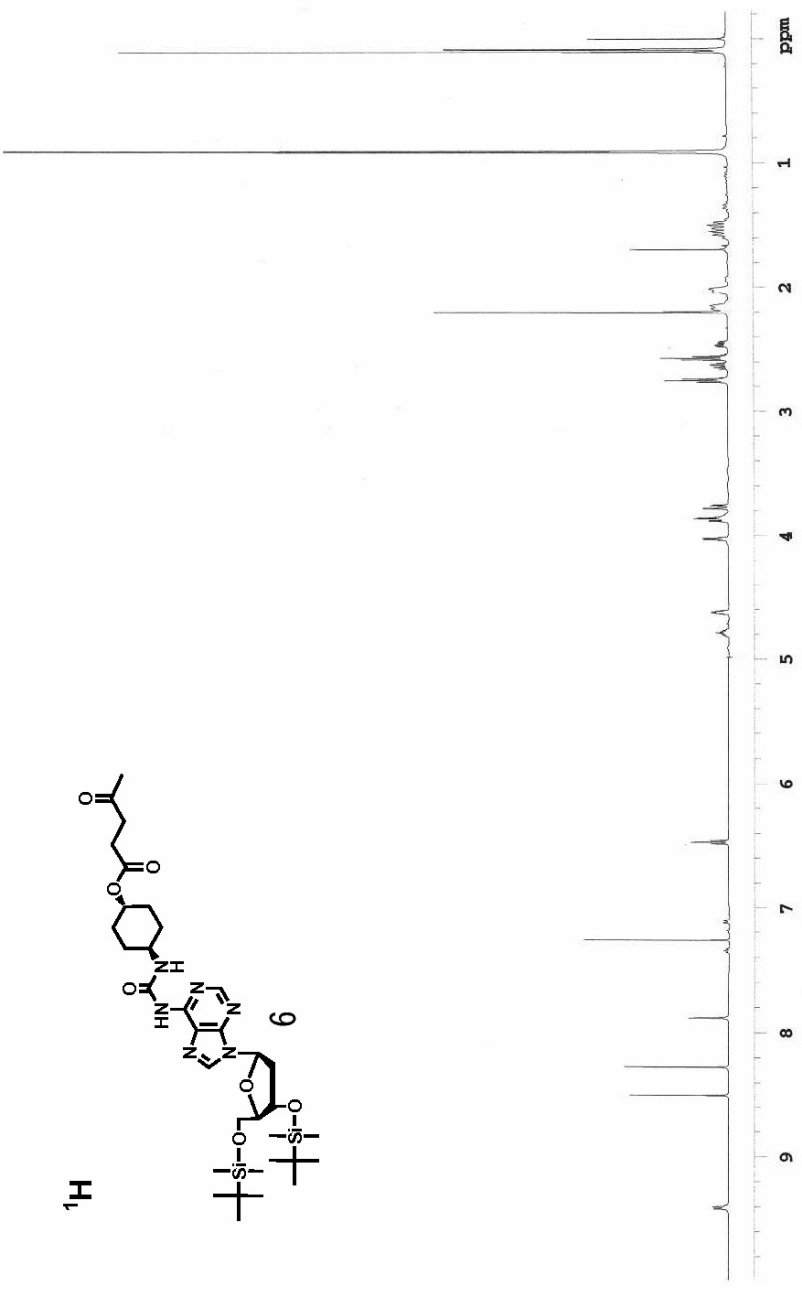
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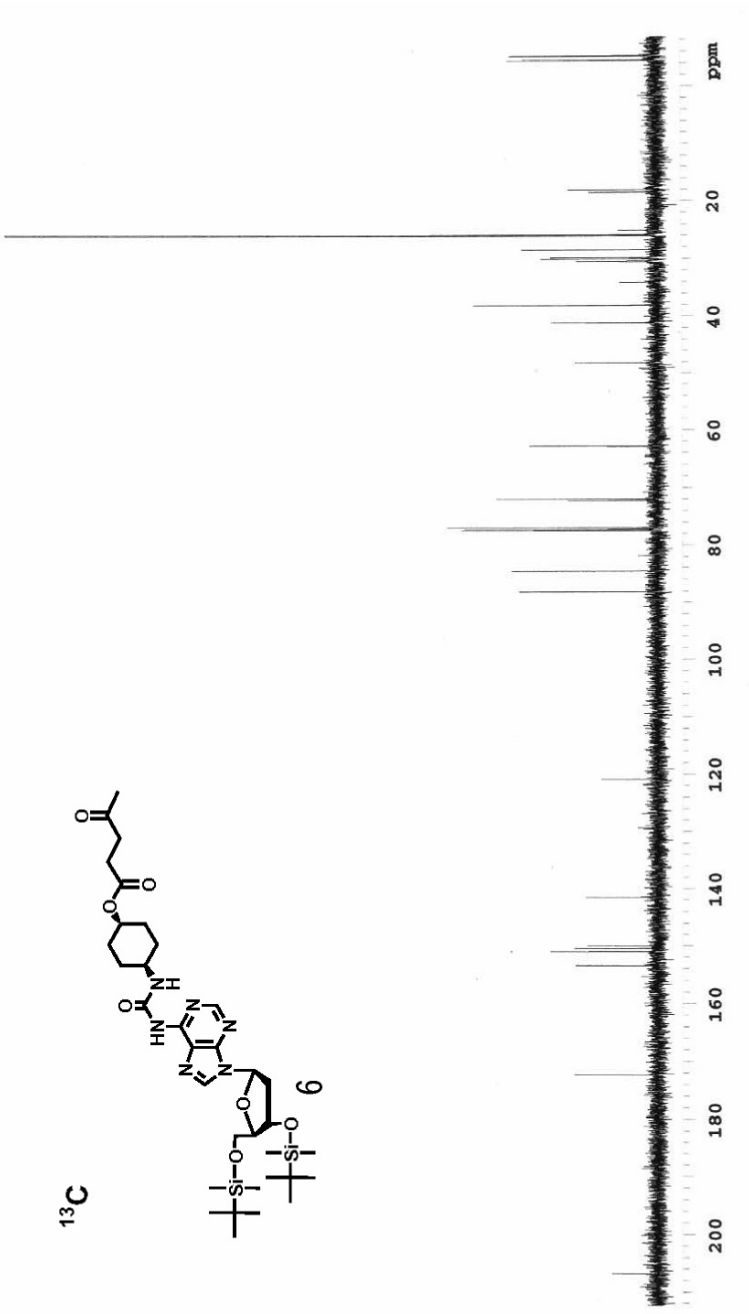
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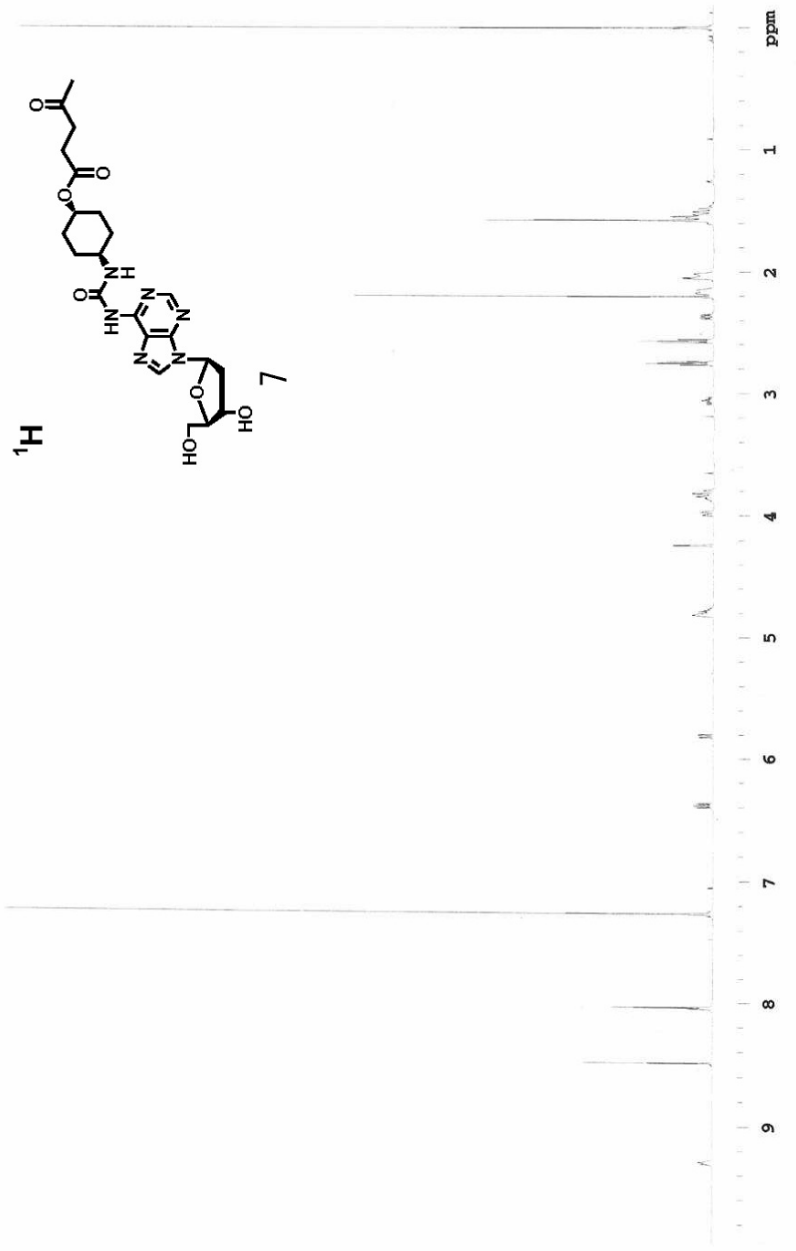
^{1}H
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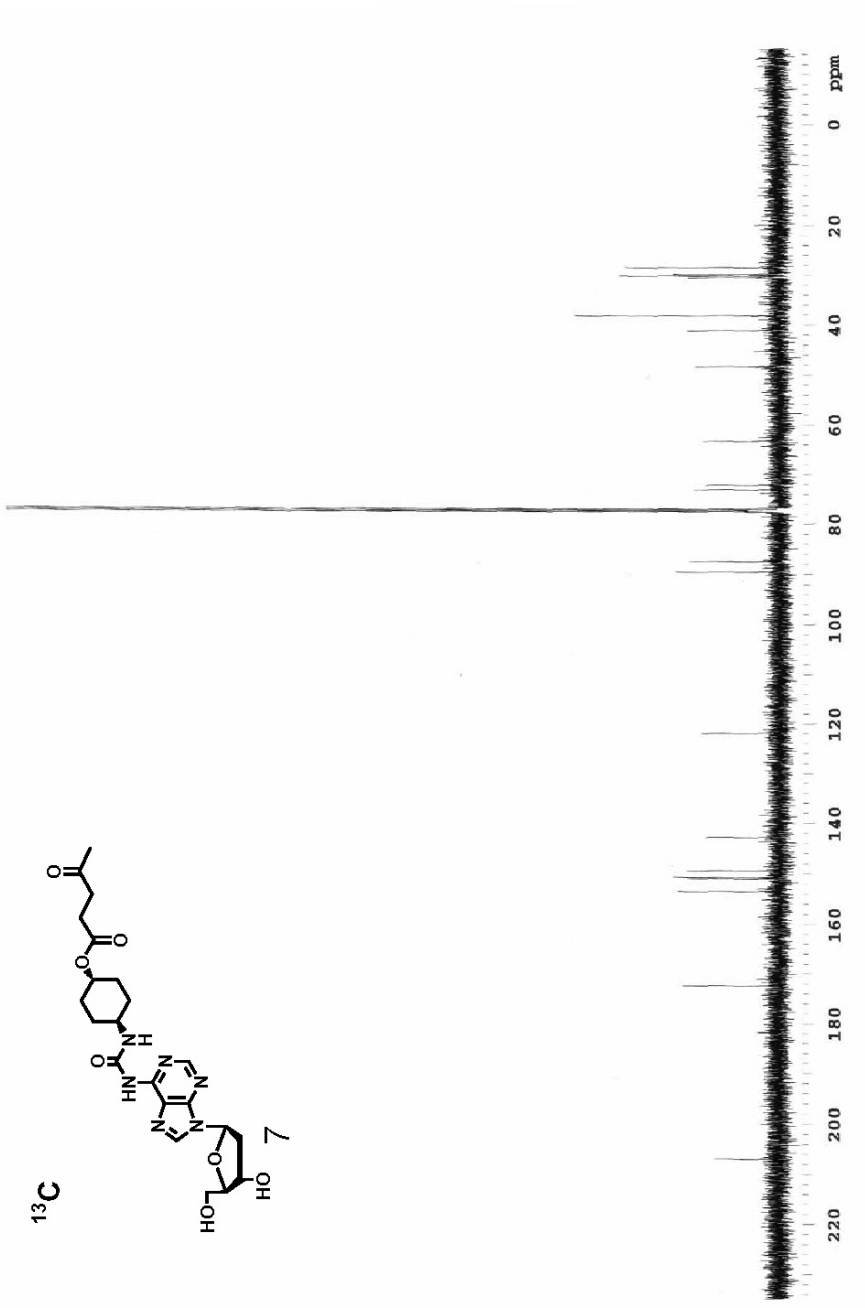
2
3
4
5
6
7
8
9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60
80
100
120
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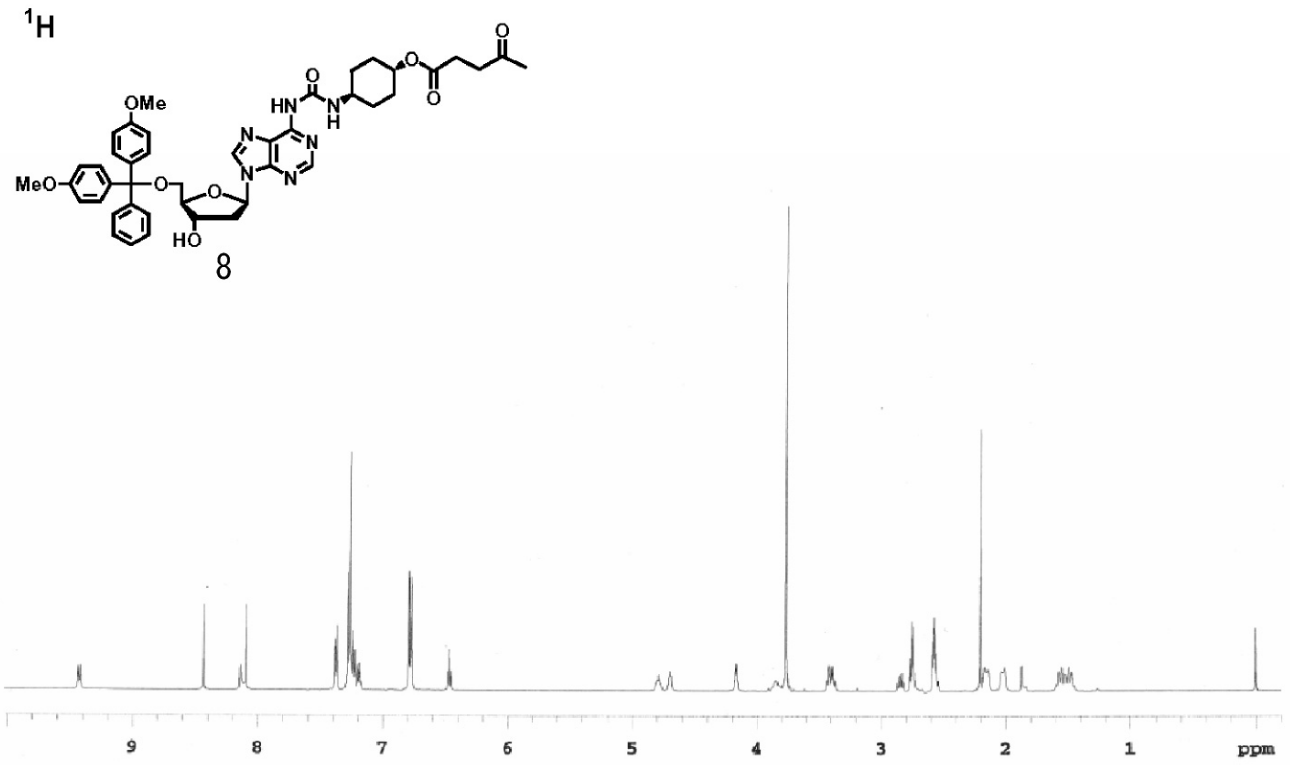
160
180
200
220


1H
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MeO
HO
HN
N
H
O
8
9
8
7
6
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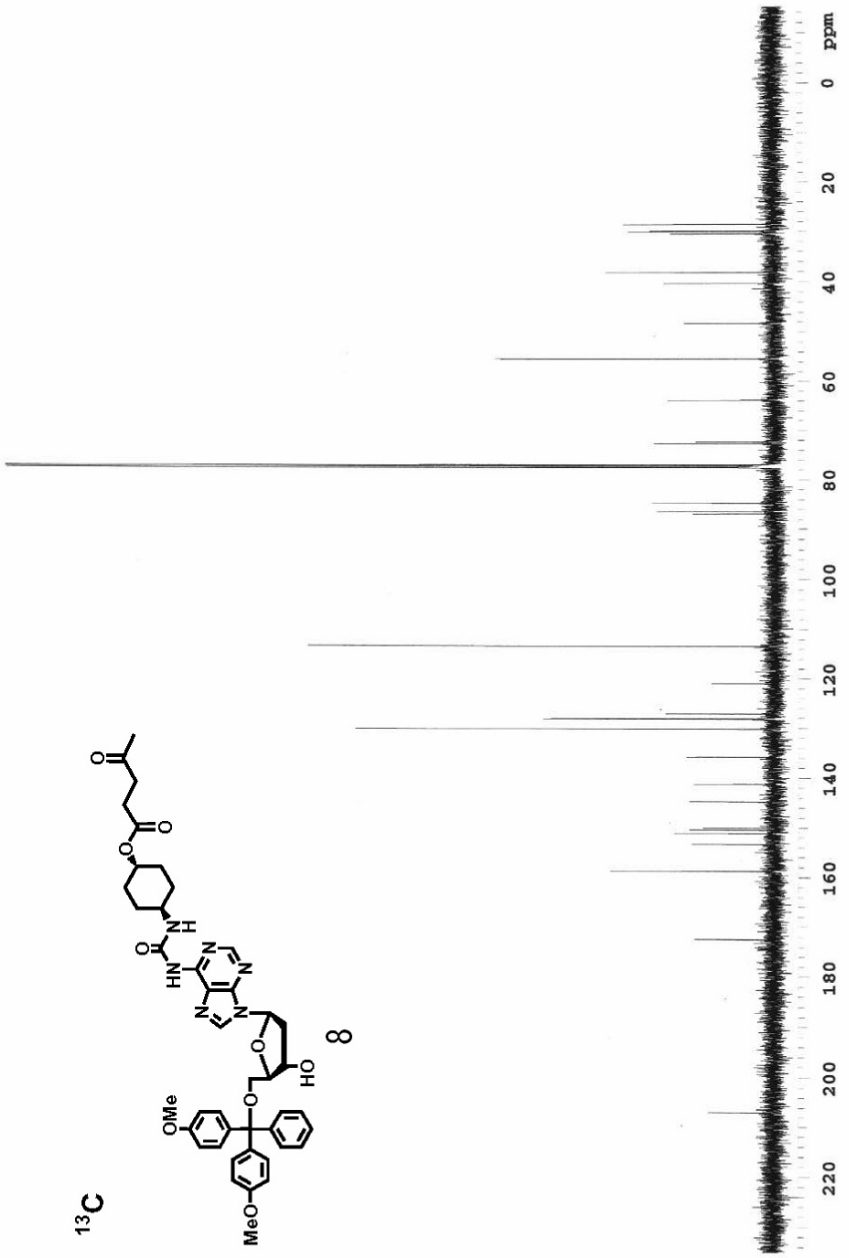
4
3
2
1
ppm


^{13}C
8
ppm
0
20
40
60
80
100
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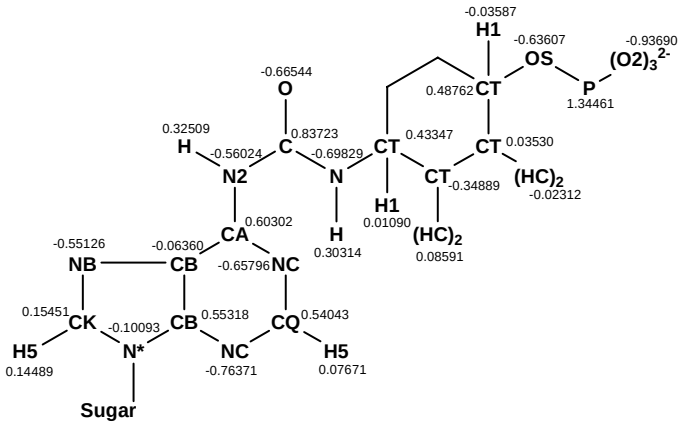

Fig. S1. Atom types and the atomic charges of the modified base incorporated to **probe7**

Table S1. Bond, angle and dihedral parameters for the modified base.

bond[a]	K_r (kcal mol^{-1} Å^{-2})	r_{eq} (Å)	
N2-C	490.00	1.335	
angle[b]	K_θ (kcal mol^{-1} deg^{-2})	θeq (deg)	
CA-N2-C	67.400	119.630	
N2-C -N	75.400	111.700	
N2-C -O	74.100	122.260	
H -N2-C	50.000	120.000	
dihedral[c]	V_n (kcal mol^{-1})	γ (deg)	n
CA-N2-C-N	10.000	180.0	2.0
CA-N2-C-O	10.000	180.0	2.0
H -N2-C-N	2.000	0.0	1.0
H -N2-C-O	2.000	0.0	1.0

a) $E_{bond} = K_r(r-r_{eq})^2$; b) $E_{angle} = K_\theta(\theta-\theta_{eq})^2$; c) $E_{dihedral} = 0.5V_n[1+\cos(n\phi-\gamma)]$

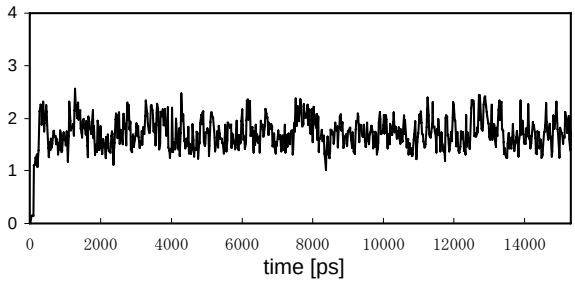

Fig. S2 RMS deviations (Å) during the MD simulation