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Supplementary Information

Investigation of the Interaction of 2-(2'-Hydroxyphenyl)-benzoxazoles and their Derivatives with B-DNA by Docking and Molecular Dynamics

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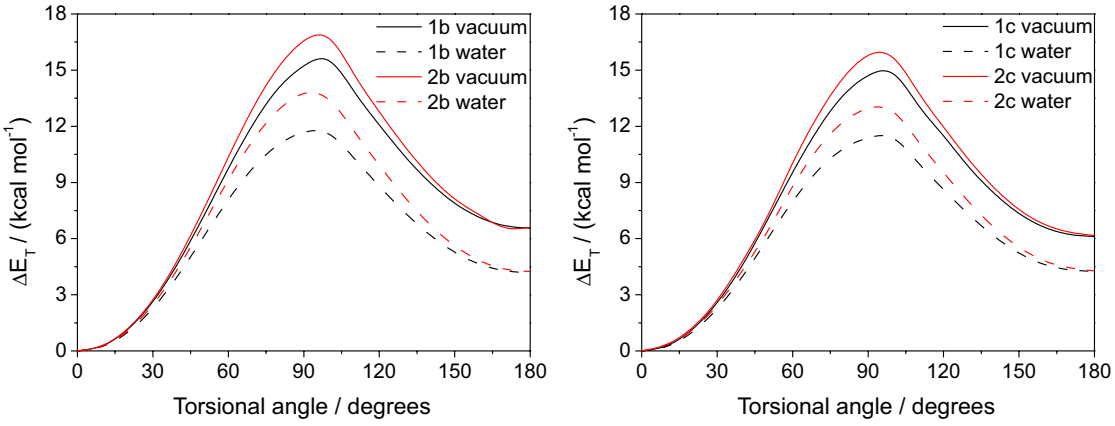

Figure S1. Relative energy (kcal mol^{-1}) × dihedral angle (degrees) obtained for the ligands 1b and 2b (left) and 1c and 2c (right) in vacuum and the aqueous medium (DFT/B3LYP with the basis set 6-31G (d)).

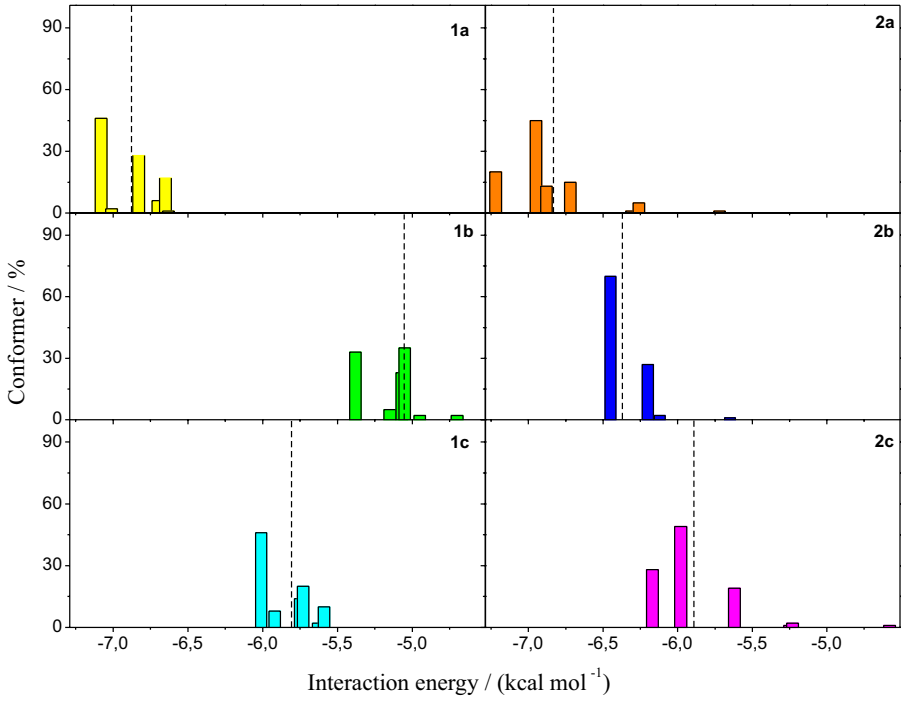

Figure S2. Interaction energy (Auto Dock) of the ligands with the B-DNA (X3DNA) and the average interaction energy (---).

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Table S1. Results of molecular docking calculations, analyzed by clusters as shown in Figure S2

Ligand	Interaction type	
	Interaction energy / (kcal mol^{-1})	(%)
1a	–7.08	Minor groove (46)
	–7.01	Minor groove (2)
	–6.83	Intercalation (28)
	–6.70	Intercalation (6)
	–6.65	Intercalation (17)
	–6.63	Intercalation (1)
2a	–7.22	Minor groove (20)
	–6.95	Intercalation (45)
	–6.88	Intercalation (13)
	–6.72	Minor groove (15)
	–6.31	Intercalation (1)
	–6.26	Intercalation (5)
	–5.72	Minor groove (1)
1b	–5.38	Minor groove (33)
	–5.15	Minor groove (5)
	–5.07	Intercalation (23)
	–5.05	Intercalation (35)
	–4.95	Intercalation (2)
	–4.70	Intercalation (2)
2b	–6.45	Intercalation (70)
	–6.20	Minor groove (27)
	–6.12	Intercalation (2)
	–5.65	Minor groove (1)
1c	–6.01	Minor groove (46)
	–5.92	Minor groove (8)
	–5.75	Intercalation (14)
	–5.73	Intercalation (20)
	–5.63	Intercalation (2)
	–5.59	Intercalation (10)
2c	–6.17	Intercalation (28)
	–5.98	Minor groove (49)
	–5.62	Intercalation (19)
	–5.25	Minor groove (1)
	–5.23	Intercalation (2)
	–4.58	Minor groove (1)

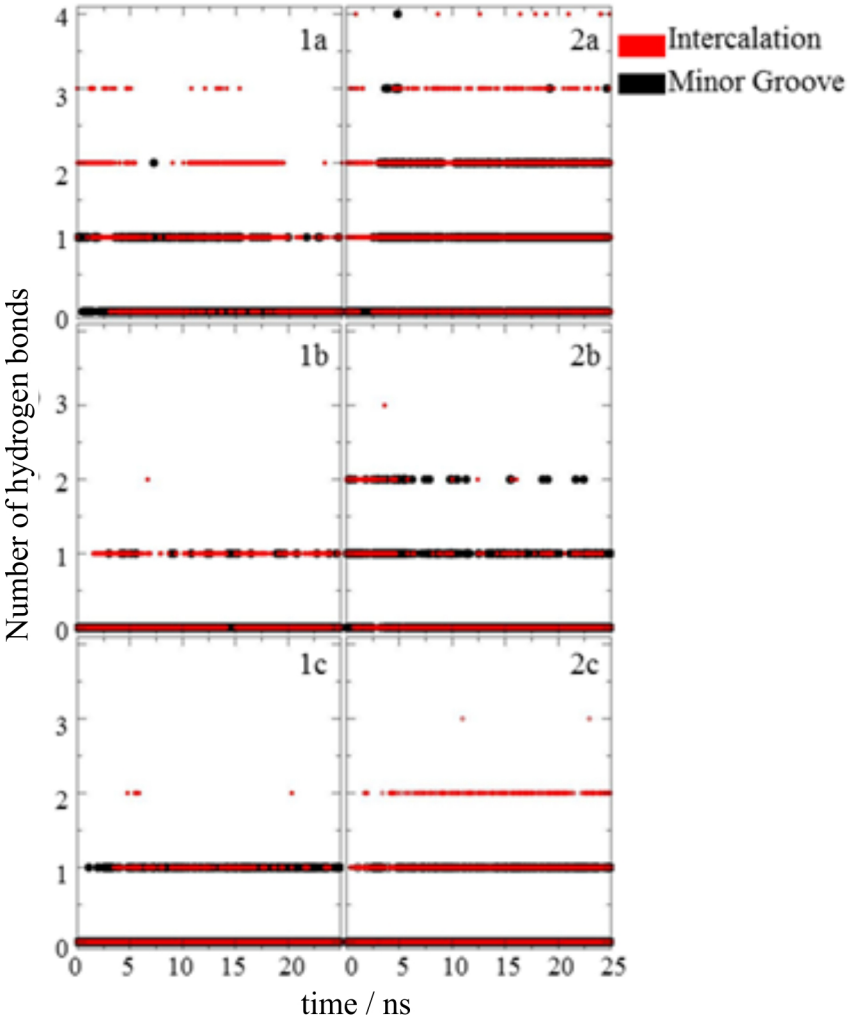

Figure S3. Number of hydrogen bonds of ligands with DNA throughout the simulation.

Table S2. Average values of the RMSD parameter for all base-pair steps (BPS). Results for the oligonucleotide without ligand (B-DNA), intercalation and minor groove binding mode complexes

System evaluated	RMSD
B-DNA	0.20 ± 0.04
1aI	0.39 ± 0.12
1aG	0.28 ± 0.04
2aI	0.37 ± 0.12
2aG	0.30 ± 0.03
1bI	0.36 ± 0.08
1bG	0.28 ± 0.03
2bI	0.29 ± 0.05
2bG	0.30 ± 0.04
1cI	0.35 ± 0.05
1cG	0.32 ± 0.04
2cI	0.37 ± 0.10
2cG	0.33 ± 0.04

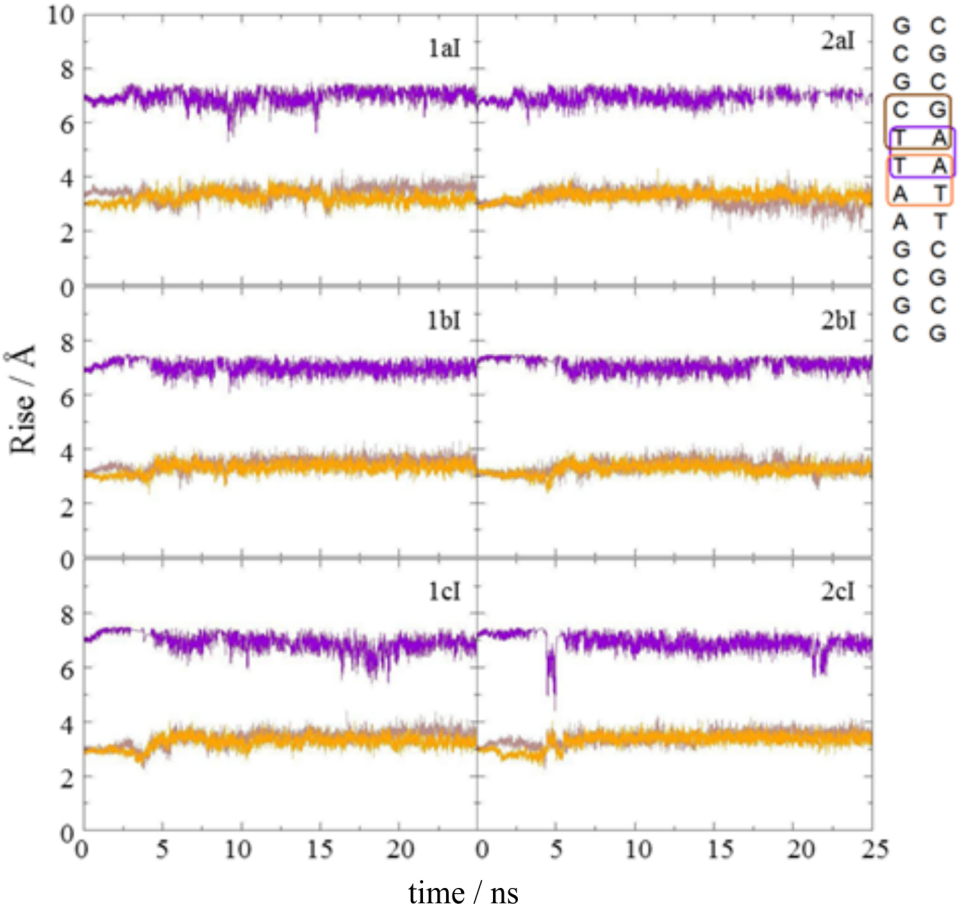

Figure S4. Rise parameter for some relevant base-pair steps for the intercalation binding mode complexes.

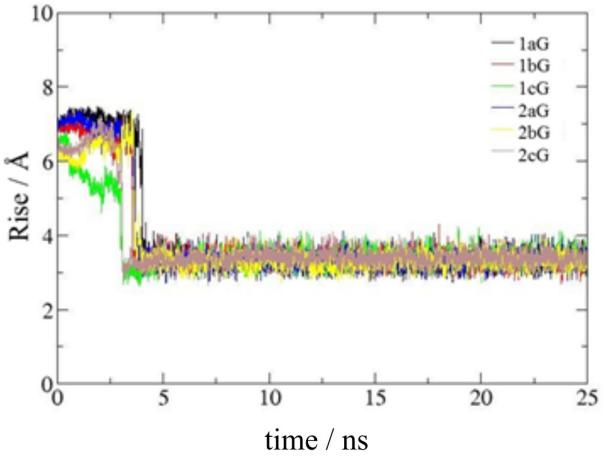

Figure S5. Rise parameter for the base-pair step AATT for the minor groove binding mode complexes.

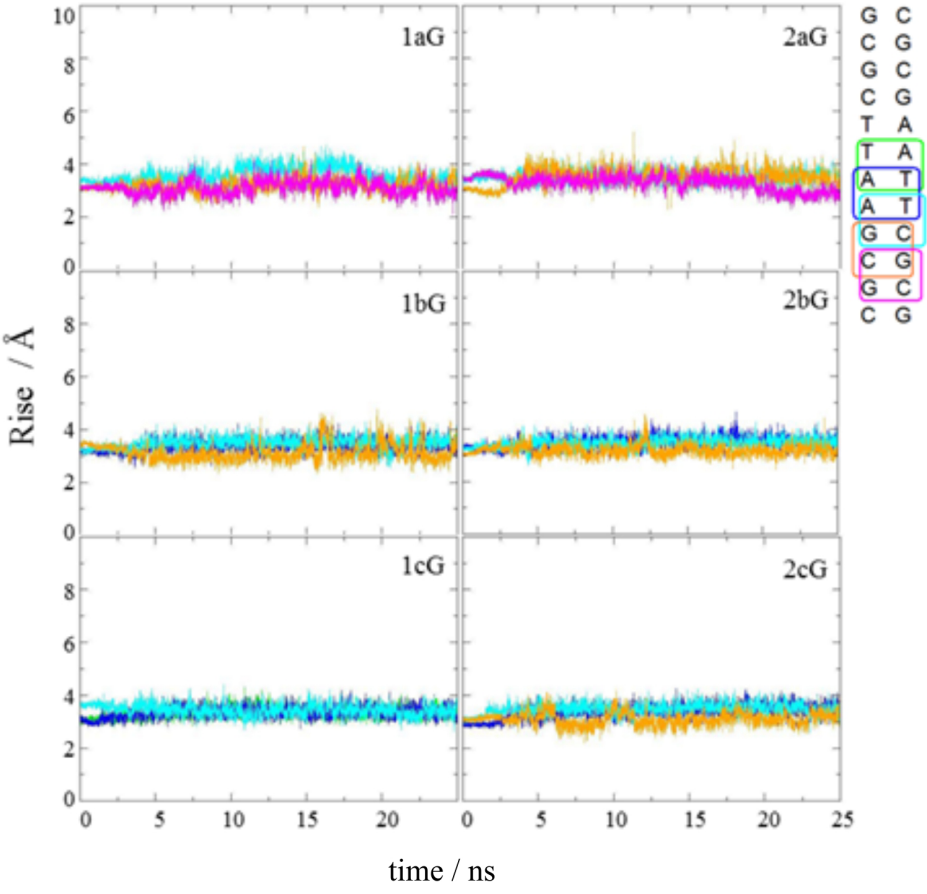

Figure S6. Rise parameter for some relevant base-pair steps for the minor groove binding mode complexes.

Table S3. Average values of the Rise parameter for all base-pair steps (BPS). Sequence-dependent experimental results are shown, along with the simulation results for the oligonucleotide without ligand (B-DNA) and minor groove binding mode complexes

BPS	Exp.[30]	B-DNA	**1aG**	**2aG**	**1bG**	**2bG**	**1cG**	**2cG**
CGCG1	3.36 ± 0.01	3.35 ± 0.41	3.36 ± 0.37	3.64 ± 0.43	3.67 ± 0.39	3.39 ± 0.37	3.40 ± 0.74	3.60 ± 0.41
GCGC1	3.38 ± 0.08	3.34 ± 0.24	3.39 ± 0.20	3.29 ± 0.24	3.47 ± 0.20	3.46 ± 0.18	3.40 ± 0.23	3.43 ± 0.21
CGCG2	3.26 ± 0.05	3.19 ± 0.33	3.11 ± 0.29	3.33 ± 0.54	3.10 ± 0.28	3.08 ± 0.28	3.16 ± 0.26	3.11 ± 0.33
GATC	3.30 ± 0.10	3.44 ± 0.21	3.45 ± 0.22	3.26 ± 0.25	3.44 ± 0.21	3.44 ± 0.21	3.44 ± 0.20	3.45 ± 0.21
AATT	3.27 ± 0.02	3.37 ± 0.20	3.34 ± 0.20	3.30 ± 0.19	3.34 ± 0.19	3.30 ± 0.19	3.30 ± 0.20	3.39 ± 0.19
ATAT	3.31 ± 0.03	3.37 ± 0.18	3.28 ± 0.20	3.28 ± 0.16	3.32 ± 0.18	3.36 ± 0.17	3.37 ± 0.19	3.20 ± 0.17
TTAA	3.29 ± 0.01	3.32 ± 0.21	3.37 ± 0.21	3.25 ± 0.18	3.46 ± 0.22	3.51 ± 0.21	3.40 ± 0.20	3.22 ± 0.18
TCGA	3.14 ± 0.02	3.36 ± 0.21	3.61 ± 0.31	3.51 ± 0.21	3.49 ± 0.20	3.48 ± 0.20	3.41 ± 0.22	3.57 ± 0.21
CGCG3	3.56 ± 0.07	3.24 ± 0.31	3.20 ± 0.27	3.61 ± 0.29	3.10 ± 0.30	3.18 ± 0.22	3.33 ± 0.26	3.62 ± 0.25
GCGC2	3.21 ± 0.18	3.45 ± 0.20	3.34 ± 0.24	3.24 ± 0.30	3.50 ± 0.19	3.38 ± 0.18	3.17 ± 0.25	3.24 ± 0.23
CGCG4	3.54 ± 0.19	3.47 ± 0.44	3.43 ± 0.40	2.73 ± 0.24	3.79 ± 0.37	3.38 ± 0.57	3.43 ± 0.35	3.40 ± 0.32

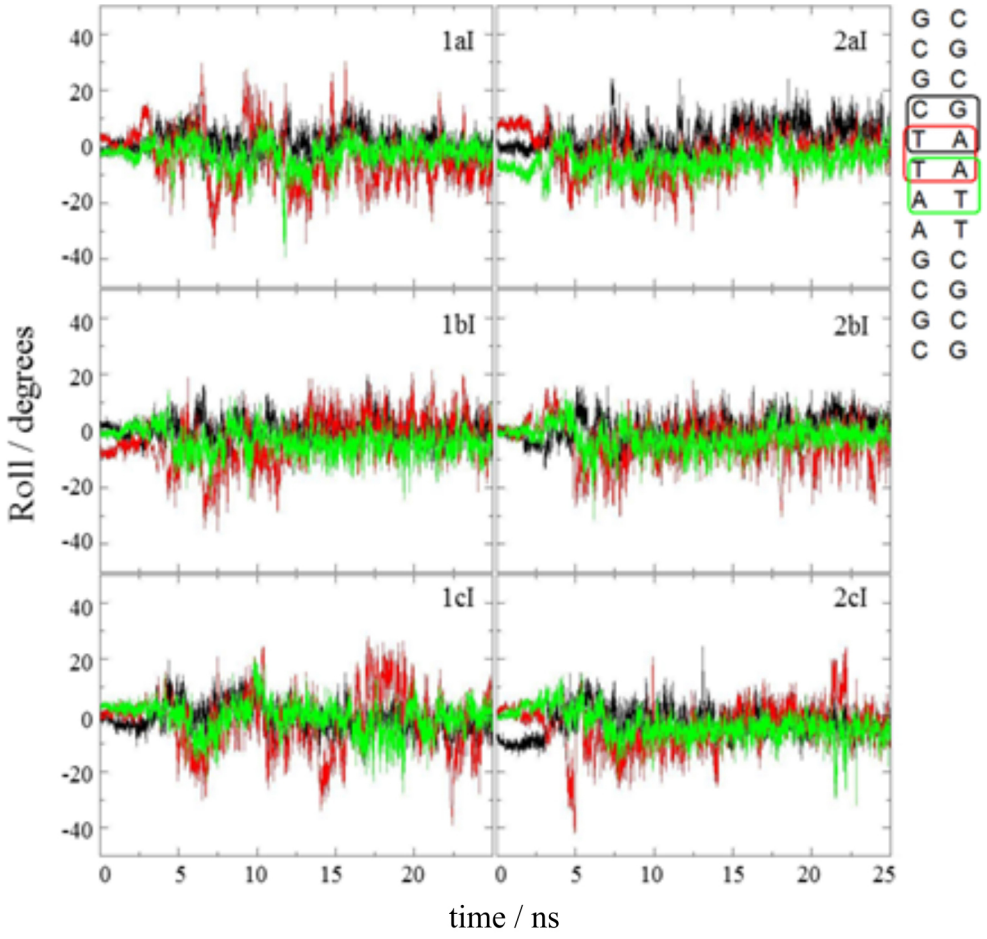

Figure S7. Roll parameter for some relevant base-pair steps for the intercalation binding mode complexes.

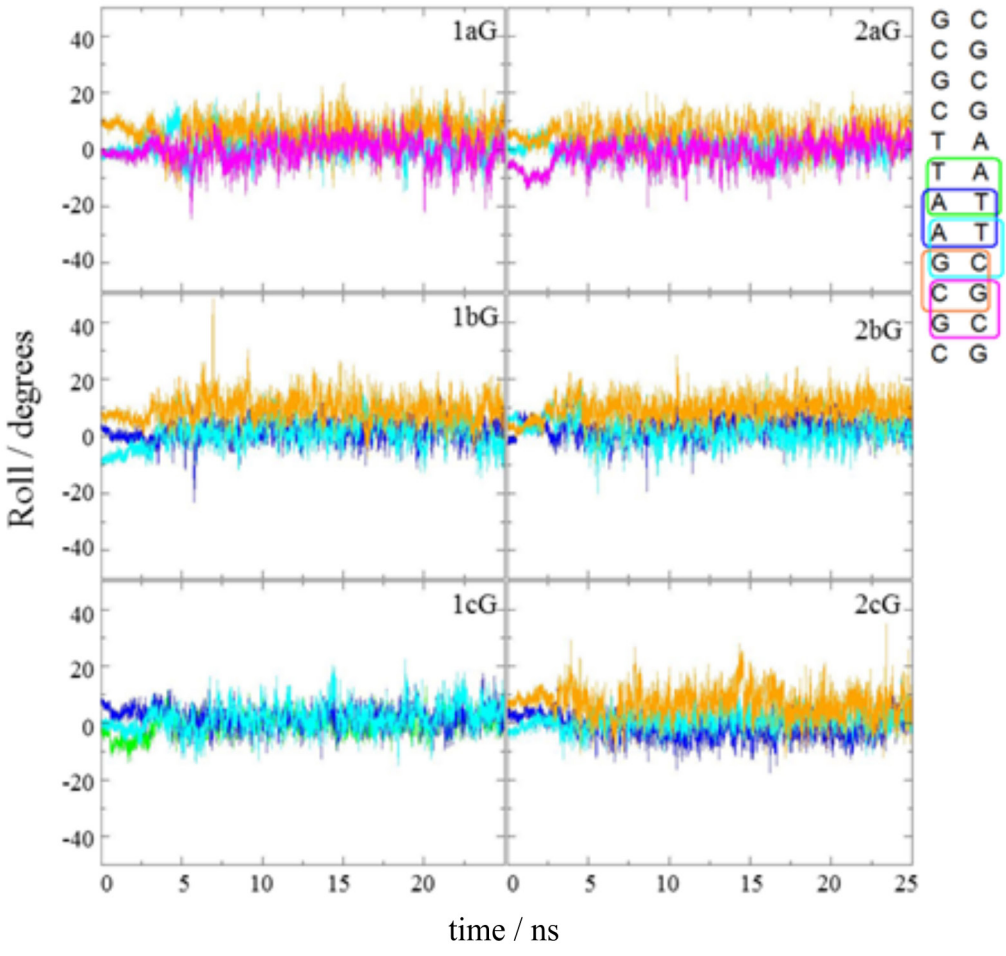

Figure S8. Roll parameter for some relevant base-pair steps for the minor groove binding mode complexes.

Table S4. Average values of the Roll parameter for all base-pair steps (BPS). Results for the oligonucleotide without ligand (B-DNA) and minor groove binding mode complexes

BPS	B-DNA	**1aG**	**2aG**	**1bG**	**2bG**	**1cG**	**2cG**
ATAT	–0.58 ± 3.31	–	–	–	–	0.21 ± 3.99	–
TTAA	2.51 ± 4.13	–	–	2.01 ± 3.59	2.83 ± 3.63	1.43 ± 3.63	1.53 ± 4.72
TCGA	1.74 ± 4.52	1.88 ± 4.54	0.52 ± 3.34	0.77 ± 4.29	1.08 ± 4.04	2.27 ± 4.86	1.28 ± 3.79
CGCG3	8.11 ± 5.04	6.53 ± 4.80	5.63 ± 5.06	9.75 ± 4.70	10.15 ± 4.06	–	7.48 ± 4.83
GCGC2	–1.93 ± 4.88	–0.32 ± 4.83	–0.49 ± 4.34	–	–	–	–