

Supplementary Material

Stereoselective synthesis of tetrahydrofuranyl 1,2,3-triazolyl C-nucleoside analogues by ‘click’ chemistry and investigation of their biological activity

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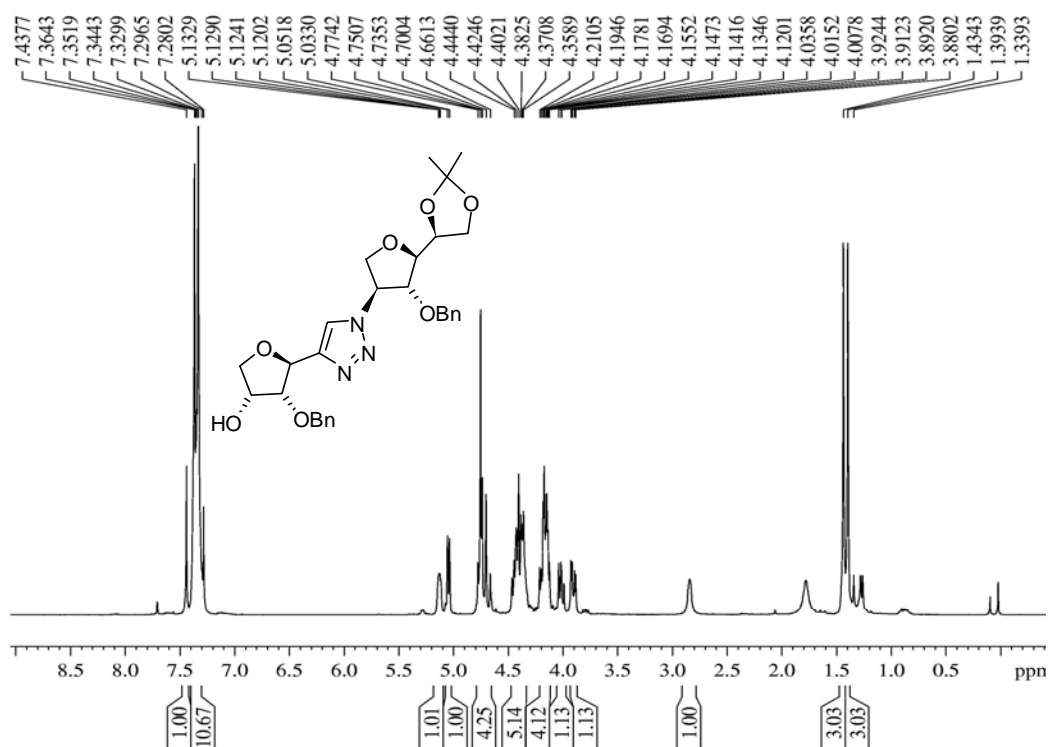
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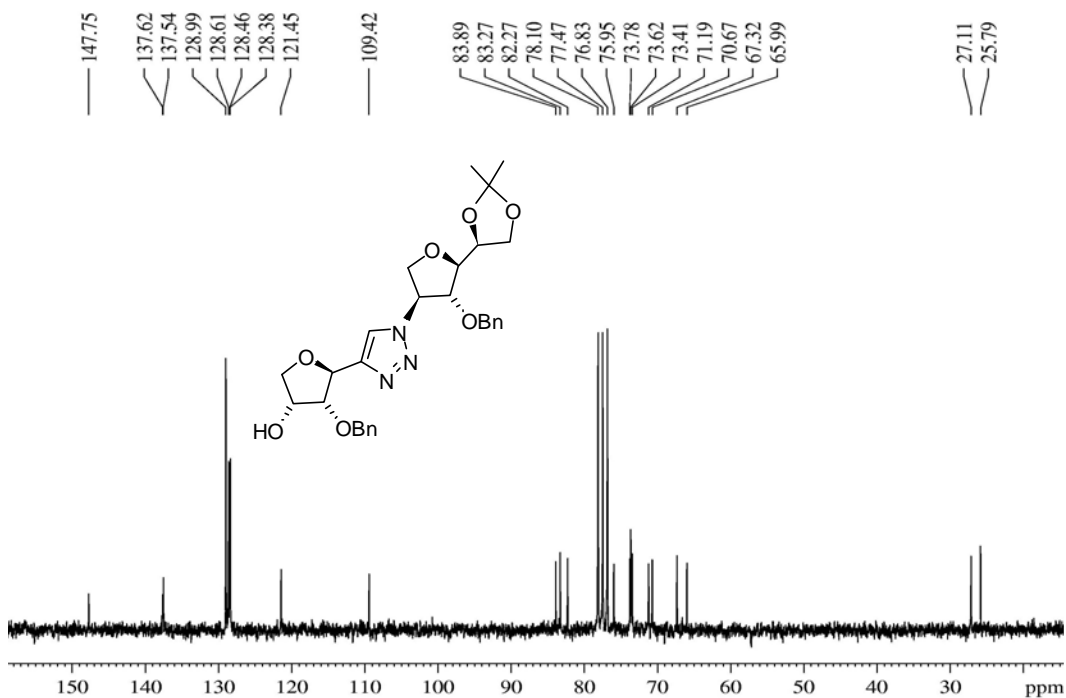
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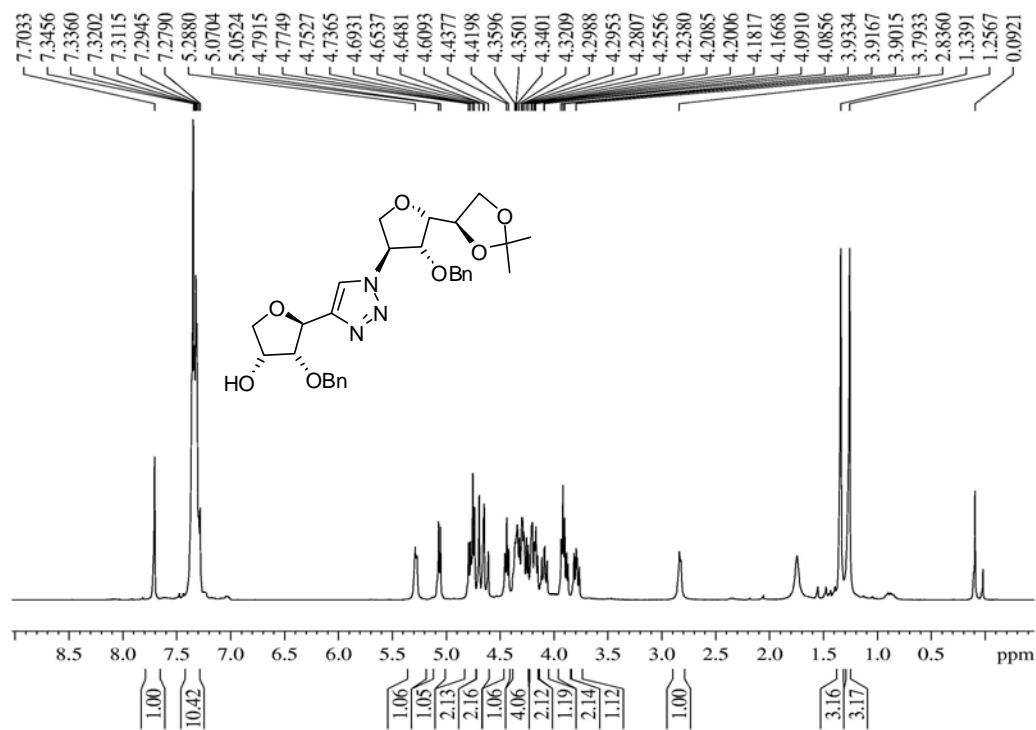
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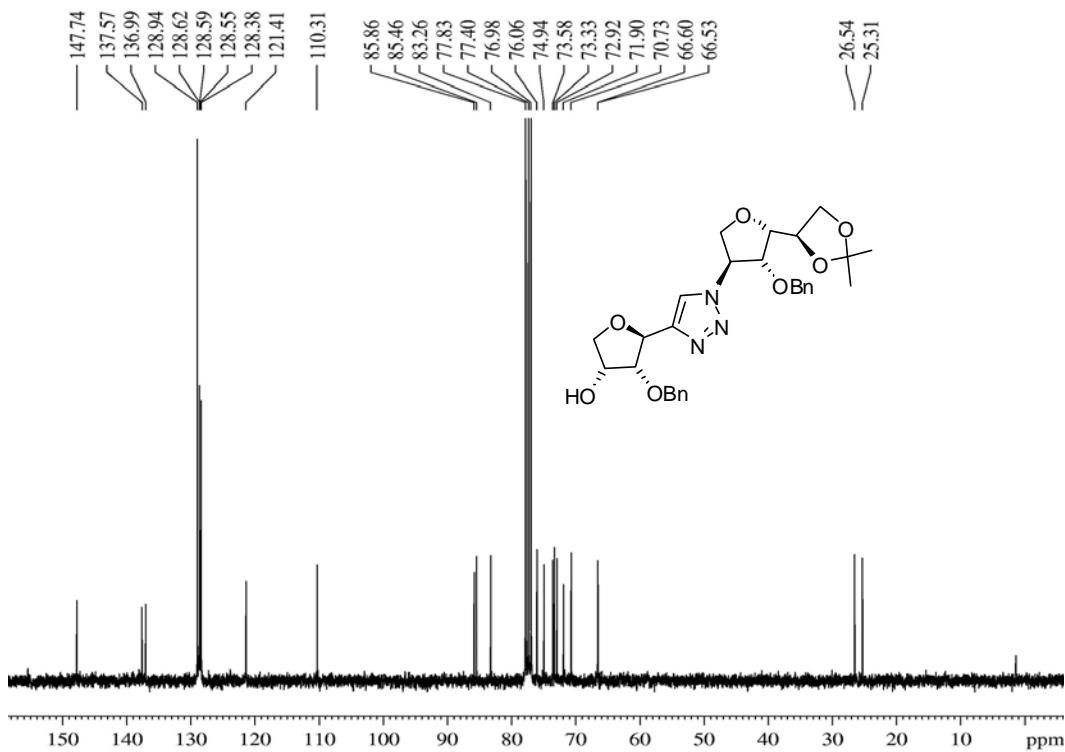
¹H NMR spectrum of compound **14**



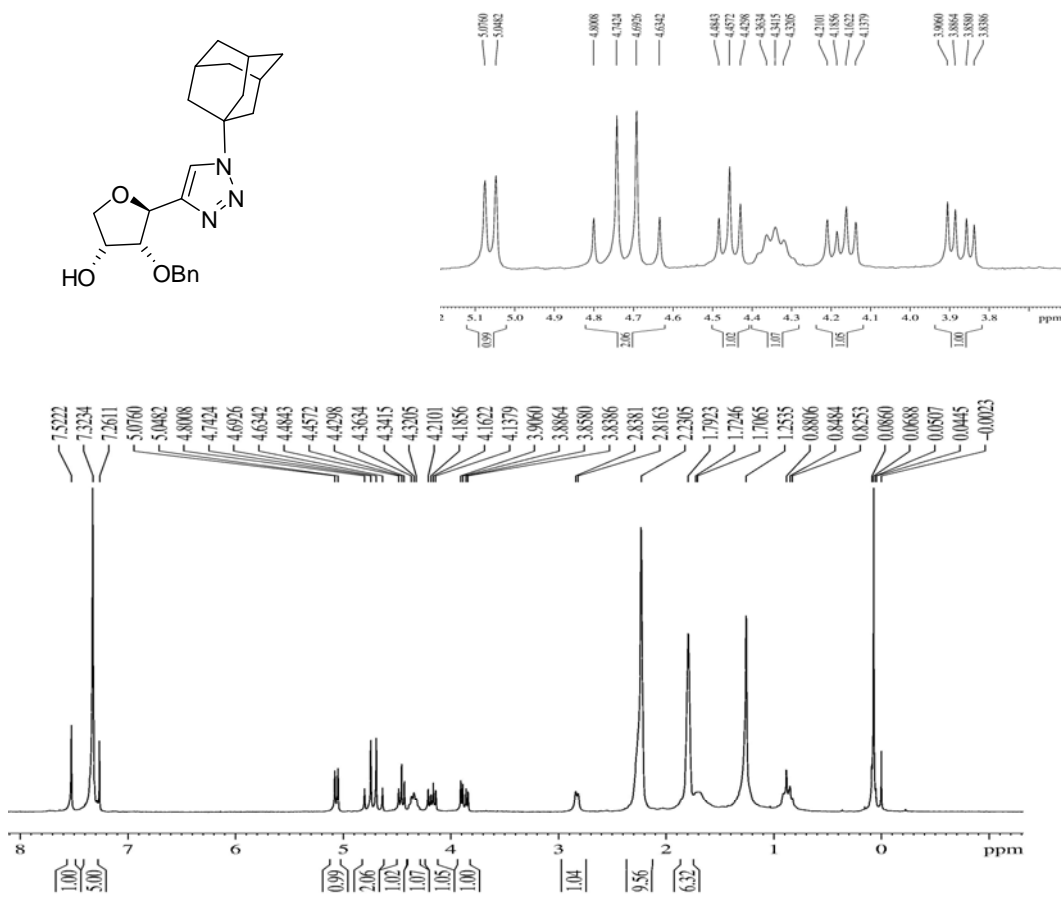
¹³C NMR spectrum of compound **14**



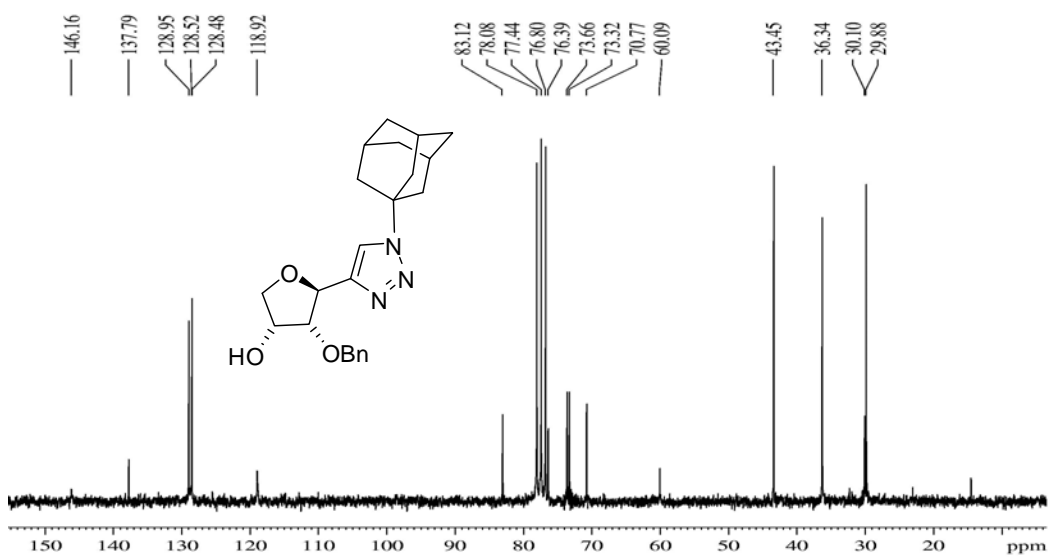
¹H NMR spectrum of compound **15**



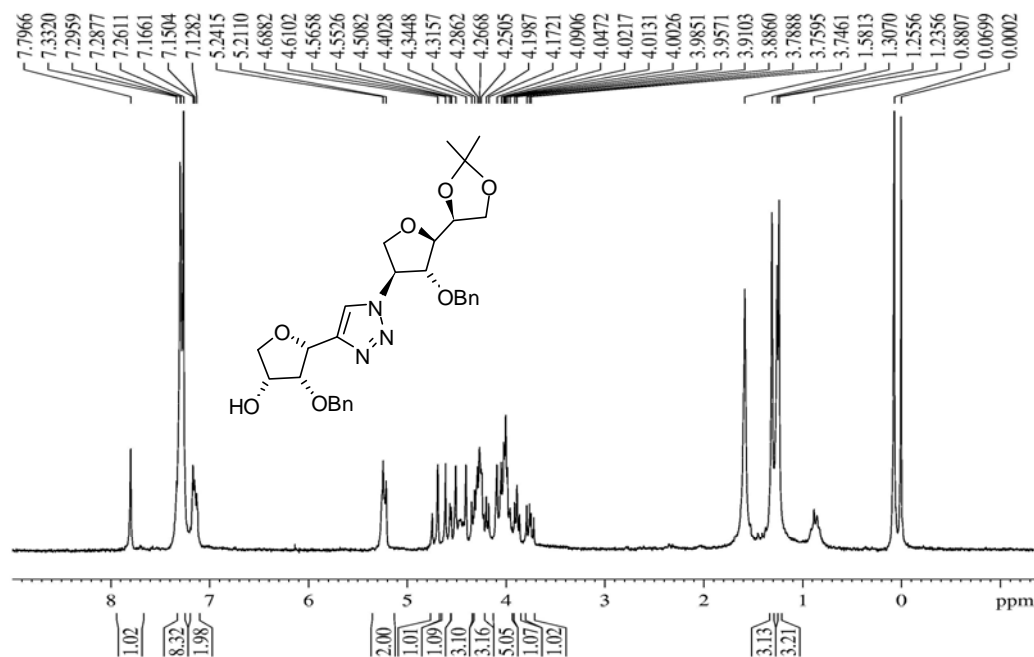
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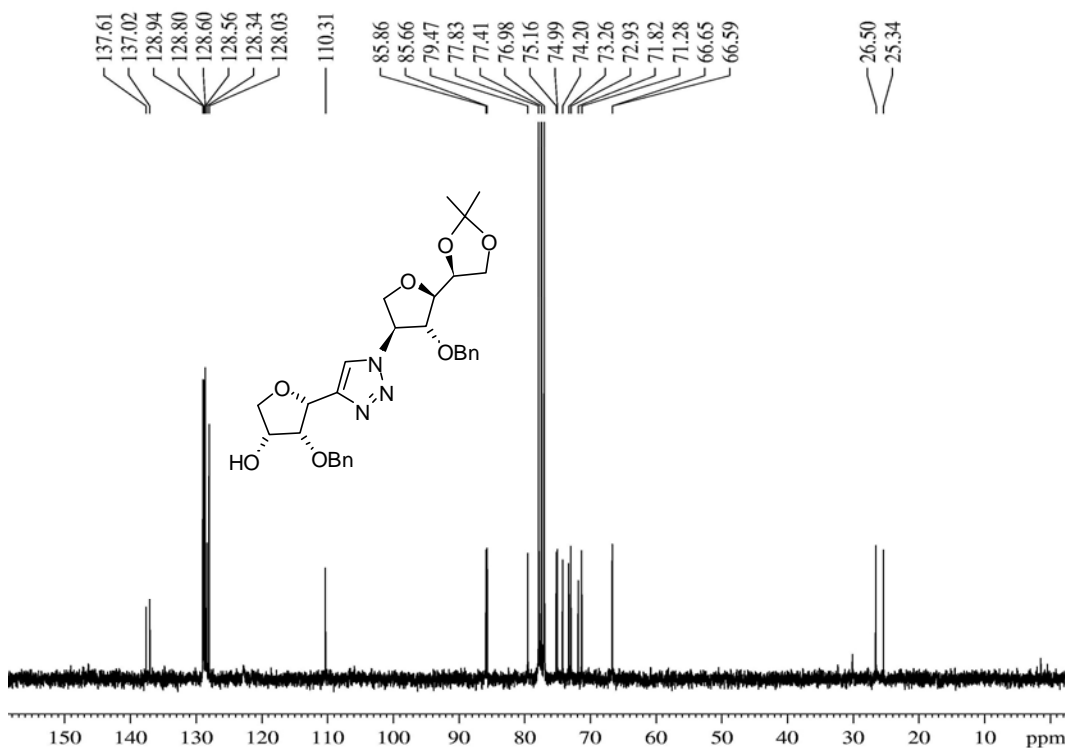
^1H NMR spectrum of compound **16** and its expansion



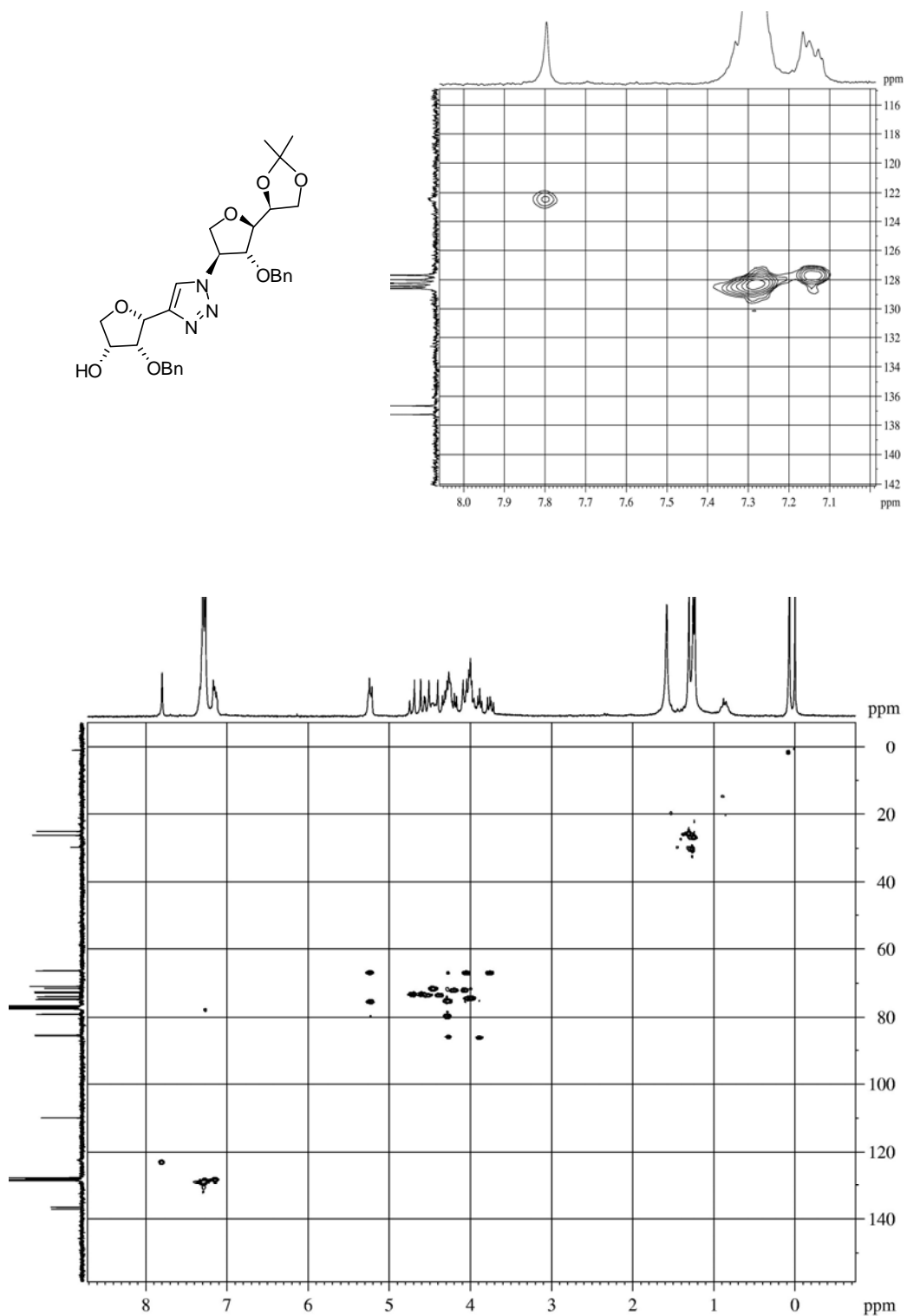
^{13}C NMR spectrum of compound **16**

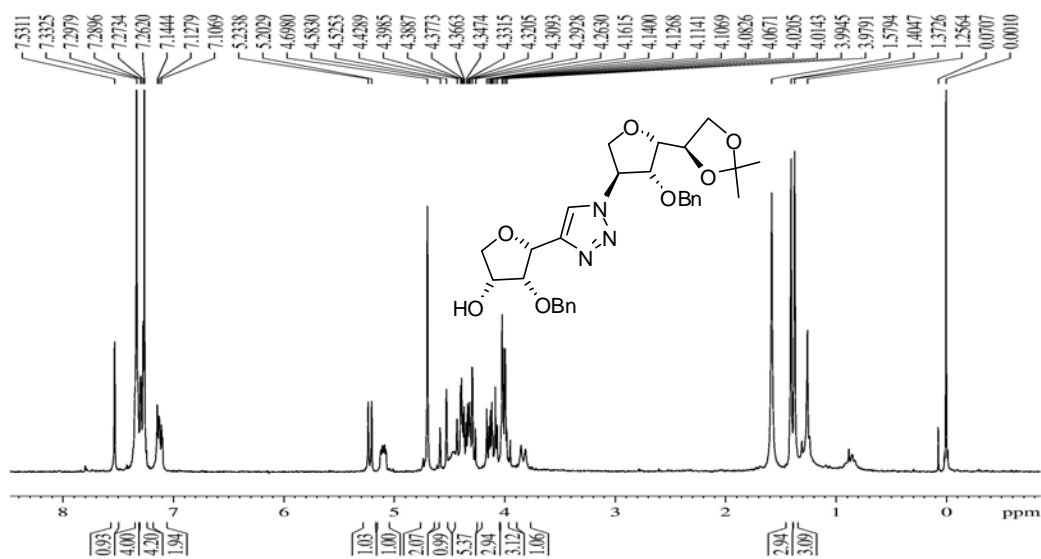


¹H NMR spectrum of compound **18**

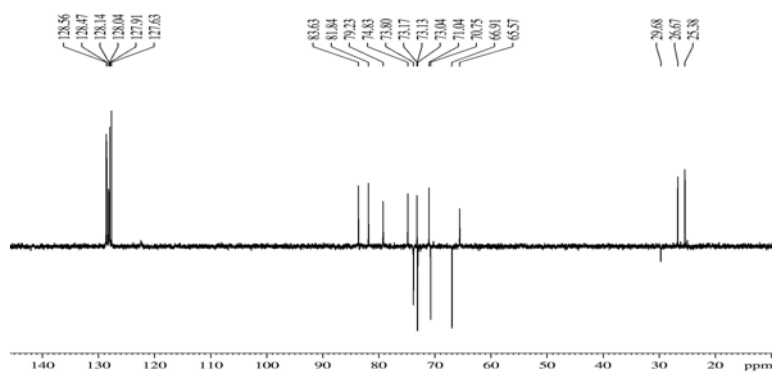


¹³C NMR spectrum of compound **18**

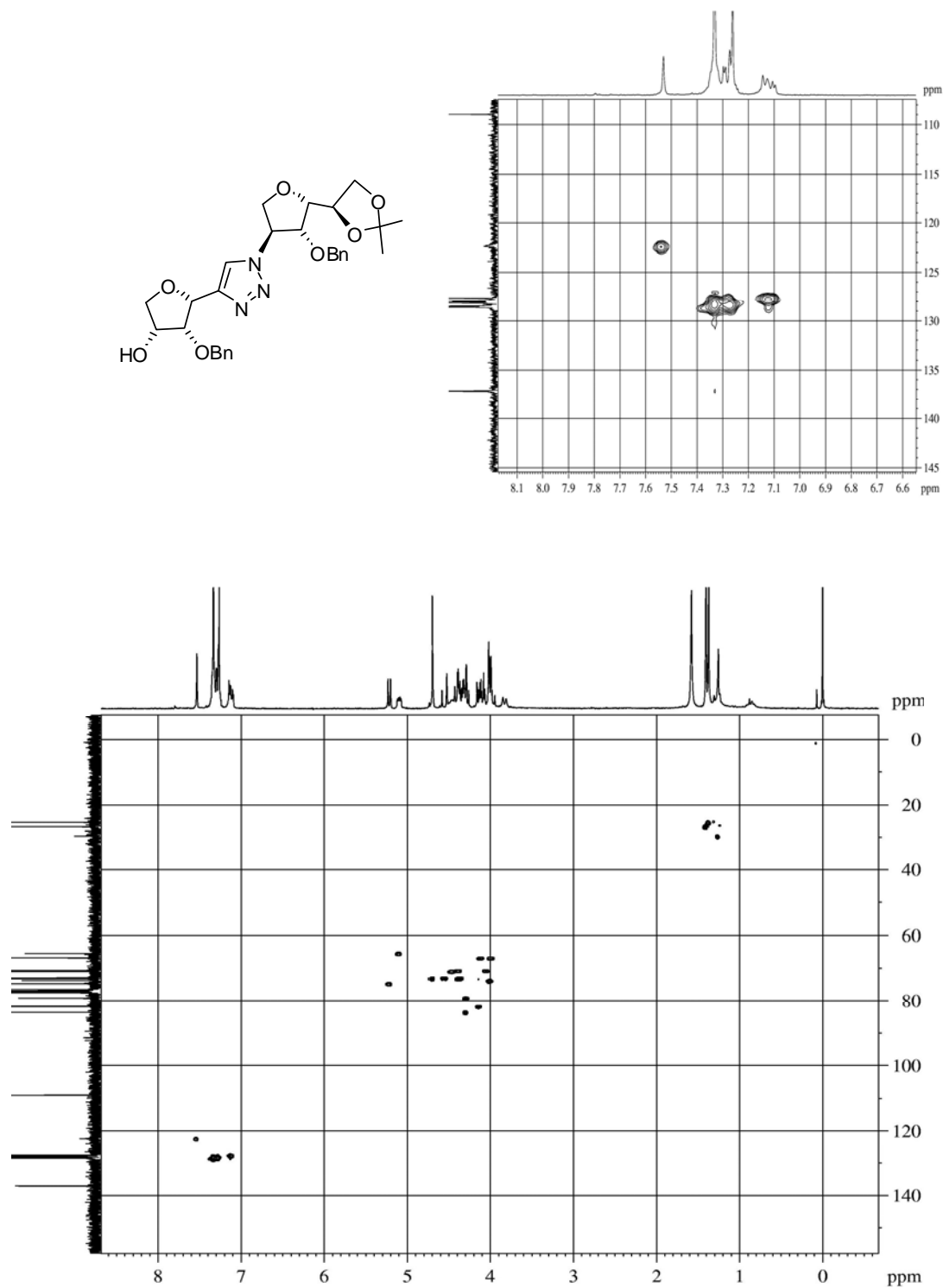
HSQC spectrum of compound **18** and its expansion

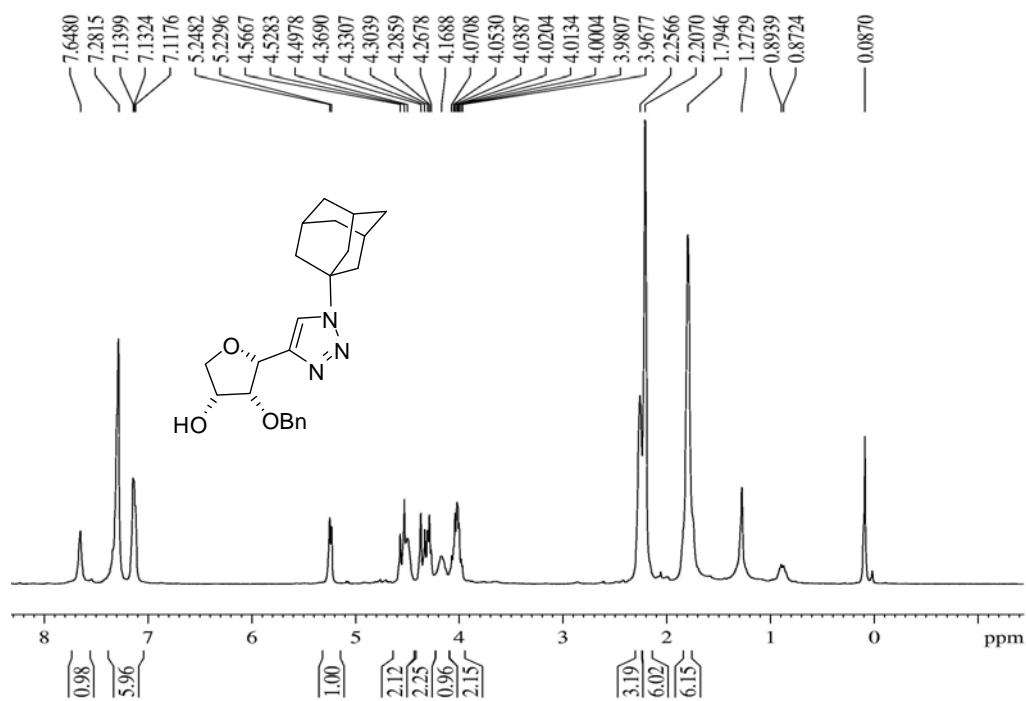


¹H NMR spectrum of compound **19**

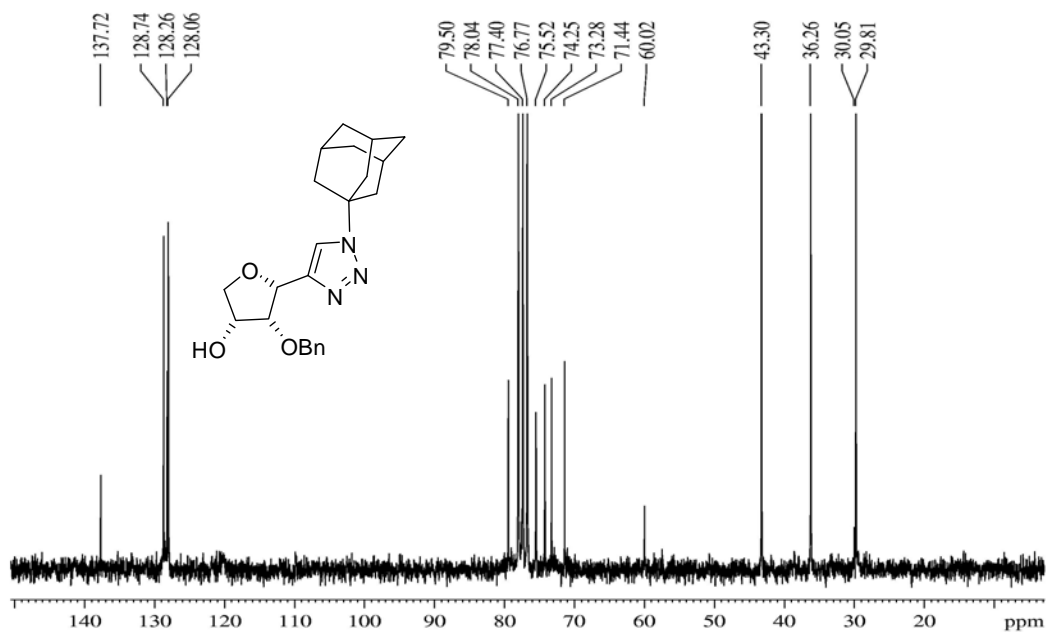


¹³C NMR spectrum of compound **19**

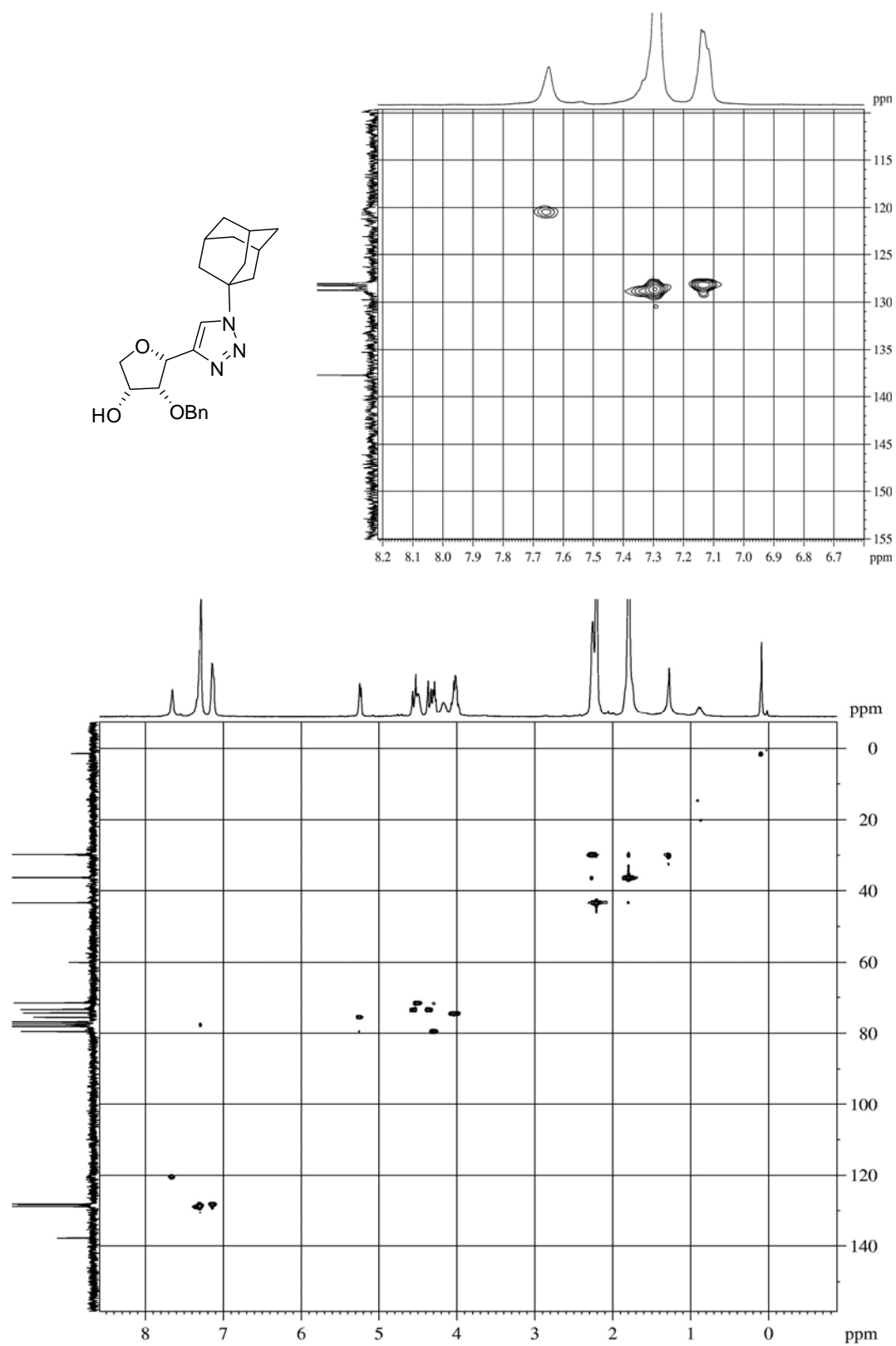
HSQC spectrum of compound **19** and its expansion

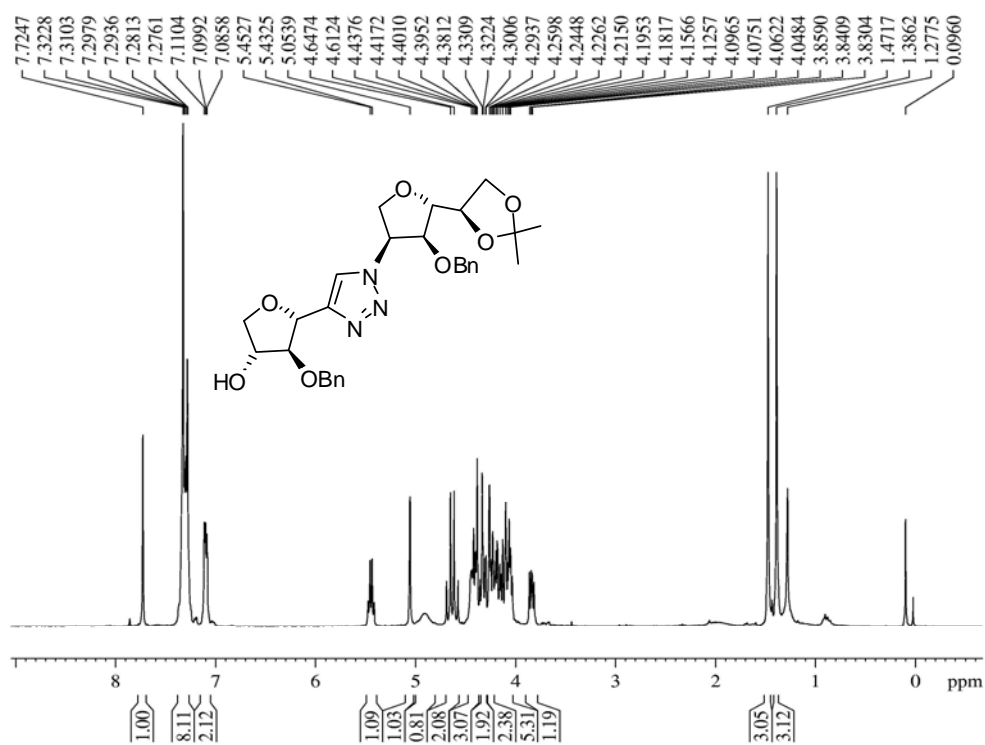


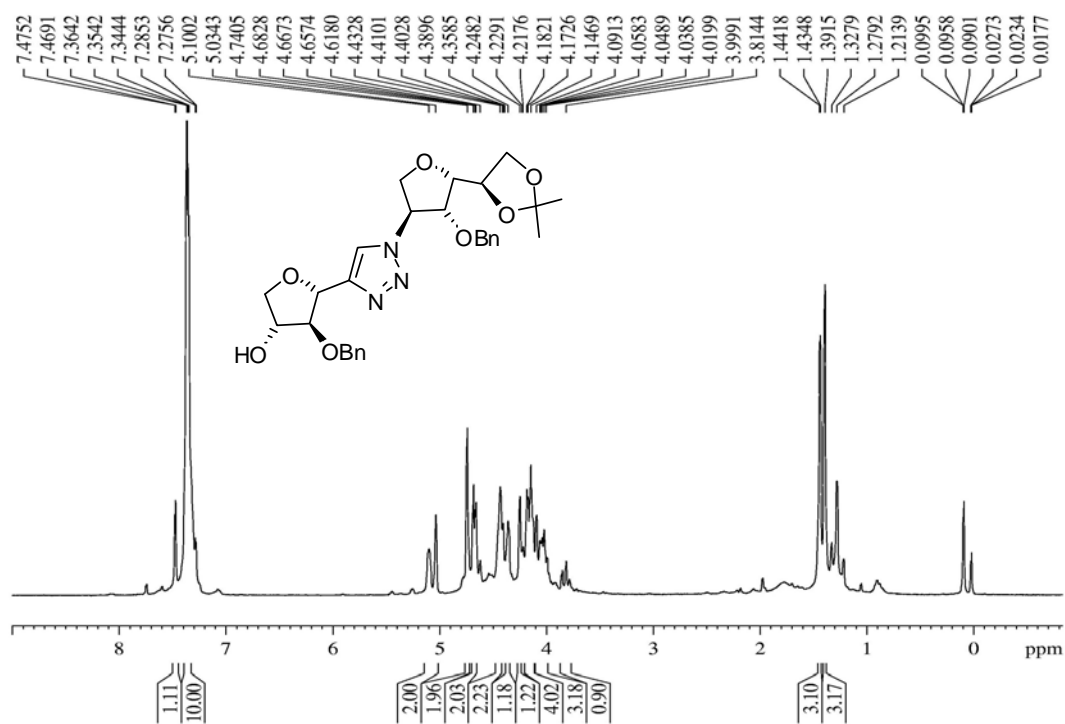
¹H NMR spectrum of compound **20**



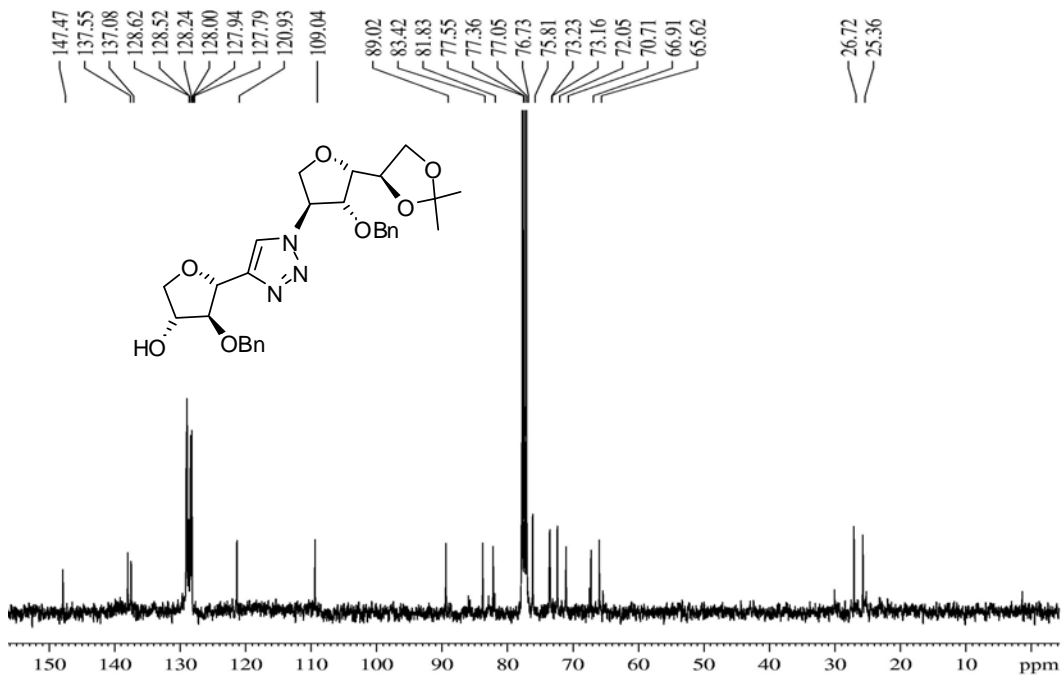
¹³C NMR spectrum of compound **20**

HSQC spectrum of compound **20** and its expansion

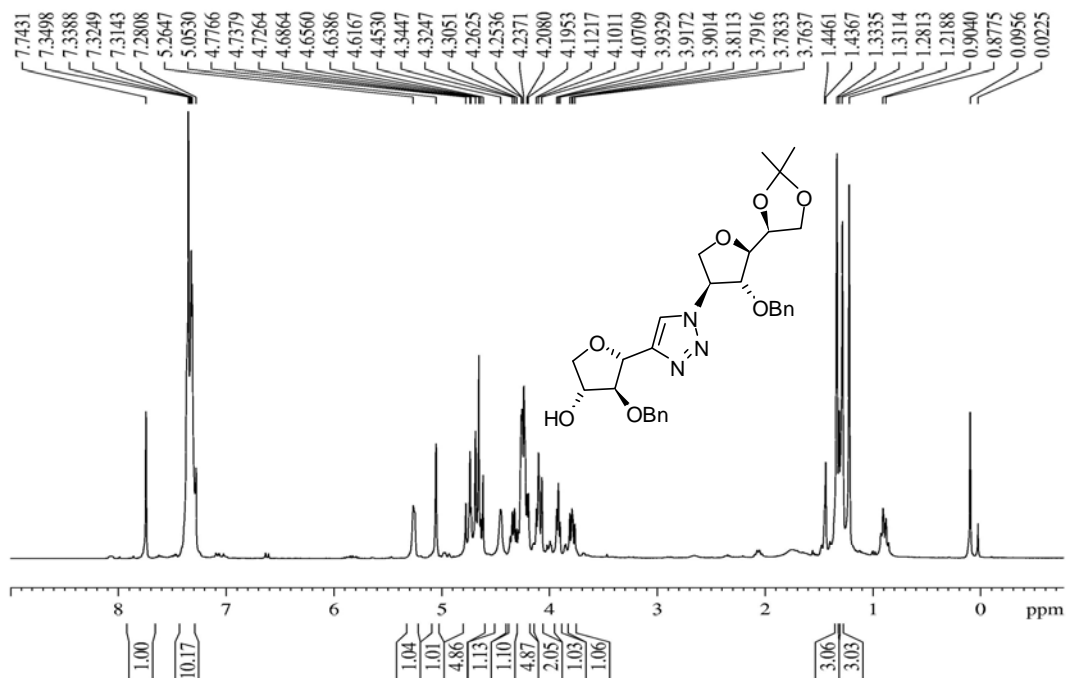




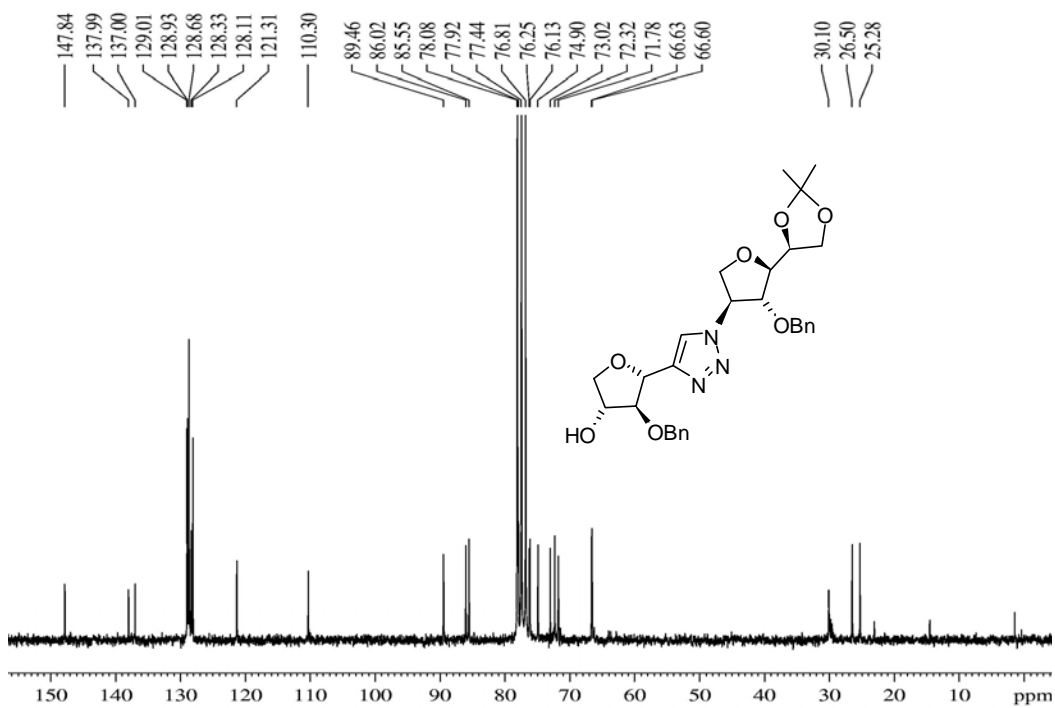
¹H NMR spectrum of compound **23**



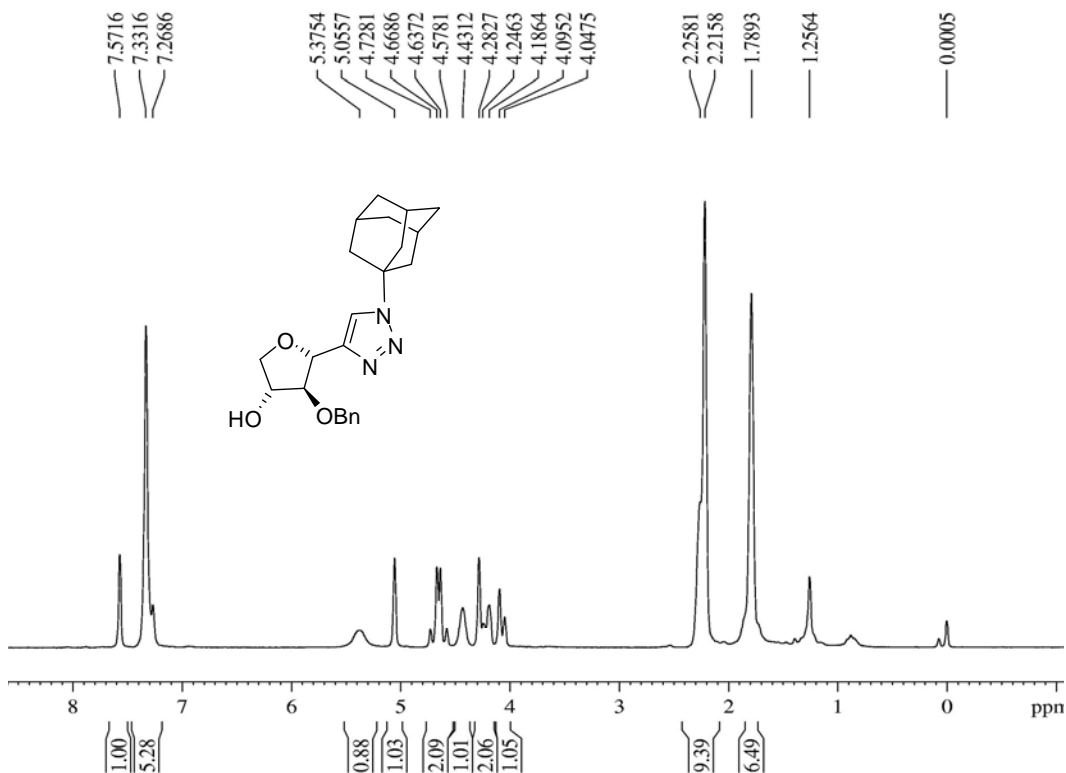
¹³C NMR spectrum of compound **23**

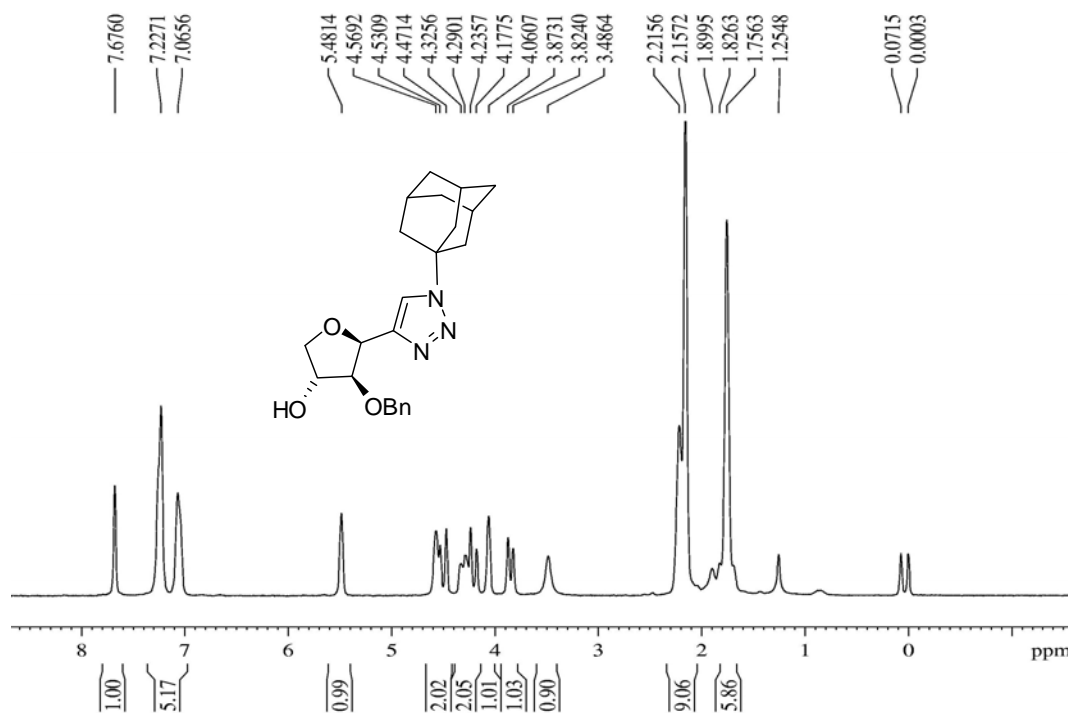


¹H NMR spectrum of compound **24**



¹³C NMR spectrum of compound **24**





Experimental Section – Biology

***In vitro* anti-bacterial and anti-fungal activity evaluation**

All the prepared tetrahydrofuranyl 1,2,3-triazolyl C-nucleoside analogues were evaluated for their *in vitro* antifungal activity against *Candida albicans*, *Cryptococcus neoformans*, *Sporothrix schenckii*, *Trichophyton mentagrophytes*, *Aspergillus fumigatus* and *Candida parapsilosis* (ATCC 22019) and antibacterial activity against *Escherichia coli*, *Pseudomonas aeruginosa* (ATCC BAA-427), *Staphylococcus aerus* (ATCC 25923) and *Klebsiella pneumoniae* (ATCC 27736). In this process, minimum inhibitory concentration of compounds was tested according to standard microbroth dilution technique as per NCCLS guidelines.²³ Briefly, testing was performed in flat bottom 96 well tissue culture plates (CELLSTAR® Greiner bio-one GmbH, Germany) in RPMI 1640 medium buffered with MOPS (3-[N-morpholino]propanesulfonic acid) (Sigma chem. Co., MO, USA) for fungal strains and in Muller Hinton broth (Titan Biotech Ltd, India) for bacterial strains. The concentration range of test compounds was 50-0.36 and 32-0.0018 µg/mL for standard compounds. Initial inocula of fungal and bacterial strain were maintained at $1-5 \times 10^3$ cells/mL. These plates were incubated in a moist chamber at 35 °C and absorbance at 492 nm was recorded on VersaMax microplate reader (Molecular devices, Sunnyvale, USA) after 48 h for *C. albicans* and *C. parapsilosis*, 72 h for *A. fumigatus*, *S. schenckii*, and *C. neoformans* and 96 h for *T. mentagrophytes* while bacterial strains were incubated for 24 h. MIC was determined as 90% inhibition of growth with respect to the growth control was observed by using SOFTmax Pro 4.3 Software (Molecular Devices, Sunnyvale, USA).

Table S1. *In vitro* anti-bacterial activity of 1,2,3-triazolyl C-nucleosides

Compound	Minimum inhibitory conc (MIC) in µg/ml			
	<i>Ec</i> ^a	<i>Pa</i>	<i>Sa</i>	<i>Kp</i>
14	>50	>50	>50	>50
15	>50	>50	>50	>50
16	>50	>50	>50	>50
18	>50	>50	>50	>50
19	>50	>50	>50	>50
20	>50	>50	>50	>50
22	>50	>50	>50	>50
23	>50	>50	>50	>50
24	>50	>50	>50	>50
25	>50	>50	1.56	0.78
27	>50	>50	0.78	0.78
28	>50	>50	>50	>50
29	>50	>50	>50	>50
Gentamycin	0.18	25	6.25	0.78
Ampicillin	12.5	>50	12.5	>50
Vancomycin	50	>50	0.045	>50
Ciprofloxacin	0.0112	0.09	0.78	0.045

^aEscherichia coli (Ec), Pseudomonas aeruginosa (Pa), Staphylococcus aureus (Sa), Klebsiella pneumoniae (Kp)

Table S2. *In vitro* anti-fungal activity of 1,2,3-triazolyl C-nucleosides

Compound	Minimum inhibitory concentration (MIC) in µg/ml					
	<i>Ca</i> ^a	<i>Cn</i>	<i>Ss</i>	<i>Tm</i>	<i>Af</i>	<i>Cp</i>
14	>50	>50	>50	>50	>50	>50
15	50	50	>50	>50	>50	>50
16	50	50	>50	25	>50	>50
18	>50	>50	>50	12.5	>50	>50
19	>50	>50	>50	25	>50	>50
20	>50	>50	>50	25	>50	>50
22	>50	>50	>50	>50	>50	>50
23	>50	>50	>50	>50	>50	>50
24	>50	>50	>50	>50	>50	>50
25	>50	>50	>50	>50	>50	>50
27	>50	>50	>50	>50	>50	>50
28	>50	>50	>50	>50	>50	>50
29	>50	>50	>50	>50	>50	>50
Amphotericin B	0.016	0.062	0.062	0.062	0.125	0.031
Fluconazole	1	2	4	16	>32	0.5

^a*Candida albicans* (Ca), *Cryptococcus neoformans* (Cn), *Sporothrix schenckii* (Ss), *Trichophyton mentagrophytes* (Tm), *Aspergillus fumigatus* (Af)