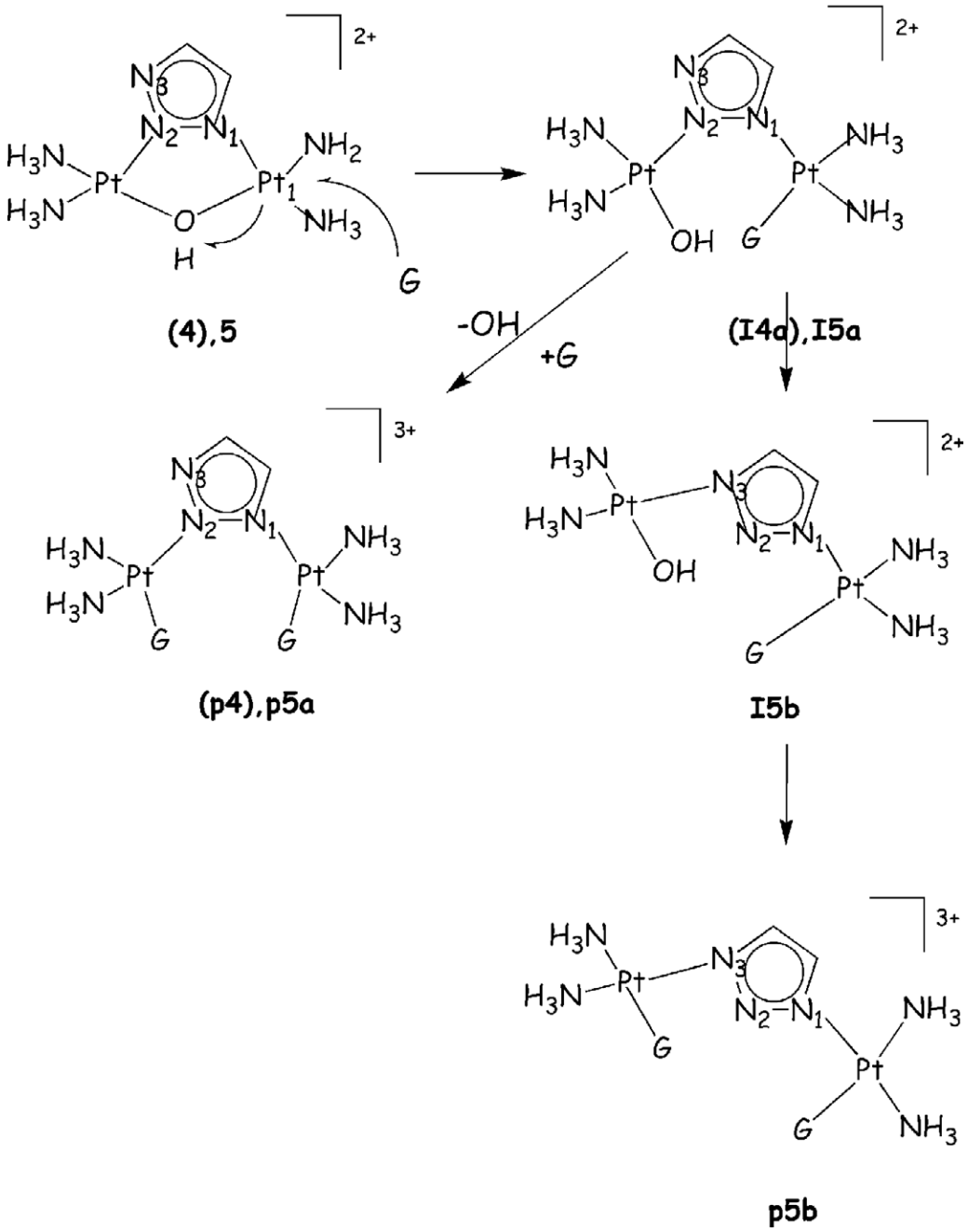

Figure S1 Mechanism of binding of the azole bridged diplatinum drugs to guanine bases. The mechanism is shown for **5** and the corresponding compounds of **4** are indicated in parenthesis. These complexes are equivalent to the ones depicted in this picture, with N3 replaced by a C3-H group.

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	***DSI NMR***	***DSA-DNA***		***DSI-DNA***		***NBOC-DSA-DNA***
	Covalent	Covalent	Covalent	Non-covalent	Covalent	Non-covalent	Non-covalent
χ_1	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
χ_3	11.4	9.7	8.4	9.0	4.7	6.6	-