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Figure S1 Mechanism of binding of the azole bridged diplatinum drugs to guanine bases. The mechanism is shown for **5** and the corresponding compounds of **4** are indicated in parenthesis. These complexes are equivalent to the ones depicted in this picture, with N3 replaced by a C3-H group.

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Table S1: Dihedral angles around amide link taken from classical simulation: χ_1 = C7-C8-N12-C14, χ_2 = C8-N12-C14-O14, χ_3 = N12-C14-C15-C18-C19.

	DSA NMR Covalent	DSI NMR Covalent	DSA-DNA		DSI-DNA		NBOC- DSA-DNA
			Covalent	Non- covalent	Covalent	Non- covalent	Non- covalent
χ1	22.4	14.2	14.8	20.9	15.3	20.2	11.7
χ ₂	11.0	13.5	13.4	14.4	20.5	16.9	-2.3
χ3	11.4	9.7	8.4	9.0	4.7	6.6	-