Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

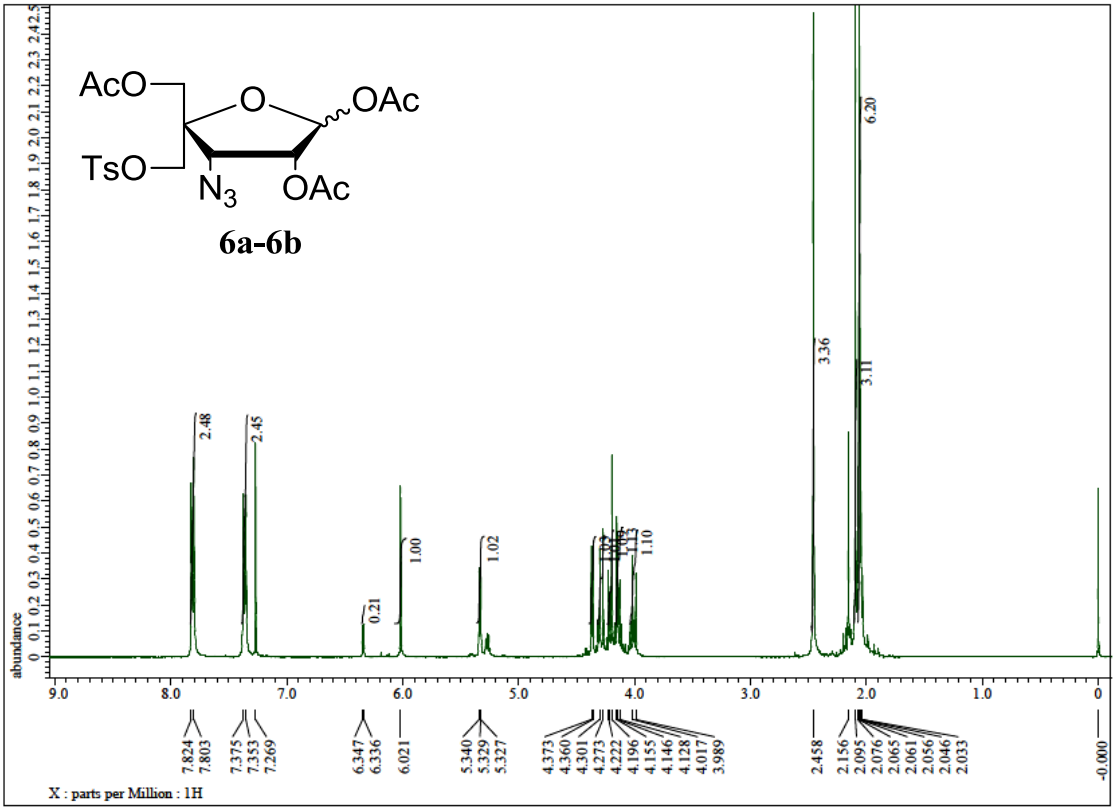
## Chemo-enzymatic synthesis of bicyclic 3'-azido- and 3'-amino-nucleoside

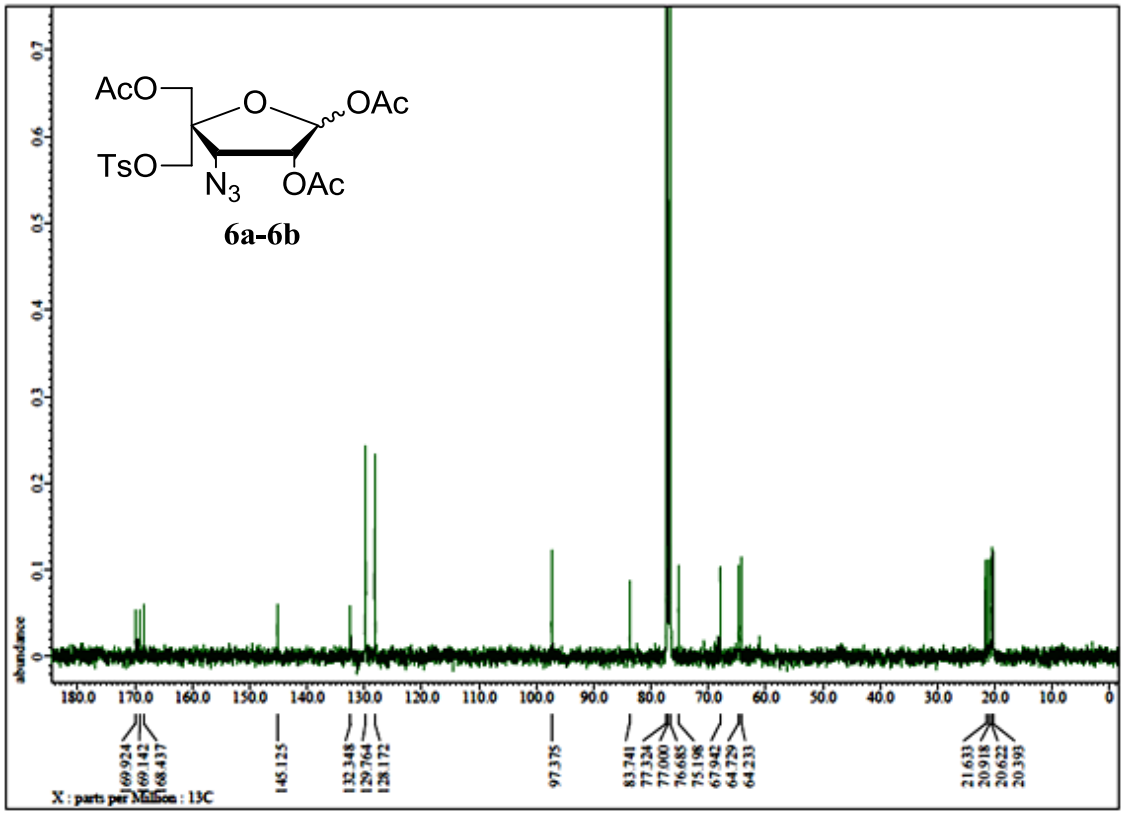
Manish Kumar,[a] Vivek K. Sharma,[a] Carl E. Olsen[b] and Ashok K. Prasad[a,*]

[a]Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi-110 007; [b]Faculty of Life Sciences, Department of Plant and Environmental Sciences, University of Copenhagen, DK- 1871 Frederiksberg C, Denmark

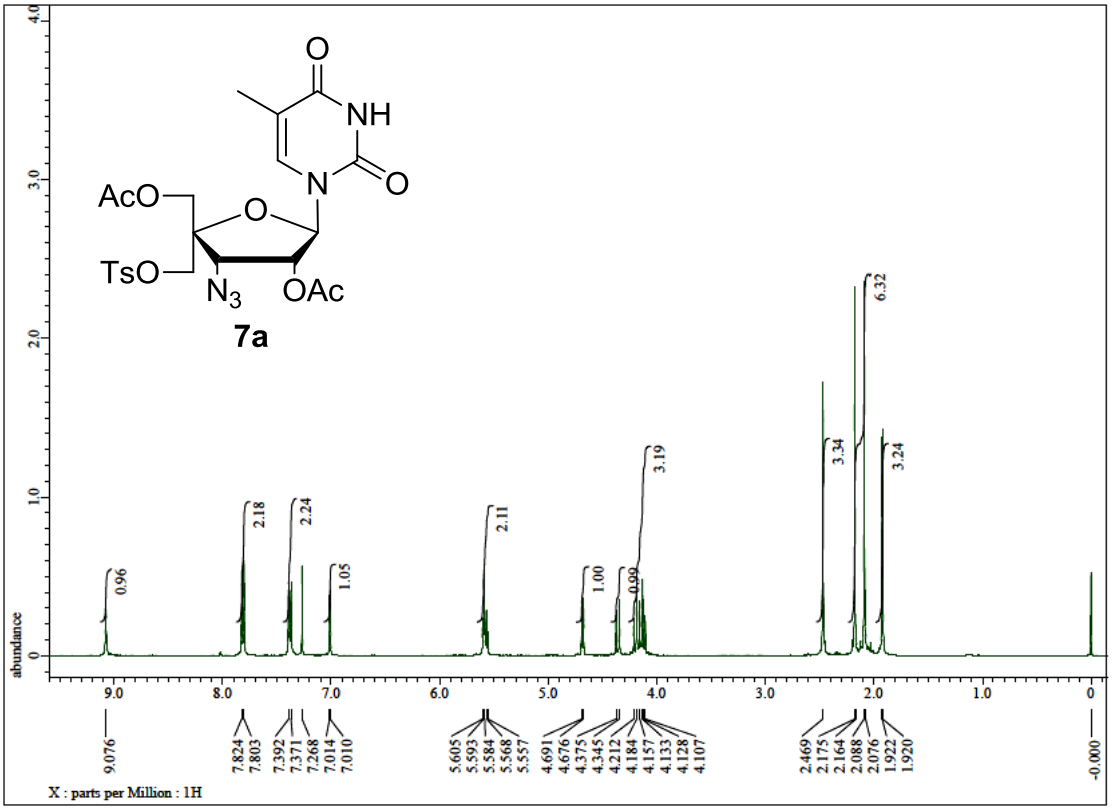
*ashokenzyme@yahoo.com*

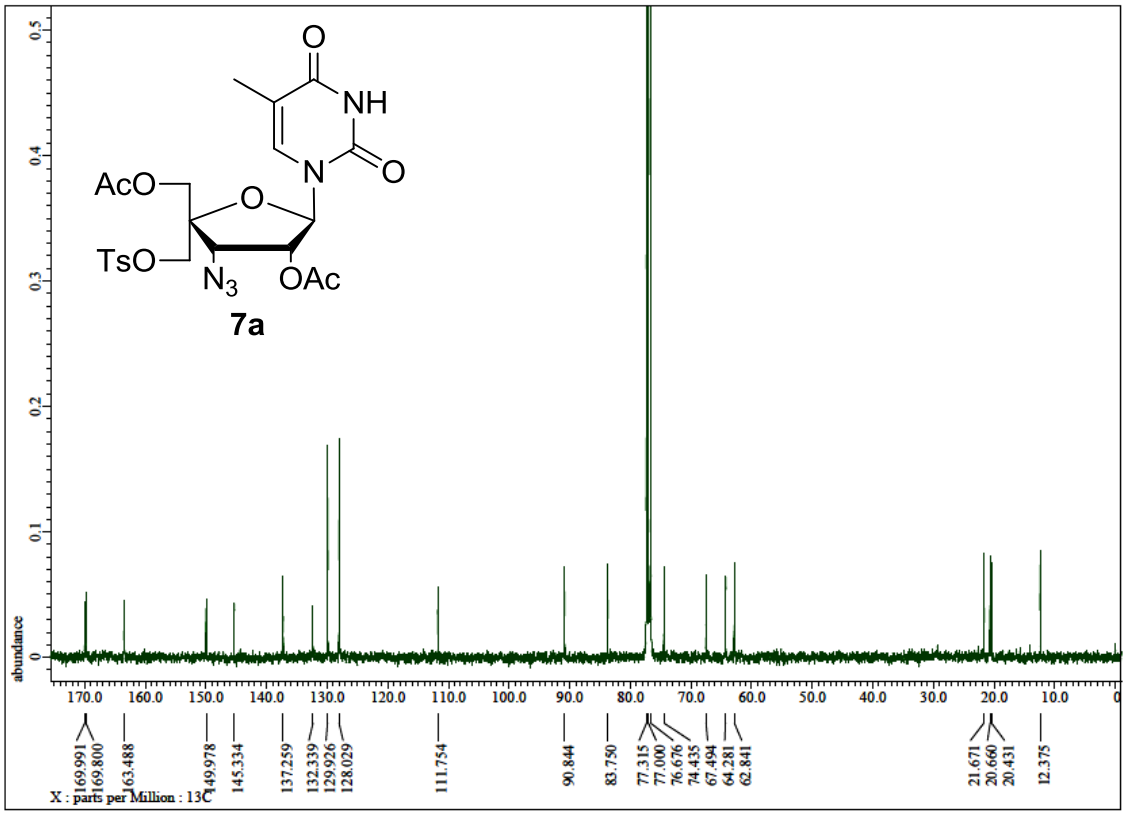
**$^{1}$H- and $^{13}$C NMR Spectrum of compound 6a-6b**



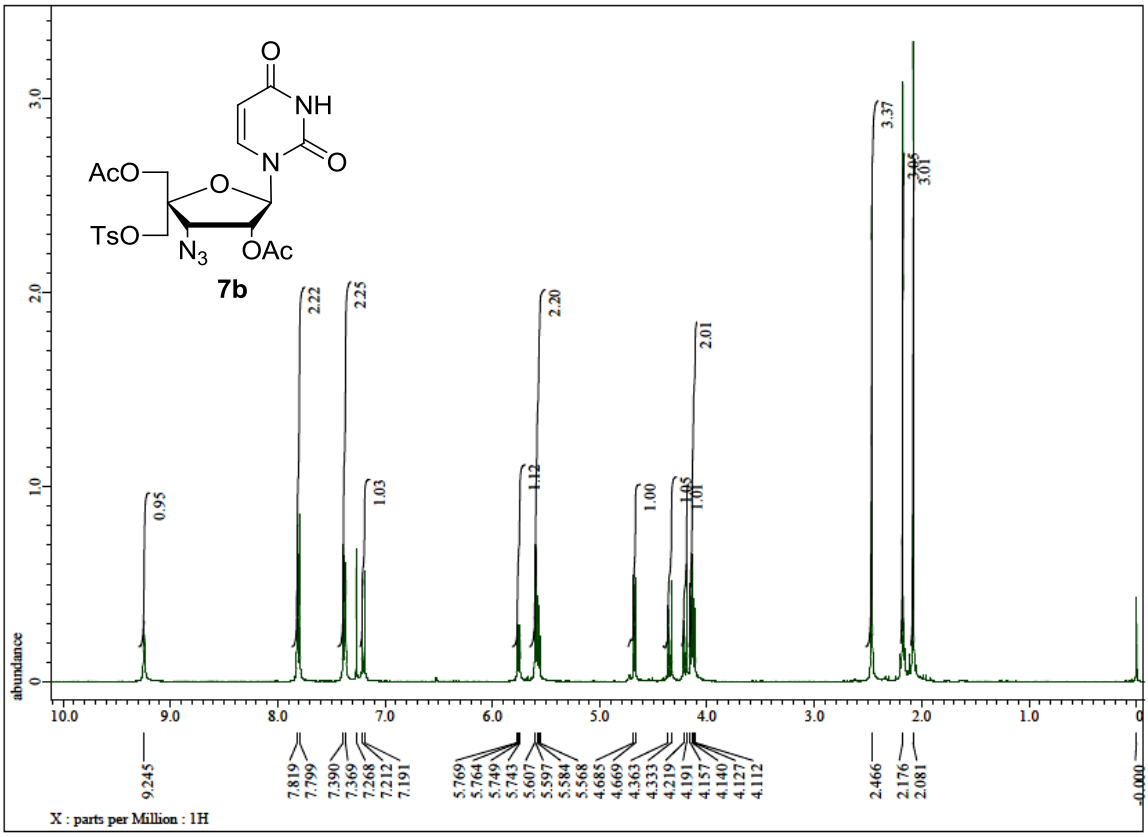



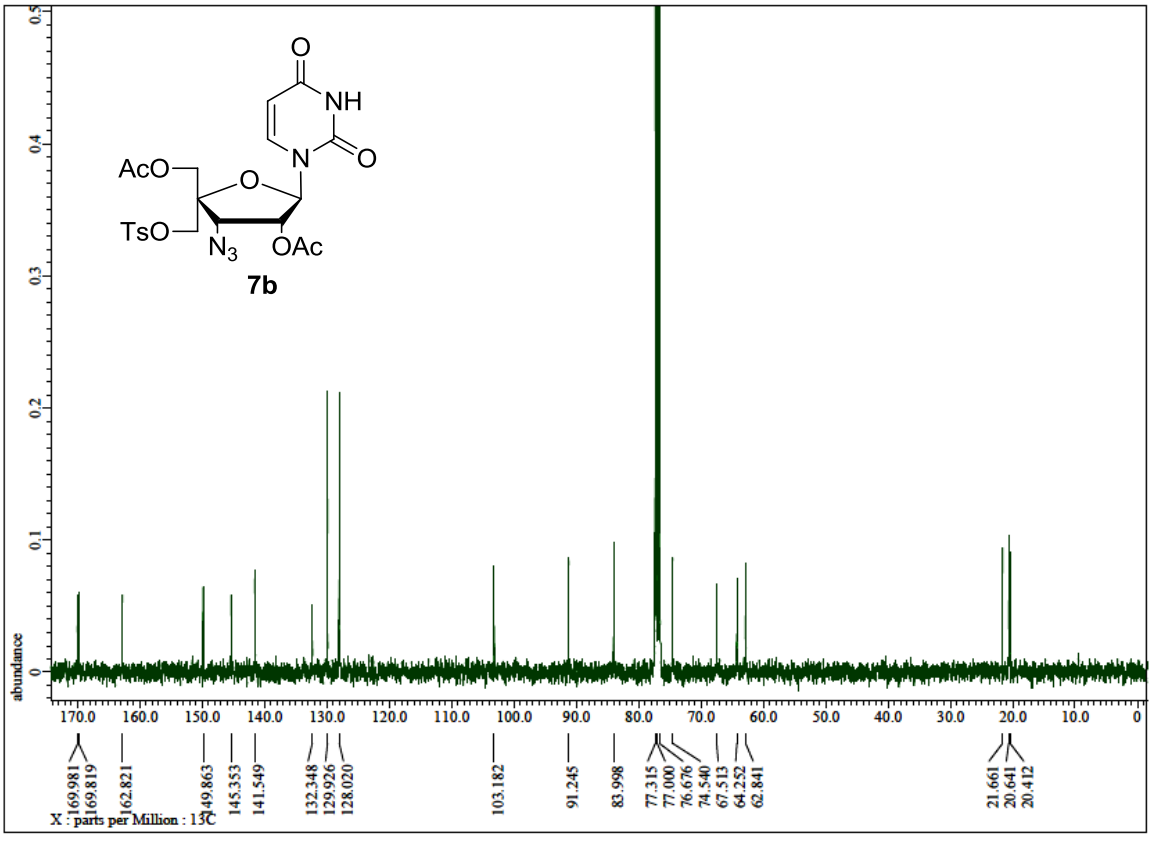
**$^{1}$H- and $^{13}$C NMR Spectrum of compound 7a**



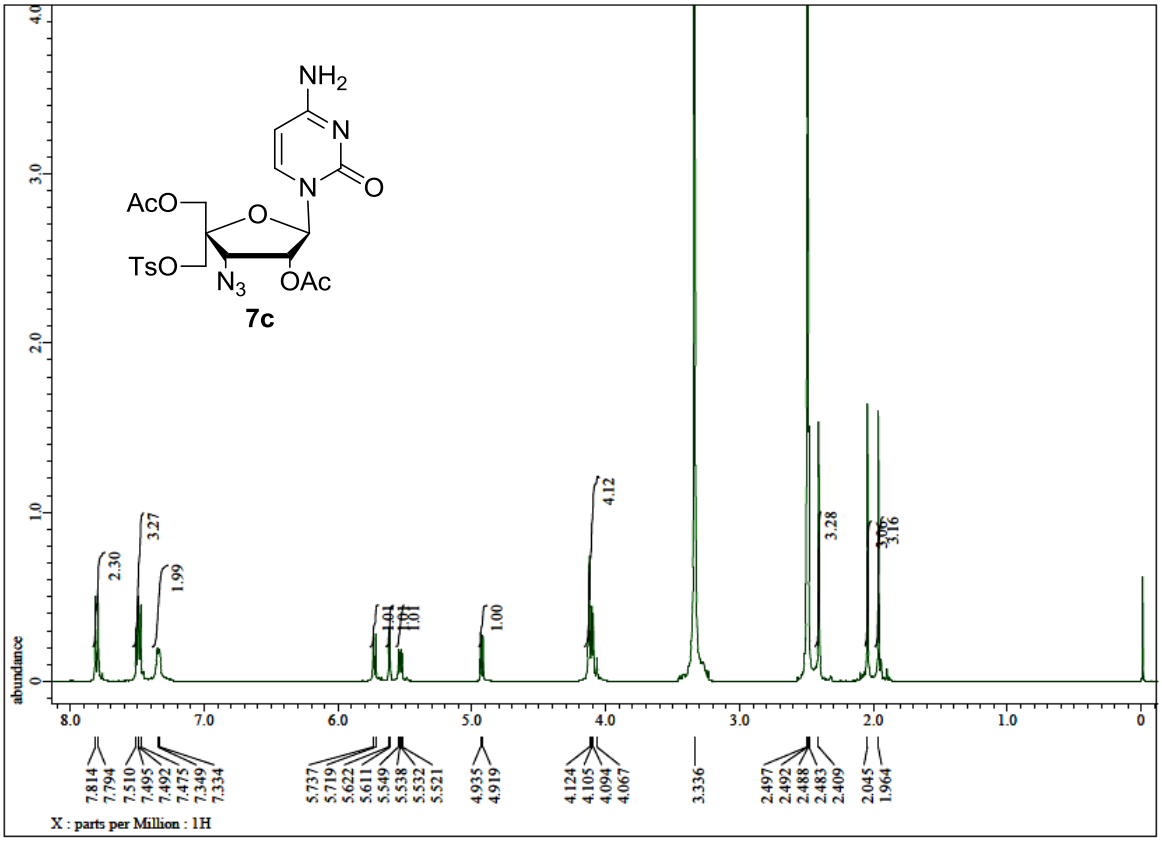



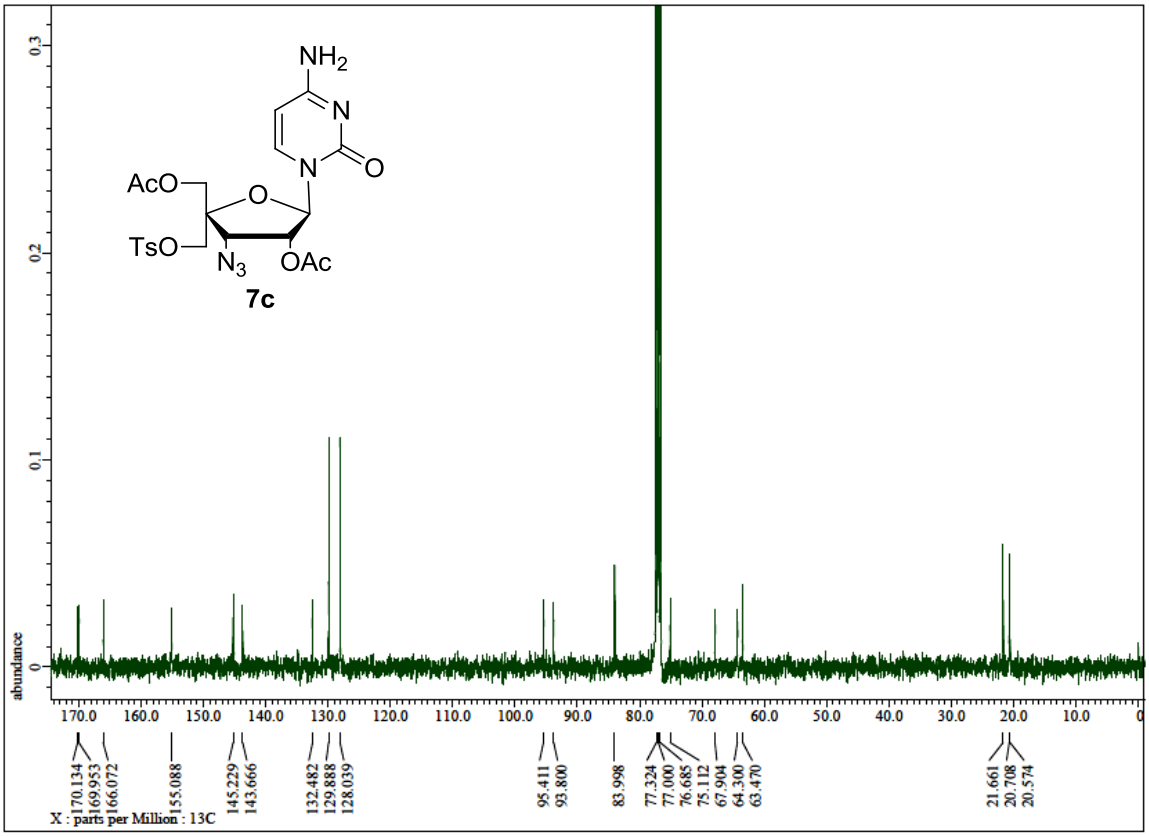
## $^{1}$H- and $^{13}$C NMR Spectrum of compound 7b



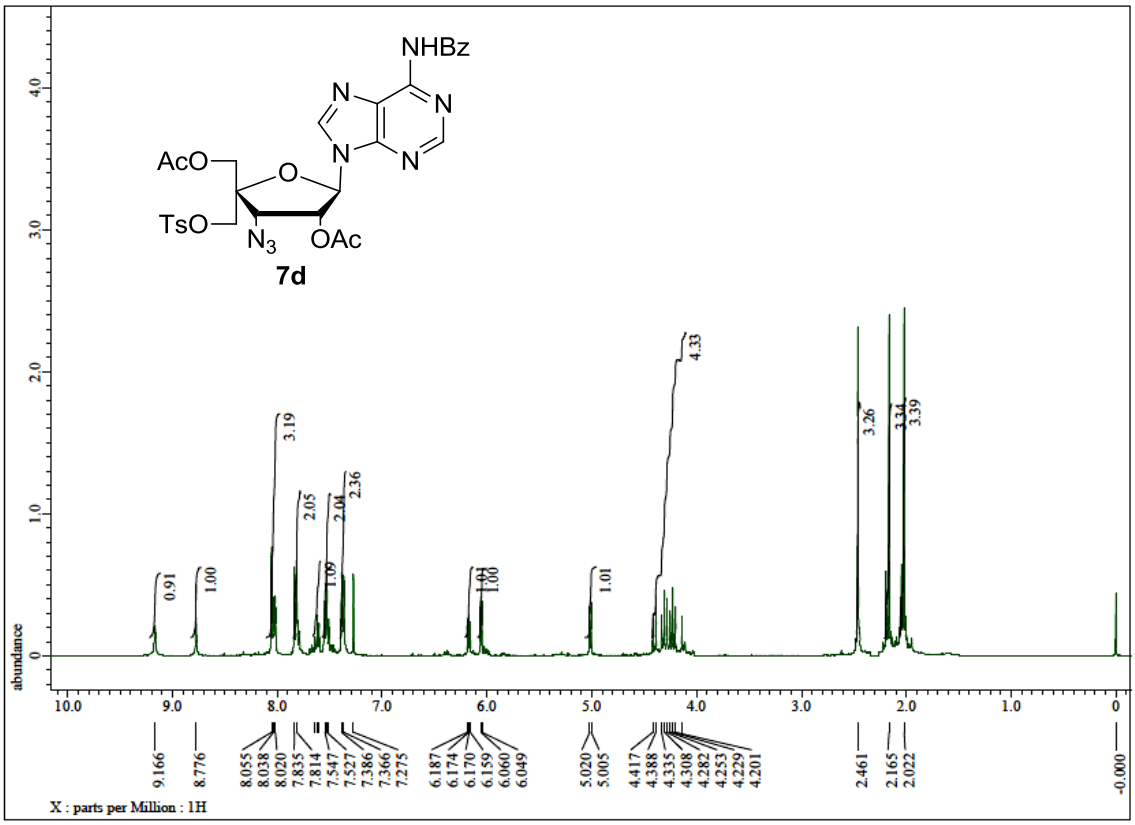



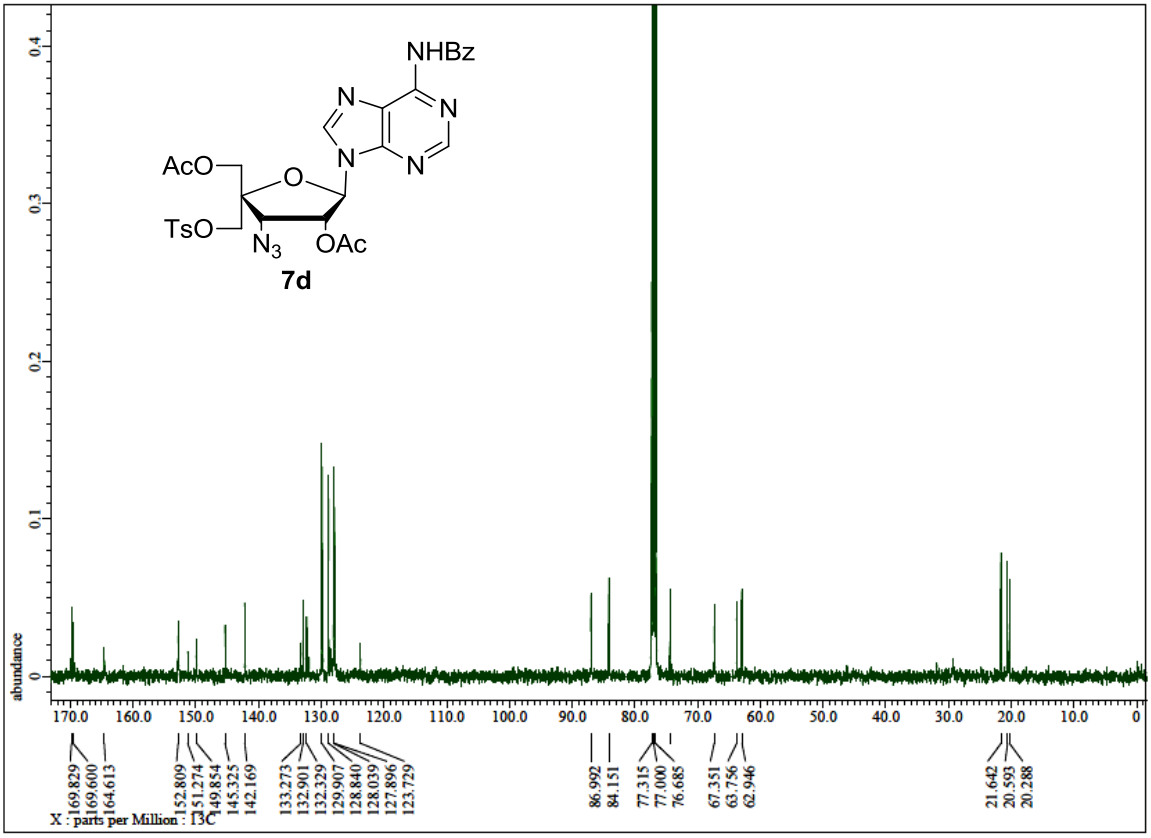
## $^{1}$H- and $^{13}$C NMR Spectrum of compound 7c



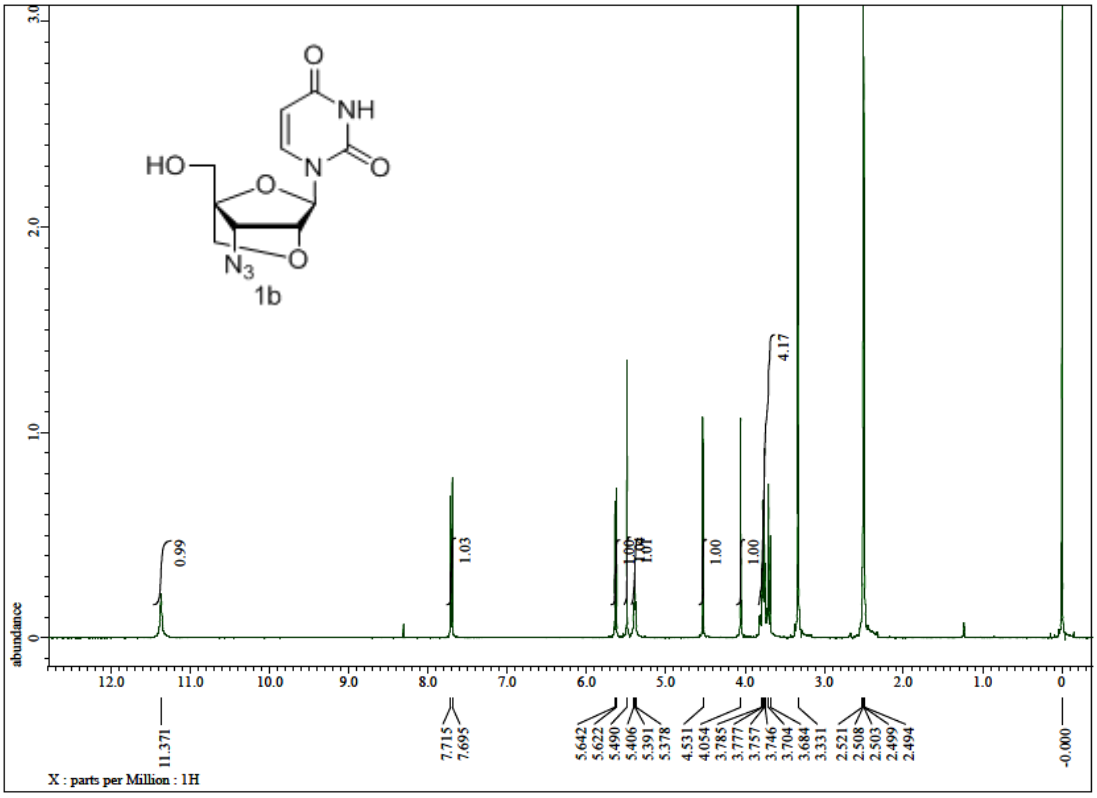



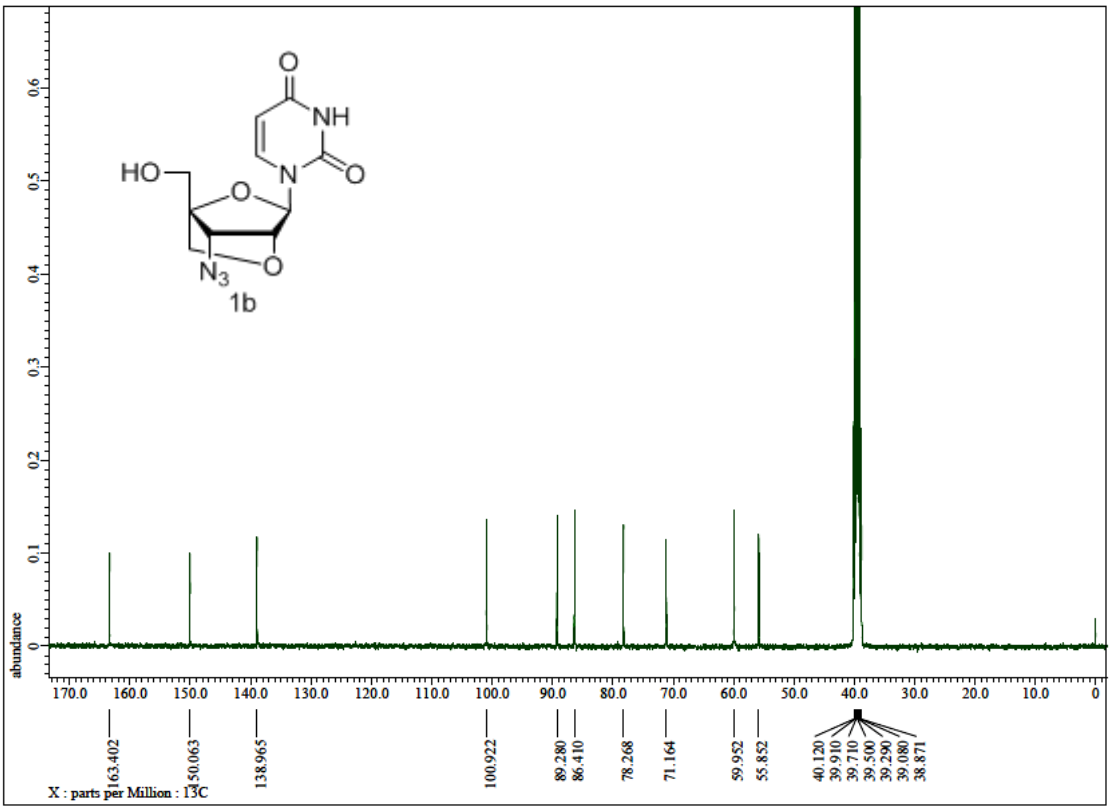
## $^{1}$H- and $^{13}$C NMR Spectrum of compound 7d



## $^{1}$H- and $^{13}$C NMR Spectrum of compound 1b



**Single Crystal X-Ray structure and data of compound 5.**

Single crystal suitable for X-ray diffraction was grown by dissolving compound **5** in THF and allowing it to evaporate slowly at room temperature. X-ray diffraction data was collected on an Oxford Diffraction XCalibur CCD diffractometer with graphite monochromated Cu Kα radiation (λ = 1.54184 Å) at temperature 298 K. The structure was solved by direct methods using SHELXS-97 and refined by full-matrix least-squqres method on $F^2$ (SHELXL-97). All calculations were carried out using the WinGX package of the crystallographic programs. For the molecular graphics, the program DIAMOND-2 and Mercury was used. Further information on the crystal structure determination (excluding structure factors) has been deposited in the Cambridge Crystallographic Data Centre as supplementary publications no.**995894**. Molecular structure have been drawn using ORTEP as software as given in **Figure S1**. The selected bond lengths, bond angles, *etc*. are given in **Table S1**.

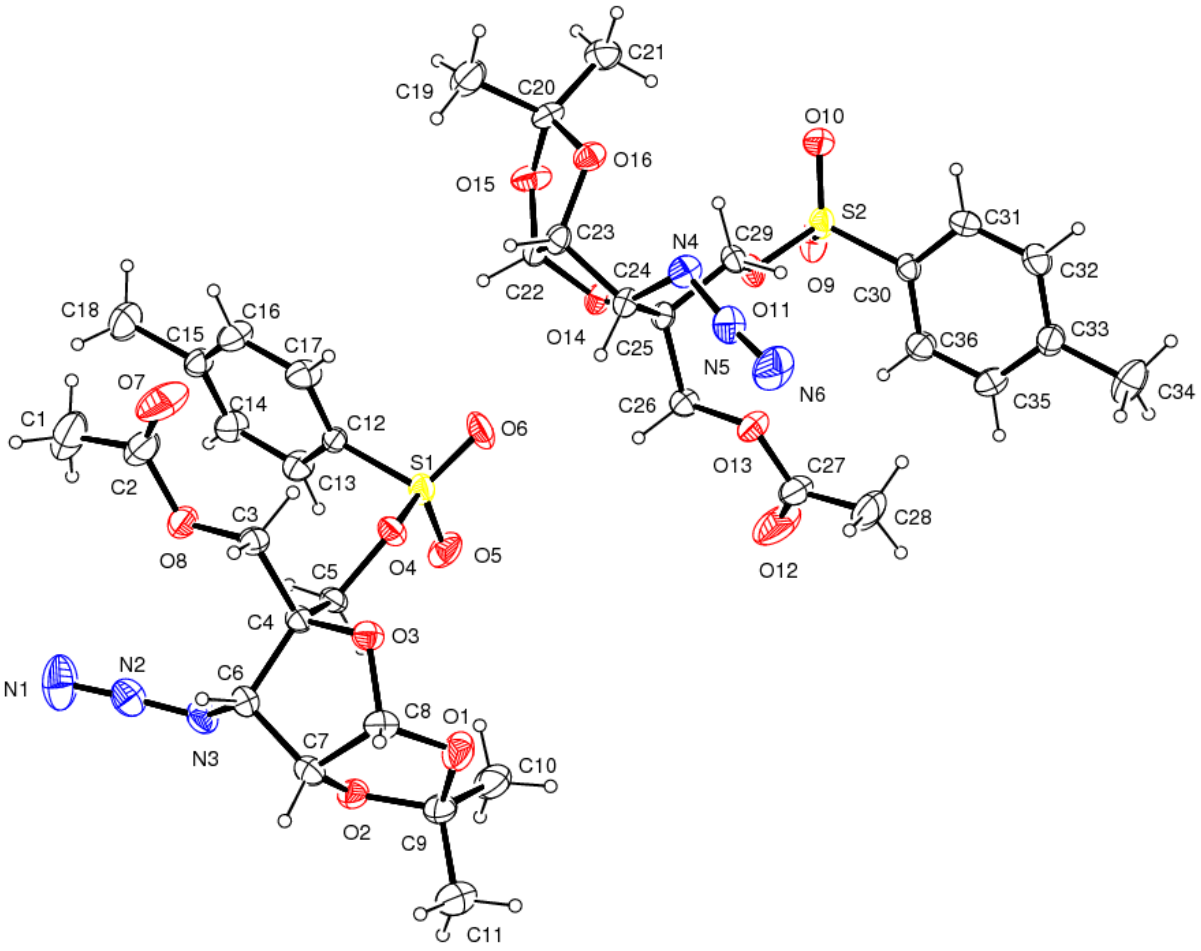



**Figure S1.** ORTEP diagram of the compound **5** drawn in 20% thermal probability ellipsoids with atomic numbering scheme showing two crystallographically independent units.

**Table 1**: Single crystal X-ray diffraction data of compound **5**

| **Compound** | **5** |
|---|---|
| **Empirical formula** | $C_{18}H_{23}N_3O_8S$ |
| **Formula weight** | 441.45 |
| **Temperature** | 298(2) K |
| **Wavelength** | 0.71073 Å |
| **Crystal system** | Monoclinic |
| **Space group** | P 21 |
| **Unit cell dimensions** | a = 9.9038(14) Å<br>α = 90° |
| | b = 13.785(3) Å<br>β = 101.077(15)° |
| | c = 16.1493(3) Å<br>γ = 90° |
| **Volume** | 2163.7(6) $Å^3$ |
| **Z** | 4 |
| **Density (calculated)** | 1.355 $Mg/m^3$ |
| **Absorption coefficient** | 0.198 $mm^{-1}$ |
| **F(000)** | 928 |
| **Crystal size** | 0.24 x 0.18 x 0.14 $mm^3$ |
| **Theta range for data collection** | 2.97 to 25.00°. |
| **Index ranges** | -10<=h<=11,<br>-16<=k<=16,<br>-19<=l<=17 |
| **Reflections collected** | 13901 |
| **Independent reflections** | 6745 [R(int) = 0.0420] |
| **Completeness to theta = 25.00 º** | 98.4 % |

| | |
|---|---|
| **Max. and min. transmission** | 0.9728 and 0.9540 |
| **Refinement method** | Full-matrix least-squares on $F^2$ |
| **Data / restraints / parameters** | 6745 / 1 / 549 |
| **Goodness-of-fit on $F^2$** | 0.990 |
| **Final R indices [I>2sigma(I)]** | R1 = 0.0545,<br>wR2 = 0.0992 |
| **R indices (all data)** | R1 = 0.0845,<br>wR2 = 0.1118 |
| **Absolute structure parameter** | 0.05(8) |
| **Largest diff. peak and hole** | 0.190 and -0.173 e.Å$^{-3}$ |
| **CCDC** | **995894** |