

Supporting Information

Selective Formation of Intermolecular Hydrogen-bonding Palladium(II) Complexes with Nucleosides Using Unsymmetrical Tridentate Ligands

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1. X-Ray crystallography

Table S1. Hydrogen-bond distances and angles.

	D–H···A			D–H / Å	H···A / Å	D···A / Å	D–H···A / °
1	N2	H2A	O2 ⁱ	0.91	1.95	2.8609(18)	177.1
	O3	H3A	O1	0.975(19)	1.82(2)	2.785(2)	169(4)
1'	N2	H2A	O2 ⁱⁱ	0.91	2.07	2.969(3)	171.9
	N2	H2B	O2 ⁱⁱⁱ	0.91	2.06	2.904(3)	153.3
2	O1	H1	O2	0.84	1.87	2.608(6)	146.7
	N2	H2A	O3 ^{iv}	0.91	2.24	3.078(7)	153.1
	O3	H3A	O4	0.84	1.86	2.595(6)	146.0
	N5	H5A	O1	0.91	2.18	2.974(5)	145.3

Symmetry code: (i = '–x+1, y–1/2, –z+3/2', ii = 'x, –y+1/2, z+1/2', iii = '–x+1, y+1/2, –z+1/2', iv = x–1, y–1, z+1).

2. ^1H NMR Spectroscopy

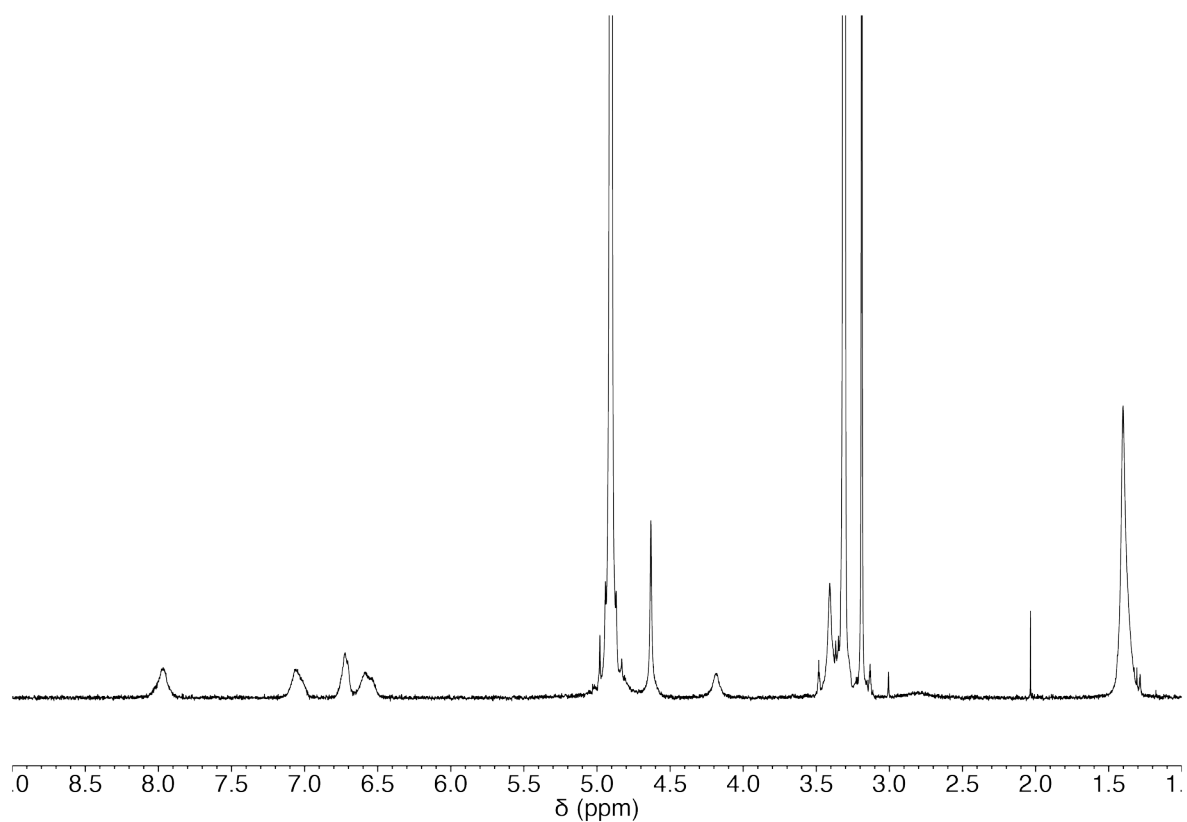


Figure S1. ^1H NMR spectra of (a) reaction mixture of **1** in CD_3OD .

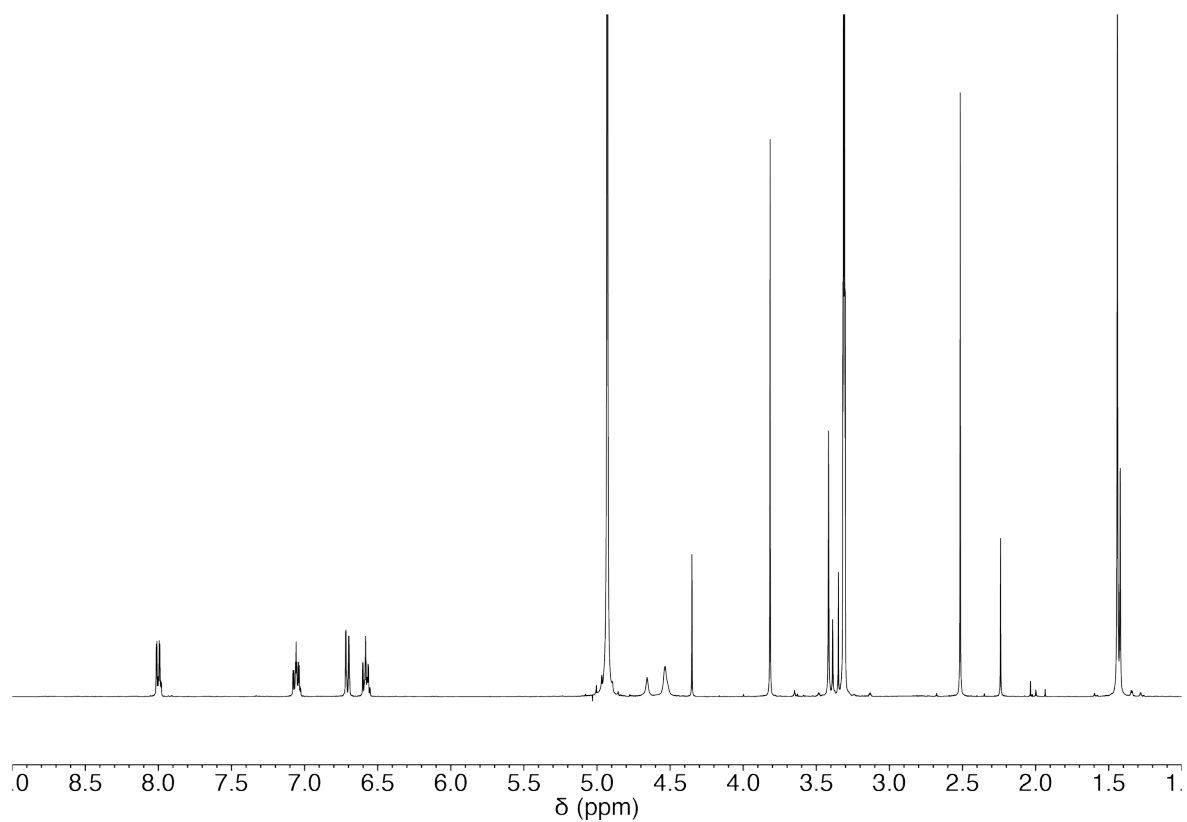


Figure S2. ^1H NMR spectra of (a) reaction mixture of **1'** in CD_3OD .

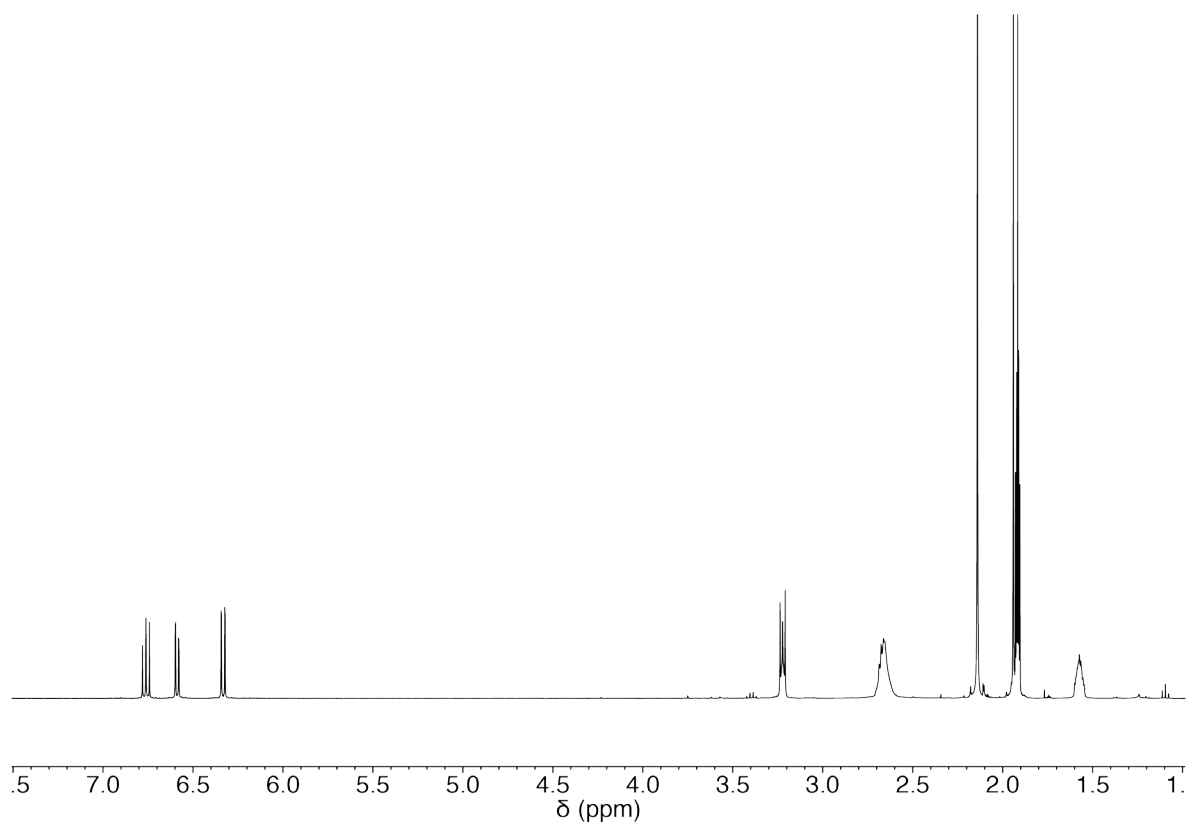


Figure S3. ^1H NMR spectra of (a) reaction mixture of **2** in CD_3CN .

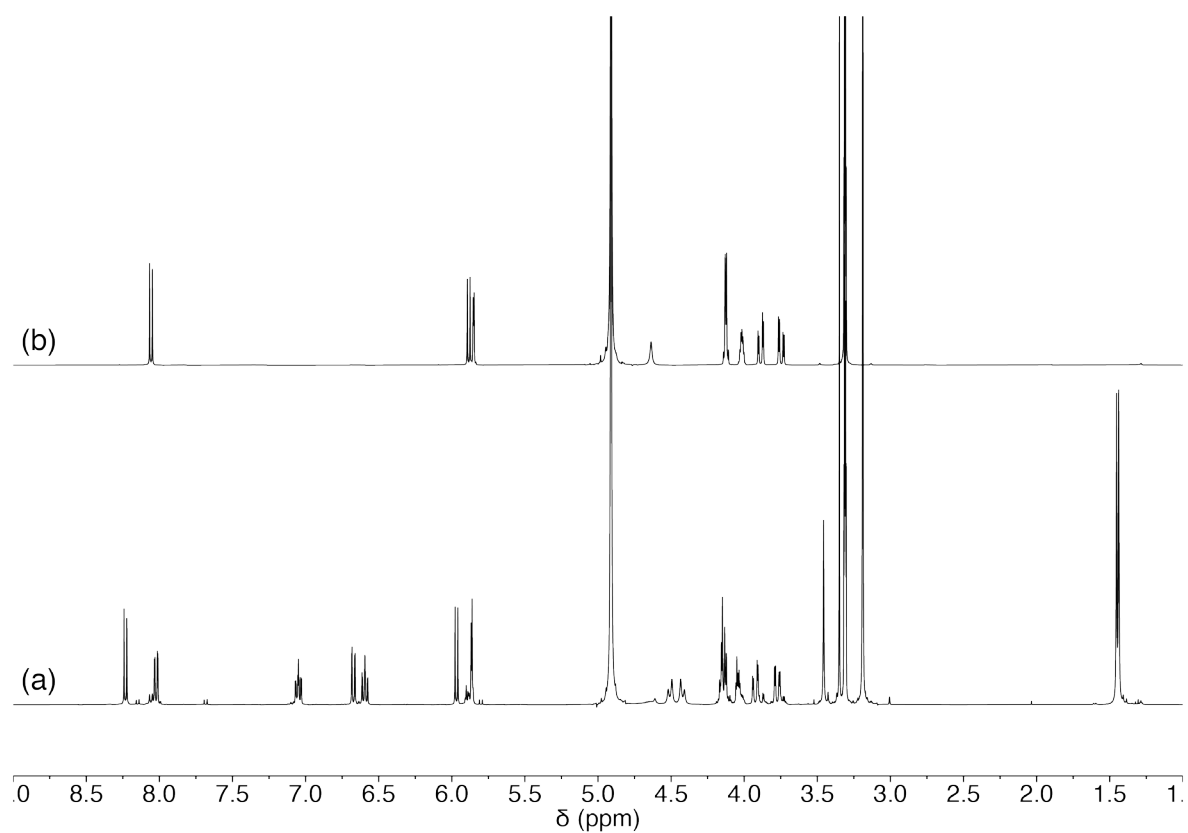


Figure S4. ^1H NMR spectra of (a) reaction mixture of **1** and cytidine, and (b) cytidine in CD_3OD .

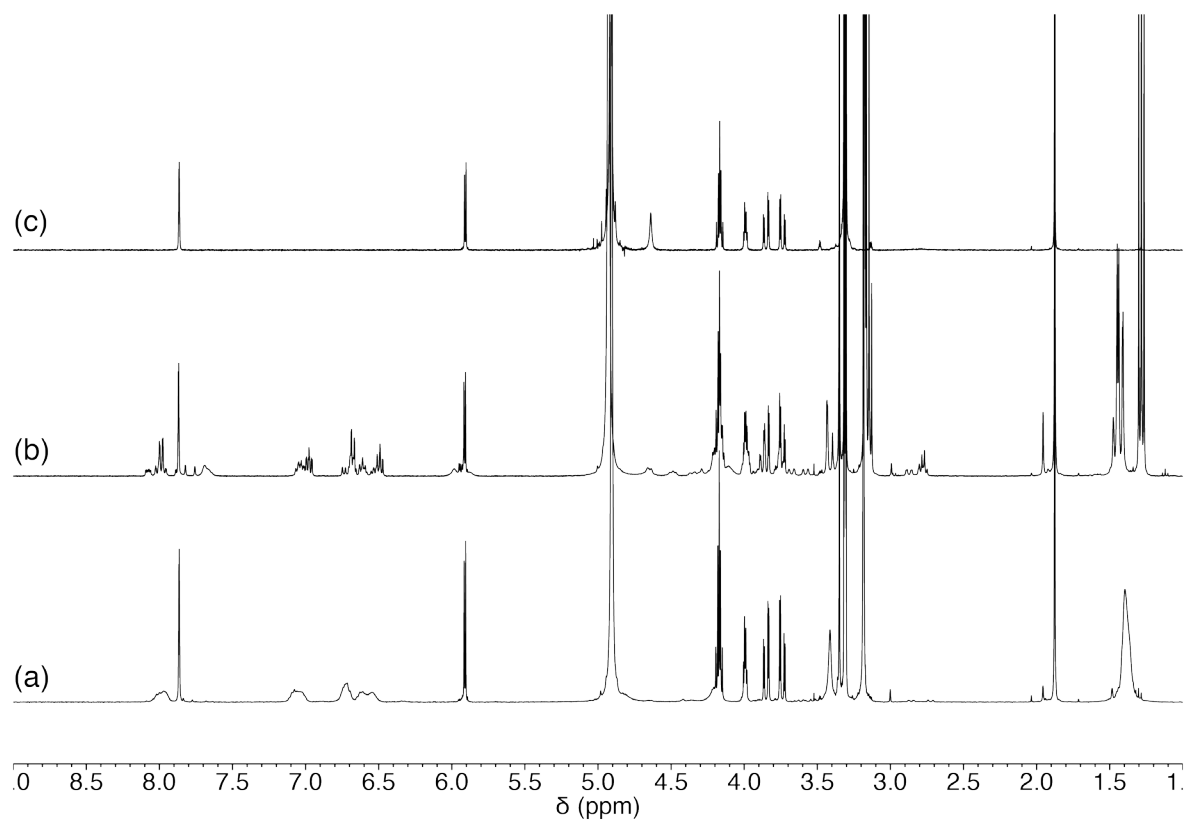


Figure S5. ^1H NMR spectra of (a) reaction mixture of **1** and 5-methyluridine, (b) **1**, 5-methyluridine and triethylamine, and (c) 5-methyluridine in CD_3OD .

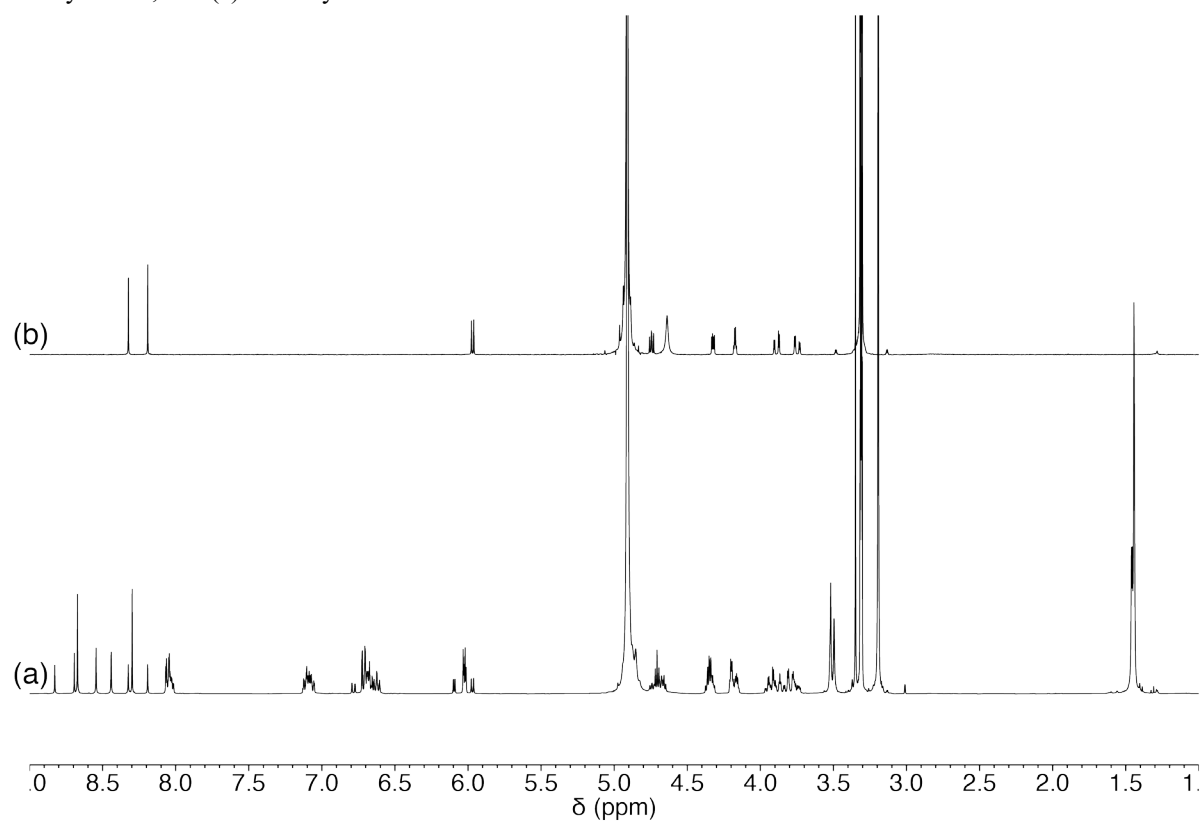


Figure S6. ^1H NMR spectra of (a) reaction mixture of **1** and adenosine, (b) adenosine in CD_3OD .

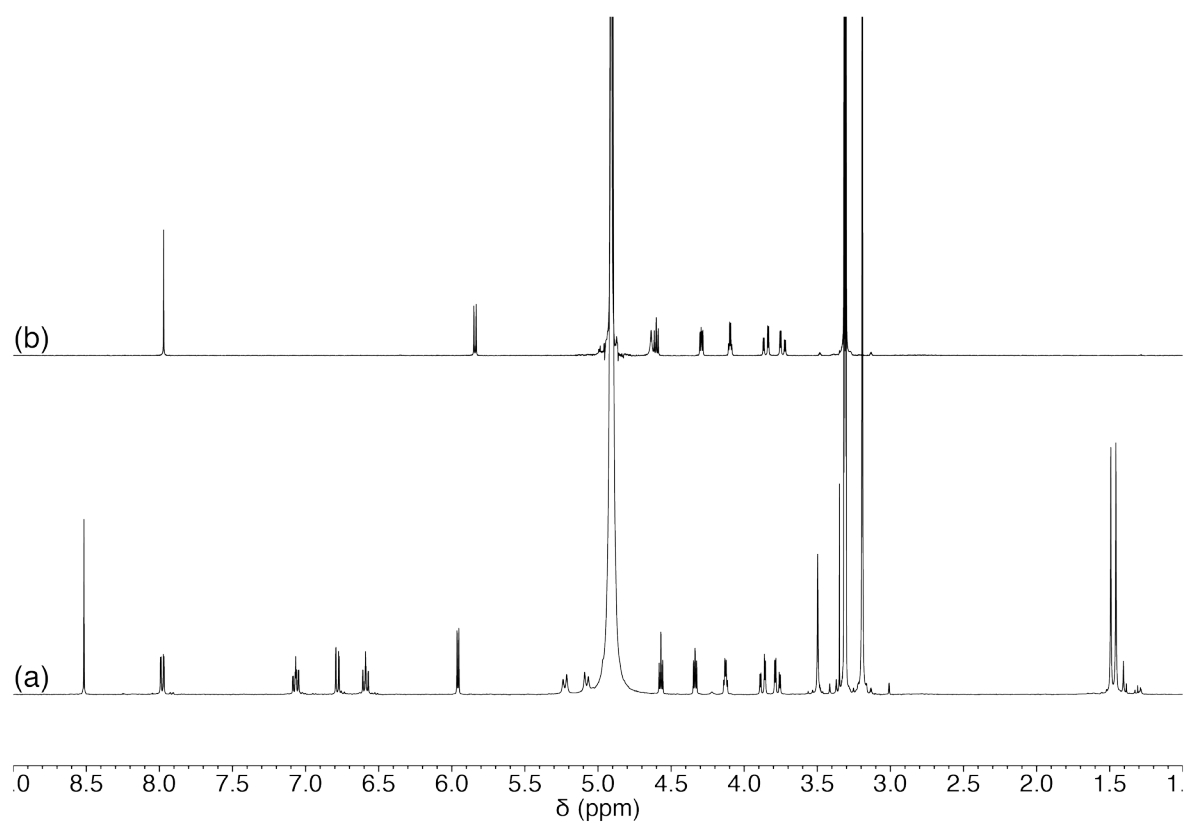


Figure S7. ^1H NMR spectra of (a) reaction mixture of **1** and guanosine, (b) guanosine in CD_3OD .