Supporting Information

for

Pyrrolidine nucleotide analogs with a tunable conformation

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Additional experimental data

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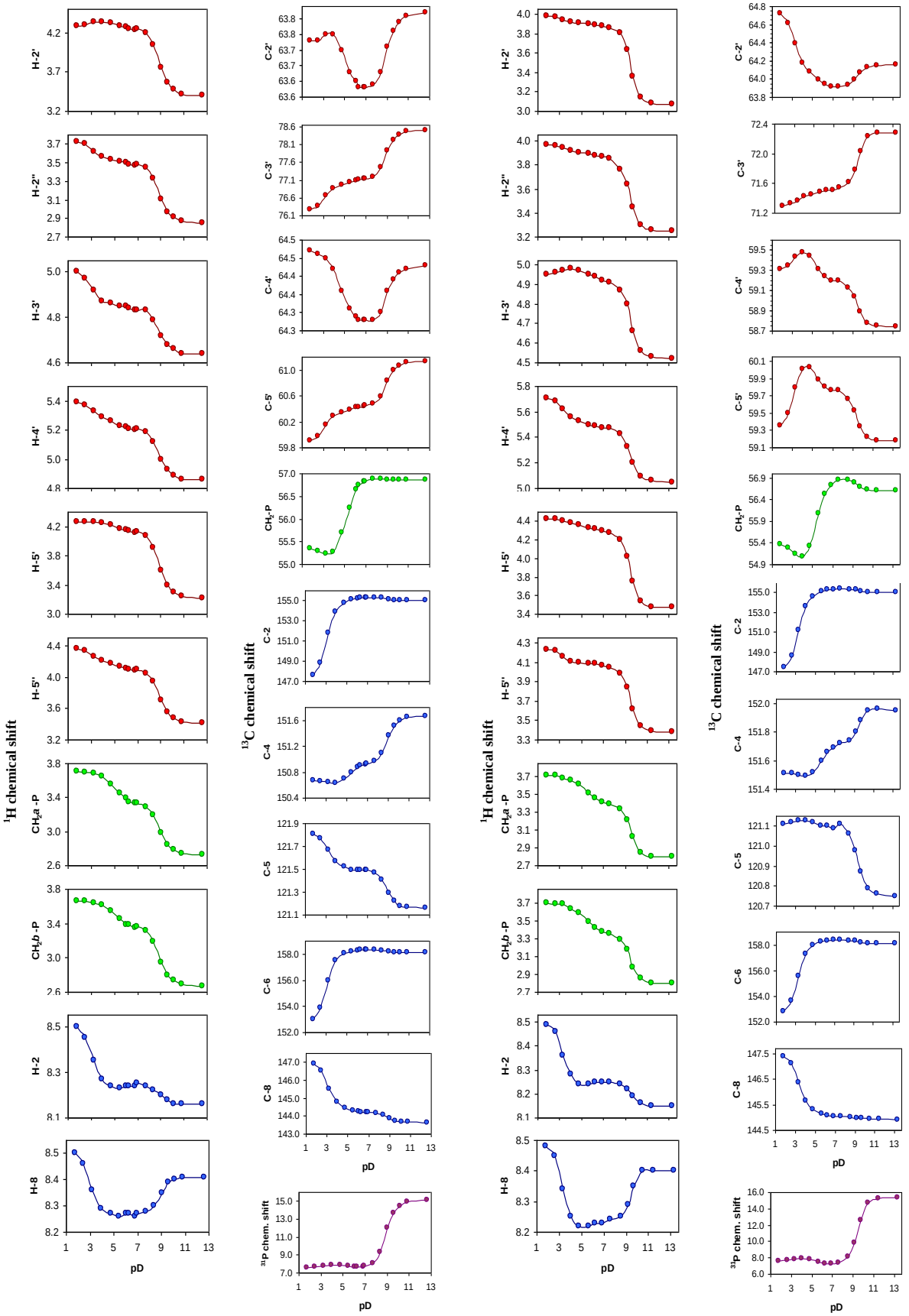
The pD titration curves for compounds 9 and 10

Compound 9

Compound 10



Variable temperature ^{31}P NMR of 14

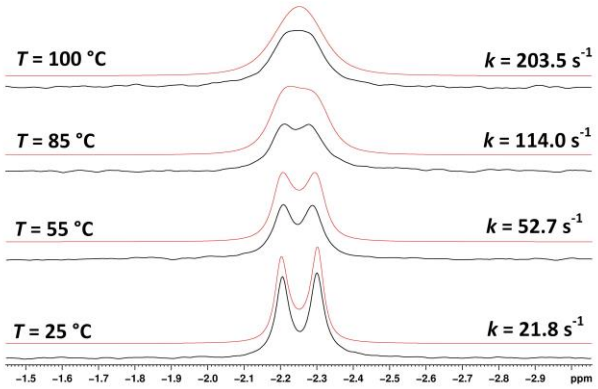


Figure S1: ^{31}P NMR spectra (202.3 MHz) of **14** measured (black curve) and simulated (red curve) at various temperatures.

Table S1: Rate constant values obtained by lineshape analysis of the spectra measured at various temperatures for **14**.

T (°C)	*T* (K)	1/*T* (K^{-1})	*k* (s^{-1})	ln(*k*/*T*)
25	298.15	0.003354	21.8	-2.61569
35	308.15	0.003245	30.1	-2.32606
45	318.15	0.003143	42.2	-2.02010
55	328.15	0.003047	52.7	-1.82886
65	338.15	0.002957	69.7	-1.57929
75	348.15	0.002872	98.5	-1.26258
85	358.15	0.002792	114.0	-1.14475
95	368.15	0.002716	164.5	-0.80558
100	373.15	0.002680	203.5	-0.60631

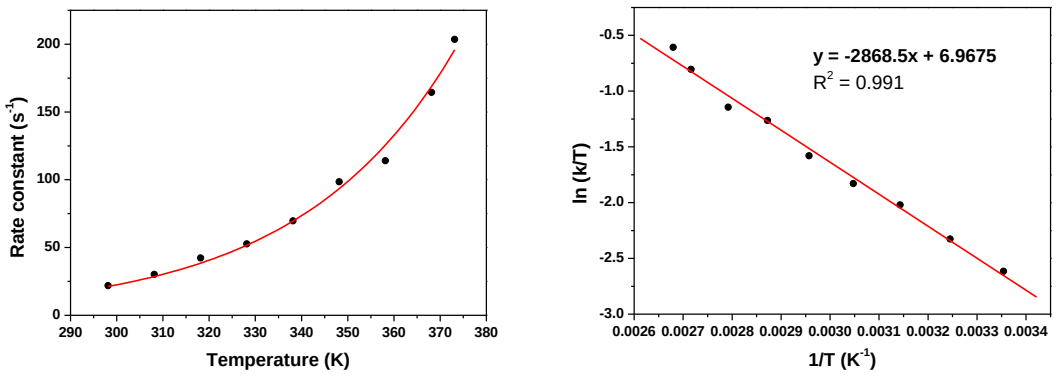


Figure S2: The plot of *T* vs. *k* and 1/*T* vs. ln(*k*/*T*) for compound **14**.

The parametrization of the pyrrolidine ring

The relation between exocyclic ϕ_{exo} and endocyclic ϕ_{endo} dihedral angles ($\phi_{exo} = A\phi_{endo} + B$) extracted from DFT B3LYP/6-31G* optimized geometries of 20 conformers.

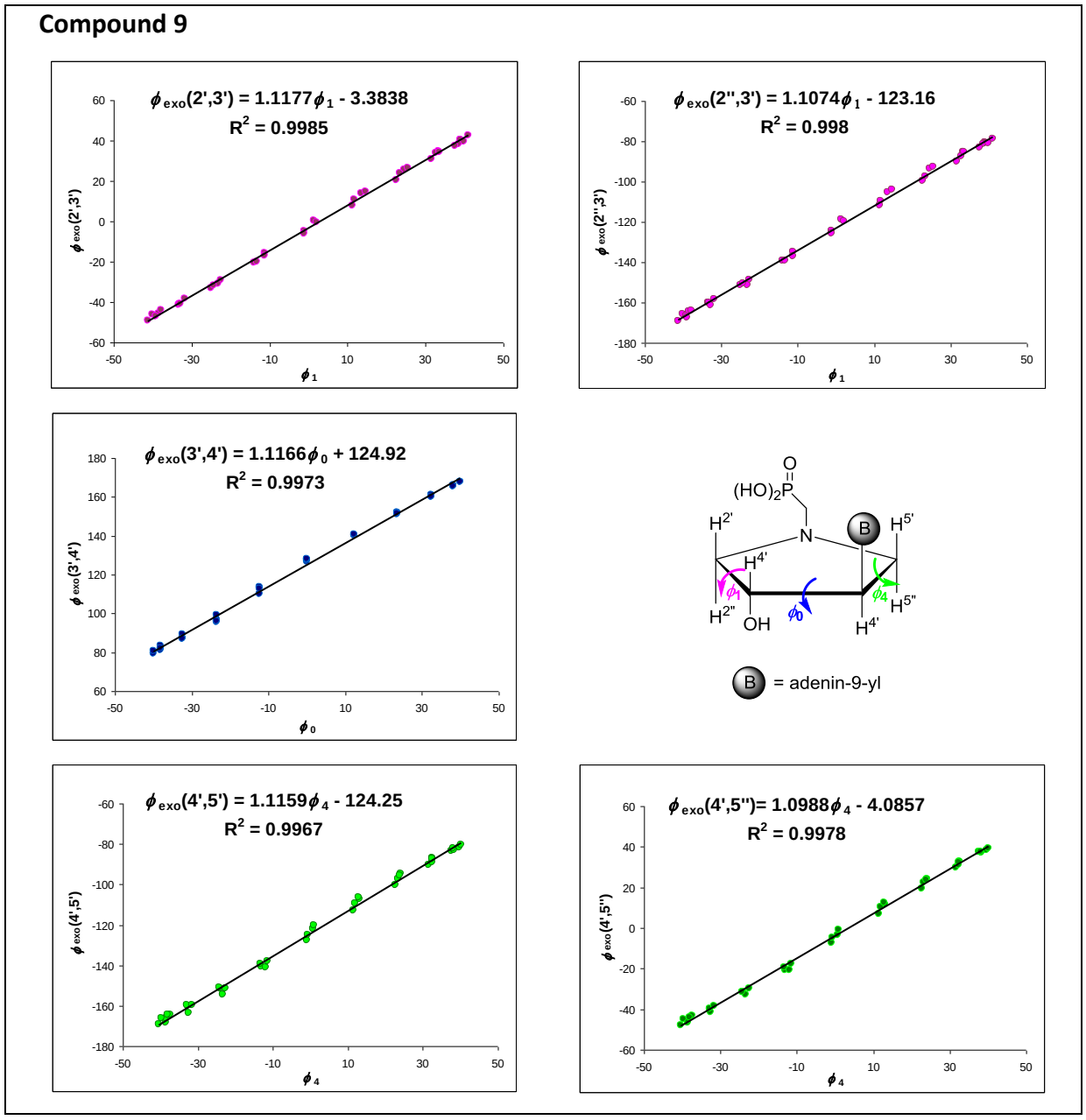


Figure S3: The ring parametrization for compound **9**.

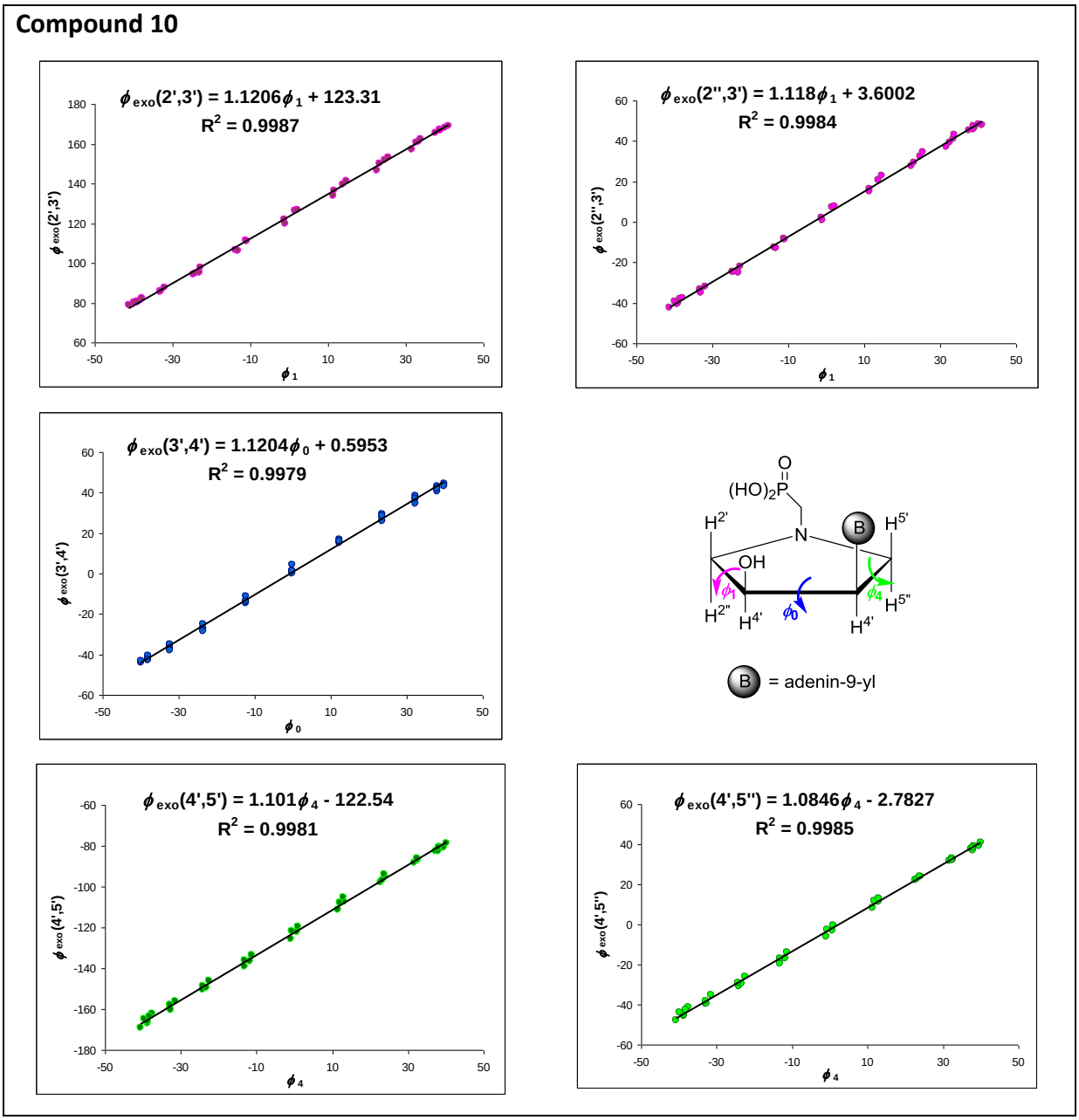


Figure S4: The ring parametrization for compound **10**.

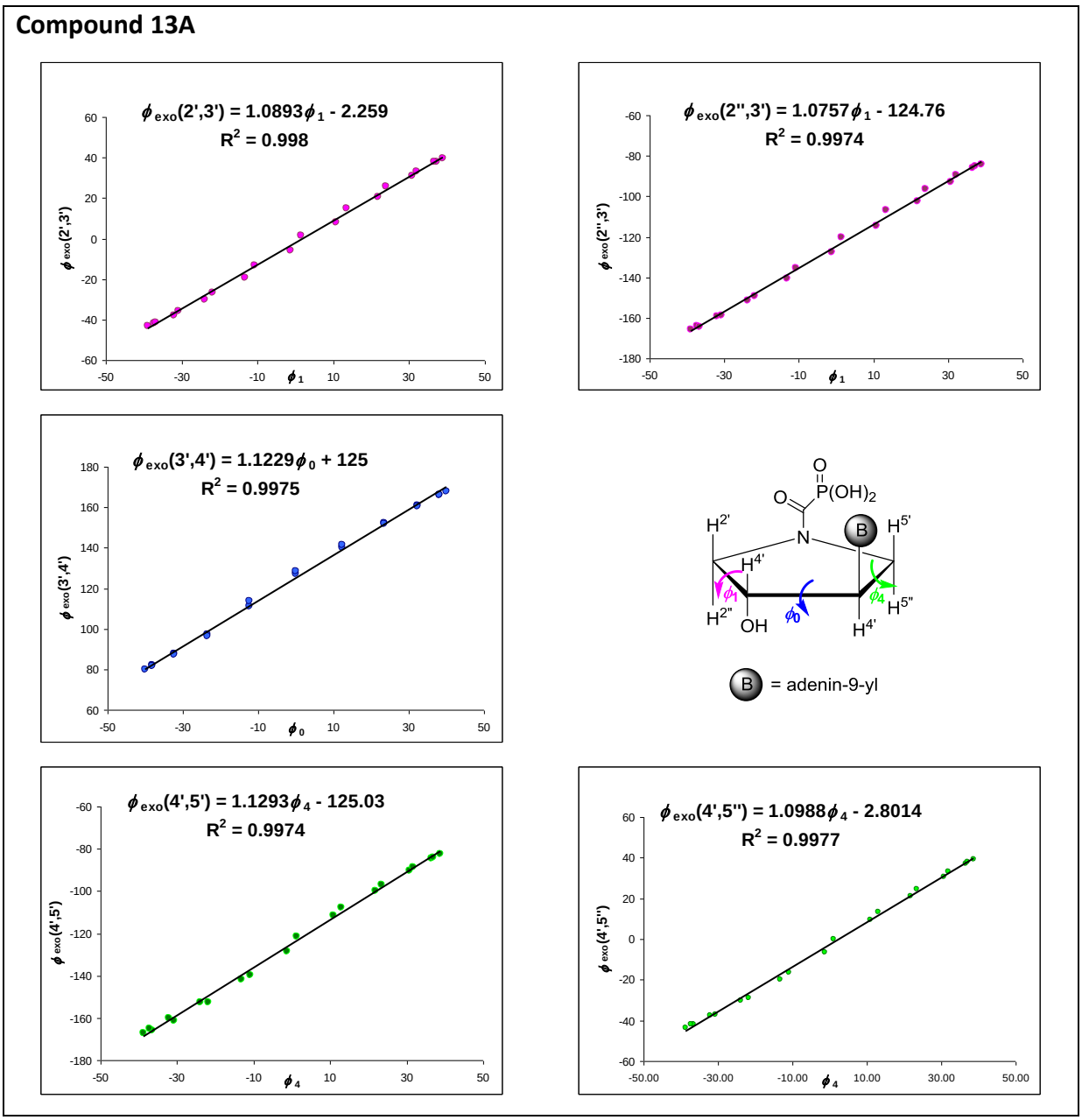


Figure S5: The ring parametrization for compound **13A**.

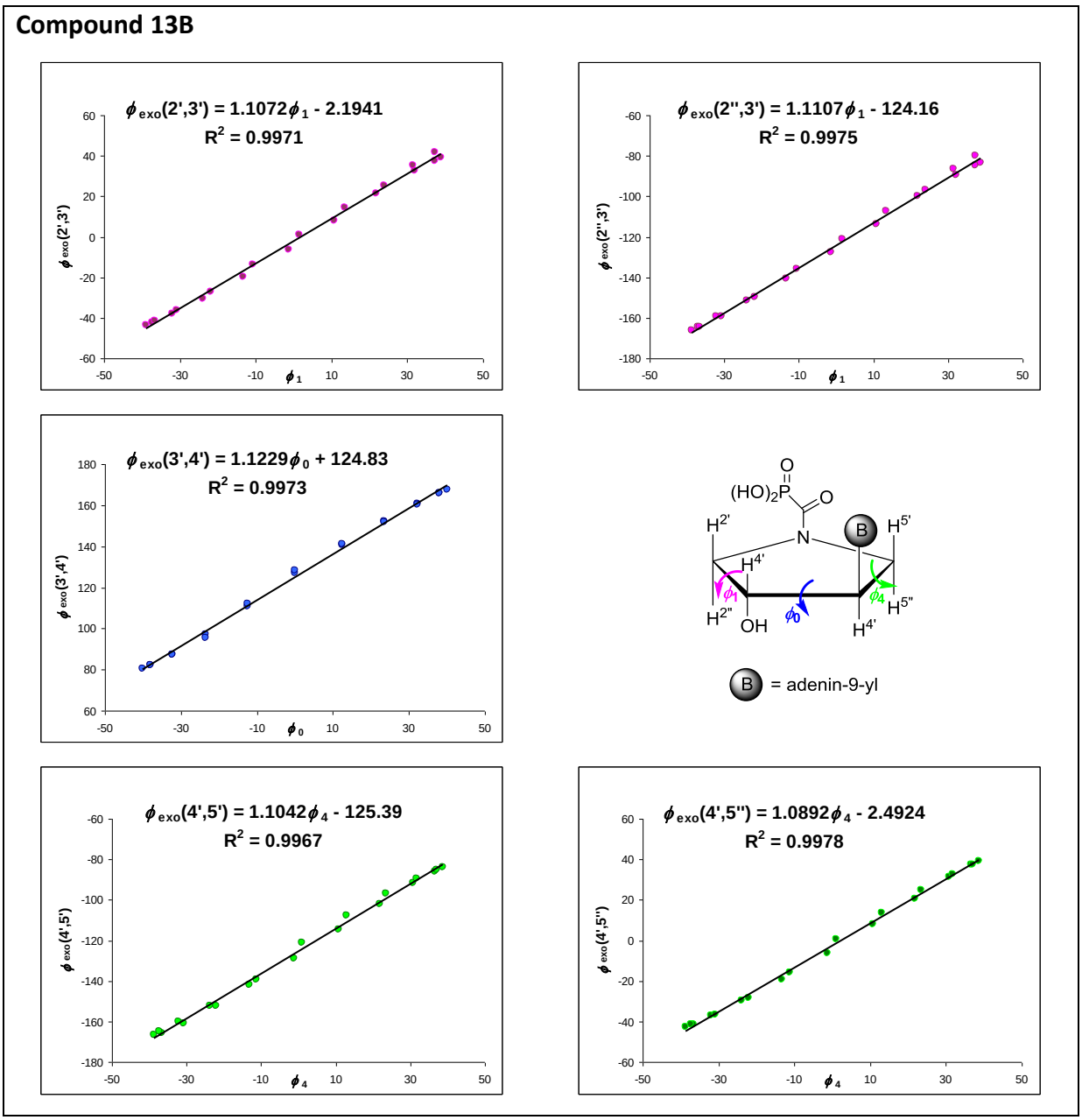


Figure S6: The ring parametrization for compound **13B**.

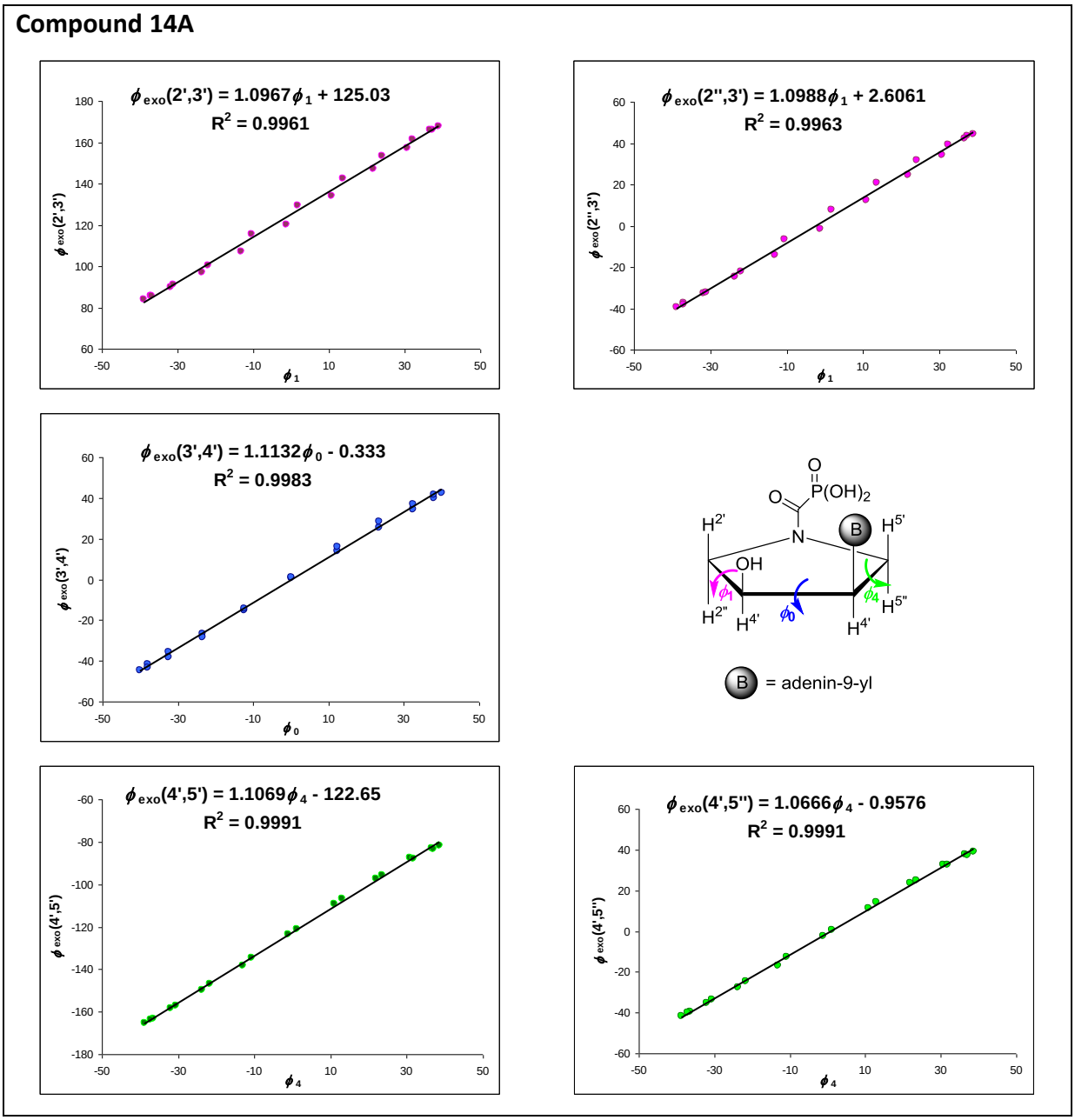


Figure S7: The ring parametrization for compound **14A**.

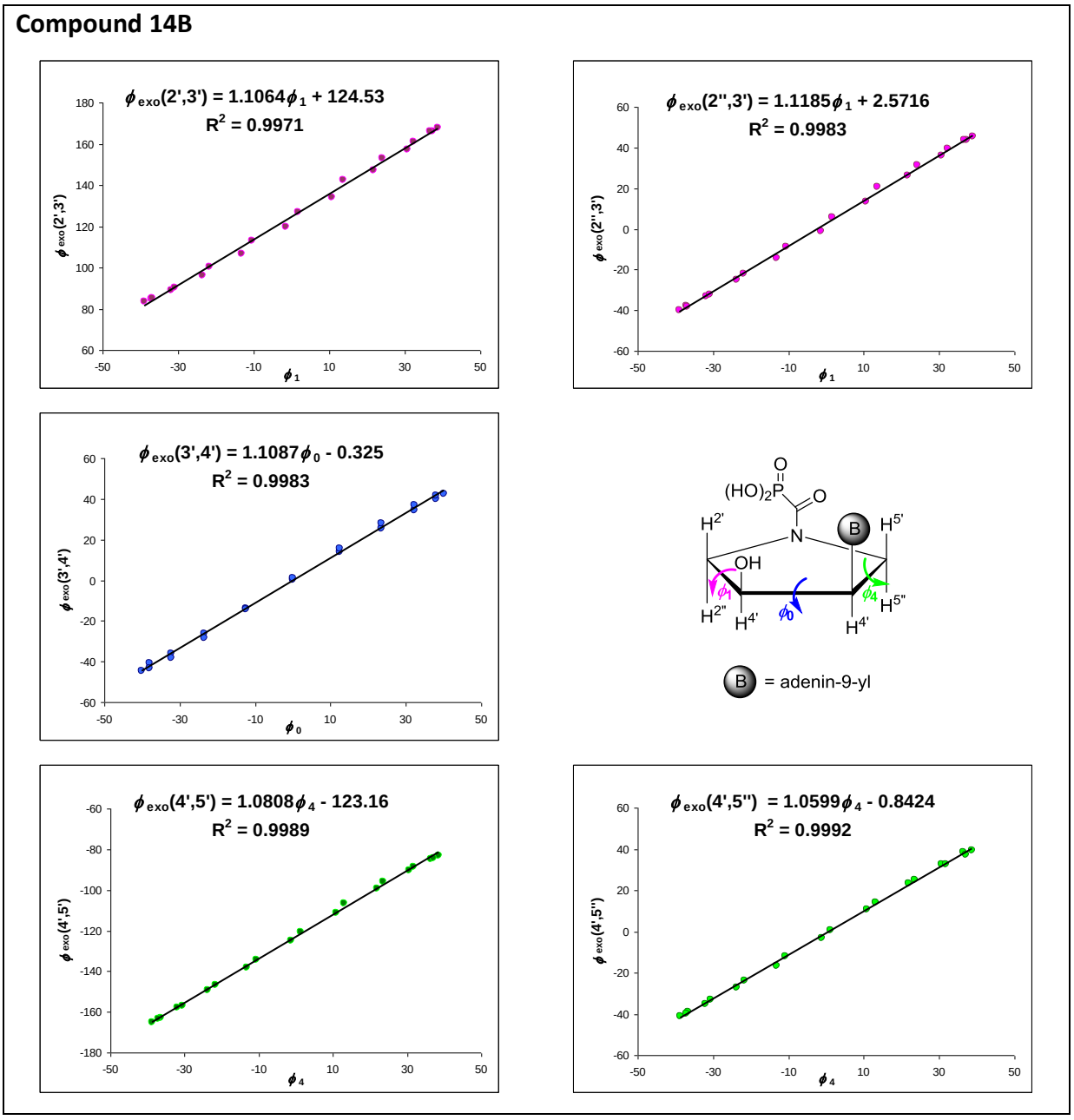
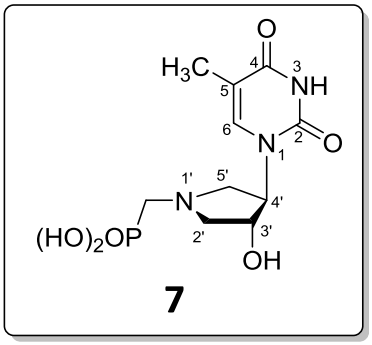


Figure S8: The ring parametrization for compound **14B**.

NMR signals assignment and copies of ^{1}H, ^{13}C and ^{31}P NMR spectra

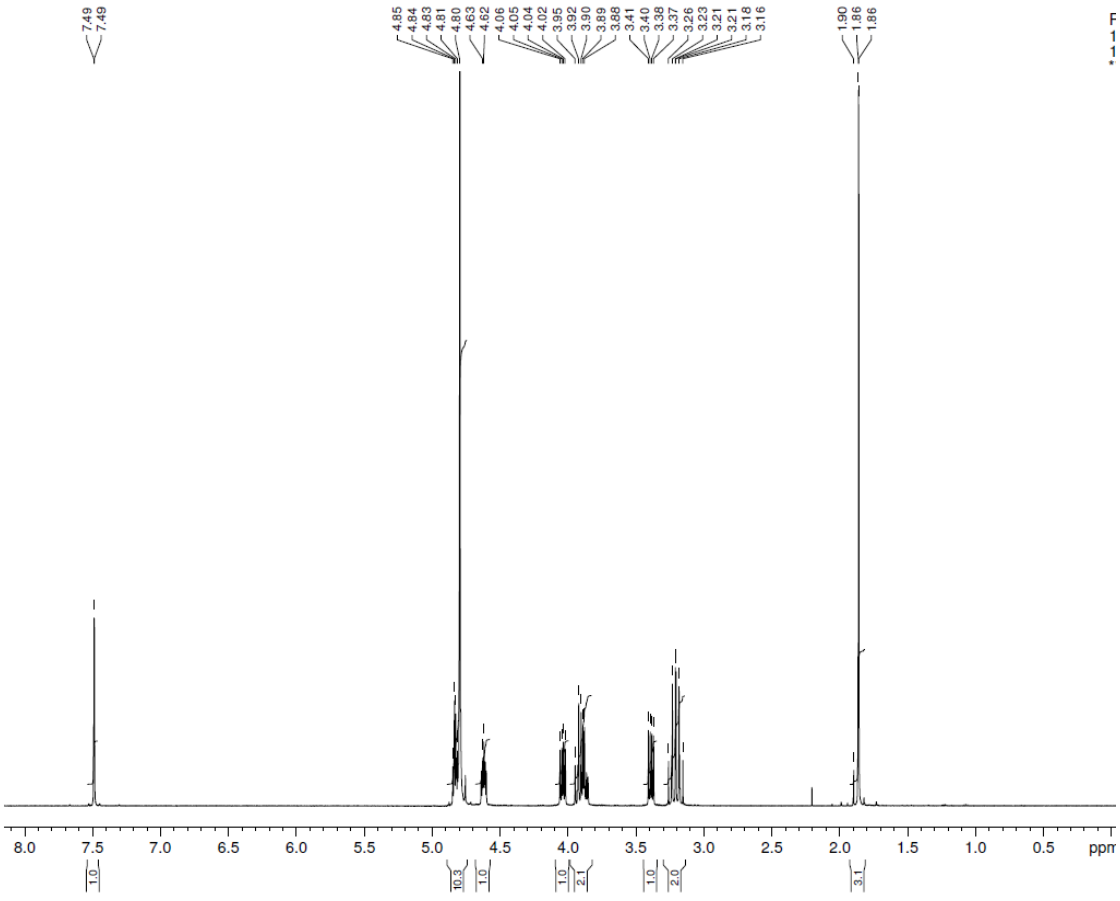


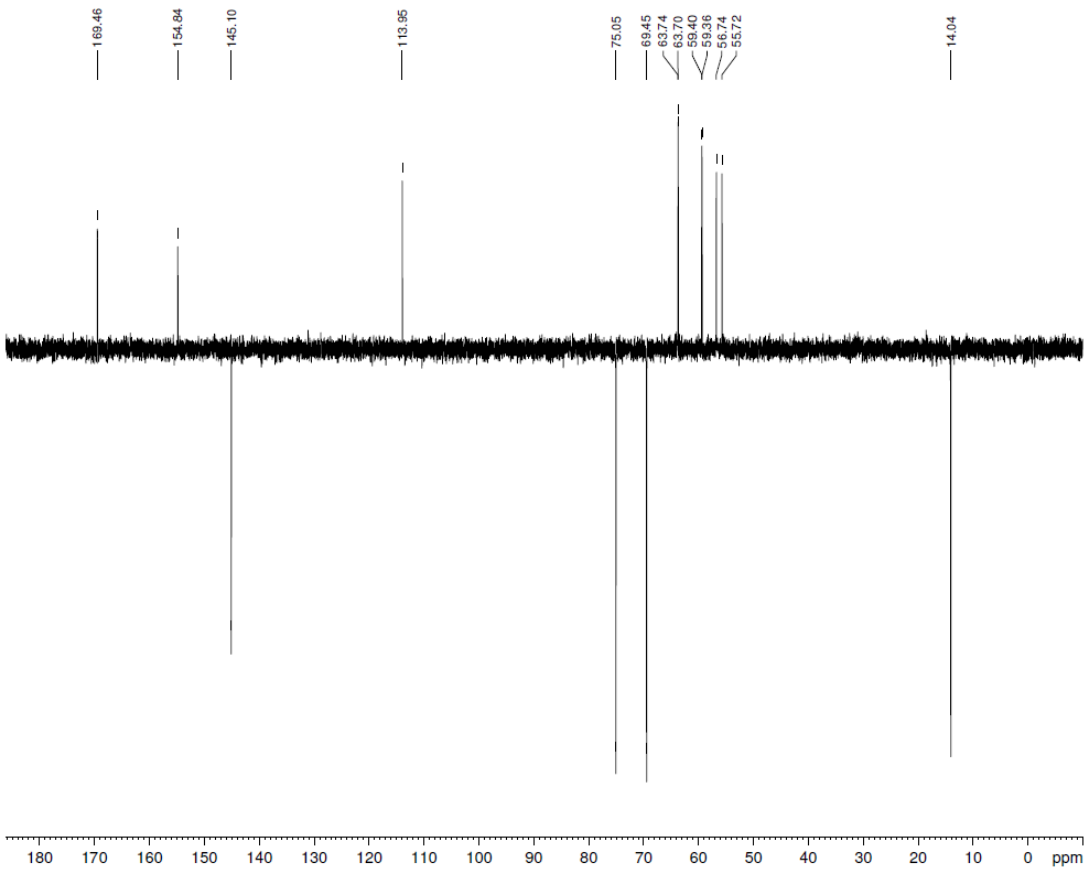
7

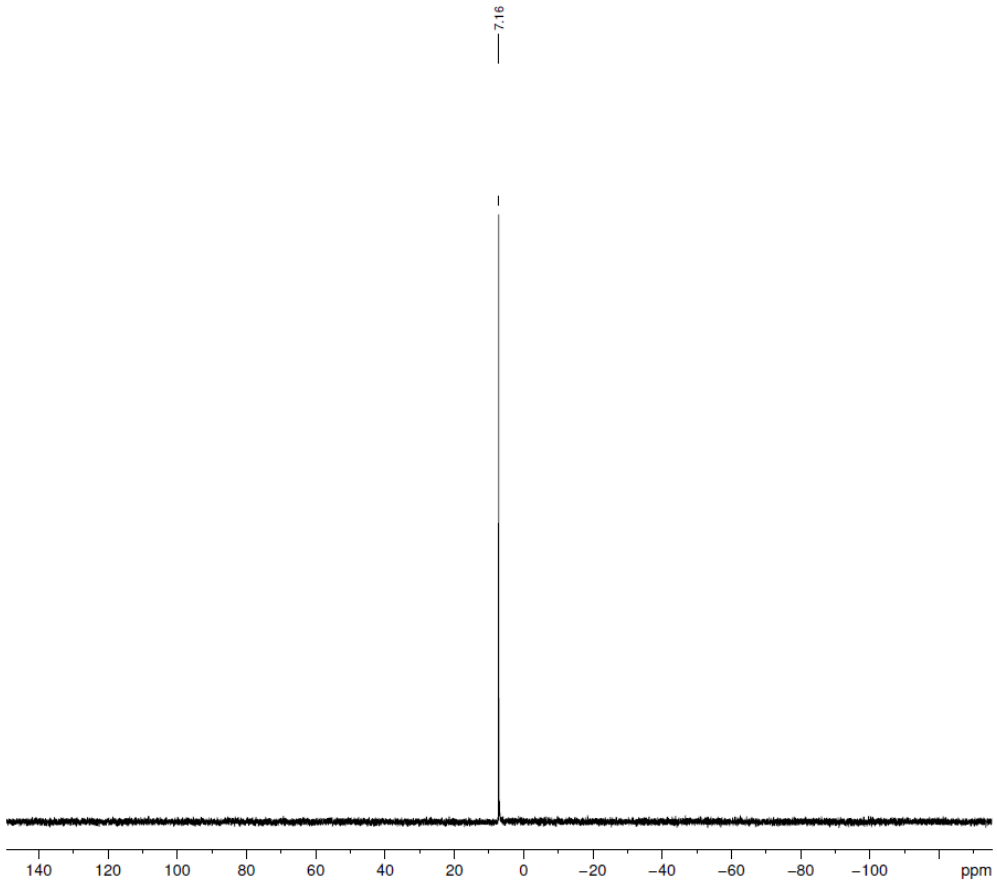
^{1}H NMR (499.8 MHz, D_2O, *T* = 25 °C, pD = 6.4): 1.86 (d, 3H, ^{4}J = 1.2, CH_3); 3.18 (dd, 1H, J_{gem} = 14.2, $J_{H,P}$ = 11.3, $CH_a\mathbf{H_b}P$); 3.24 (dd, 1H, J_{gem} = 14.2, $J_{H,P}$ = 11.7, $CH_a\mathbf{H_b}P$); 3.39 (dd, 1H, J_{gem} = 12.0, $J_{2'',3'}$ = 6.4, H-2''); 3.87 (dd, 1H, J_{gem} = 12.8, $J_{5',4'}$ = 5.6, H-5'); 3.93 (dd, 1H, J_{gem} = 12.8, $J_{5'',4'}$ = 9.1, H-5''); 4.04 (dd, 1H, J_{gem} = 12.0, $J_{2',3'}$ = 6.9, H-2'); 4.62 (ddd, 1H, $J_{4',5''}$ = 9.1, $J_{4',5'}$ = 5.6, $J_{4',3'}$ = 4.1, H-4'); 4.83 (ddd, 1H, $J_{3',2'}$ = 6.9, $J_{3',2''}$ = 6.4, $J_{3',4'}$ = 4.1, H-3'); 7.49 (q, 1H, ^{4}J = 1.2, H-6).

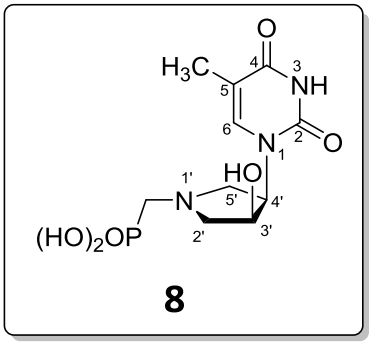
^{13}C NMR (125.7 MHz, D_2O, *T* = 25 °C, pD = 6.4): 14.04 (CH_3); 56.23 (d, $J_{C,P}$ = 128.1, CH_2P); 59.38 (d, $J_{C,P}$ = 4.6, C-5'); 63.72 (d, $J_{C,P}$ = 5.1, C-2'); 69.45 (C-4'); 75.05 (C-3'); 113.95 (C-5); 145.10 (C-6); 154.84 (C-2); 169.46 (C-4);.

$^{31}P\{1H\}$ NMR (202.3 MHz, D_2O, *T* = 25 °C, pD = 6.4): 7.16.




169.46
154.84
145.10
113.95
75.05
69.45
63.74
63.70
59.40
59.36
56.74
55.72
14.04
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.16
140 120 100 80 60 40 20 0 −20 −40 −60 −80 −100 ppm

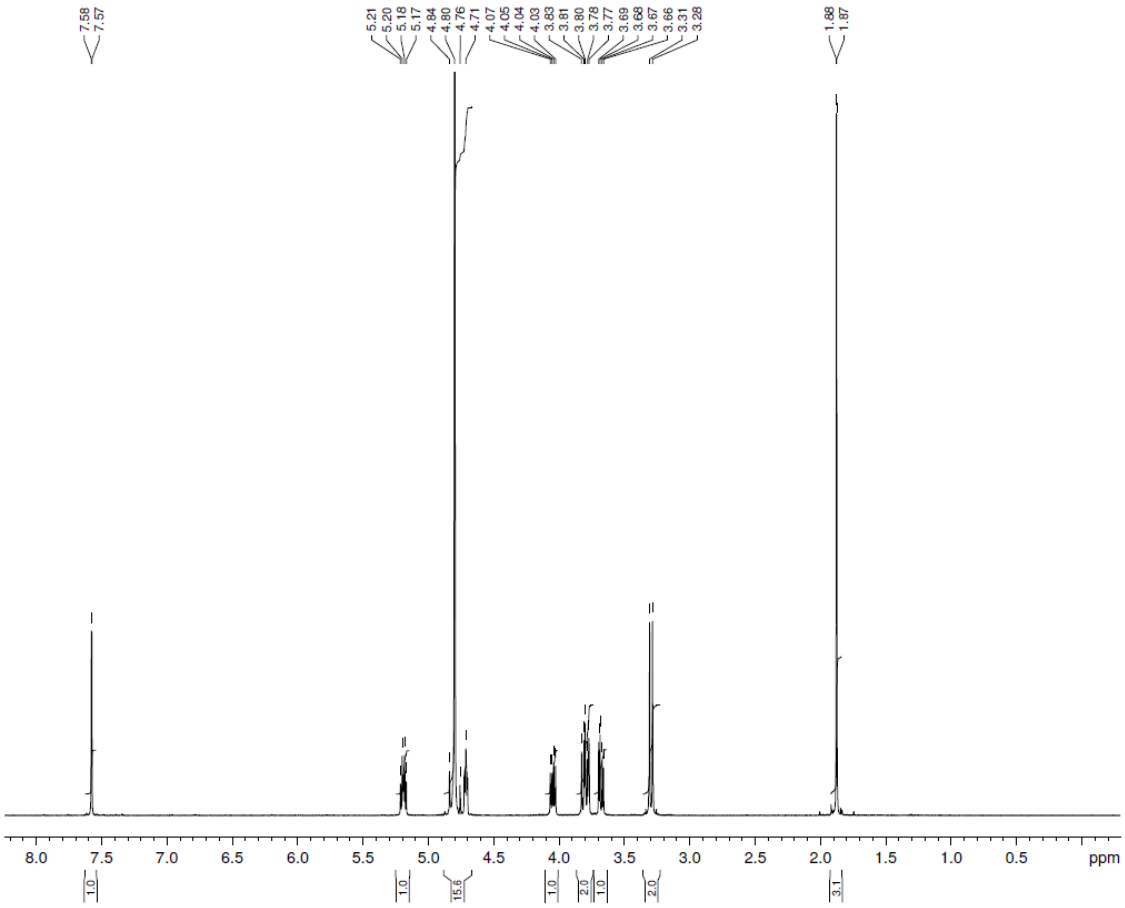


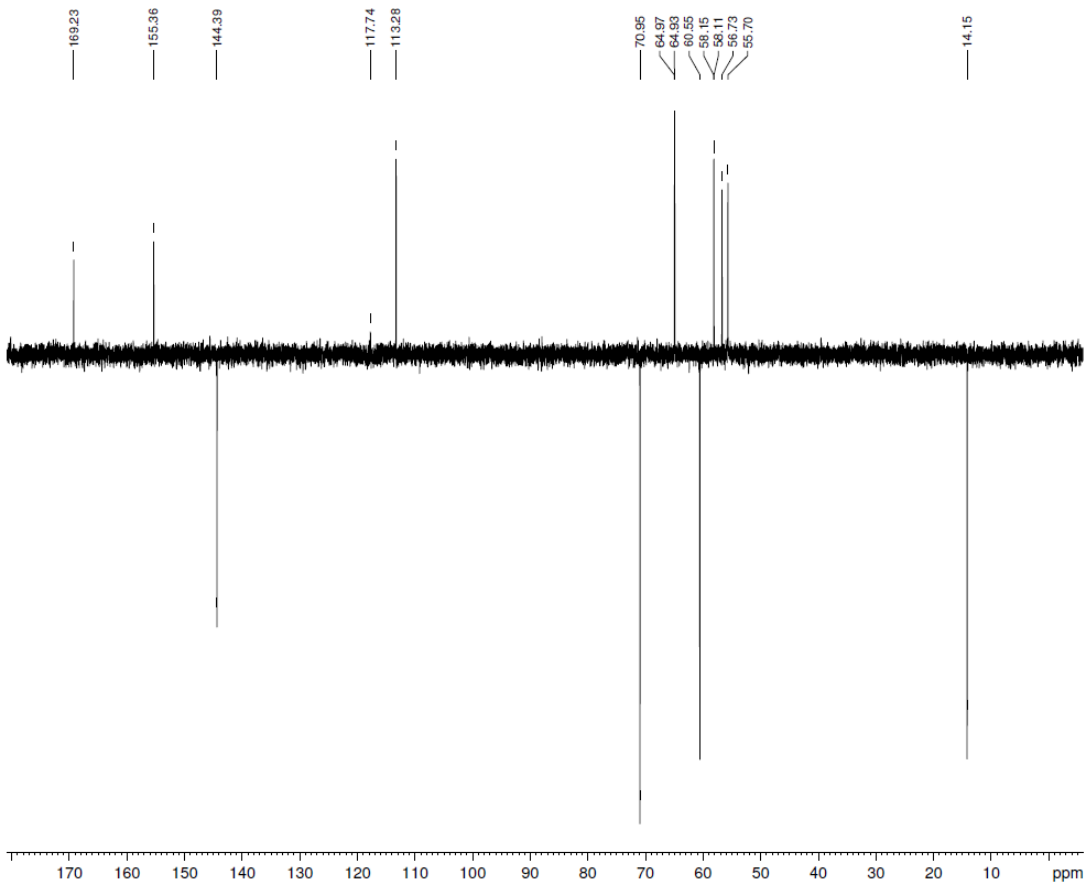
8

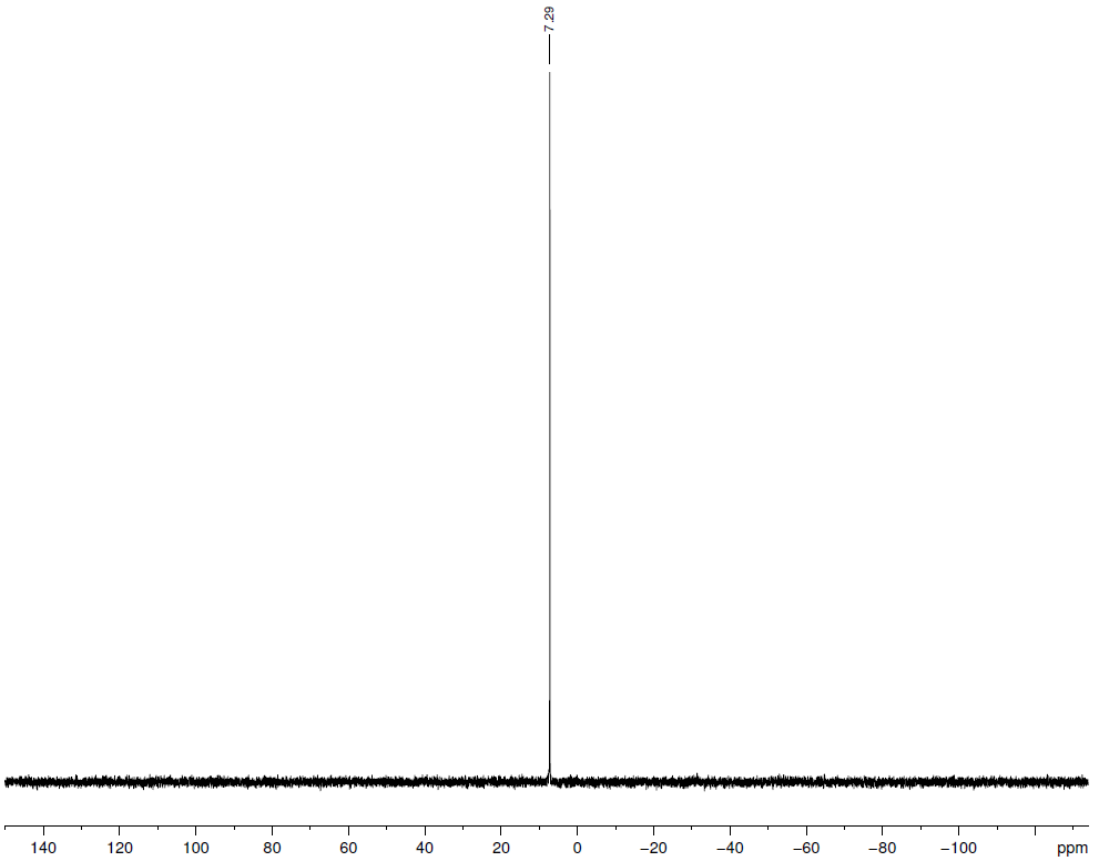
^{1}H NMR (499.8 MHz, D_2O, *T* = 25 °C, pD = 5.7): 1.88 (d, 3H, ^{4}J = 1.2, CH_3); 3.28, 3.31 (2 × dd, 2 × 1H, J_{gem} = 14.4, $J_{H,P}$ = 11.7, CH_2P); 3.68 (dd, 1H, J_{gem} = 12.7, $J_{2",3'}$ = 5.2, H-2"); 3.78 (dd, 1H, J_{gem} = 12.7, $J_{2',3'}$ = 2.0, H-2'); 3.80 (dd, 1H, J_{gem} = 12.8, $J_{5",4'}$ = 9.4, H-5"); 4.05 (dd, 1H, J_{gem} = 12.8, $J_{5',4'}$ = 6.9, H-5'); 4.71 (ddd, 1H, $J_{3',4'}$ = 6.0, $J_{3',2"}$ = 5.2, $J_{3',2'}$ = 2.0, H-3'); 5.19 (ddd, 1H, $J_{4',5"}$ = 9.4, $J_{4',5'}$ = 6.9, $J_{4',3'}$ = 6.0, H-4'); 7.58 (q, 1H, ^{4}J = 1.2, H-6).

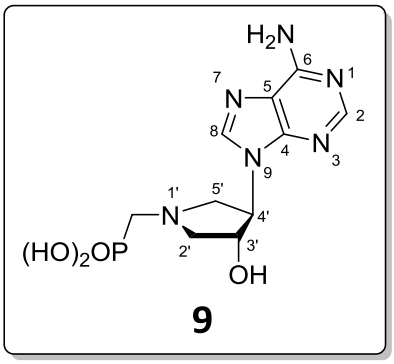
^{13}C NMR (125.7 MHz, D_2O, *T* = 25 °C, pD = 5.7): 14.15 (CH_3); 56.21 (d, $J_{C,P}$ = 130.0, CH_2P); 58.13 (d, $J_{C,P}$ = 4.9, C-5'); 60.55 (C-4'); 64.95 (d, $J_{C,P}$ = 5.0, C-2'); 70.95 (C-3'); 113.28 (C-5); 144.39 (C-6); 155.36 (C-2); 169.23 (C-4);.

^{31}P{1H} NMR (202.3 MHz, D_2O, *T* = 25 °C, pD = 5.7): 7.29.




169.23
155.36
144.39
117.74
113.28
70.95
64.97
64.83
60.55
58.15
58.11
56.73
55.70
14.15
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.29
140 120 100 80 60 40 20 0 −20 −40 −60 −80 −100 ppm

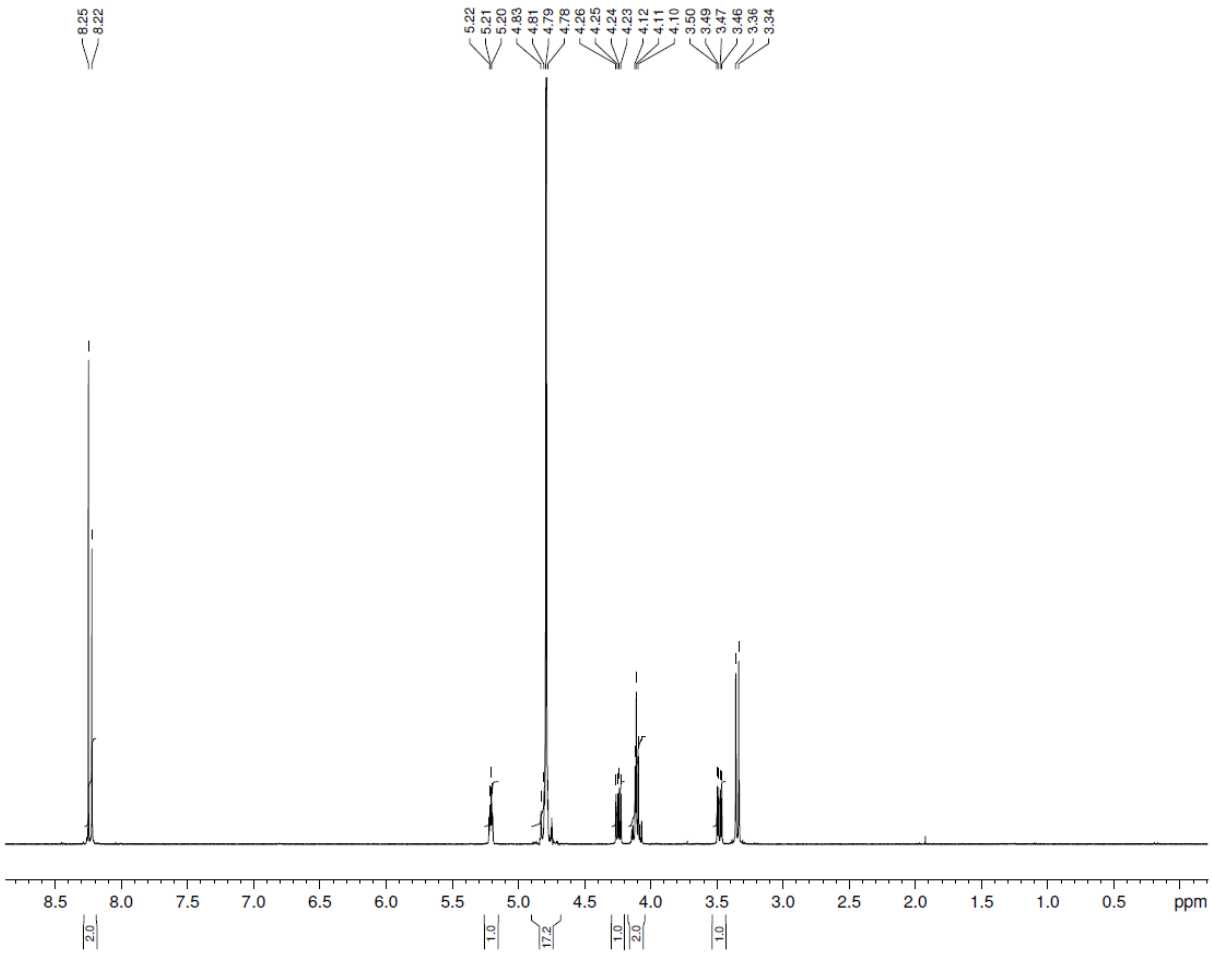


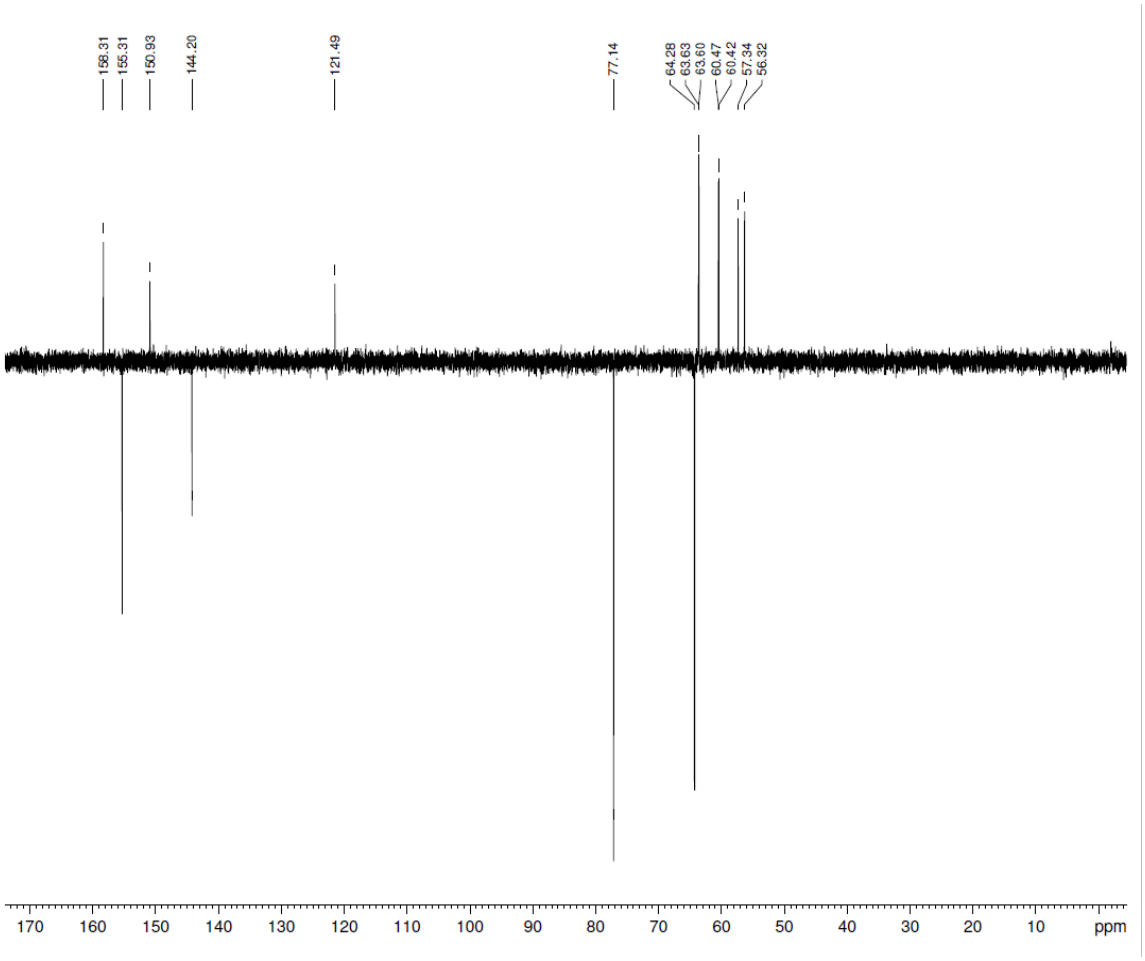
9

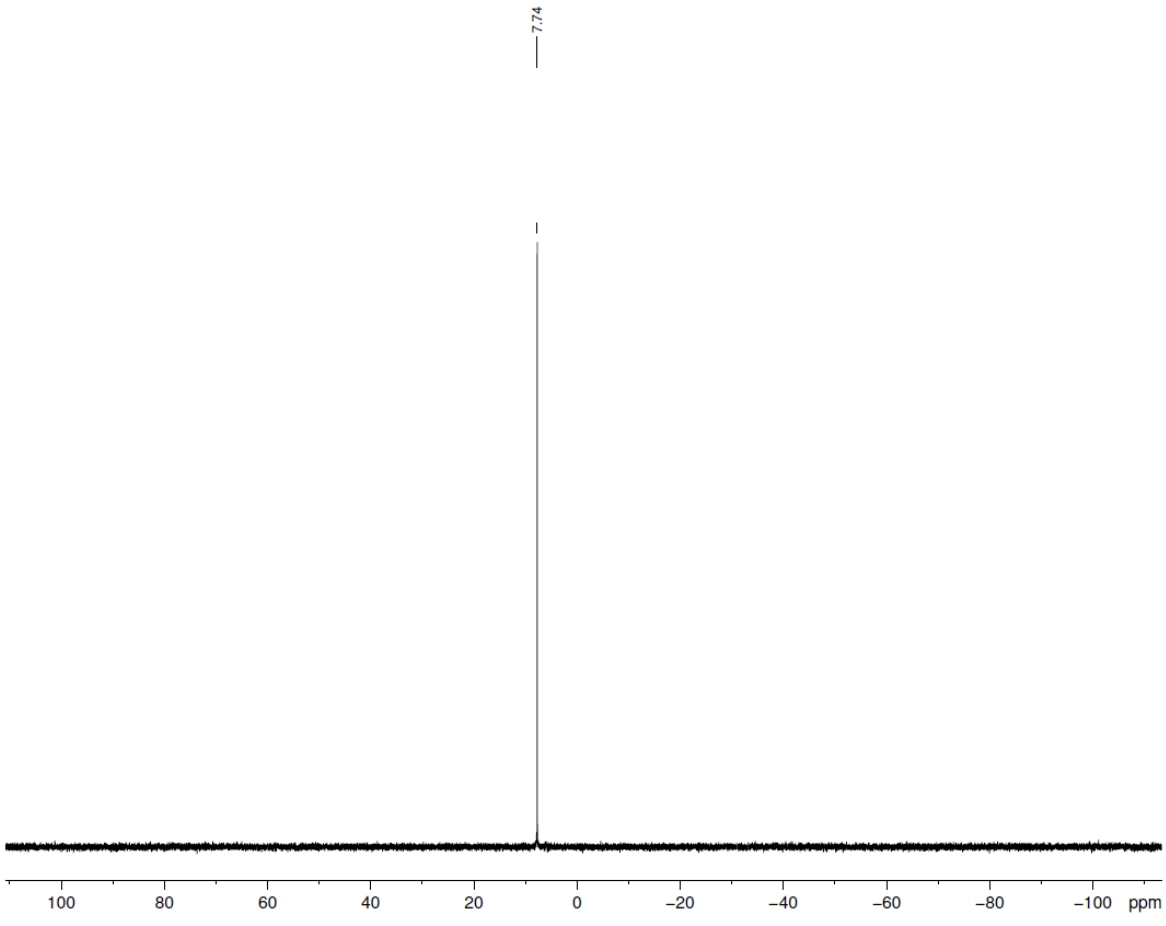
^{1}H NMR (499.8 MHz, D_2O, *T* = 25 °C, pD = 6.9): 3.33 (dd, 1H, J_{gem} = 14.4, $J_{H,P}$ = 11.3, $CH_a\mathbf{H_b}P$); 3.36 (dd, 1H, J_{gem} = 14.4, $J_{H,P}$ = 11.4, $C\mathbf{H_a}H_bP$); 3.48 (dd, 1H, J_{gem} = 12.6, $J_{2'',3'}$ = 5.1, H-2''); 4.09 (dd, 1H, J_{gem} = 13.0, $J_{5'',4'}$ = 7.3, H-5''); 4.13 (dd, 1H, J_{gem} = 13.0, $J_{5',4'}$ = 4.4, H-5'); 4.25 (dd, 1H, J_{gem} = 12.6, $J_{2',3'}$ = 6.5, H-2'); 4.78 (overlap with HDO signal, H-3'); 5.21 (ddd, 1H, $J_{4',5''}$ = 7.3, $J_{4',5'}$ = 4.4, $J_{4',3'}$ = 3.0, H-4'); 8.22 (s, 1H, H-8); 8.25 (s, 1H, H-2).

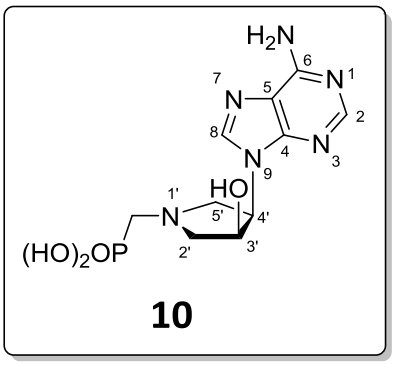
^{13}C NMR (125.7 MHz, D_2O, *T* = 25 °C, pD = 6.9): 56.83 (d, $J_{C,P}$ = 128.5, CH_2P); 60.45 (d, $J_{C,P}$ = 6.0, C-5'); 63.61 (d, $J_{C,P}$ = 4.3, C-2'); 64.28 (C-4'); 77.14 (C-3'); 121.49 (C-5); 144.20 (C-8); 150.93 (C-4); 155.31 (C-2); 158.31 (C-6).

^{31}P{1H} NMR (202.3 MHz, D_2O, *T* = 25 °C, pD = 6.9): 7.74.




158.31
155.31
150.93
144.20
121.49
77.14
64.28
63.63
63.60
60.47
60.42
57.34
56.32
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.74
100 80 60 40 20 0 −20 −40 −60 −80 −100 ppm

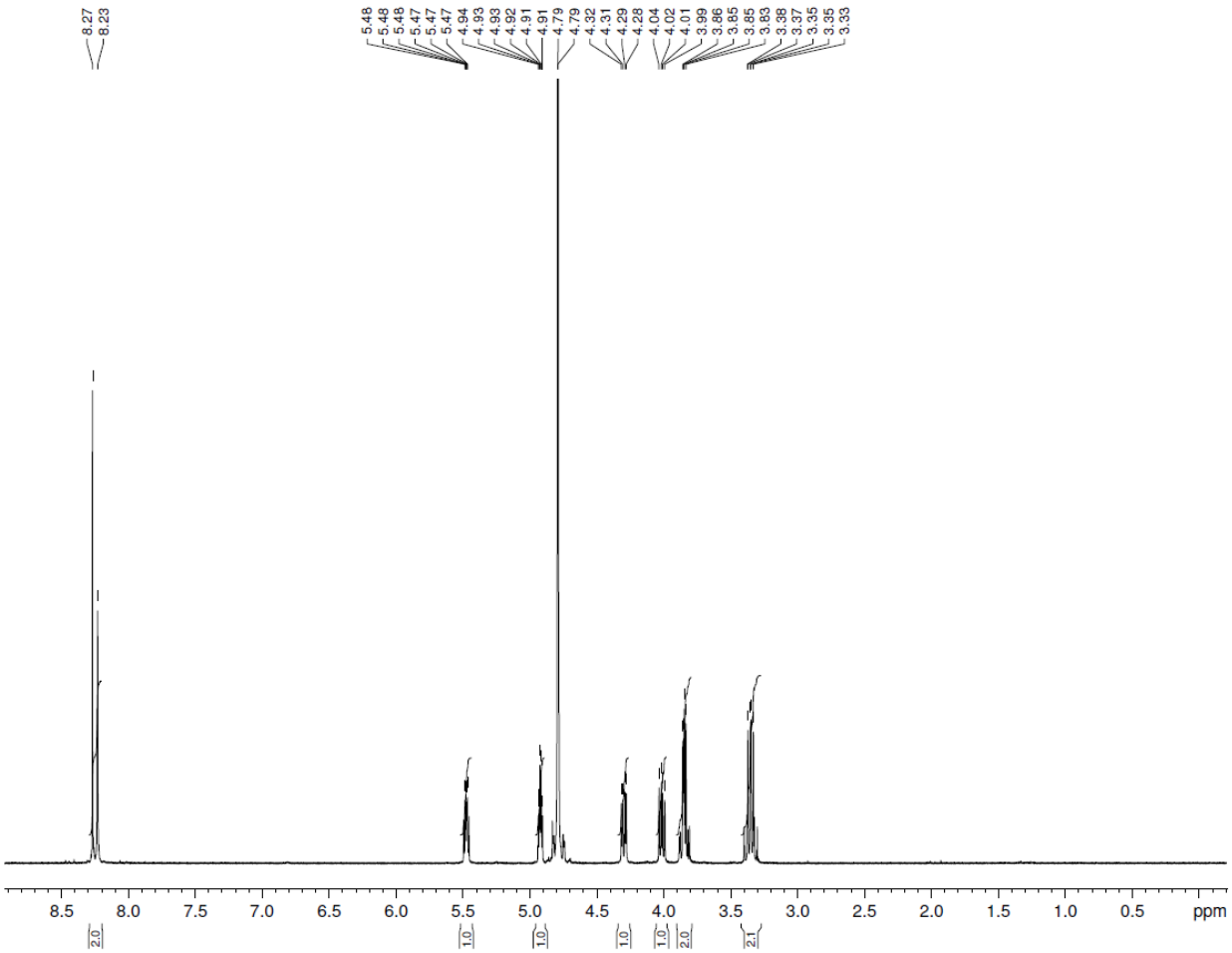


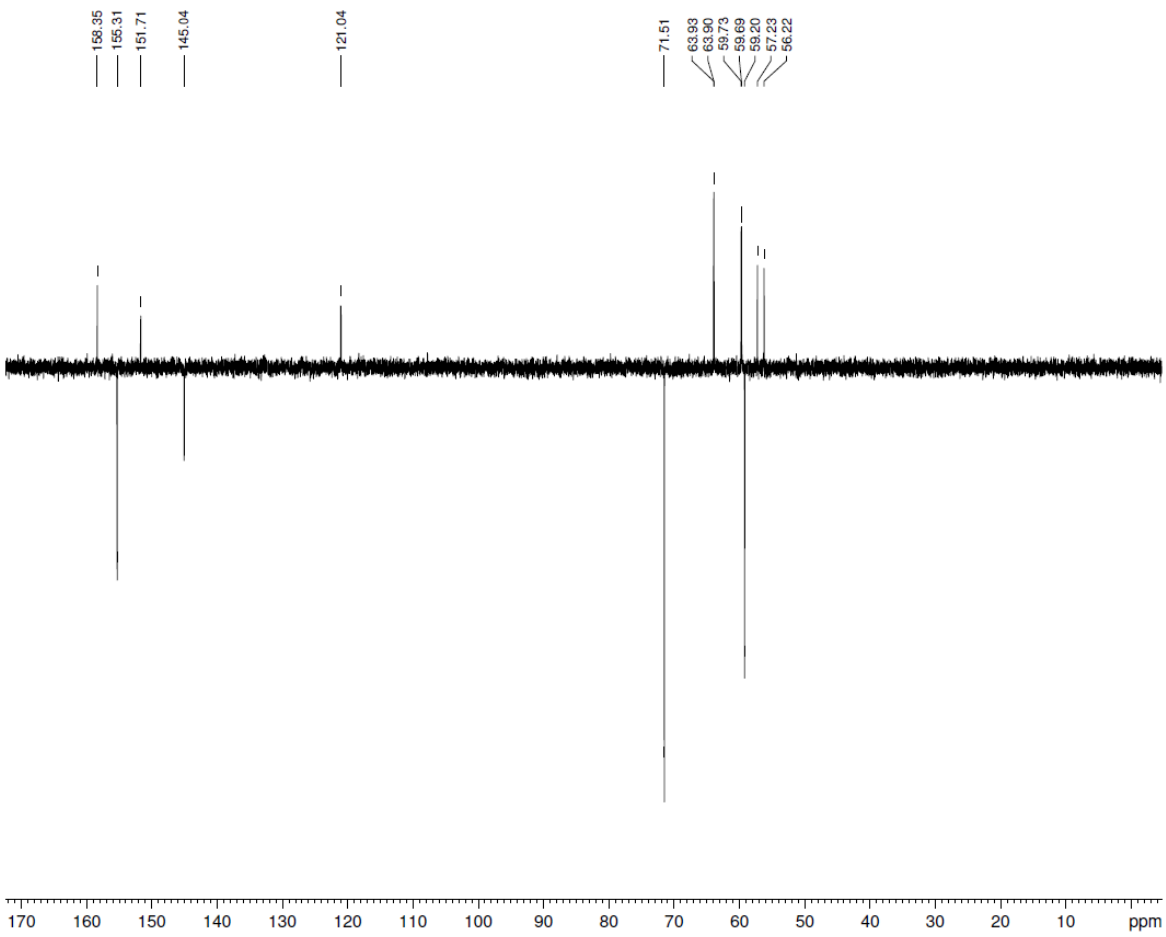
10

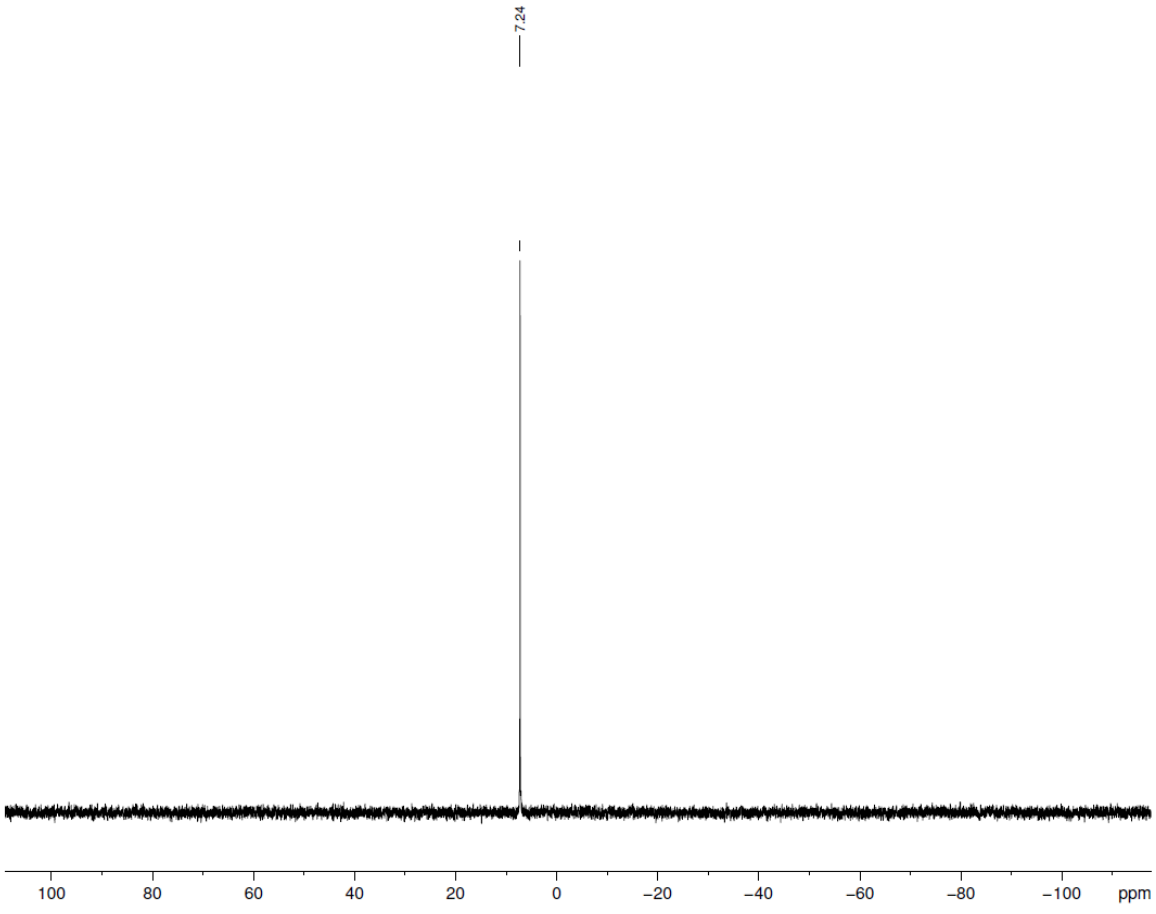
^{1}H NMR (499.8 MHz, D_2O, *T* = 25 °C, pD = 6.7): 3.33 (dd, 1H, J_{gem} = 14.1, $J_{H,P}$ = 11.2, $CH_a\mathbf{H_b}P$); 3.37 (dd, 1H, J_{gem} = 14.1, $J_{H,P}$ = 11.6, $C\mathbf{H_a}H_bP$); 3.83 (dd, 1H, J_{gem} = 13.0, $J_{2'',3'}$ = 6.1, H-2''); 3.87 (dd, 1H, J_{gem} = 13.0, $J_{2',3'}$ = 3.5, H-2'); 4.01 (dd, 1H, J_{gem} = 12.8, $J_{5'',4'}$ = 7.9, H-5''); 4.30 (dd, 1H, J_{gem} = 12.8, $J_{5',4'}$ = 5.0, H-5'); 4.25); 4.92 (td, 1H, $J_{3',4'}$ = $J_{3',2''}$ = 6.1, $J_{3',2'}$ = 3.5, H-3'); 5.47 (ddd, 1H, $J_{4',5''}$ = 7.9, $J_{4',3'}$ = 6.2, $J_{4',5'}$ = 5.0, H-4'); 8.23 (s, 1H, H-8); 8.27 (s, 1H, H-2).

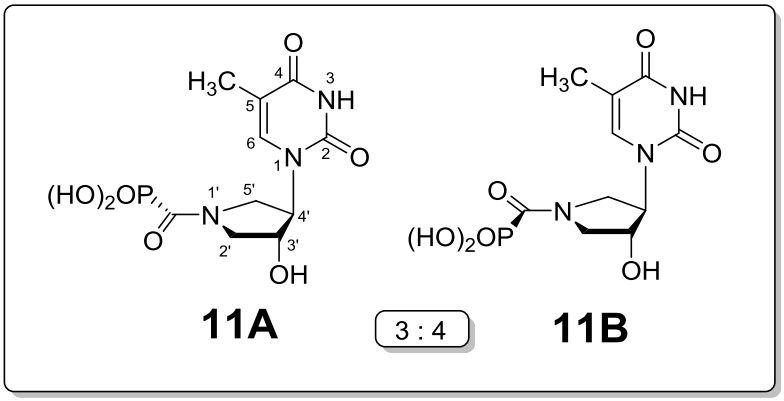
^{13}C NMR (125.7 MHz, D_2O, *T* = 25 °C, pD = 6.7): 56.73 (d, $J_{C,P}$ = 127.6, CH_2P); 59.20 (C-4'); 59.71 (d, $J_{C,P}$ = 5.8, C-5'); 63.92 (d, $J_{C,P}$ = 4.0, C-2'); 71.51 (C-3'); 121.04 (C-5); 145.04 (C-8); 151.71 (C-4); 155.31 (C-2); 158.35 (C-6).

^{31}P{1H} NMR (202.3 MHz, D_2O, *T* = 25 °C, pD = 6.7): 7.24.




158.35
155.31
151.71
145.04
121.04
71.51
63.93
63.90
59.73
59.69
59.20
57.23
56.22
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.24
100
80
60
40
20
0
−20
−40
−60
−80
−100
ppm



Rotamer A:

^{1}H NMR (400.1 MHz, D_2O, *T* = 25 °C, pD = 6.4): 1.88 (d, 3H, ^{4}J = 1.2, CH_3); 3.47 (ddd, 1H, J_{gem} = 13.6, $J_{2",3'}$ = 4.8, $J_{H,P}$ = 1.7, H-2"); 3.85 (ddd, 1H, J_{gem} = 13.6, $J_{2',3'}$ = 6.8, $J_{H,P}$ = 1.6, H-2'); 4.12 (dd, 1H, J_{gem} = 12.9, $J_{5',4'}$ = 6.2, H-5'); 4.41 (dd, 1H, J_{gem} = 12.9, $J_{5",4'}$ = 7.7, H-5"); 4.59 (ddd, 1H, $J_{3',2'}$ = 6.8, $J_{3',4'}$ = 5.4, $J_{3',2"}$ = 4.8, H-3'); 4.91 (ddd, 1H, $J_{4',5"}$ = 7.7, $J_{4',5'}$ = 6.2, $J_{4',3'}$ = 5.4, H-4'); 7.43 (q, 1H, ^{4}J = 1.2, H-6).

^{13}C NMR (100.6 MHz, D_2O, *T* = 25 °C, pD = 6.4): 14.24 (CH_3); 50.26 (C-5'); 52.88 (d, $J_{C,P}$ = 4.7, C-2'); 64.31 (C-4'); 73.07 (C-3'); 114.39 (C-5); 141.28 (C-6); 155.03 (C-2); 169.15 (C-4); 177.87 (d, $J_{C,P}$ = 202.7, P-CO).

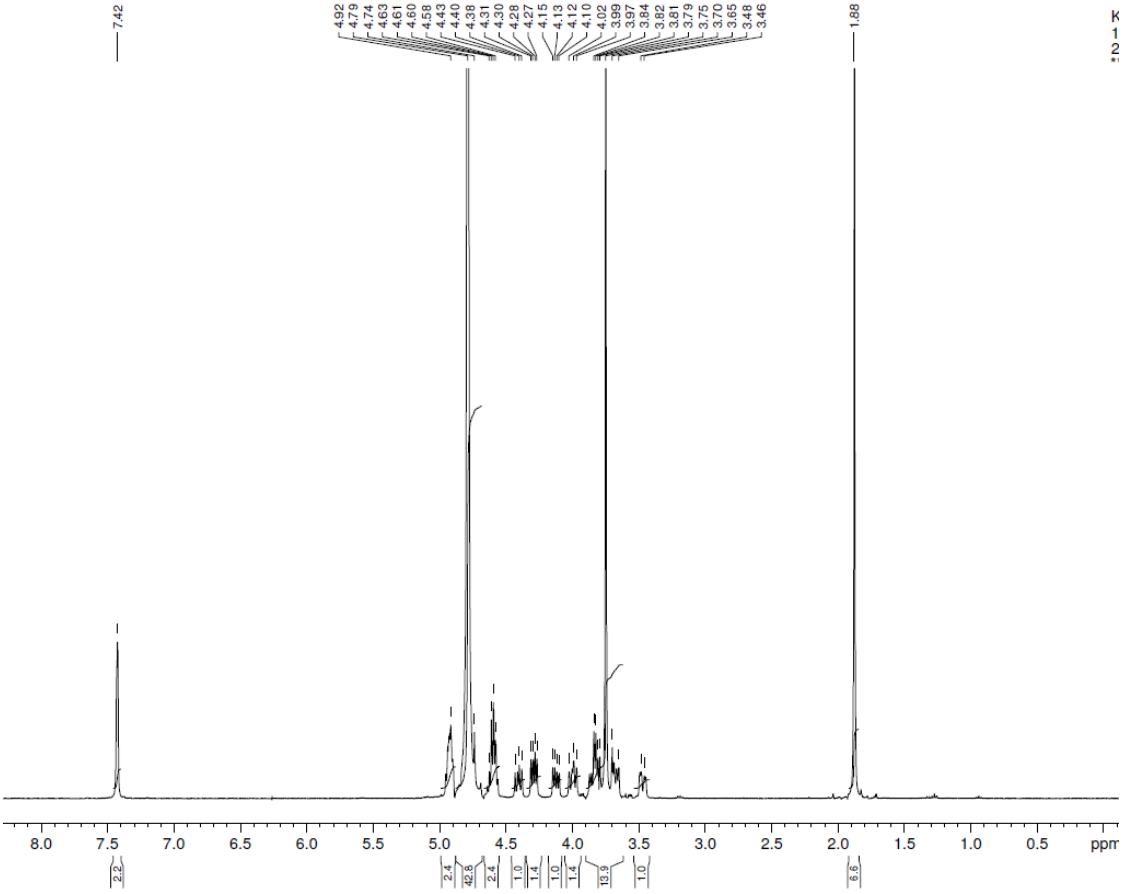
^{31}P{1H} NMR (162.0 MHz, D_2O, *T* = 25 °C, pD = 6.4): -2.72.

Rotamer B:

^{1}H NMR (400.1 MHz, D_2O, *T* = 25 °C, pD = 6.4): 1.88 (d, 3H, ^{4}J = 1.2, CH_3); 3.68 (ddd, 1H, J_{gem} = 13.6, $J_{5',4'}$ = 6.1, $J_{H,P}$ = 1.6, H-5'); 3.81 (dd, 1H, J_{gem} = 12.3, $J_{2",3'}$ = 5.7, H-2"); 4.00 (ddd, 1H, J_{gem} = 13.6, $J_{5",4'}$ = 8.5, $J_{H,P}$ = 1.6, H-5"); 4.29 (dd, 1H, J_{gem} = 12.3, $J_{2',3'}$ = 6.1, H-2'); 4.60 (ddd, 1H, $J_{3',2'}$ = 6.1, $J_{3',2"}$ = 5.7, $J_{3',4'}$ = 5.5, H-3'); 4.94 (ddd, 1H, $J_{4',5"}$ = 8.5, $J_{4',5'}$ = 6.1, $J_{4',3'}$ = 5.5, H-4'); 7.42 (q, 1H, ^{4}J = 1.2, H-6).

^{13}C NMR (100.6 MHz, D_2O, *T* = 25 °C, pD = 6.4): 14.17 (CH_3); 48.81 (d, $J_{C,P}$ = 5.3, C-5'); 54.44 (C-2'); 62.37 (C-4'); 74.64 (C-3'); 114.45 (C-5); 141.35 (C-6); 155.08 (C-2); 169.14 (C-4); 177.87 (d, $J_{C,P}$ = 202.7, P-CO).

^{31}P{1H} NMR (162.0 MHz, D_2O, *T* = 25 °C, pD = 6.4): -2.63.


7.42
4.92
4.79
4.74
4.63
4.61
4.60
4.58
4.43
4.40
4.38
4.31
4.30
4.28
4.27
4.15
4.13
4.12
4.10
4.02
3.99
3.97
3.84
3.82
3.81
3.79
3.75
3.70
3.65
3.48
3.46
1.88
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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1.0
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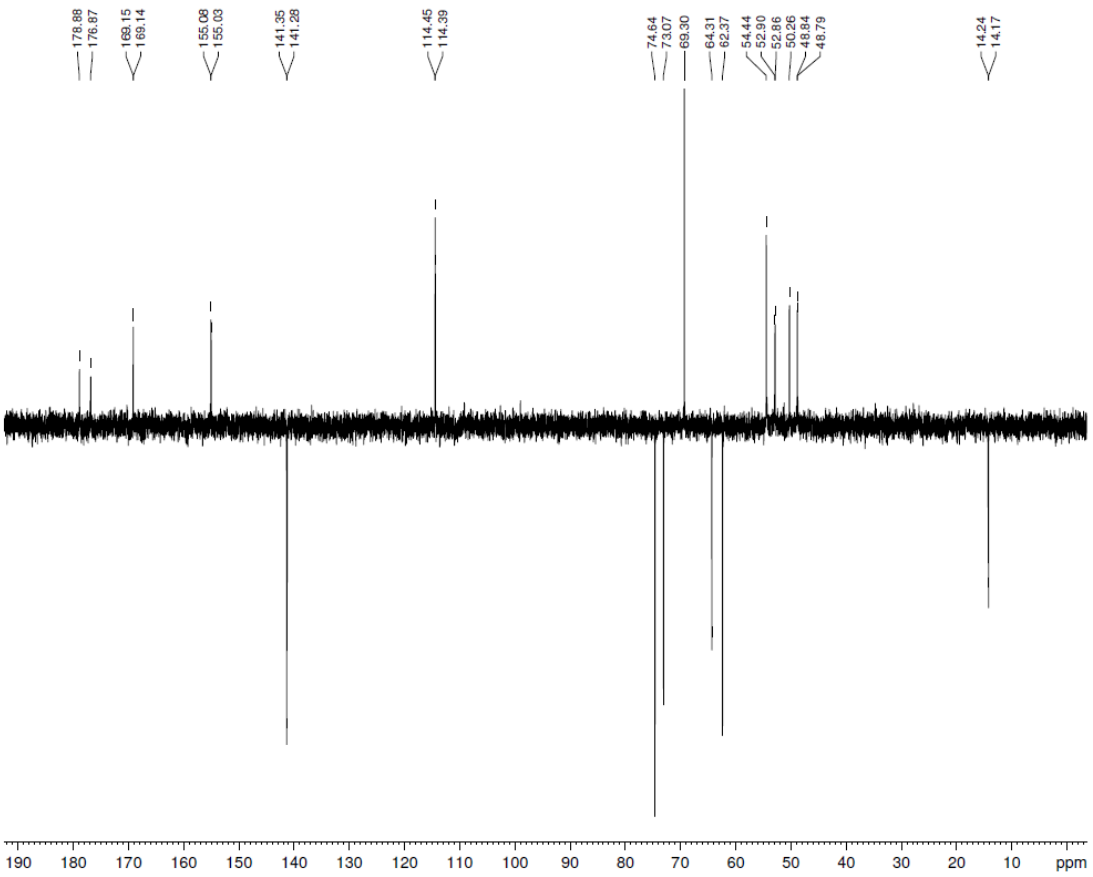
13.9
1.0
6.6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62.37
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52.90
52.86
50.26
48.84
48.79
14.24
14.17
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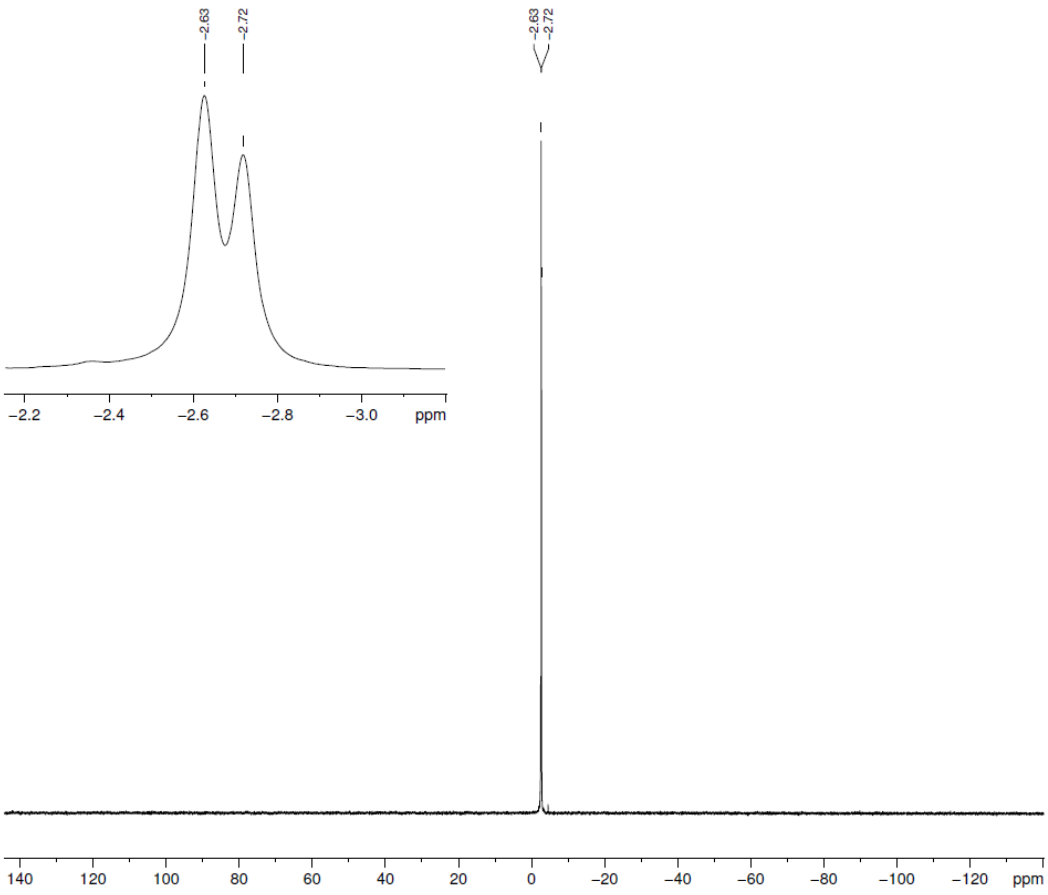
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60
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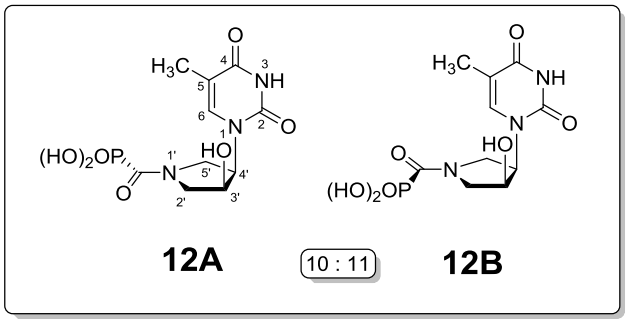


Rotamer A:

^{1}H NMR (600.1 MHz, D_2O, *T* = 25 °C, pD = 5.9): 1.891 (d, 3H, ^{4}J = 1.2, CH_3); 3.57 (dt, 1H, J_{gem} = 13.7, $J_{2',3'}$ = $J_{H,P}$ = 2.1, H-2'); 3.79 (ddd, 1H, J_{gem} = 13.7, $J_{2'',3'}$ = 5.2, $J_{H,P}$ = 2.0, H-2''); 4.17 (dd, 1H, J_{gem} = 11.7, $J_{5',4'}$ = 9.5, H-5'); 4.42 (dd, 1H, J_{gem} = 11.7, $J_{5'',4'}$ = 8.1, H-5''); 4.58 (ddd, 1H, $J_{3',2''}$ = 5.2, $J_{3',4'}$ = 4.5, $J_{3',2'}$ = 2.1, H-3'); 5.09 (ddd, 1H, $J_{4',5'}$ = 9.5, $J_{4',5''}$ = 8.1, $J_{4',3'}$ = 4.5, H-4'); 7.60 (q, 1H, ^{4}J = 1.2, H-6).

^{13}C NMR (150.9 MHz, D_2O, *T* = 25 °C, pD = 5.9): 14.22 (CH_3); 48.94 (C-5'); 54.51 (d, $J_{C,P}$ = 4.5, C-2'); 59.37 (C-4'); 70.15 (C-3'); 113.06 (C-5); 142.98 (C-6); 155.29 (C-2); 169.16 (C-4); 178.86 (d, $J_{C,P}$ = 198.0, P-CO).

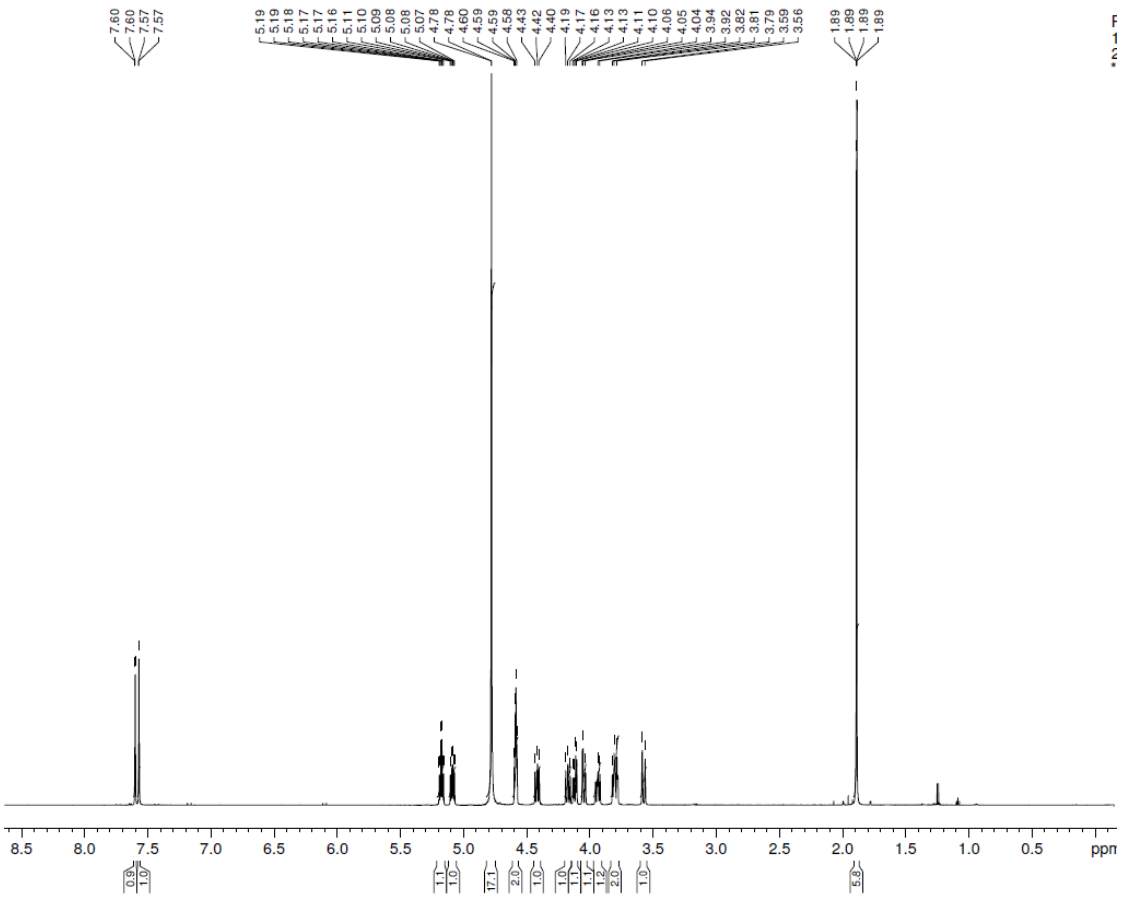
^{31}P{1H} NMR (202.3 MHz, D_2O, *T* = 25 °C, pD = 5.9): -2.16.

Rotamer B:

^{1}H NMR (600.1 MHz, D_2O, *T* = 25 °C, pD = 5.9): 1.887 (d, 3H, ^{4}J = 1.2, CH_3); 3.80 (ddd, 1H, J_{gem} = 13.0, $J_{5',4'}$ = 8.5, $J_{H,P}$ = 2.1, H-5'); 3.94 (ddd, 1H, J_{gem} = 13.0, $J_{5'',4'}$ = 8.5, $J_{H,P}$ = 2.0, H-5''); 4.05 (dd, 1H, J_{gem} = 12.7, $J_{2',3'}$ = 3.3, H-2'); 4.12 (dd, 1H, J_{gem} = 12.7, $J_{2'',3'}$ = 4.8, H-2''); 4.59 (ddd, 1H, $J_{3',2''}$ = 4.8, $J_{3',4'}$ = 4.6, $J_{3',2'}$ = 3.3, H-3'); 5.18 (dt, 1H, $J_{4',5'}$ = 8.5, $J_{4',5''}$ = 8.5, $J_{4',3'}$ = 4.6, H-4'); 7.57 (q, 1H, ^{4}J = 1.2, H-6).

^{13}C NMR (100.6 MHz, D_2O, *T* = 25 °C, pD = 5.9): 14.18 (CH_3); 48.86 (d, $J_{C,P}$ = 5.1, C-5'); 55.89 (C-2'); 57.63 (C-4'); 72.22 (C-3'); 113.14 (C-5); 142.86 (C-6); 155.37 (C-2); 169.16 (C-4); 178.88 (d, $J_{C,P}$ = 198.5, P-CO).

^{31}P{1H} NMR (162.0 MHz, D_2O, *T* = 25 °C, pD = 5.9): -2.28.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5.16
5.11
5.10
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5.08
5.08
5.07
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4.78
4.60
4.59
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4.58
4.43
4.42
4.40
4.19
4.17
4.16
4.13
4.13
4.11
4.10
4.06
4.05
4.04
3.94
3.92
3.82
3.81
3.79
3.59
3.56
1.89
1.89
1.89
1.89
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
2.0
1.5
1.0
0.5
ppm
0.9
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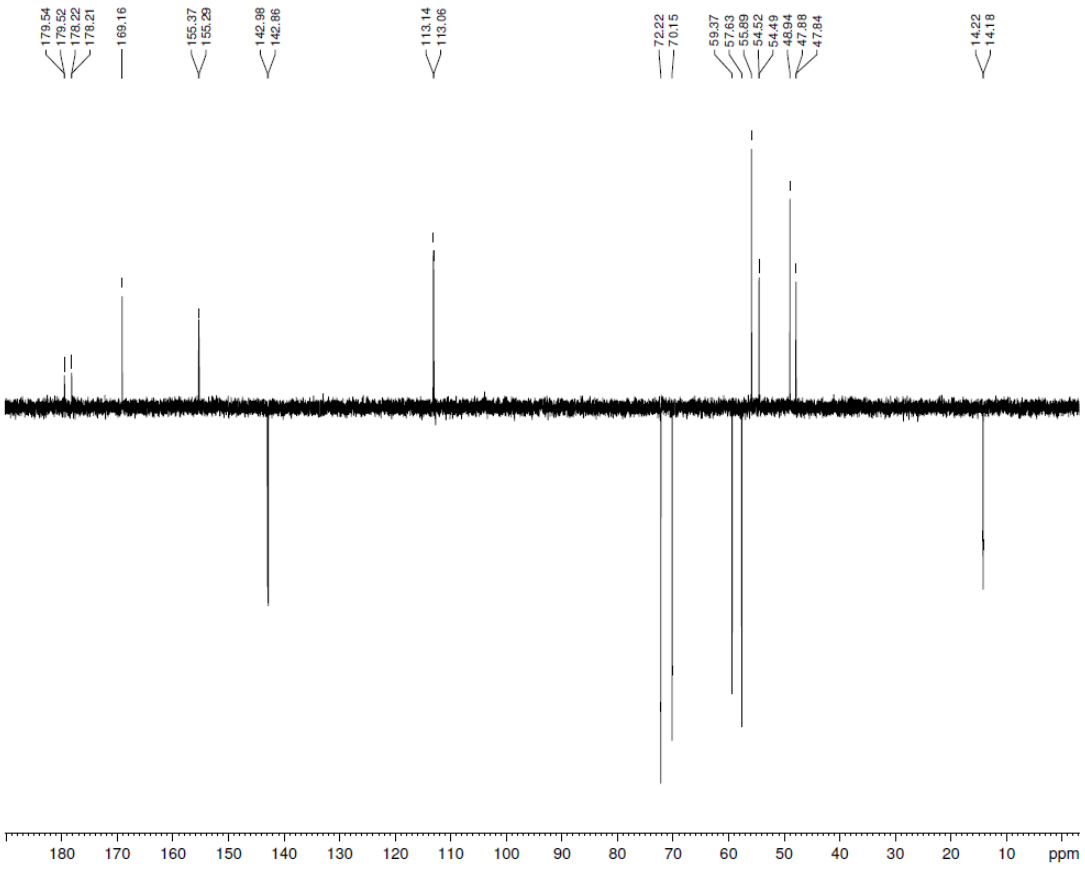
1.0
1.0
1.1
1.2
1.6
2.6
1.0
5.8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155.37
155.29
142.98
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113.14
113.06
72.22
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47.84
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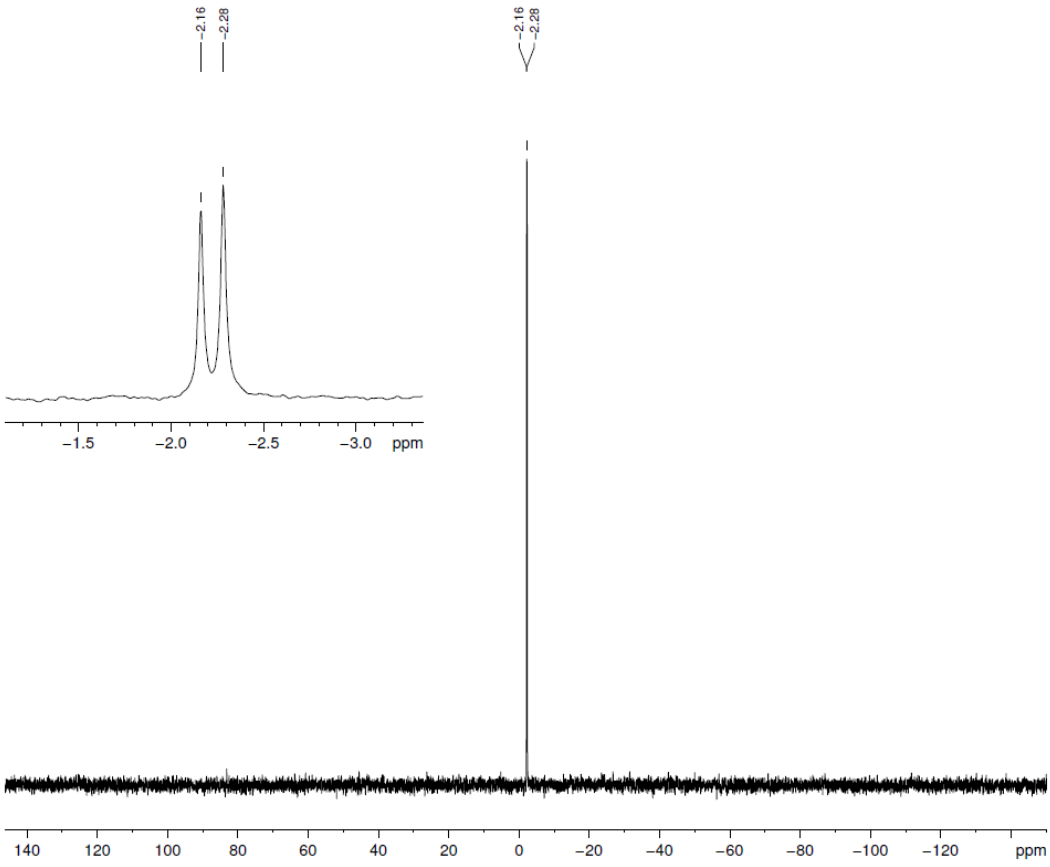
90
80
70
60
50
40
30
20
10
ppm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−2.5
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ppm
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120
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60
40
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0
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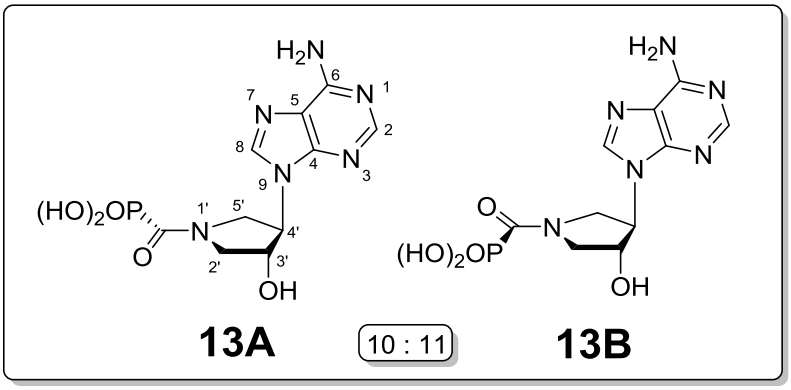
−40
−60
−80
−100
−120
ppm



Rotamer A:

^{1}H NMR (600.1 MHz, D_2O, *T* = 25 °C, pD = 6.1): 3.54 (dddd, 1H, J_{gem} = 13.6, $J_{2",3'}$ = 4.1, $J_{H,P}$ = 1.9, $J_{2",5"}$ = 0.9, H-2"); 3.83 (ddd, 1H, J_{gem} = 13.6, $J_{2',3'}$ = 6.1, $J_{H,P}$ = 1.9, H-2'); 4.55 (ddd, 1H, J_{gem} = 13.0, $J_{5',4'}$ = 5.6, $J_{5',3'}$ = 0.9, H-5'); 4.57 (ddd, 1H, J_{gem} = 13.0, $J_{5",4'}$ = 6.3, $J_{5",2"}$ = 0.9, H-5"); 4.73 (dddd, 1H, $J_{3',2'}$ = 6.1, $J_{3',4'}$ = 4.5, $J_{3',2"}$ = 4.1, $J_{3',5'}$ = 0.9, H-3'); 5.01 (ddd, 1H, $J_{4',5"}$ = 6.3, $J_{4',5'}$ = 5.6, $J_{4',3'}$ = 4.5, H-4'); 8.134 (s, 1H, H-8); 8.151 (s, 1H, H-2).

^{13}C NMR (150.9 MHz, D_2O, *T* = 25 °C, pD = 6.1): 51.65 (C-5'); 53.11 (d, $J_{C,P}$ = 4.6, C-2'); 62.87 (C-4'); 73.75 (C-3'); 121.29 (C-5); 142.56 (C-8); 151.58 (C-4); 154.92 (C-2); 157.98 (C-6); 179.15 (d, $J_{C,P}$ = 197.5, P-CO).

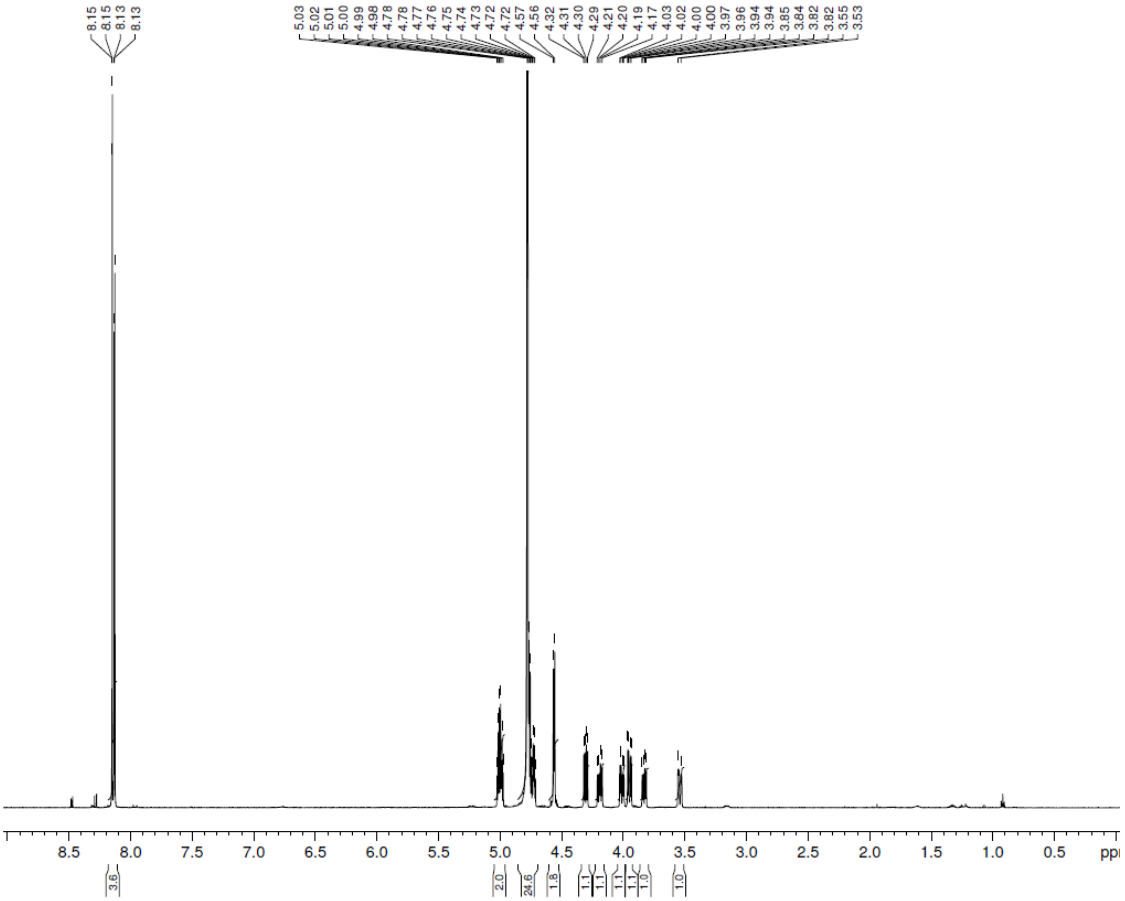
^{31}P{1H} NMR (202.3 MHz, D_2O, *T* = 25 °C, pD = 6.1): -2.25.

Rotamer B:

^{1}H NMR (600.1 MHz, D_2O, *T* = 25 °C, pD = 6.1): 3.95 (dd, 1H, J_{gem} = 12.6, $J_{2",3'}$ = 5.2, H-2"); 4.01 (ddd, 1H, J_{gem} = 13.6, $J_{5',4'}$ = 5.5, $J_{H,P}$ = 1.9, H-5'); 4.19 (ddd, 1H, J_{gem} = 13.6, $J_{5",4'}$ = 7.8, $J_{H,P}$ = 2.0, H-5"); 4.31 (ddd, 1H, J_{gem} = 12.6, $J_{2',3'}$ = 5.8, $J_{2',5'}$ = 0.8, H-2'); 4.76 (ddd, 1H, $J_{3',2'}$ = 5.8, $J_{3',4'}$ = 5.3, $J_{3',2"}$ = 5.2, H-3'); 4.99 (ddd, 1H, $J_{4',5"}$ = 7.8, $J_{4',5'}$ = 5.5, $J_{4',3'}$ = 5.3, H-4'); 8.130 (s, 1H, H-8); 8.149 (s, 1H, H-2).

^{13}C NMR (150.9 MHz, D_2O, *T* = 25 °C, pD = 6.1): 50.23 (d, $J_{C,P}$ = 4.9, C-5'); 54.64 (C-2'); 60.88 (C-4'); 75.44 (C-3'); 121.29 (C-5); 142.73 (C-8); 151.62 (C-4); 154.95 (C-2); 158.00 (C-6); 179.24 (d, $J_{C,P}$ = 197.0, P-CO).

^{31}P{1H} NMR (202.3 MHz, D_2O, *T* = 25 °C, pD = 6.1): -2.23.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4.75
4.74
4.73
4.72
4.72
4.57
4.56
4.32
4.31
4.30
4.29
4.21
4.20
4.19
4.17
4.03
4.02
4.00
4.00
3.97
3.96
3.94
3.94
3.85
3.84
3.82
3.82
3.55
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1.1
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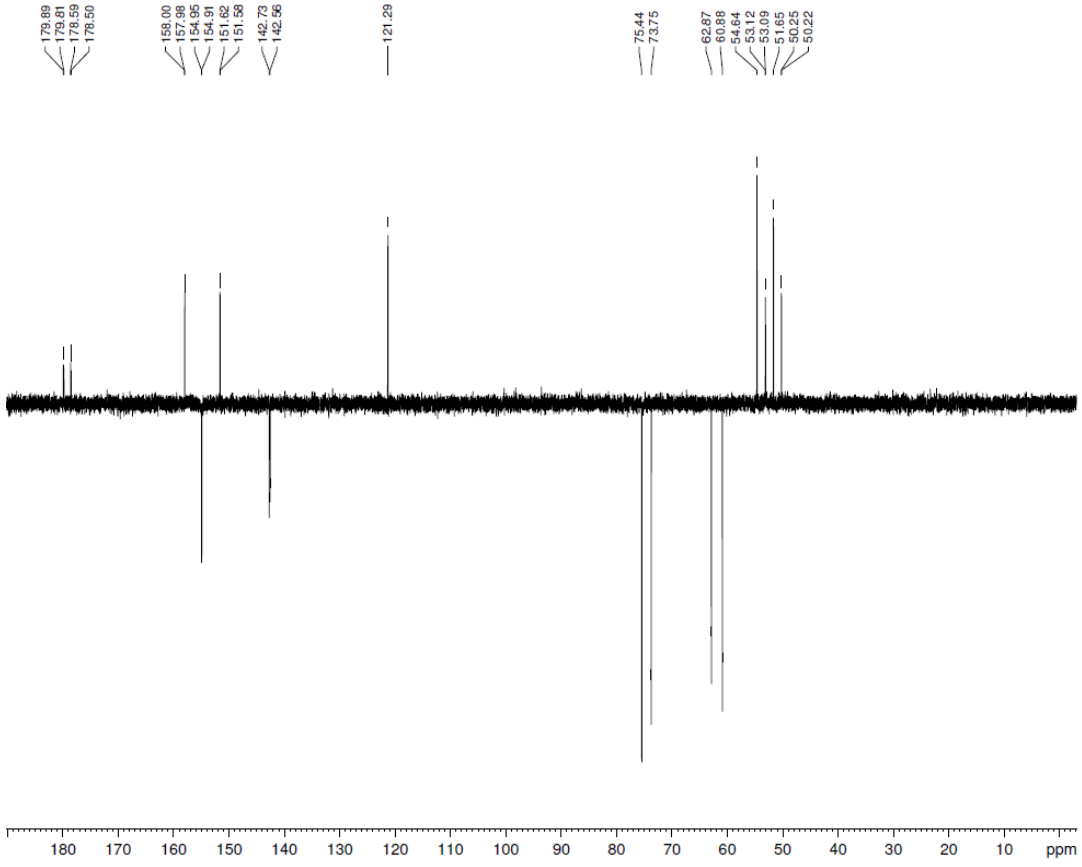
1.5
1.0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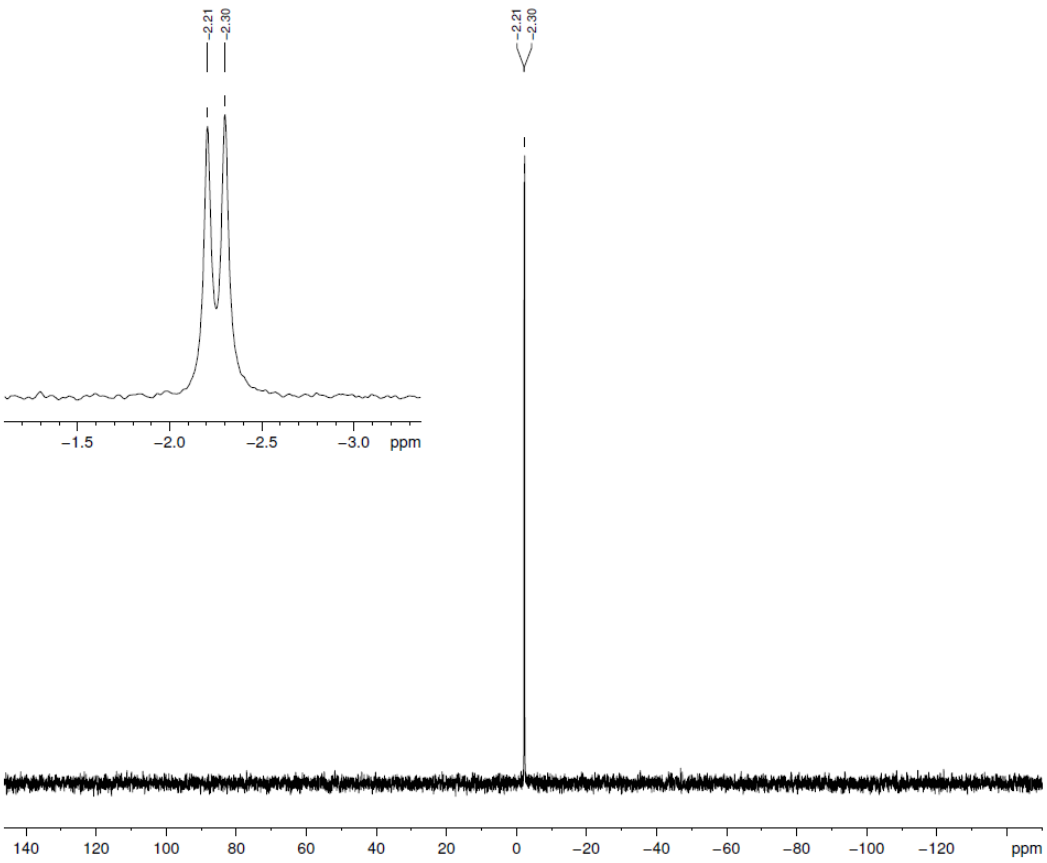
10
ppm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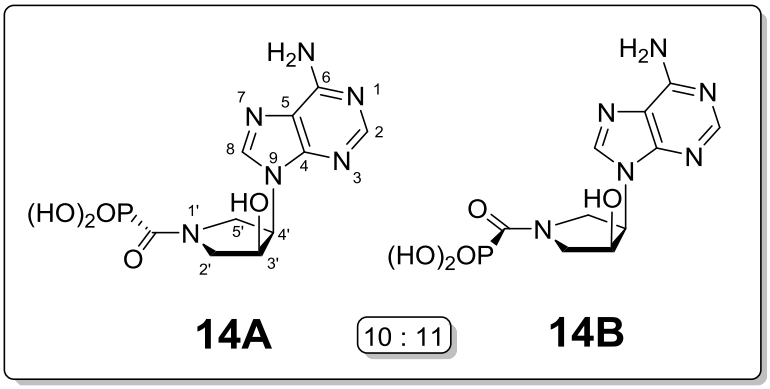


Rotamer A:

^{1}H NMR (600.1 MHz, D_2O, *T* = 25 °C, pD = 5.9): 3.65 (dt, 1H, J_{gem} = 13.7, $J_{2',3'} = J_{H,P}$ = 2.1, H-2'); 3.90 (ddd, 1H, J_{gem} = 13.7, $J_{2",3'}$ = 5.1, $J_{H,P}$ = 1.9, H-2"); 4.41 (dd, 1H, J_{gem} = 11.6, $J_{5',4'}$ = 9.2, H-5'); 4.66 (dd, 1H, J_{gem} = 11.6, $J_{5",4'}$ = 7.6, H-5"); 4.693 (ddd, 1H, $J_{3',2"}$ = 5.1, $J_{3',4'}$ = 4.2, $J_{3',2'}$ = 2.1, H-3'); 5.19 (ddd, 1H, $J_{4',5'}$ = 9.2, $J_{4',5"}$ = 7.6, $J_{4',3'}$ = 4.2, H-4'); 8.158 (s, 1H, H-2); 8.262 (s, 1H, H-8).

^{13}C NMR (150.9 MHz, D_2O, *T* = 25 °C, pD = 5.9): 50.18 (C-5'); 54.30 (d, $J_{C,P}$ = 4.5, C-2'); 58.95 (C-4'); 70.35 (C-3'); 120.80 (C-5); 143.65 (C-8); 151.93 (C-4); 154.89 (C-2); 157.95 (C-6); 178.88 (d, $J_{C,P}$ = 198.3, P-CO).

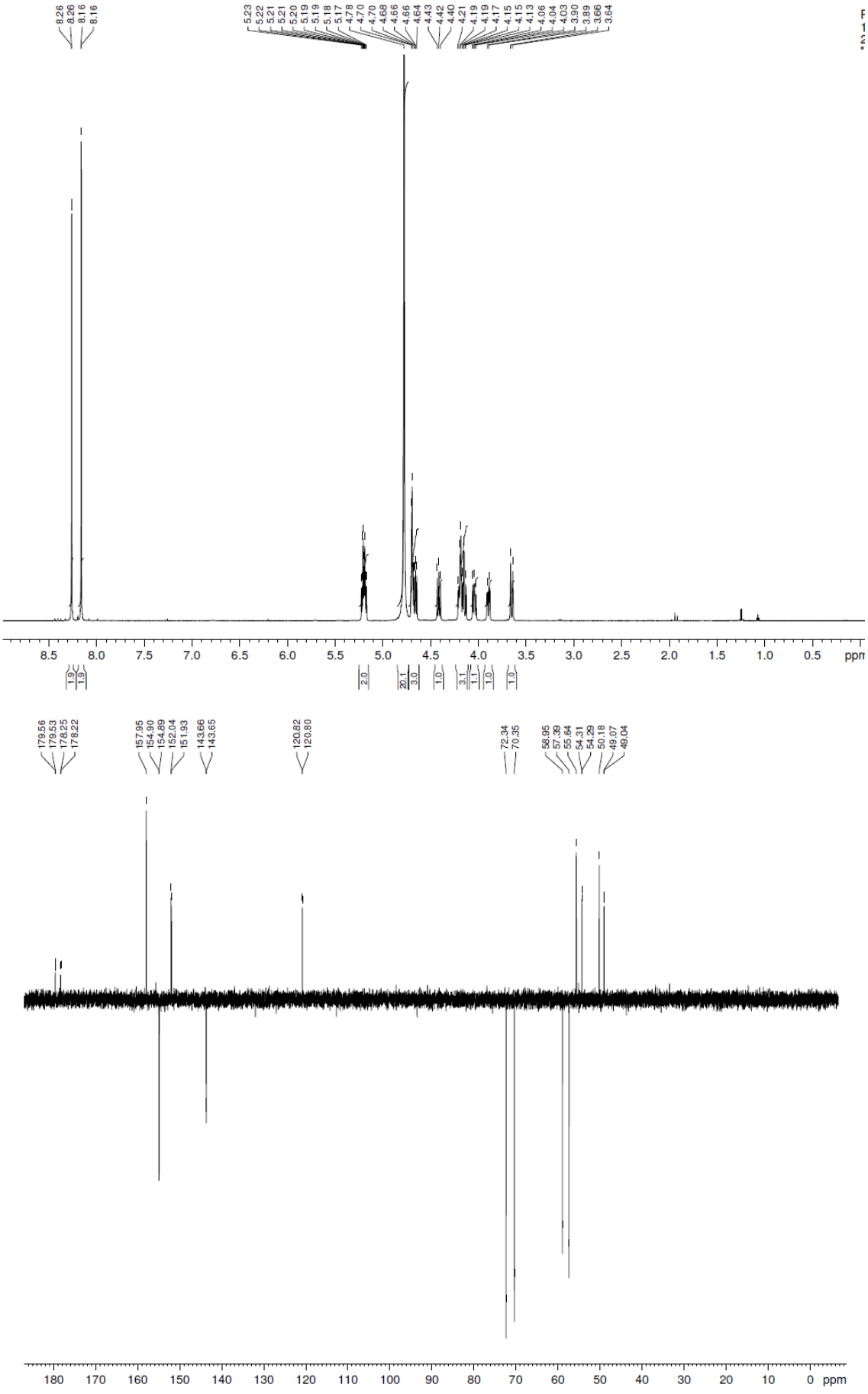
^{31}P{1H} NMR (202.3 MHz, D_2O, *T* = 25 °C, pD = 5.9): -2.21.

Rotamer B:

^{1}H NMR (600.1 MHz, D_2O, *T* = 25 °C, pD = 5.9): 4.04 (ddd, 1H, J_{gem} = 12.8, $J_{5',4'}$ = 8.3, $J_{H,P}$ = 1.9, H-5'); 4.14 (dd, 1H, J_{gem} = 13.0, $J_{2',3'}$ = 3.5, H-2'); 4.18 (ddd, 1H, J_{gem} = 12.8, $J_{5",4'}$ = 8.2, $J_{H,P}$ = 1.8, H-5"); 4.20 (dd, 1H, J_{gem} = 12.6, $J_{2",3'}$ = 4.6, H-2"); 4.698 (ddd, 1H, $J_{3',2"}$ = 4.6, $J_{3',4'}$ = 4.3, $J_{3',2'}$ = 3.5, H-3'); 5.21 (ddd, 1H, $J_{4',5'}$ = 8.3, $J_{4',5"}$ = 8.2, $J_{4',3'}$ = 4.3, H-4'); 8.163 (s, 1H, H-2); 8.261 (s, 1H, H-8).

^{13}C NMR (150.9 MHz, D_2O, *T* = 25 °C, pD = 5.9): 49.06 (d, $J_{C,P}$ = 5.2, C-5'); 55.63 (C-2'); 57.39 (C-4'); 72.34 (C-3'); 120.82 (C-5); 143.66 (C-8); 152.04 (C-4); 154.90 (C-2); 157.95 (C-6); 178.91 (d, $J_{C,P}$ = 197.9, P-CO).

^{31}P{1H} NMR (202.3 MHz, D_2O, *T* = 25 °C, pD = 5.9): -2.30.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4.68
4.66
4.66
4.64
4.43
4.42
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4.17
4.15
4.15
4.13
4.06
4.04
4.03
3.90
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1.0
0.5
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1.0
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1.1
1.0
1.0
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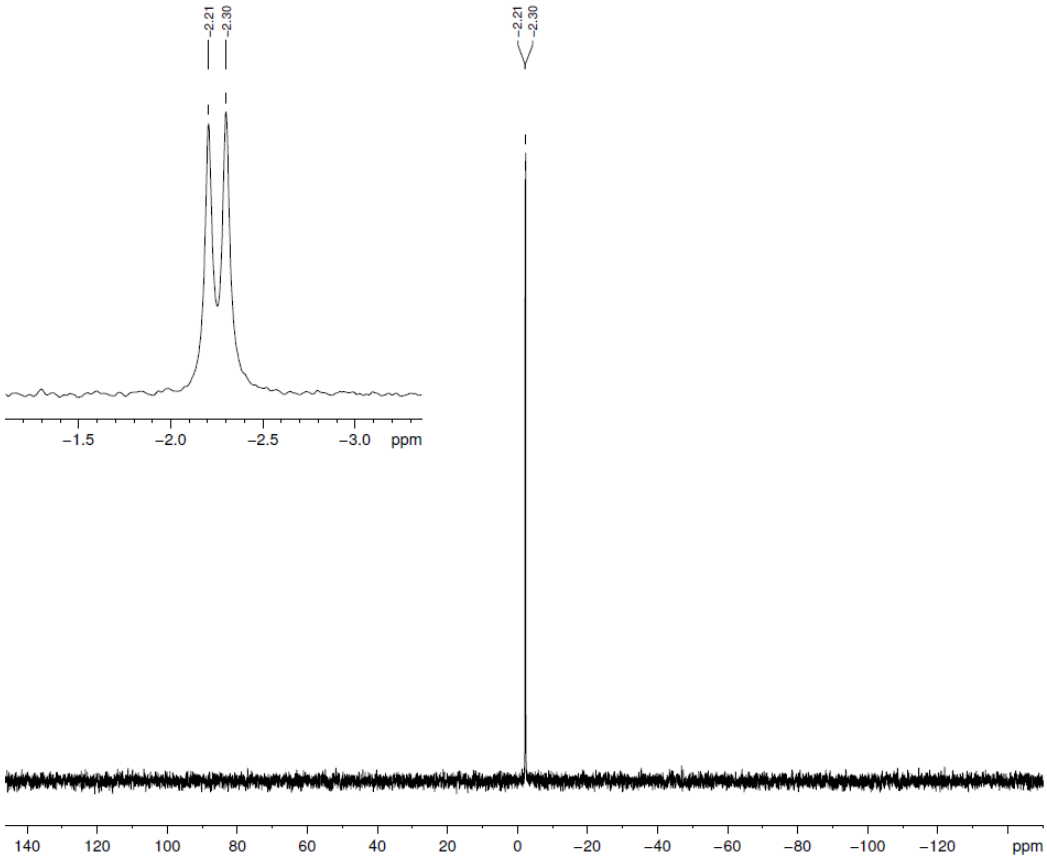
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20
0
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−40
−60
−80
−100
−120
ppm