

## Supporting Information

### Synthesis of 3'-azido/-amino-xylobicyclonucleosides

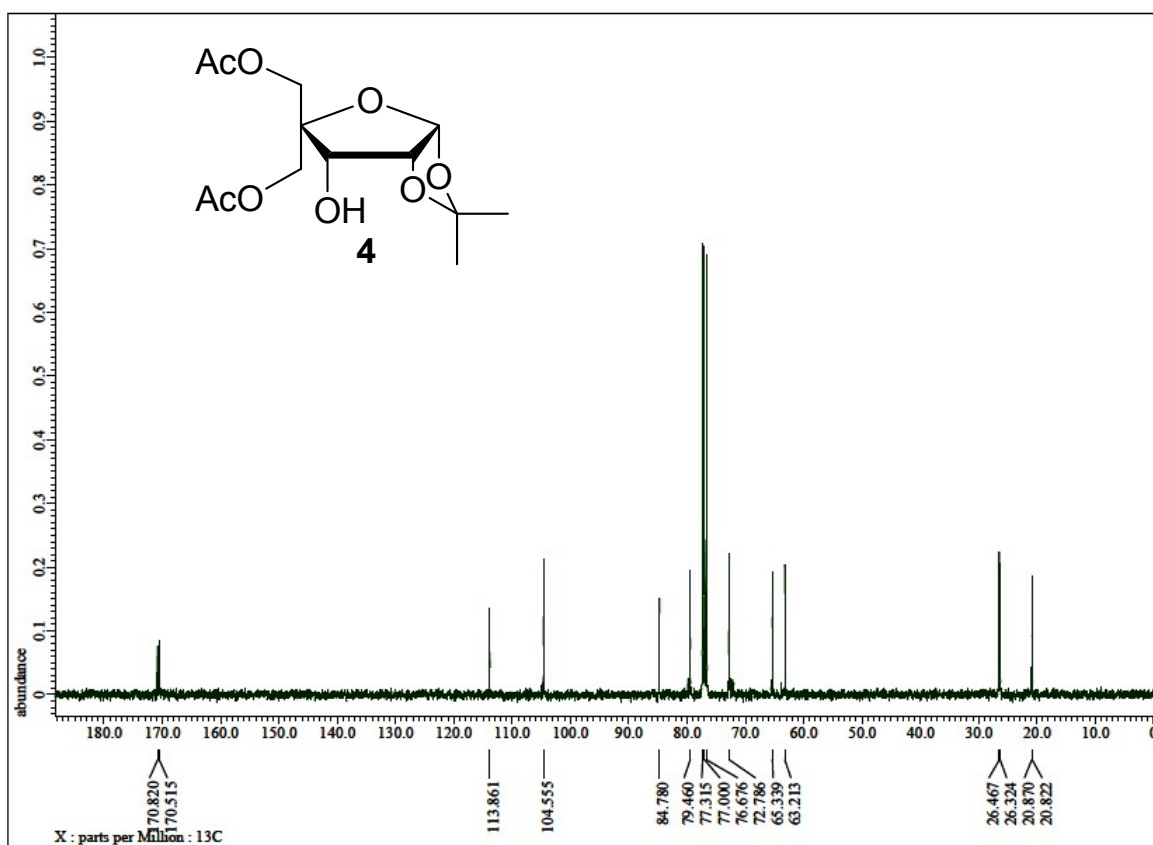
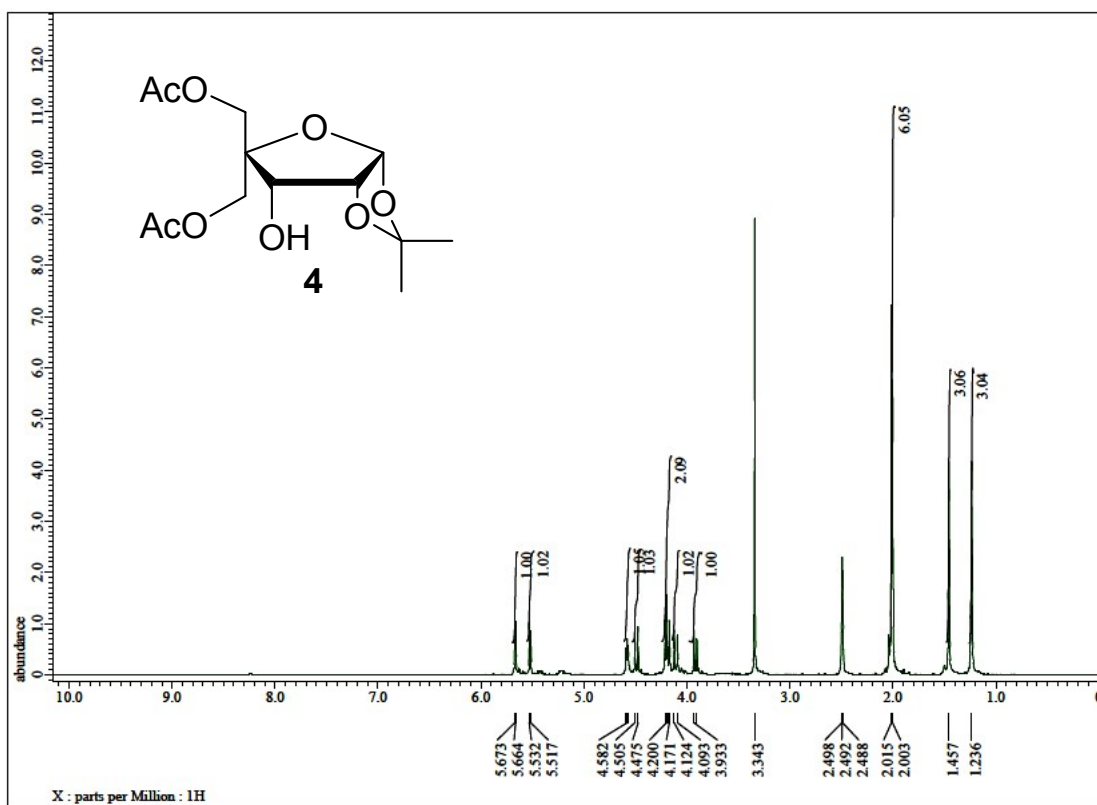
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[ashokenzyme@gmail.com](mailto:ashokenzyme@gmail.com)

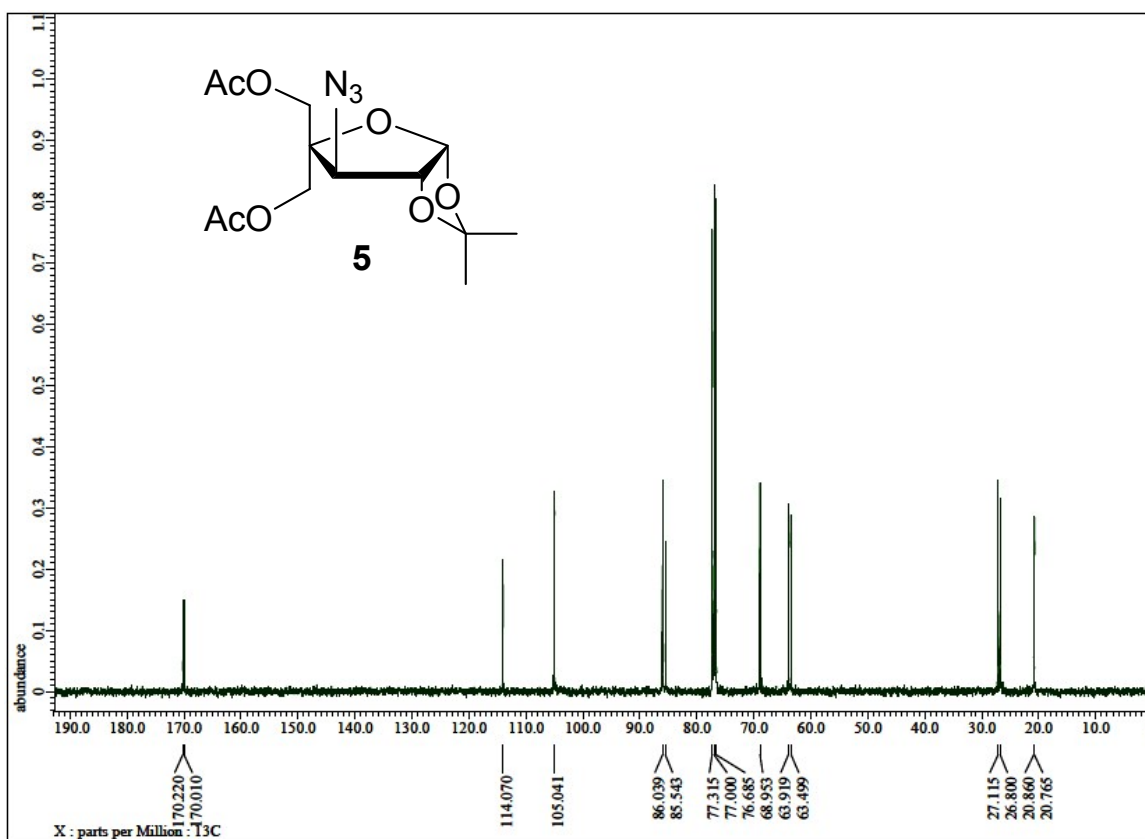
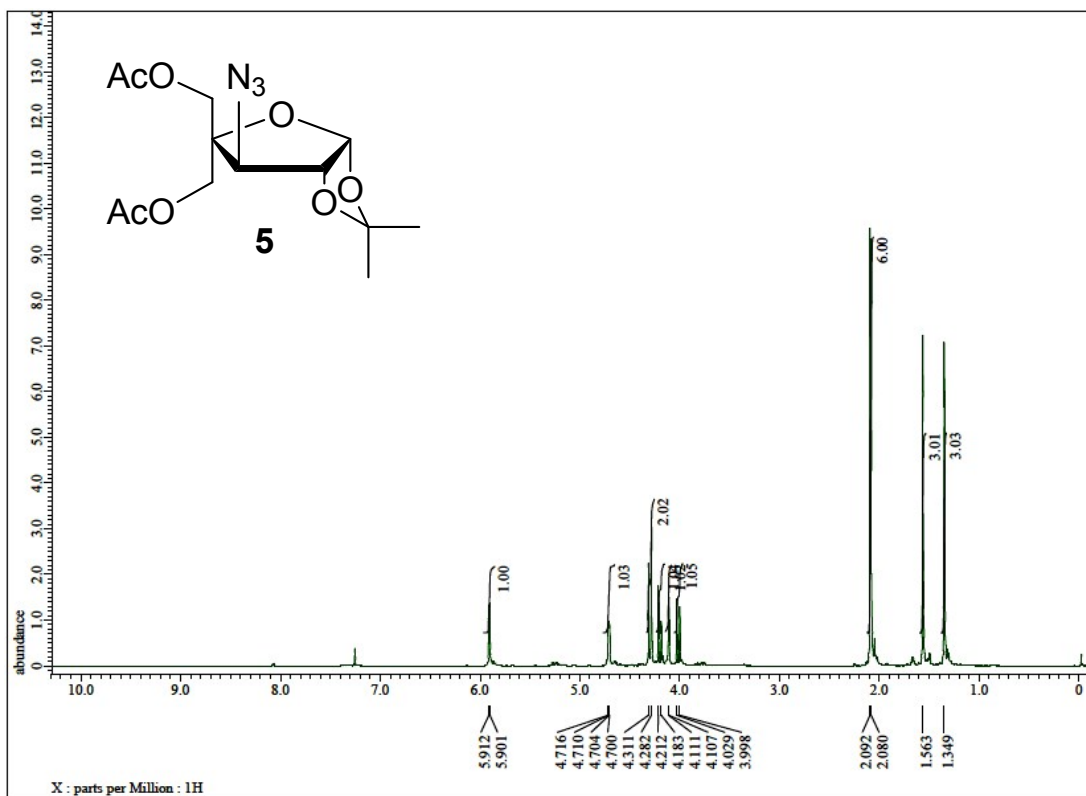
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Single crystal X-ray data of compound <b>7</b> and <b>1b</b> .....	<b>S20</b>

(Table S1)

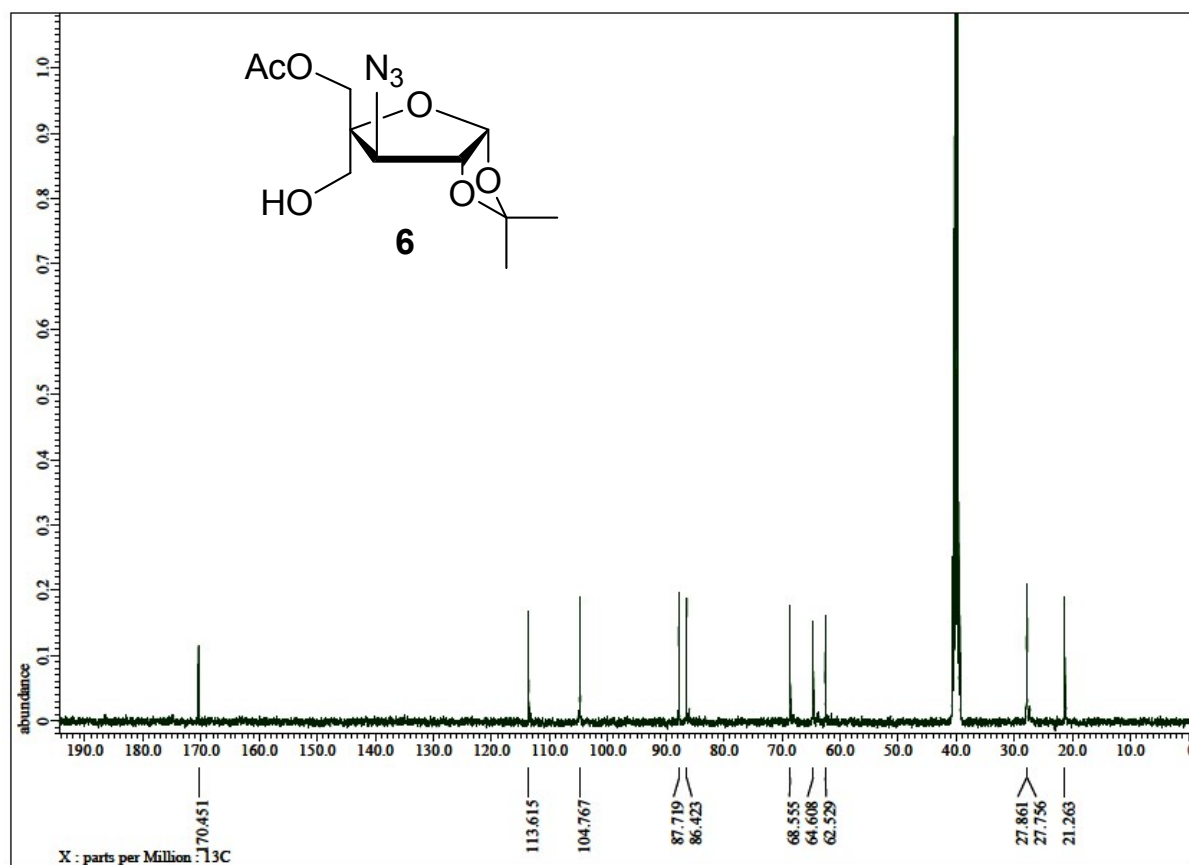
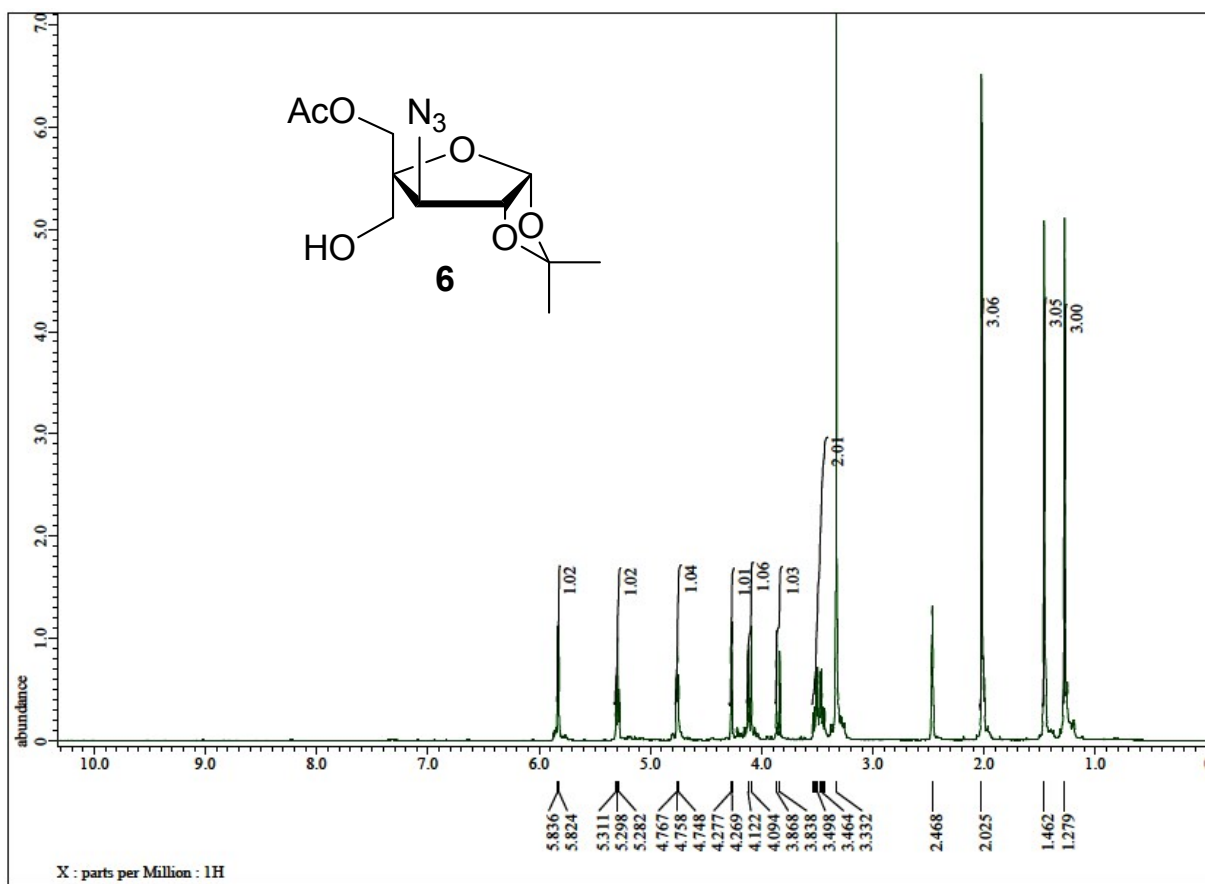
# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 4



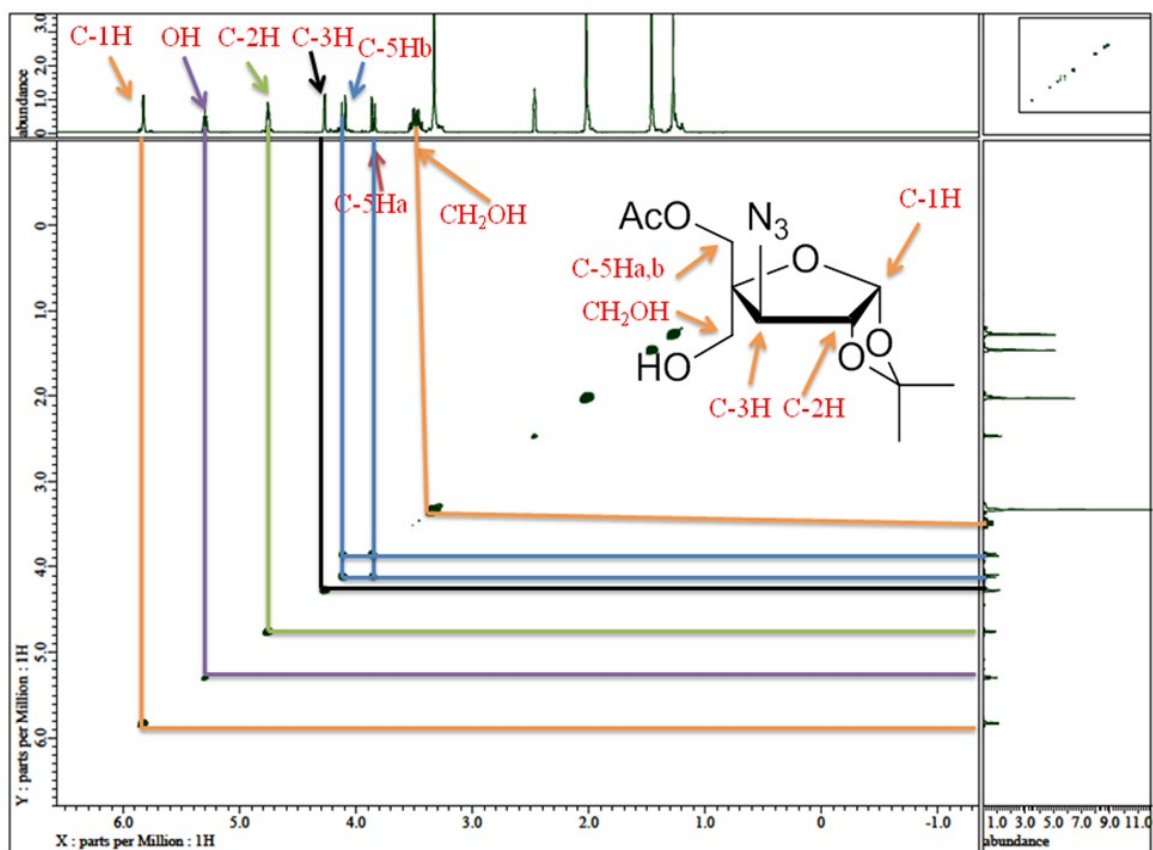
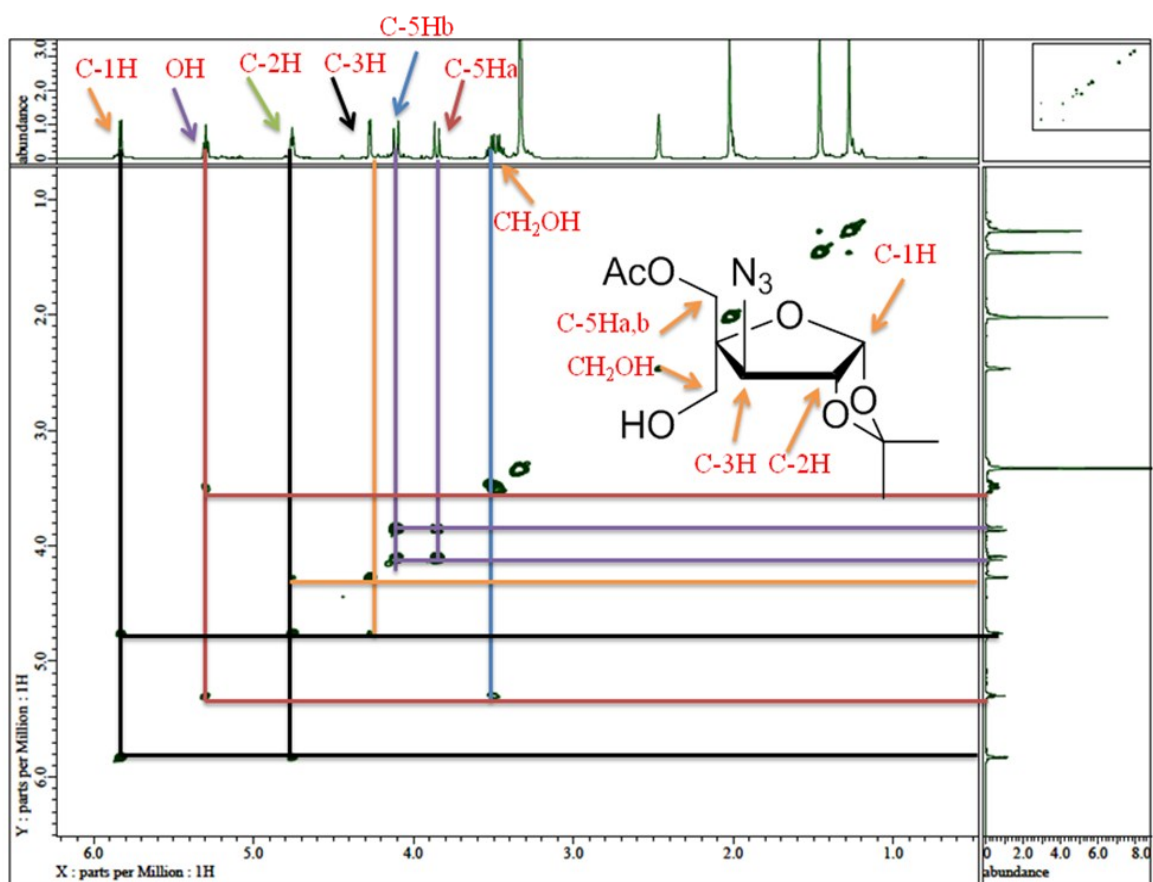
<sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 5



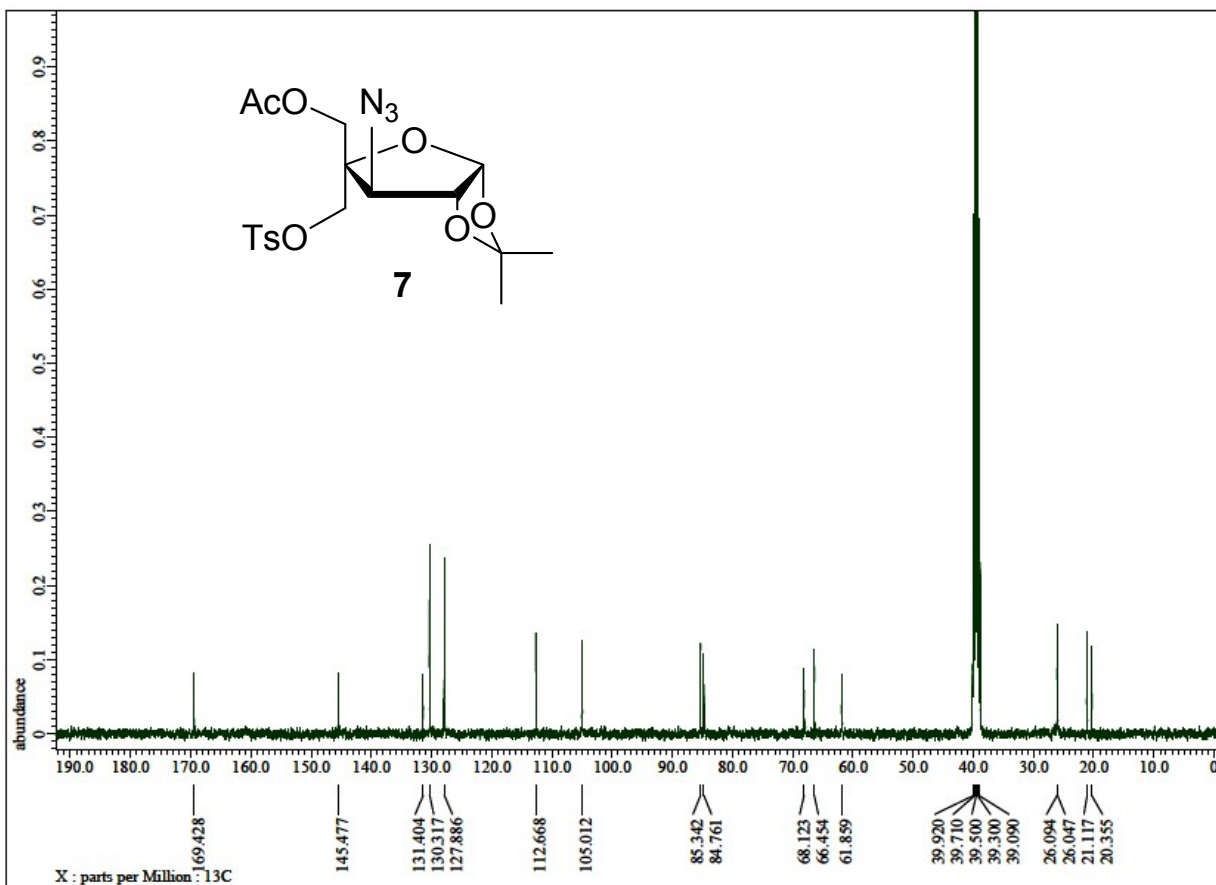
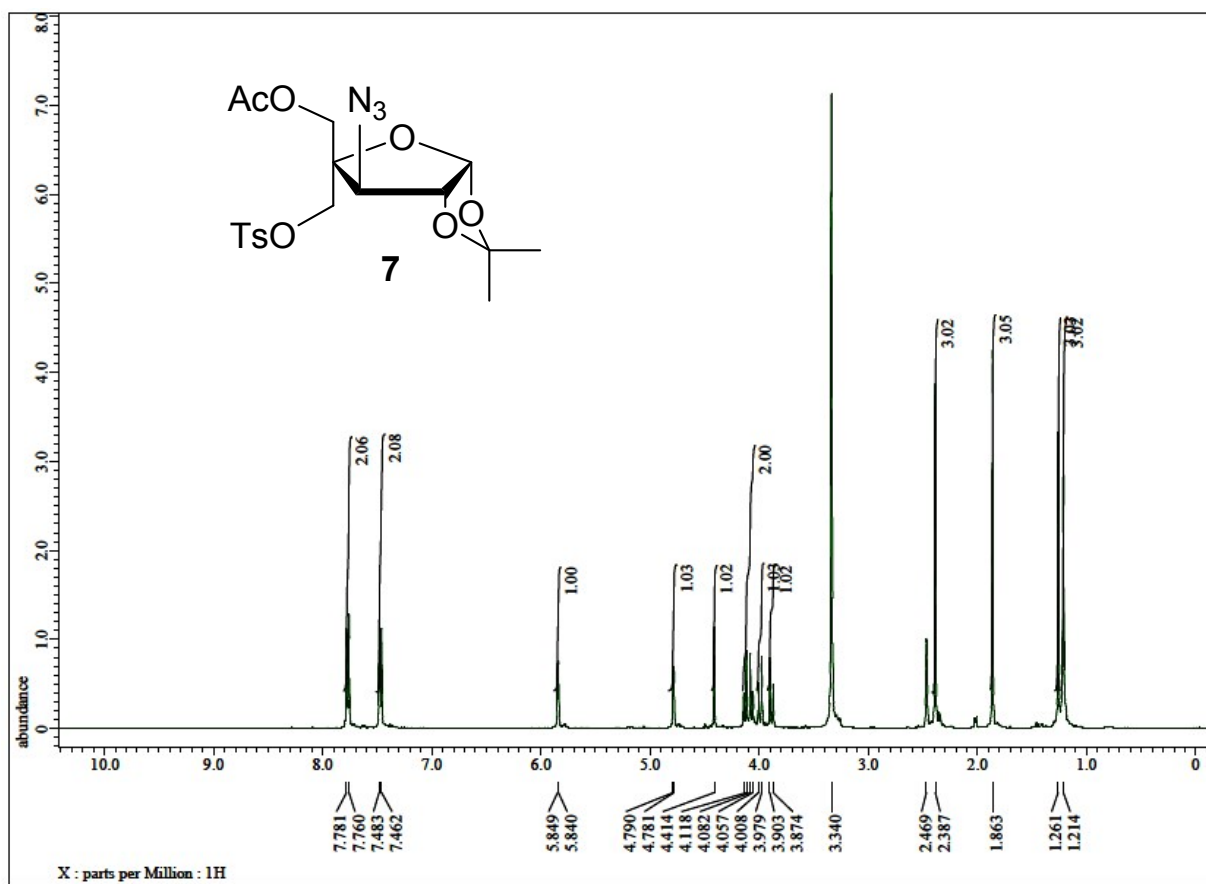
<sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 6



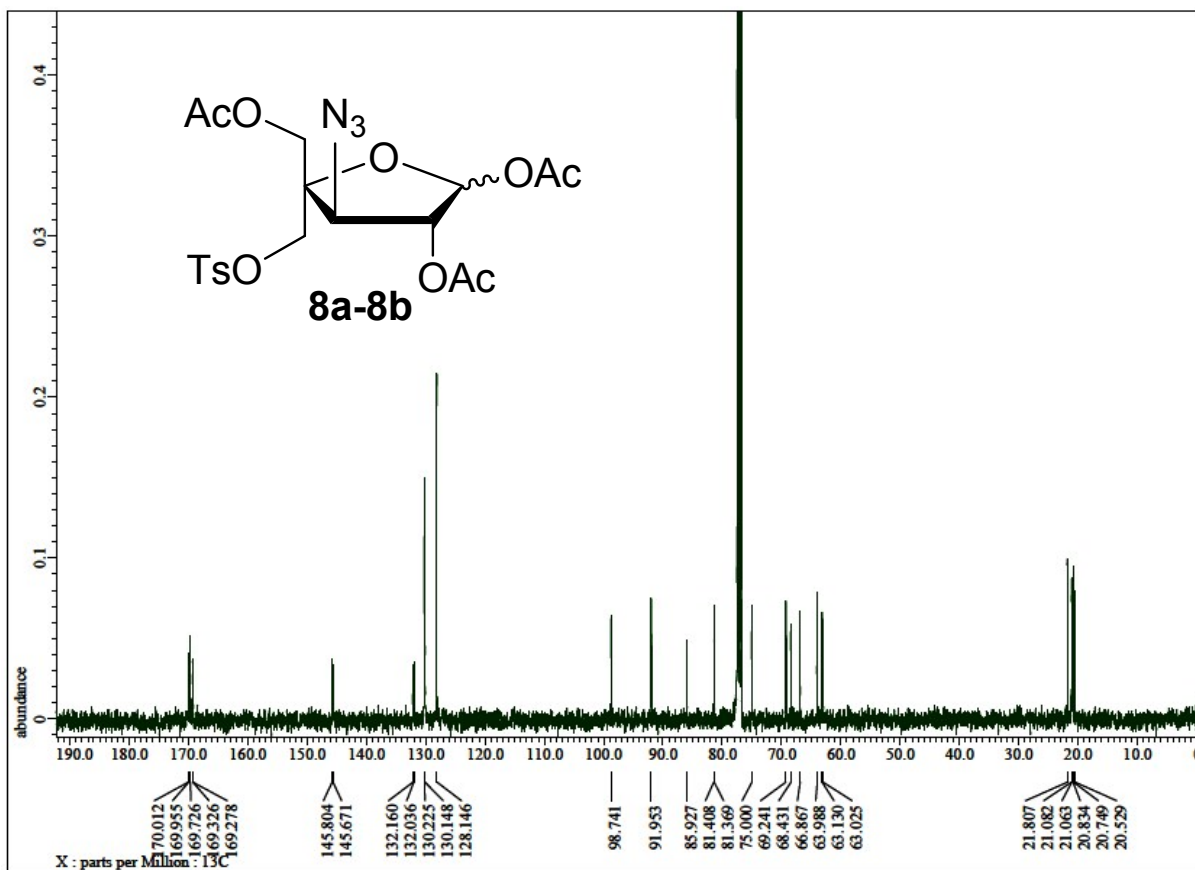
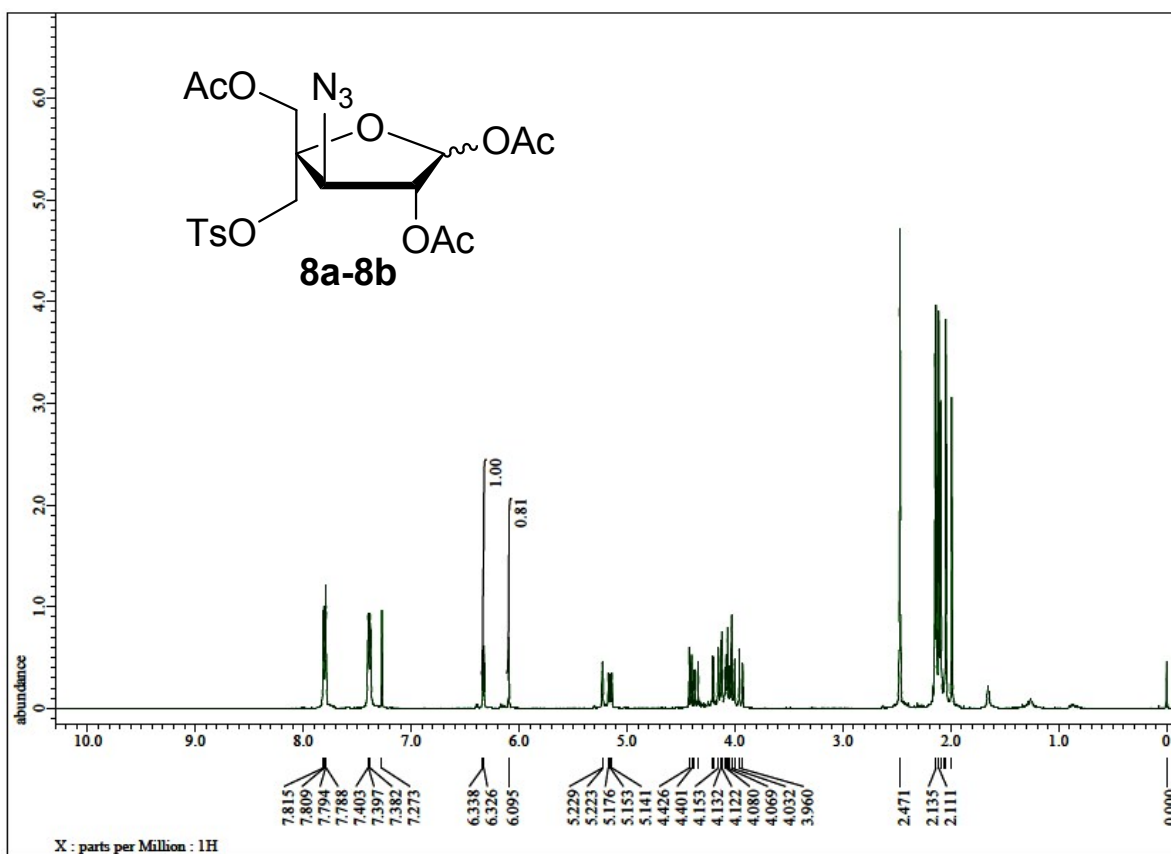
$^1\text{H}$ - $^1\text{H}$  COSY and  $^1\text{H}$ - $^1\text{H}$  NOESY NMR spectra of compound 6



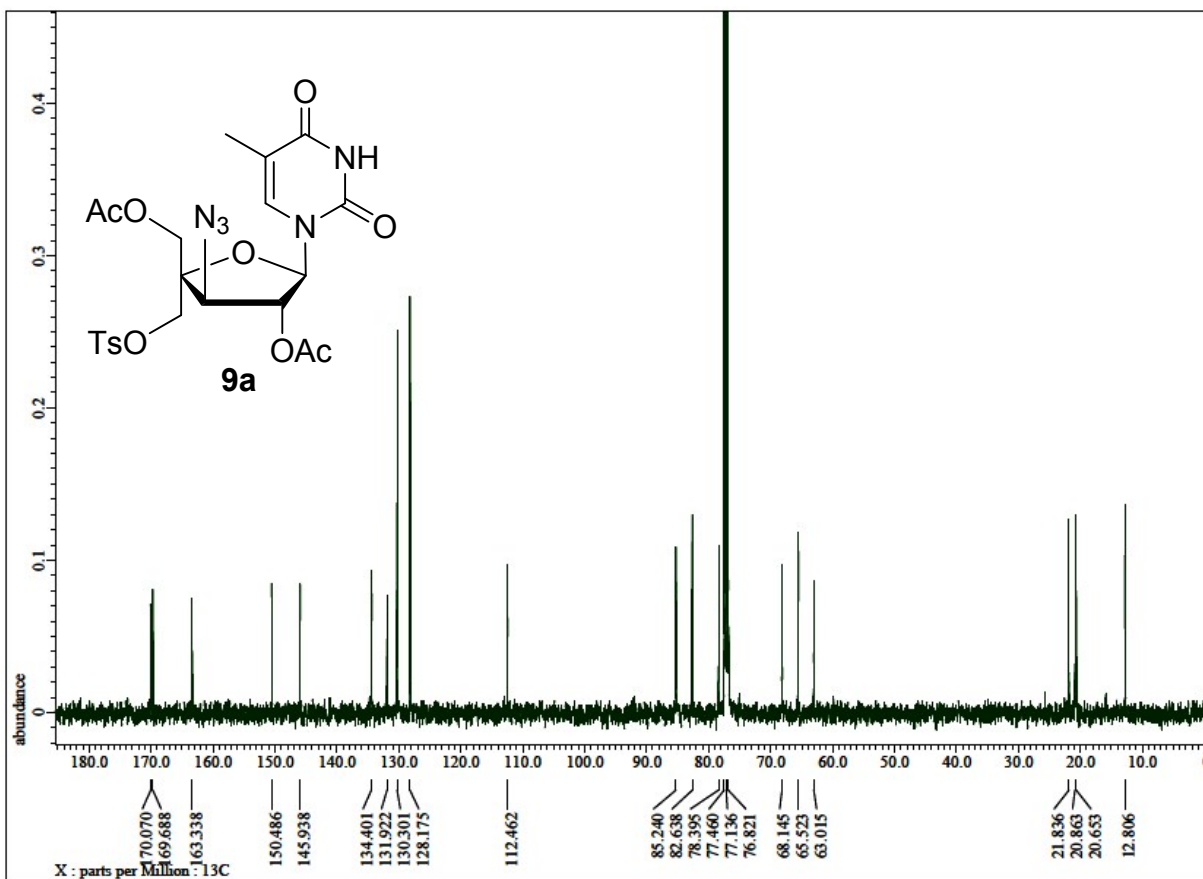
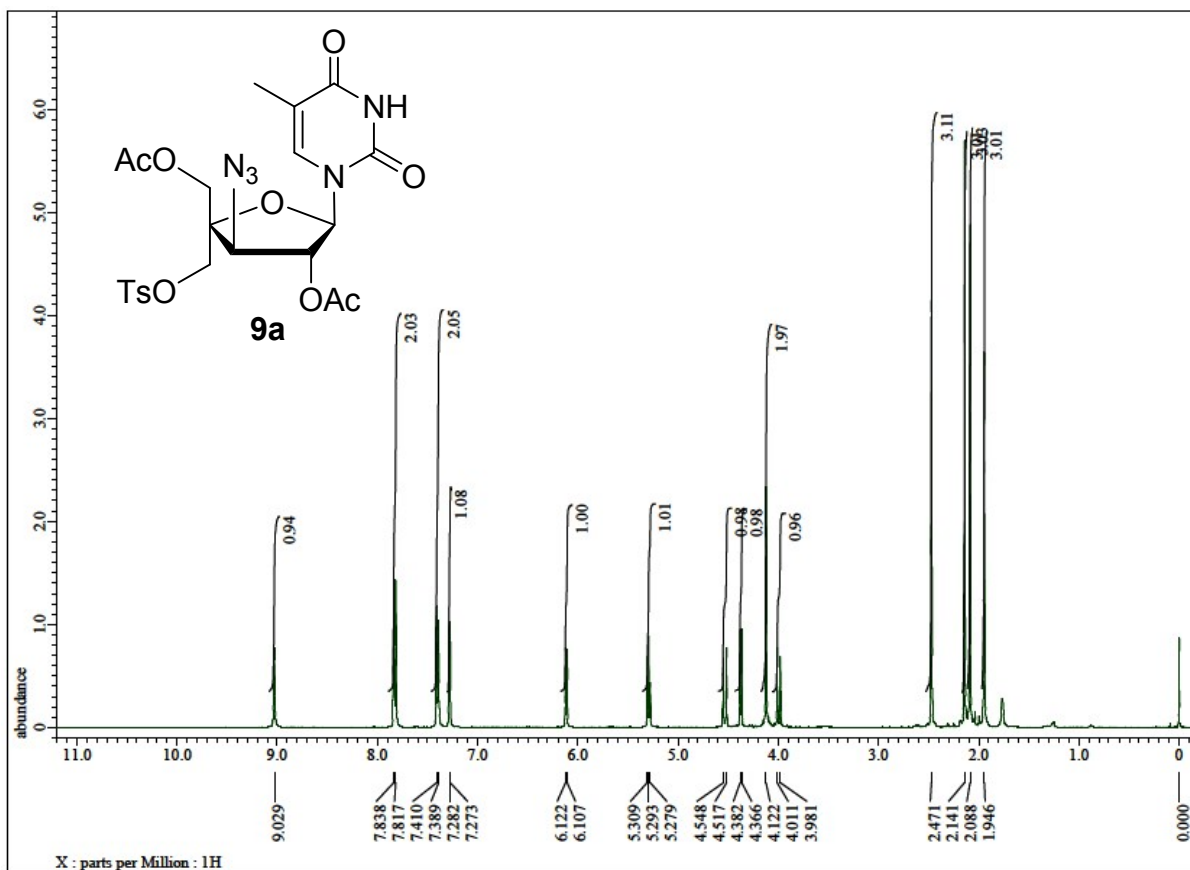
# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 7



**<sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 8a-8b**

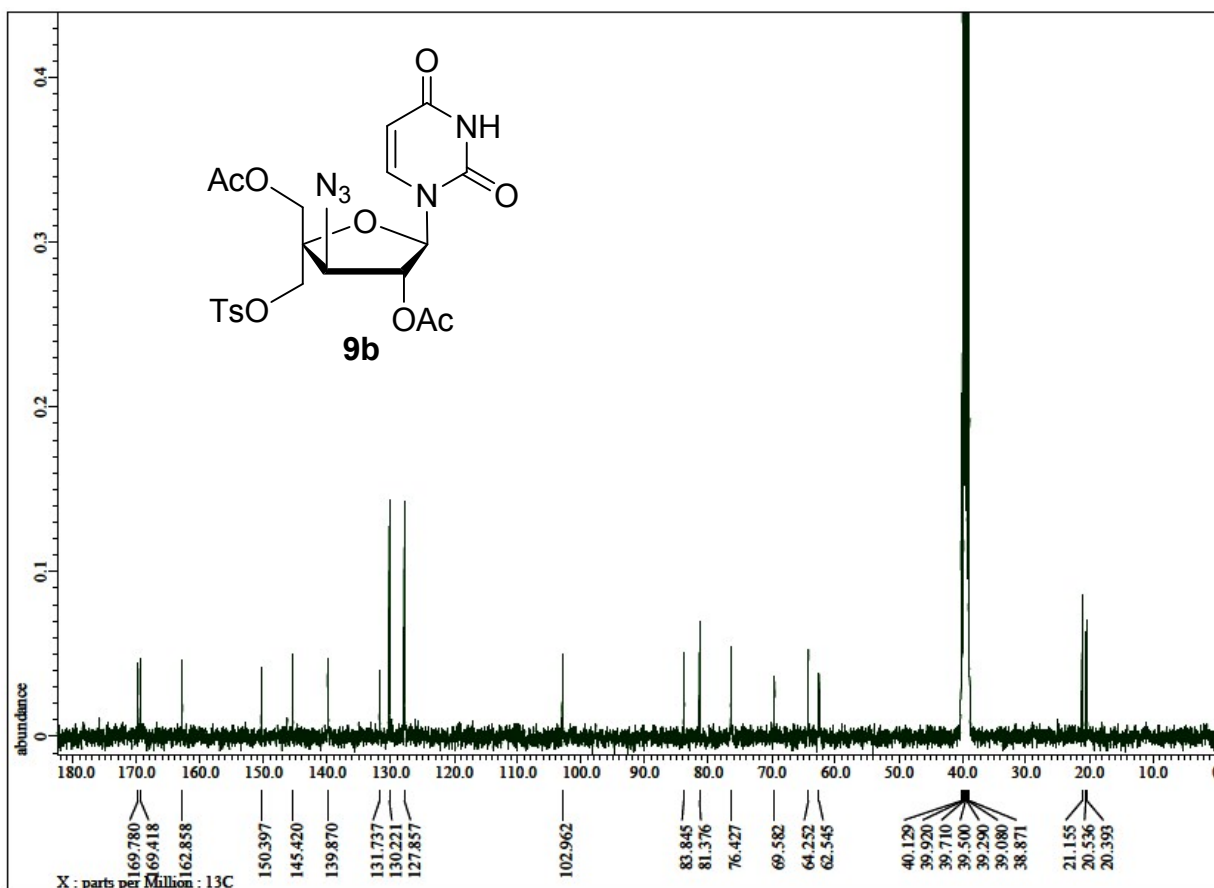
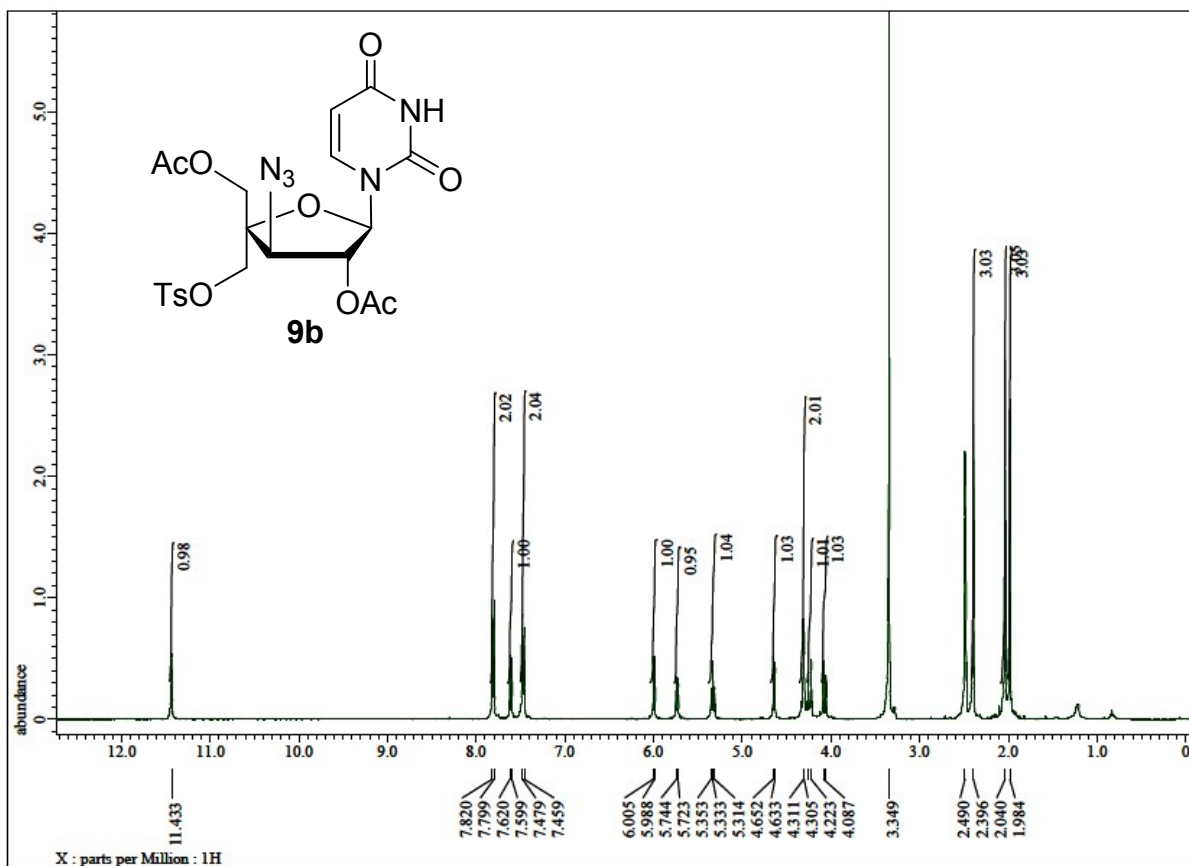


# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 9a

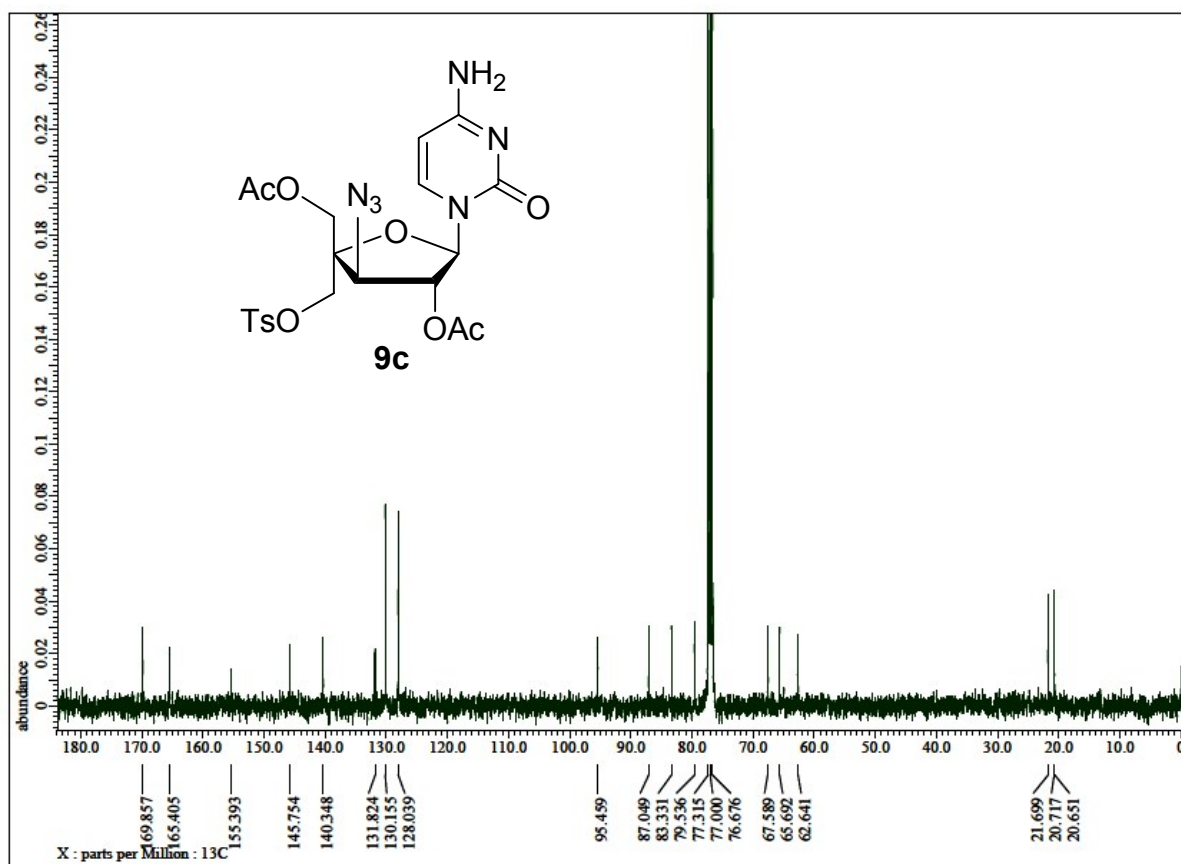
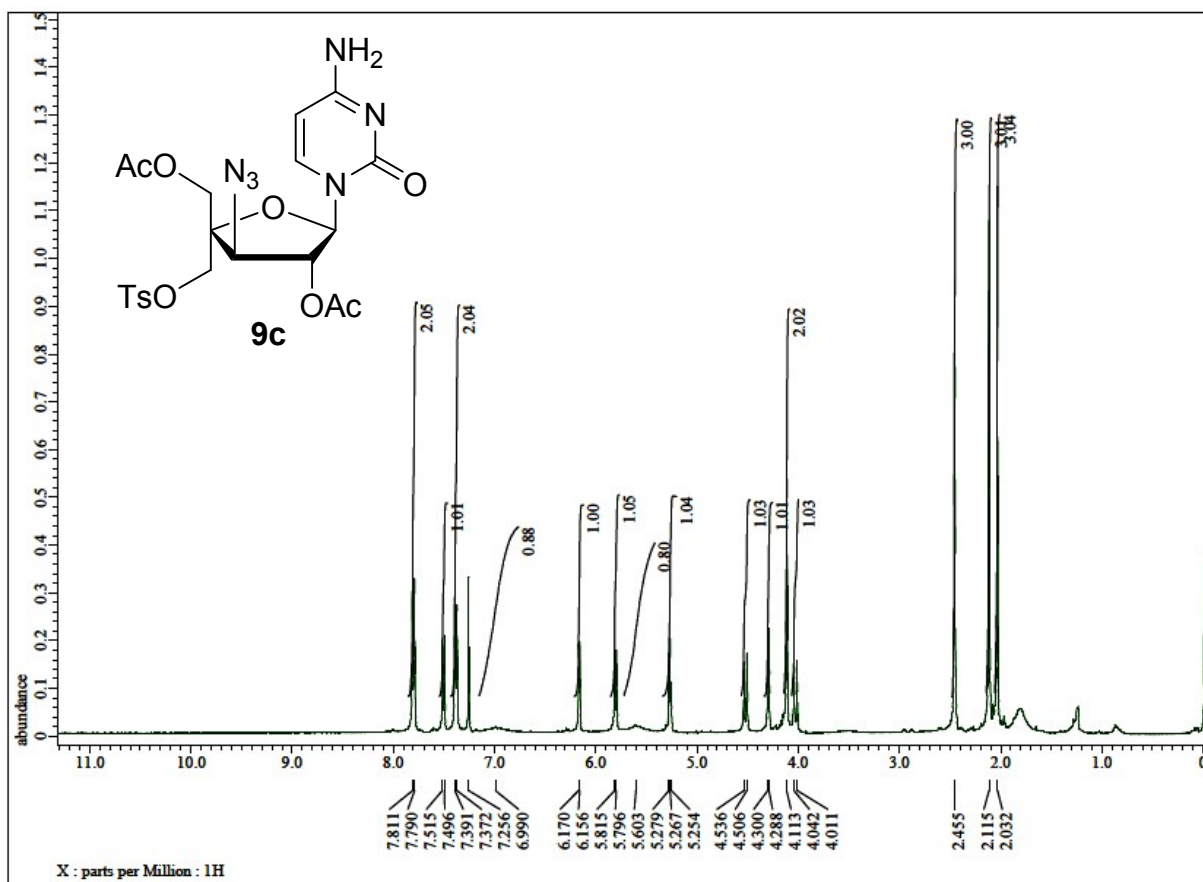




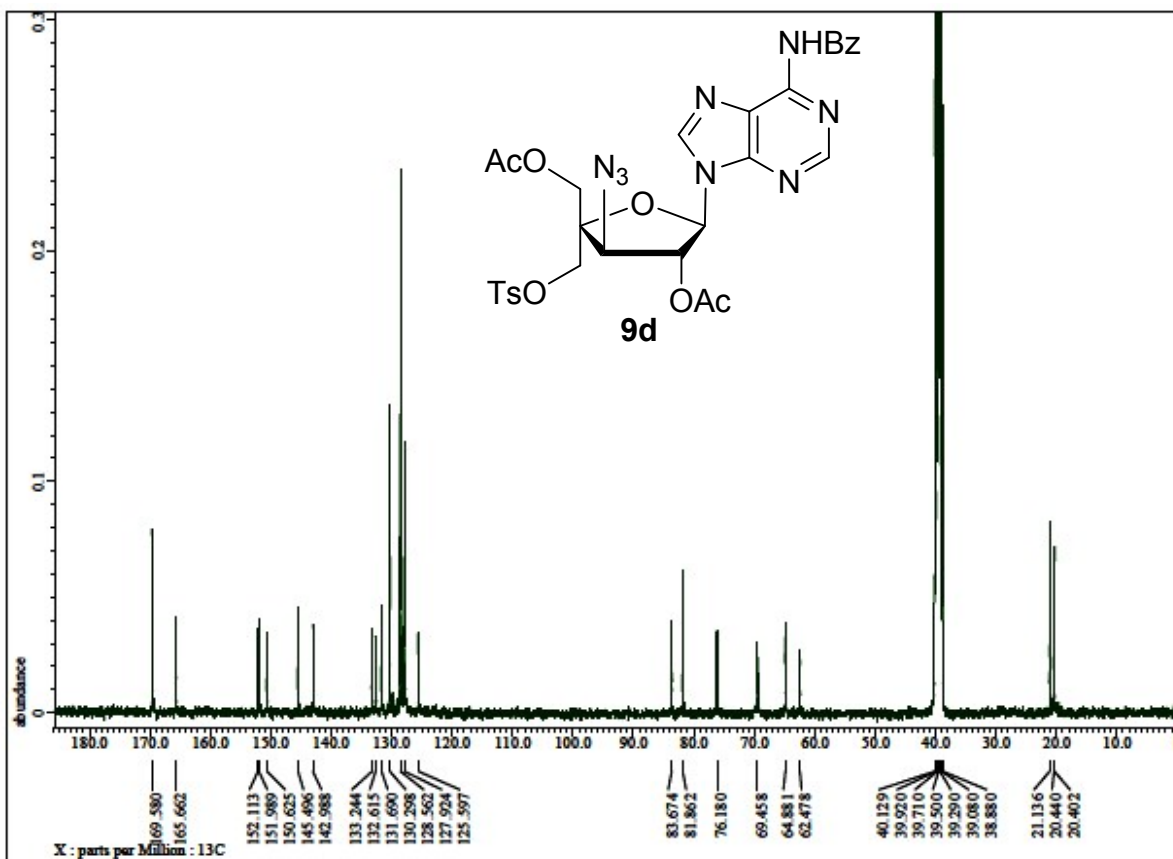
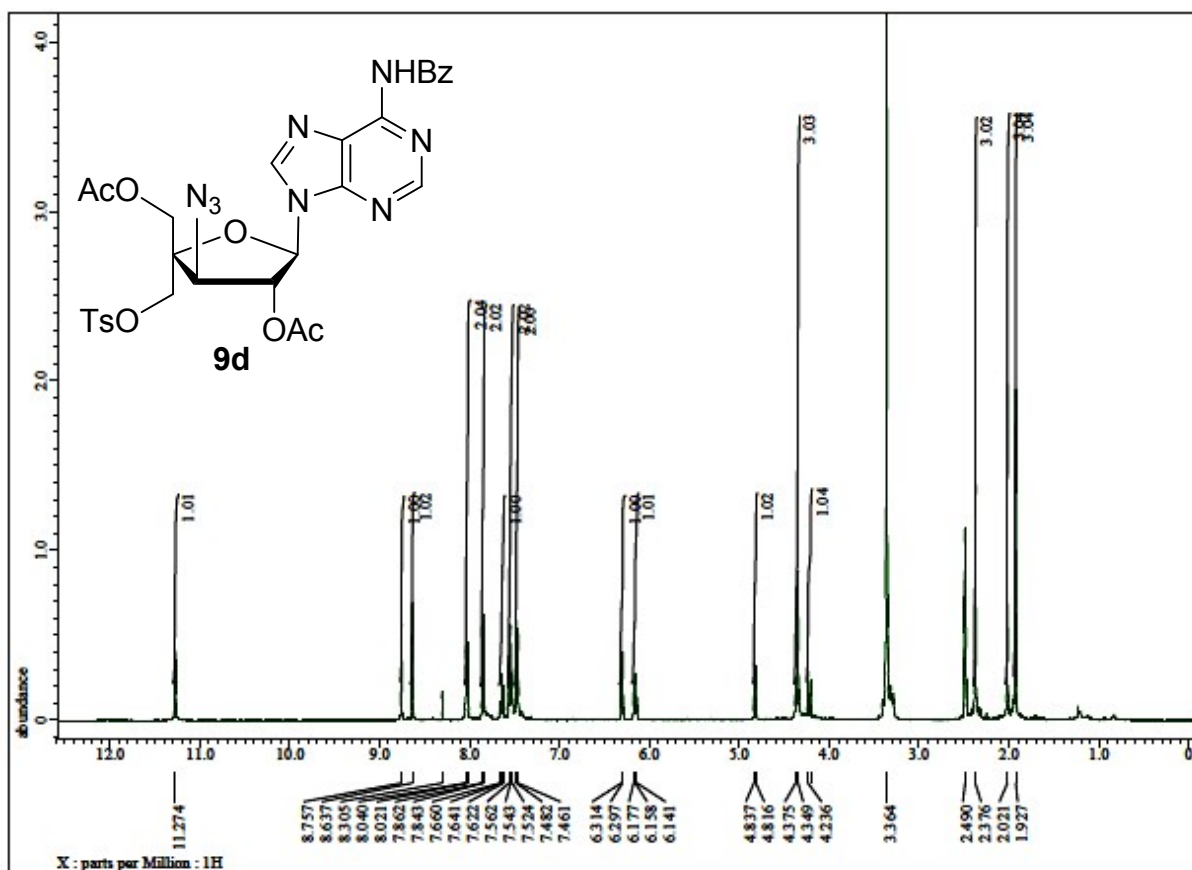
# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 9b



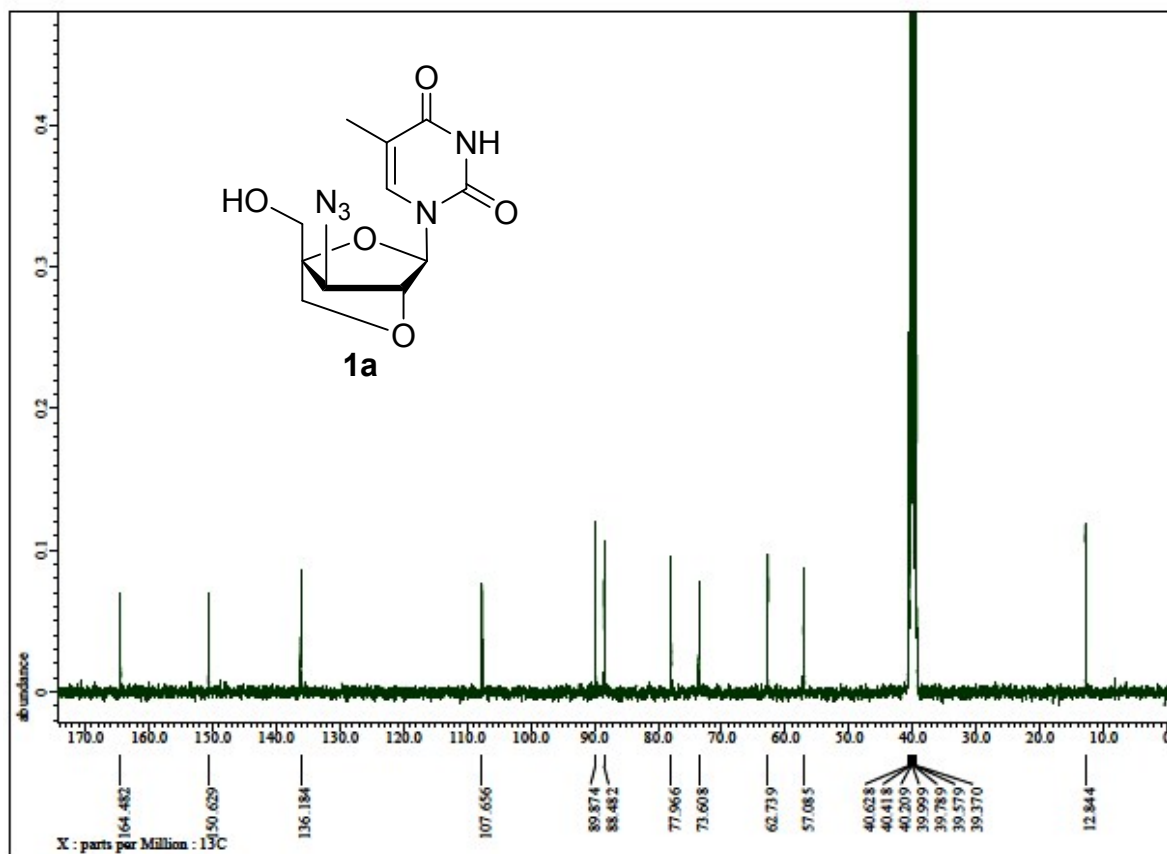
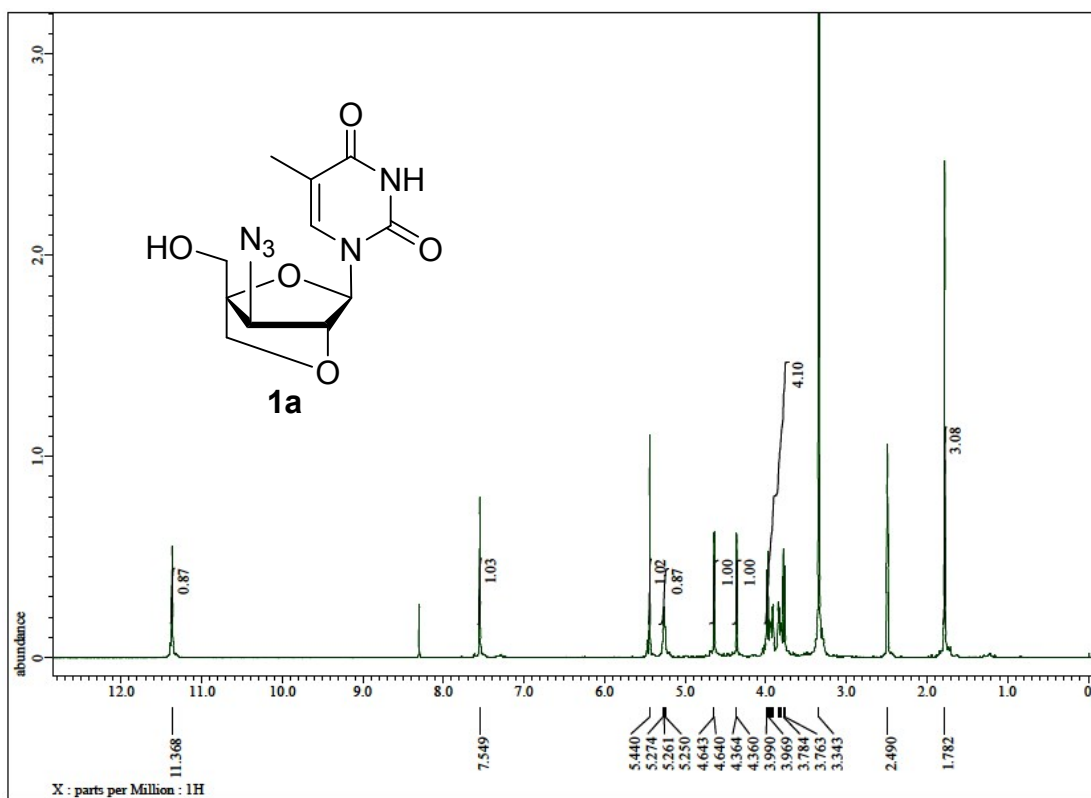
# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 9c



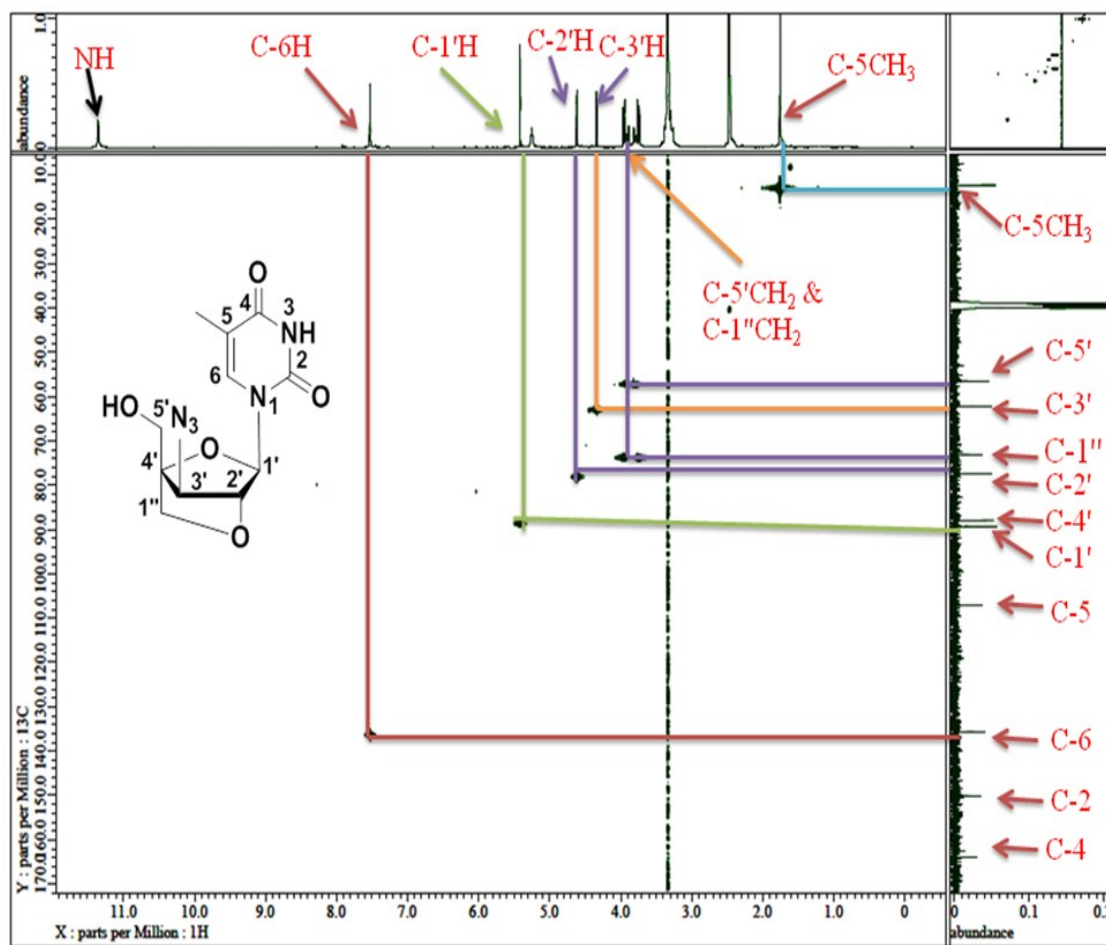
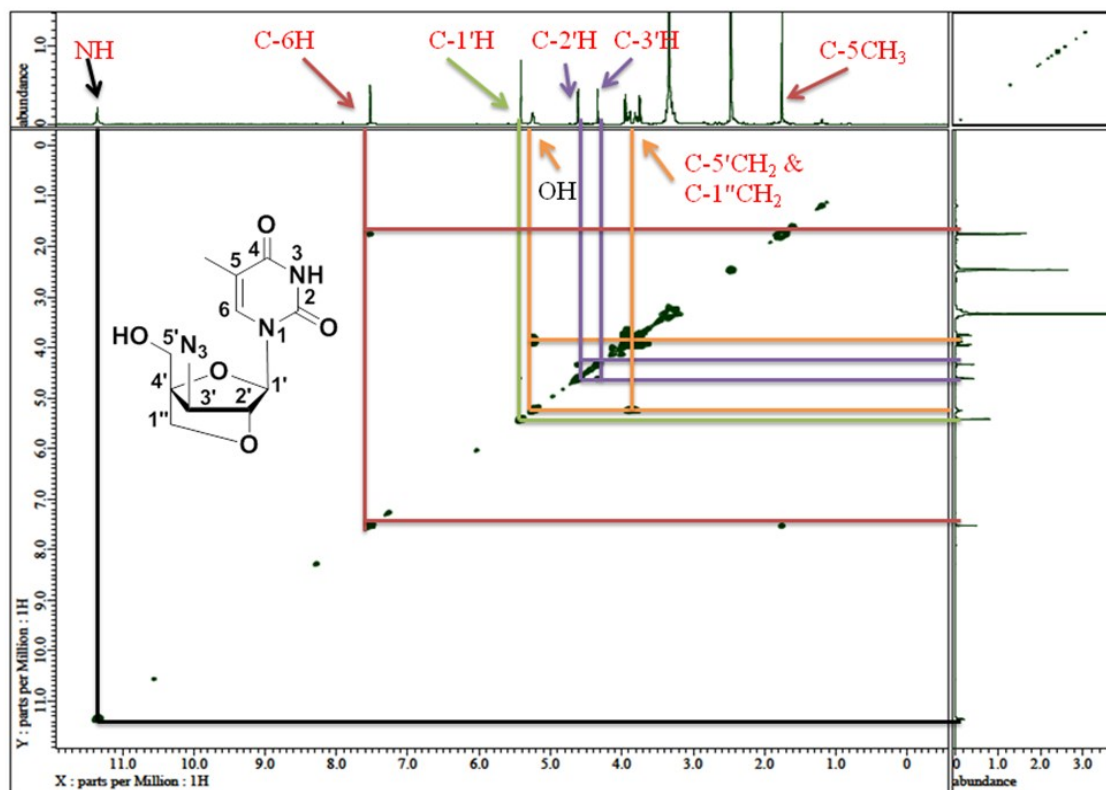
# <sup>1</sup>H- and <sup>13</sup>C- NMR spectra of compound 9d



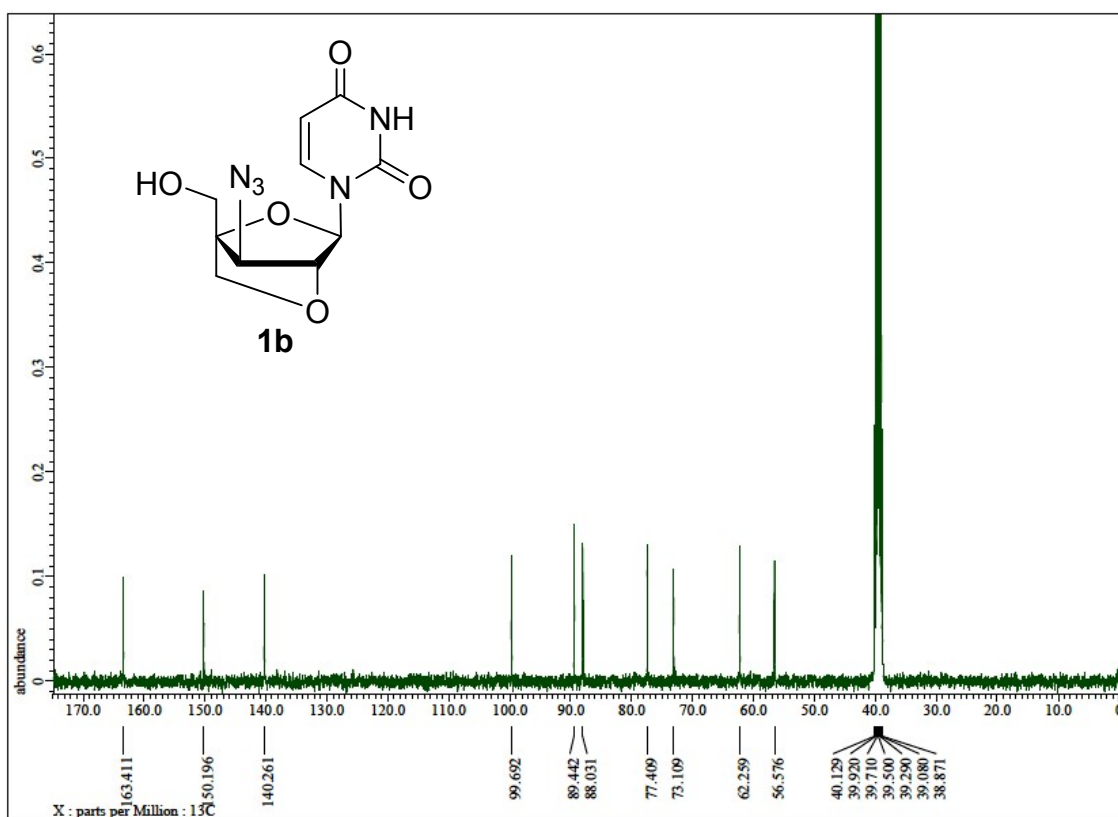
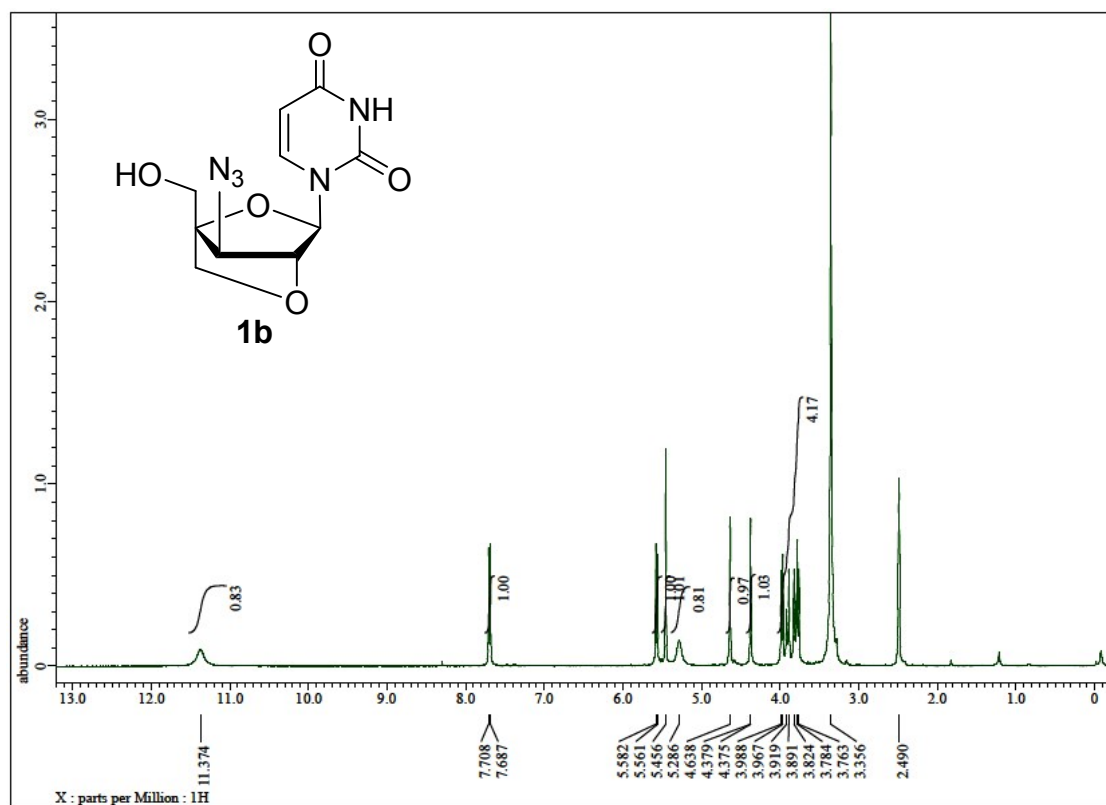
# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 1a



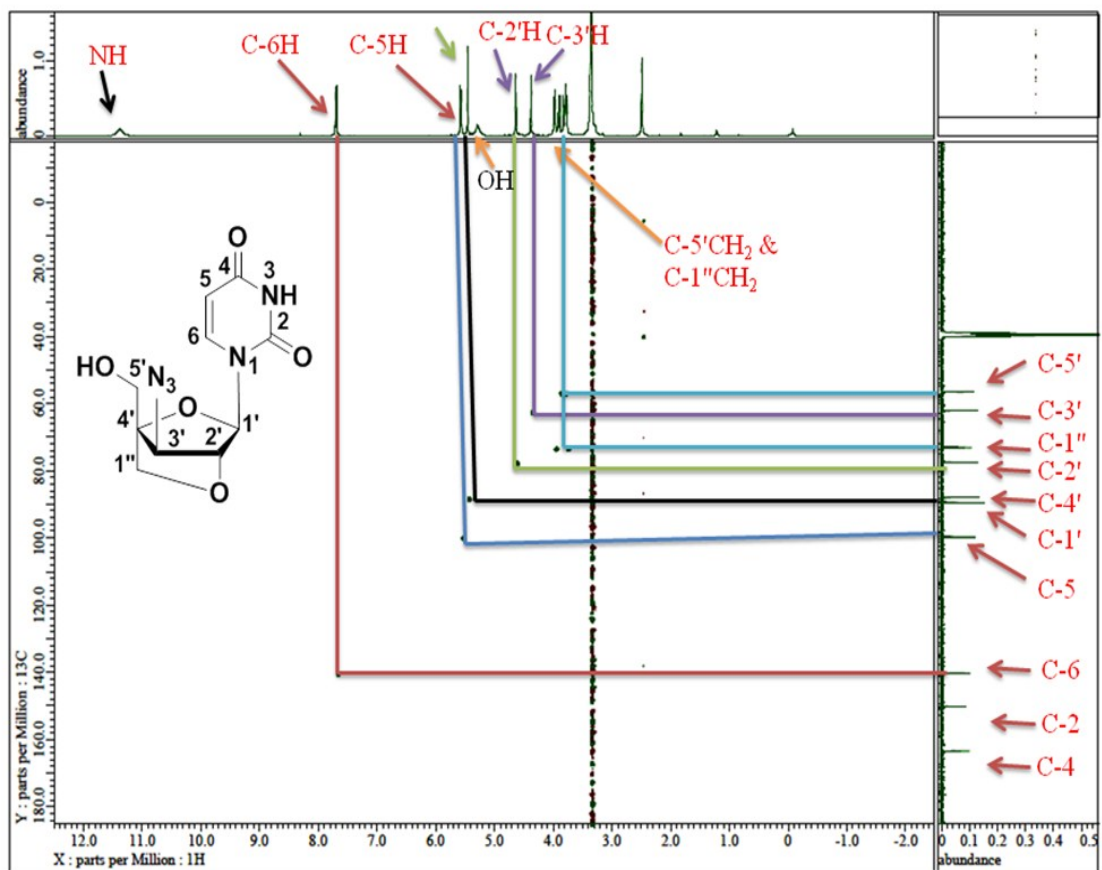
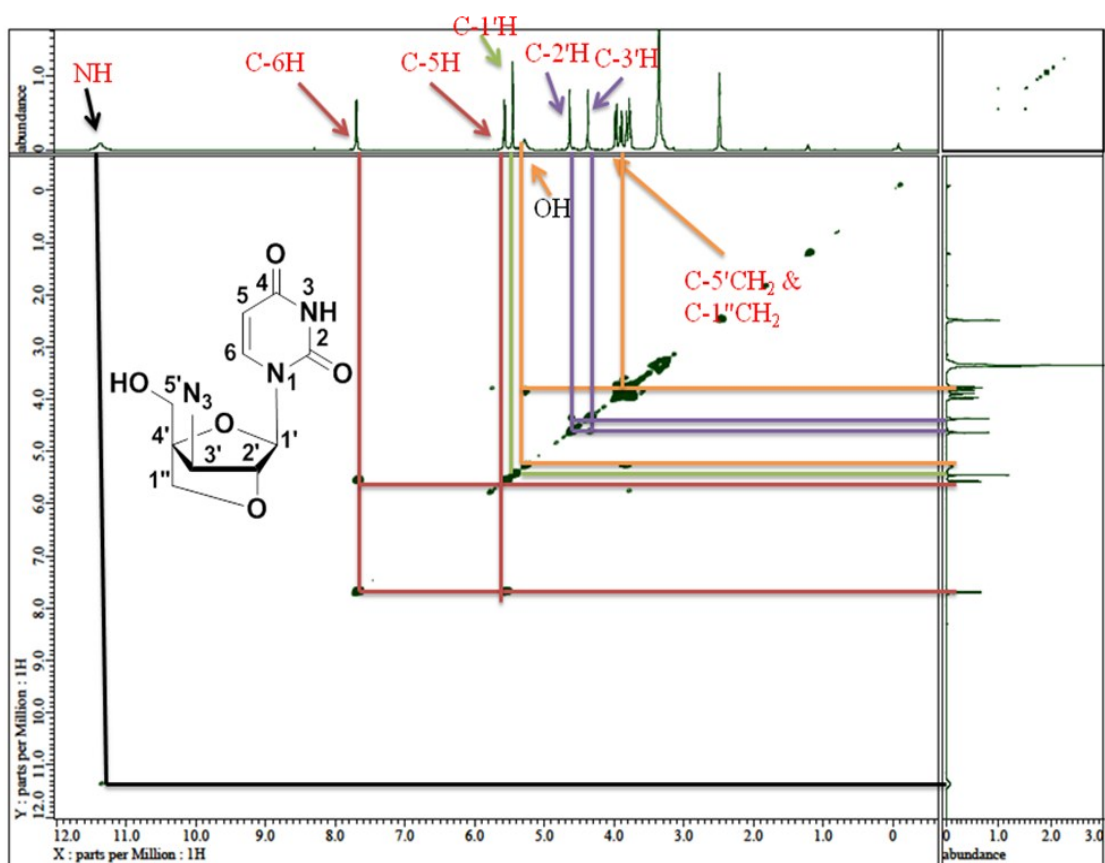
$^1\text{H}$ - $^1\text{H}$  COSY and  $^1\text{H}$ - $^{13}\text{C}$  HMQC NMR spectra of compound 1a



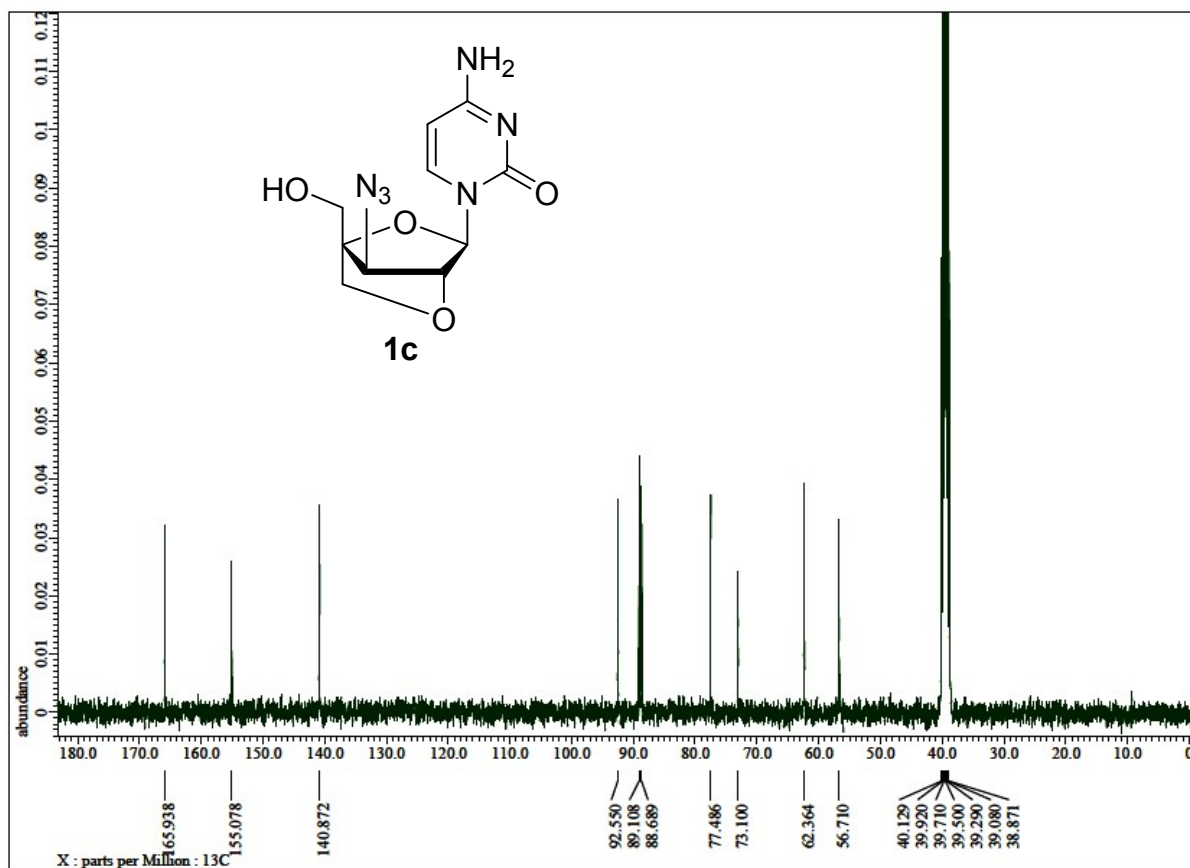
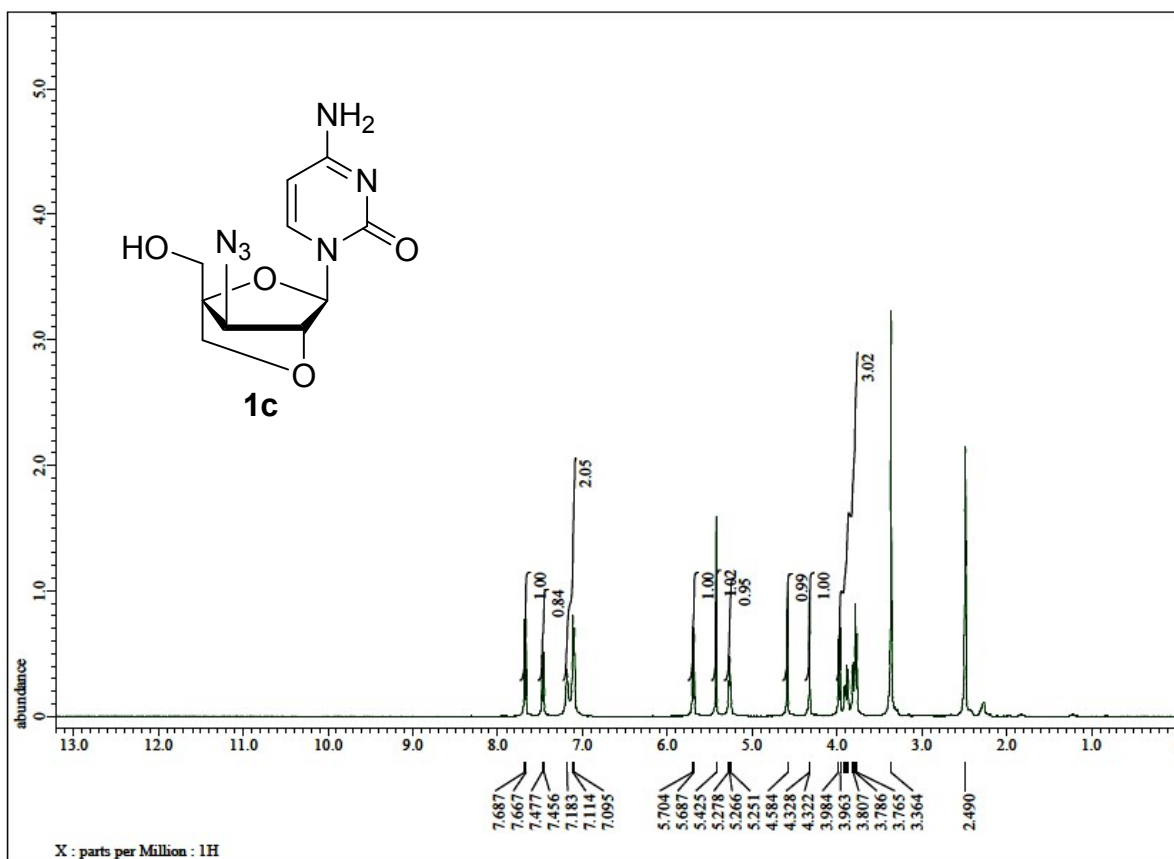
# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 1b



**$^1\text{H}$ - $^1\text{H}$  COSY and  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR spectra of compound 1b**

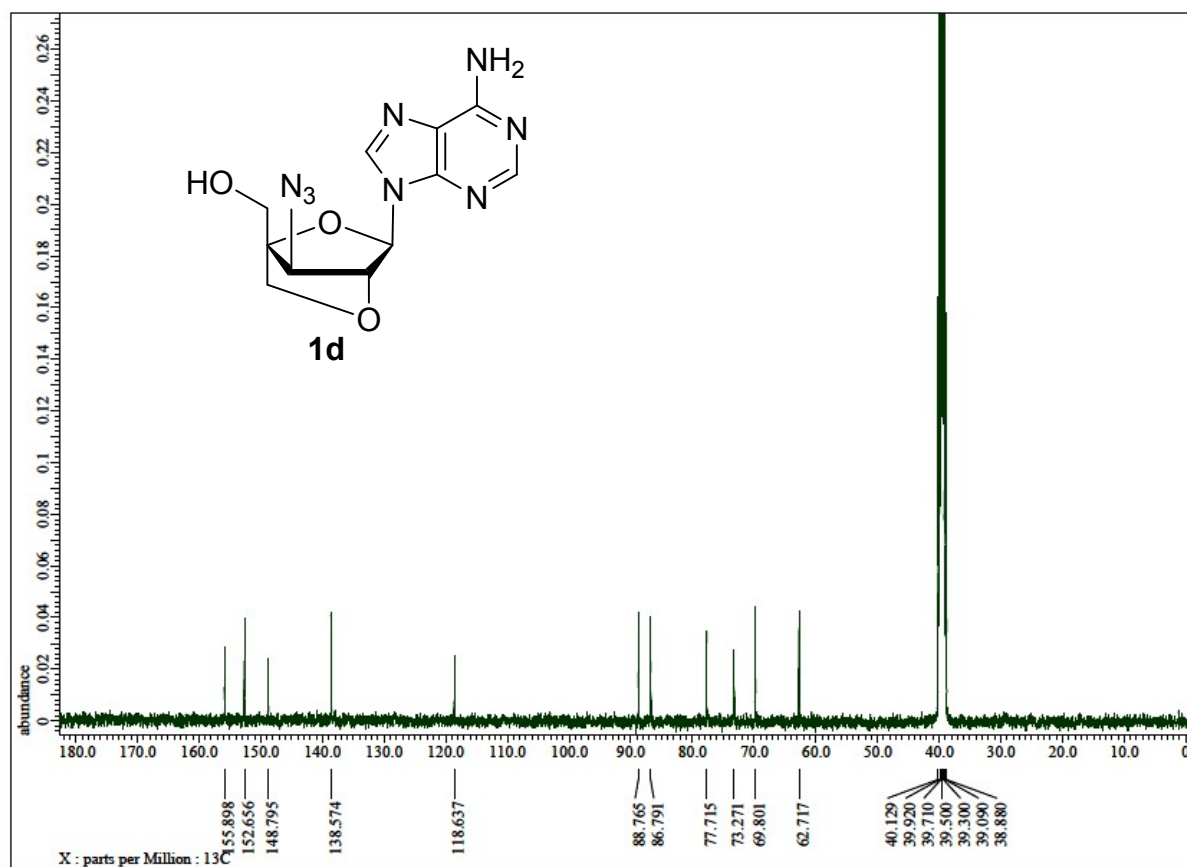
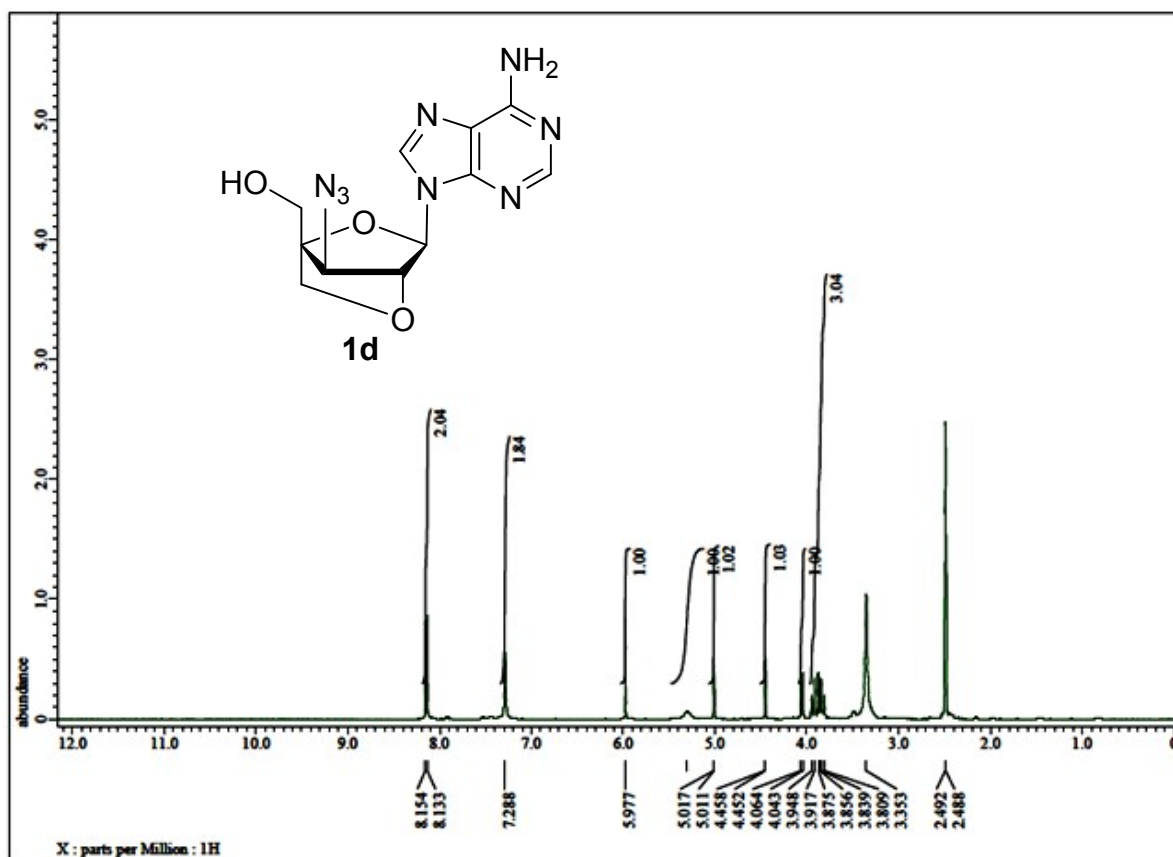


# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 1c

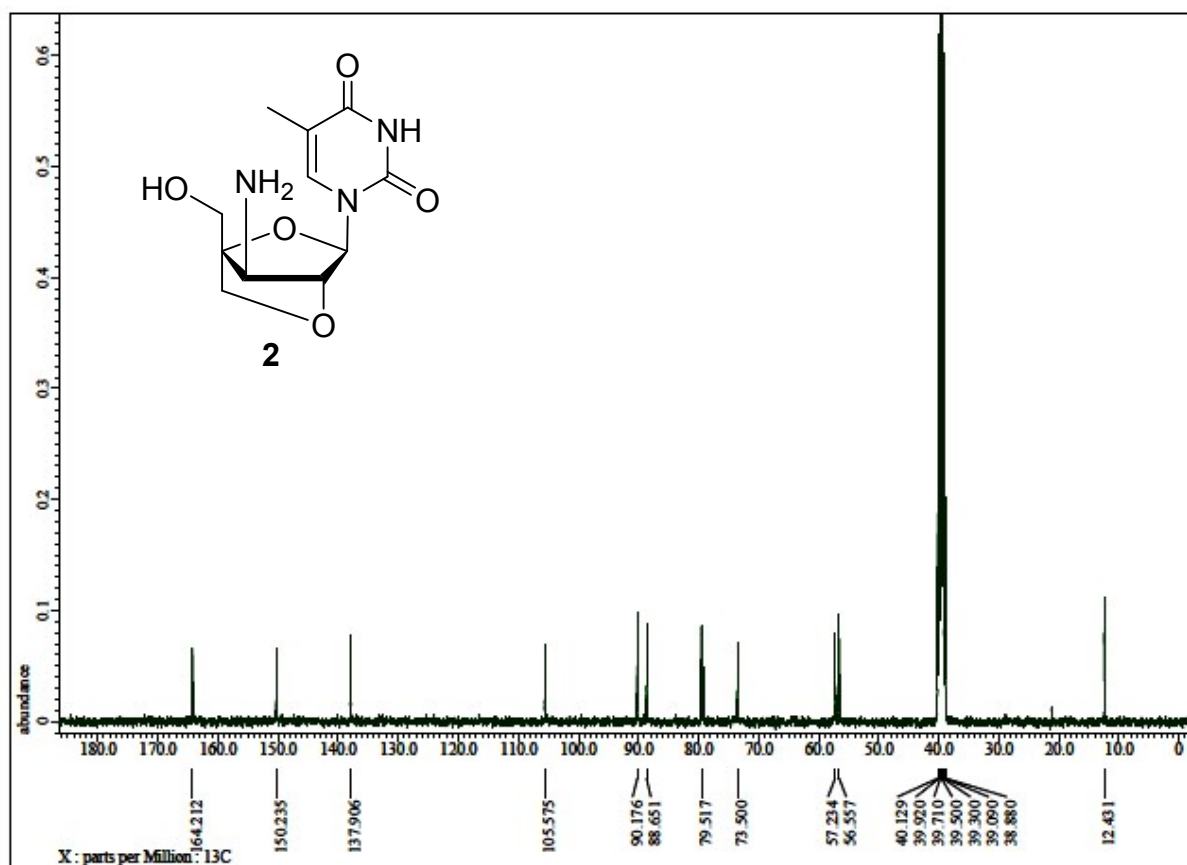
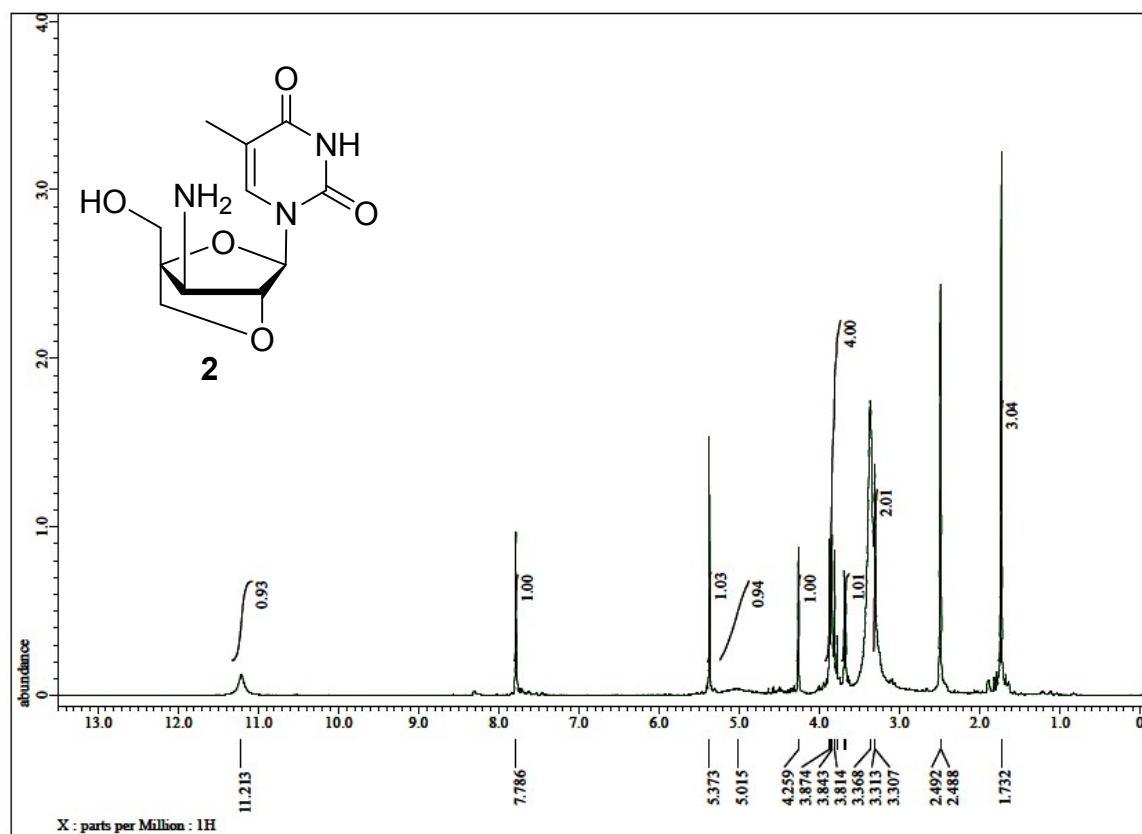


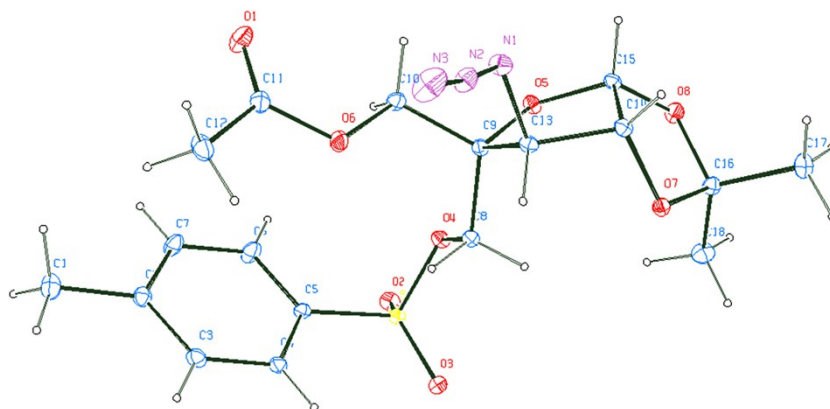


# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 1d

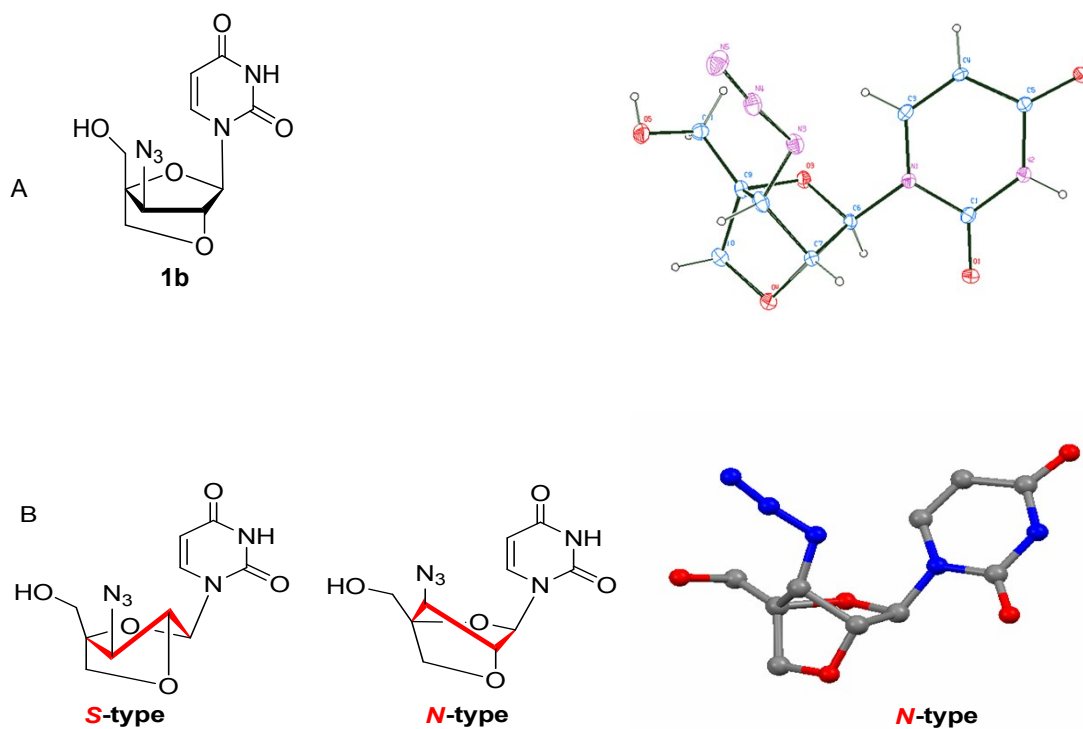


# <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 2





**Figure S1.** ORTEP diagram of tosylated sugar derivative **7**



**Figure S2.** (A) ORTEP diagram of compound 3'-azido-xylobicyclouridine **1b**; (B) Preferred *N*-type sugar pucker in compound **1b**

**Table S1.** Single crystal X-ray diffraction data of tosylated sugar derivative **7** and 3'-azido-3'-deoxy-2'-O,4'-C-methylene-xylofuranose (**1b**).

	<b>Compound 7</b>	<b>Compound 1b</b>
<b>Empirical formula</b>	C <sub>18</sub> H <sub>23</sub> N <sub>3</sub> O <sub>8</sub> S	C <sub>10</sub> H <sub>11</sub> N <sub>5</sub> O <sub>5</sub>
<b>Formula weight</b>	441.45	281.24
<b>Temperature</b>	293(2) K	293(2) K
<b>Crystal system</b>	Monoclinic	Monoclinic
<b>Space group</b>	P 21	P 21
<b>Unit cell dimensions</b>	a = 9.9041 (10) Å α = 90°	a = 6.5121(16)Å α = 90°
	b = 10.0867(9) Å β = 94.617(8)°	b = 6.8206(14) Å β = 93.72(3)°
	c = 10.6948(9) Å γ = 90°	c = 13.045(4) Å γ = 90°
<b>Volume</b>	1064.94(17) Å <sup>3</sup>	578.2(3) Å <sup>3</sup>
<b>Z</b>	2	2
<b>Density</b>	1.377 mg/m <sup>3</sup>	1.615 mg/m <sup>3</sup>
<b>Absorption coefficient</b>	0.201 mm <sup>-1</sup>	0.132 mm <sup>-1</sup>
<b>F(000)</b>	464	292
<b>Index ranges</b>	-12 ≤ h ≤ 12, -13 ≤ k ≤ 13, -14 ≤ l ≤ 14	-6 ≤ h ≤ 7, -7 ≤ k ≤ 8, -15 ≤ l ≤ 15
<b>R(int)</b>	0.0307	0.0518
<b>GOF on F<sup>2</sup></b>	0.839	0.911
<b>Final R indices</b>	R1 = 0.0496	R1 = 0.0652
<b>I&gt;2σ(I)</b>	wR2 = 0.1339	wR2 = 0.1776
<b>R indices</b>	R1 = 0.0711	R1 = 0.0867
<b>All data</b>	wR2 = 0.1647	wR2 = 0.2016
<b>CCDC</b>	<b>1414989</b>	<b>1420474</b>

