Electronic Supplementary Material (ESI) for RSC Advances

Supporting Info for

QM/MM description of platinum-DNA interactions: Comparison of binding and DNA distortion of five drugs

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Table S1: Comparison of QM/MM and crystal structure of cisplatin-d(GpG) [i]

	QM/MM	**crystal (sd)**
Pt-NH_3	2.031, 2033	2.052 (0.040)
Pt-N7	2.027, 2.024	1.992 (0.059)
N7A-Pt-N7B	90.85	88.3 (2.2)
N1-Pt-N2	92.78	91.7 (1.01)
guan/guan	86.54	81.2 (4.3)

Table S2: Selected geometrical data of platinum complexes (Å and º).[a]

	Pt-N1	Pt-N2	Pt-$N7_A$	Pt-$N7_B$	N1-Pt-N2	$N7_A$-Pt-$N7_B$
1	2.045	2.035	2.016	2.019	94.2	84.9
	2.016	2.035	2.000	2.025	89.5	88.0
2	2.035	2.025	2.023	2.026	83.4	84.2
	2.022	2.030	1.990	2.026	82.8	85.9
3	2.048	2.046	2.022	2.030	94.3	84.7
	2.050	2.054	2.006	2.039	101.3	85.1
4 RRS	2.042	2.046	2.021	2.036	97.9	84.4
	2.037	2.046	1.997	2.045	90.5	85.4
SSS	2.043	2.045	2.021	2.023	95.3	85.3
	2.046	2.054	2.005	2.038	101.5	85.0

[a] N1 and N2 refer to the carrier ligand, N7 to DNA; first line dimer, second line octamer.

[i] J.D. Orbell, L.G. Marzilli, T.J. Kistenmacher, J. Am. Chem. Soc. 103 (1981) 5126–5133.

Table 3: Base-pair geometries for platinated GC pairs (Å and °) [a]

	Shear	Stretch	Stagger	Buckle	Propeller	Opening
1	-0.58	-0.28	0.17	16.3	-20.7	1.3
	-0.41	-0.21	-0.05	0.1	0.3	0.5
2	-0.59	-0.27	0.22	19.6	-19.5	0.8
	-0.45	-0.22	-0.04	0.3	-1.0	0.8
3	-0.72	-0.30	0.23	19.6	-16.7	0.9
	-0.50	-0.25	-0.25	10.5	12.1	-0.4
4 RRS	-0.63	-0.26	0.22	20.5	-16.3	1.1
	-0.51	-0.24	-0.04	8.1	2.8	0.3
SSS	-0.61	-0.23	0.32	25.1	-17.1	1.0
	-0.51	-0.19	-0.05	9.8	6.9	1.6
GG/CC [a]	-0.28	-0.15	0.40	22.6	-1.6	-1.4
	-0.15	-0.18	-0.02	3.9	-11.1	-0.8

[a] Values reported for 5'G—3'C (first line), 3'G—5'C (second); [b] Obtained from optimisation of GC pair using the same methods.