

Coordination Pattern, Solution Structure and DNA Damage Studies of the Copper(II) Complex with the Unusual Aminoglycoside Antibiotic Hygromycin B

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Supplementary data

10 **Table S1** – ¹H-NMR parameters for HyB 1.5 mM, in the presence of Cu(II) in a 50:1 ratio, in deuterated 20 mM MES buffer at pH 8.8, ionic strength 0.1M (NaCl) and T 298K. * Fitting not good

Ring	Proton	δ (ppm)	$R_{\text{free}} (\text{s}^{-1})$	$R_{\text{obs}} (\text{s}^{-1})$	$R_{\text{ip}} (\text{s}^{-1})$
Ring I	H1	2.88	2.618	7.407	4.789
	H2ax	1.36	1.282	2.045	0.763
	H2eq	2.29	1.228	5.000	3.772
	H3	2.95	0.964	5.076	4.112
	H4	3.60	1.353	2.890	1.537
	H5	3.71	1.976	3.154	1.178
	H6	3.39	1.159	3.154	1.995
	CH ₃	2.59	1.122*	1.639*	0.517*
Ring II	H1'	5.26	1.550	3.125	1.575
	H2'	4.63	---	---	---
	H3'	4.73	---	---	---
	H4'	3.98	0.992	1.227	0.235
	H5'	3.59	1.089	1.553	0.464
	H6'a	3.91	1.153	2.512	1.359
	H6'b	3.78	1.200	2.584	1.384
Ring III	H2''	4.15	0.315	1.009	0.694
	H3''	3.95	0.750	1.927	1.177
	H4''	4.10	0.460	1.098	0.638
	H5''	4.05	1.157	2.451	1.294
	H6''	3.87	1.504	2.037	0.533
	H7''a	3.90	1.658	2.008	0.350
	H7''b	3.80	1.172	1.675	0.503