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* To whom correspondence should be addressed : l.ducasse@lpcm.u-bordeaux1.fr

Figures S1a-S1d : Dependence of the transfer integrals between first neighbour intrastrand nucleoside pairs on the RISE parameter
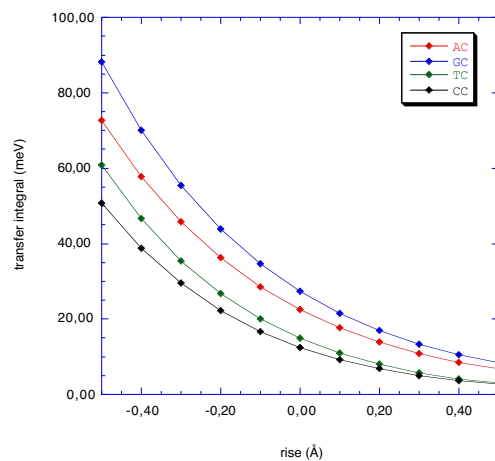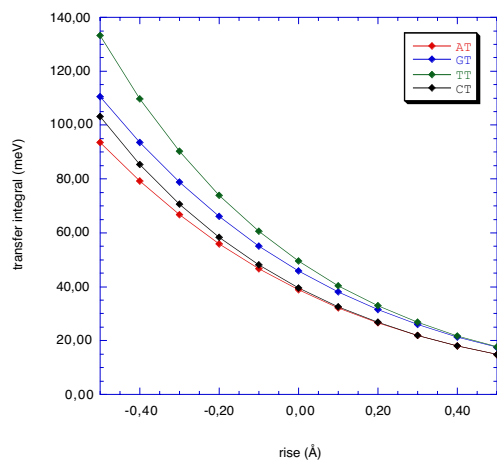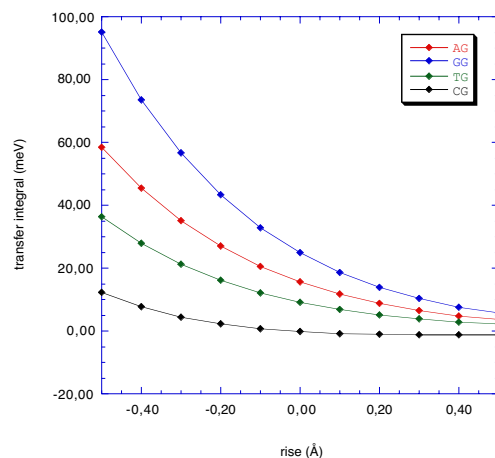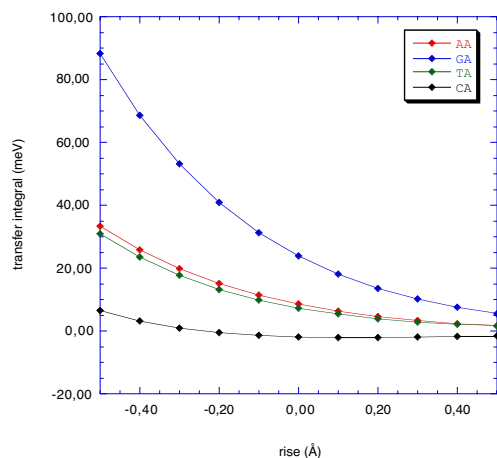
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Figures S2a-S2d : Dependence of the transfer integrals between first neighbour intrastrand nucleoside pairs on the SHIFT parameter
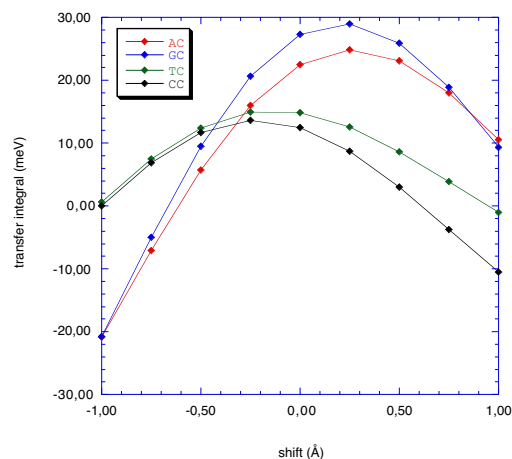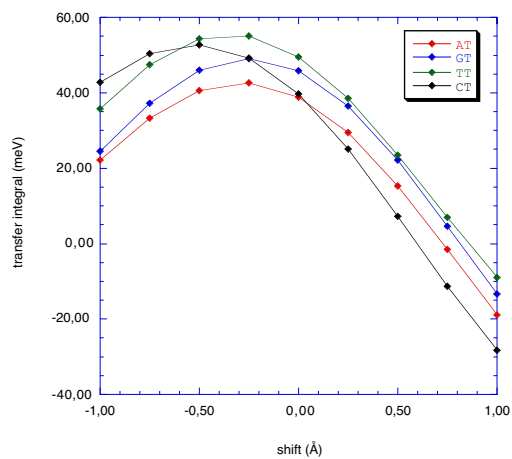
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Figures S3a-S3d : Dependence of the transfer integrals between first neighbour intrastrand nucleoside pairs on the SLIDE parameter
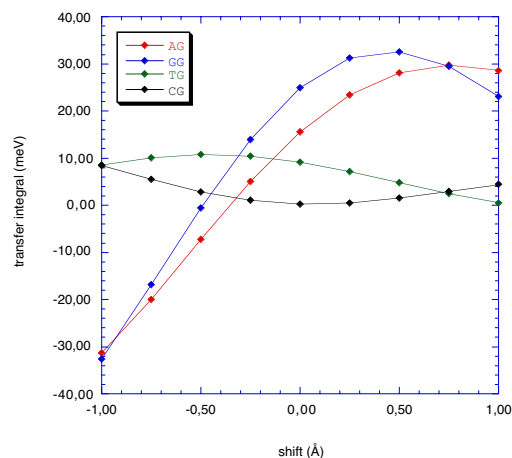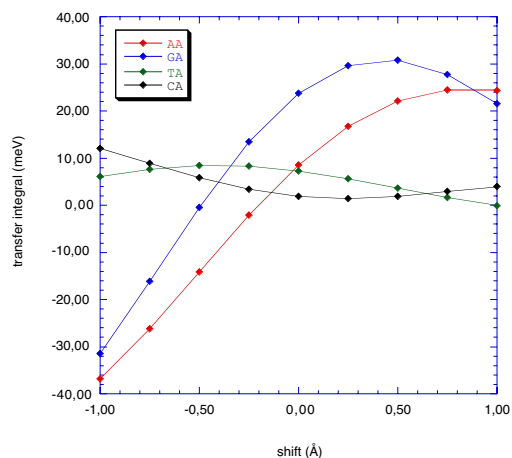
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Figures S4a-S4d : Dependence of the transfer integrals between first neighbour intrastrand nucleoside pairs on the TWIST parameter
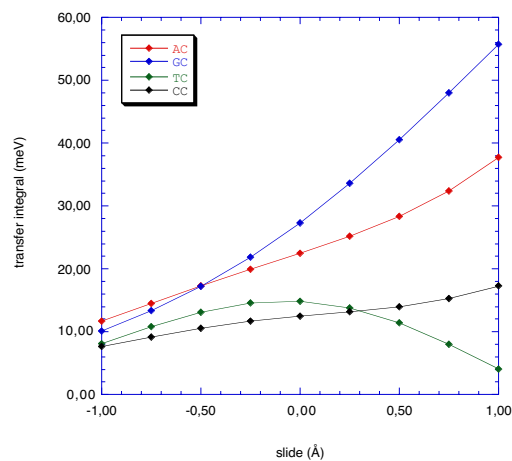
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Figures S5a-S5d : Dependence of the transfer integrals between first neighbour intrastrand nucleoside pairs on the ROLL parameter

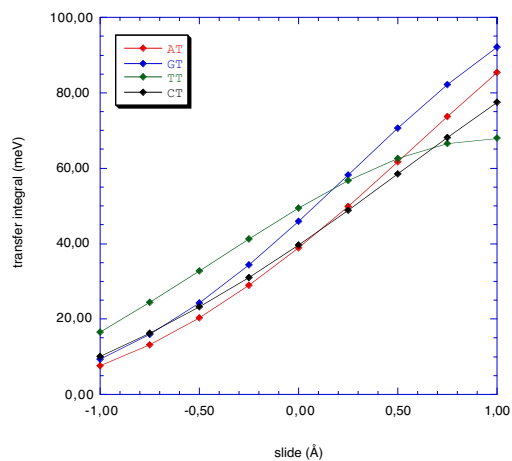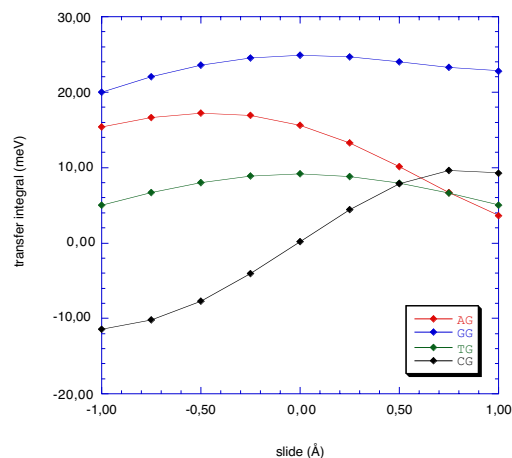ELECTRONIC SUPPLEMENTARY INFORMATION to :
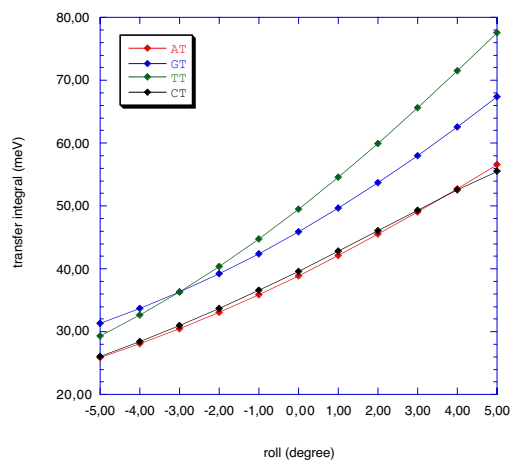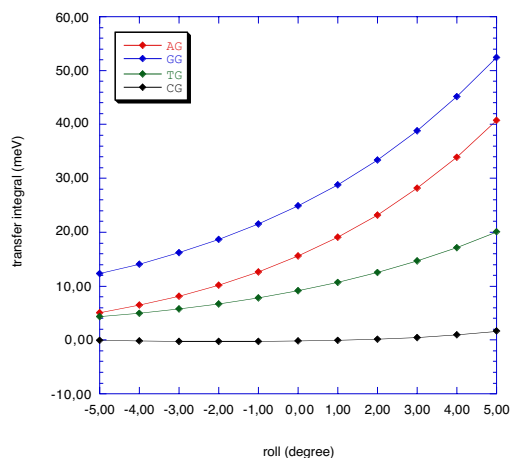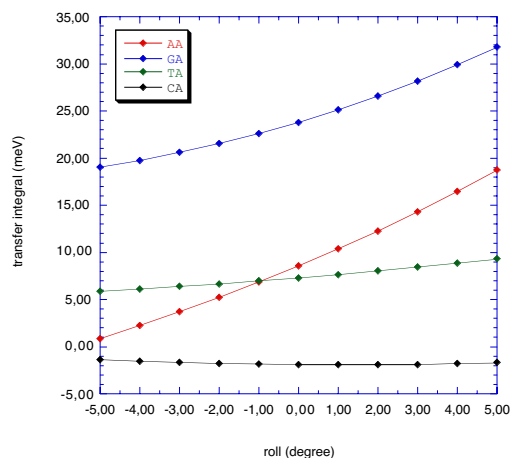
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Figures S6a-S6d : Dependence of the transfer integrals between first neighbour intrastrand nucleoside pairs on the TILT parameter
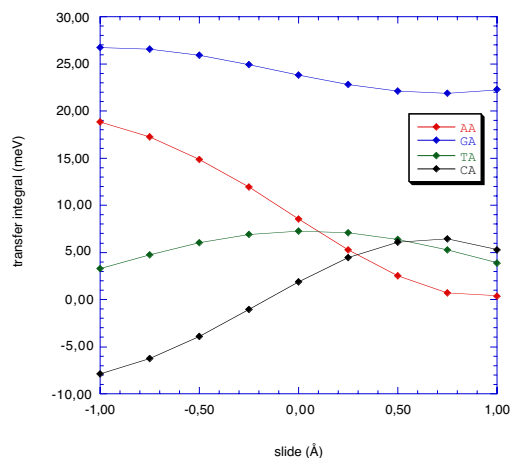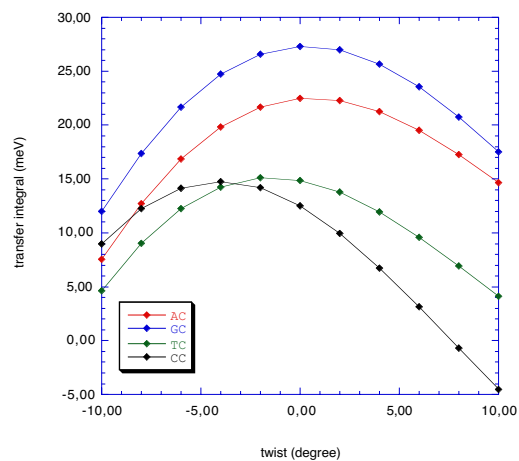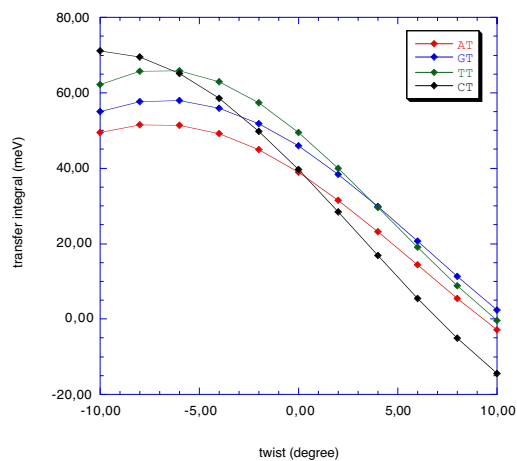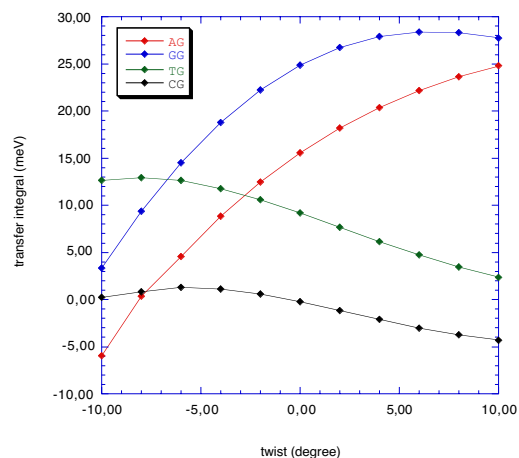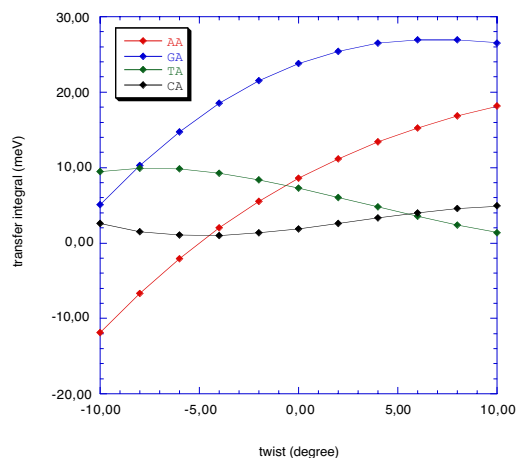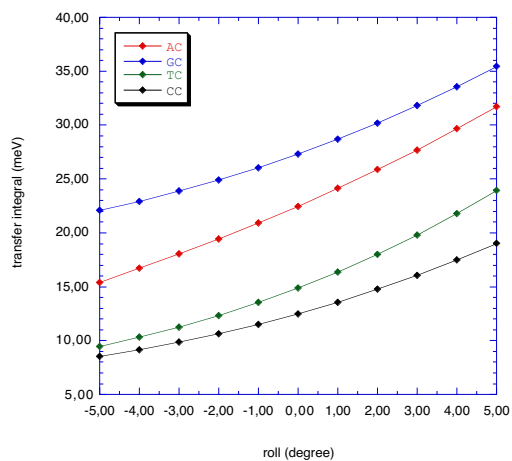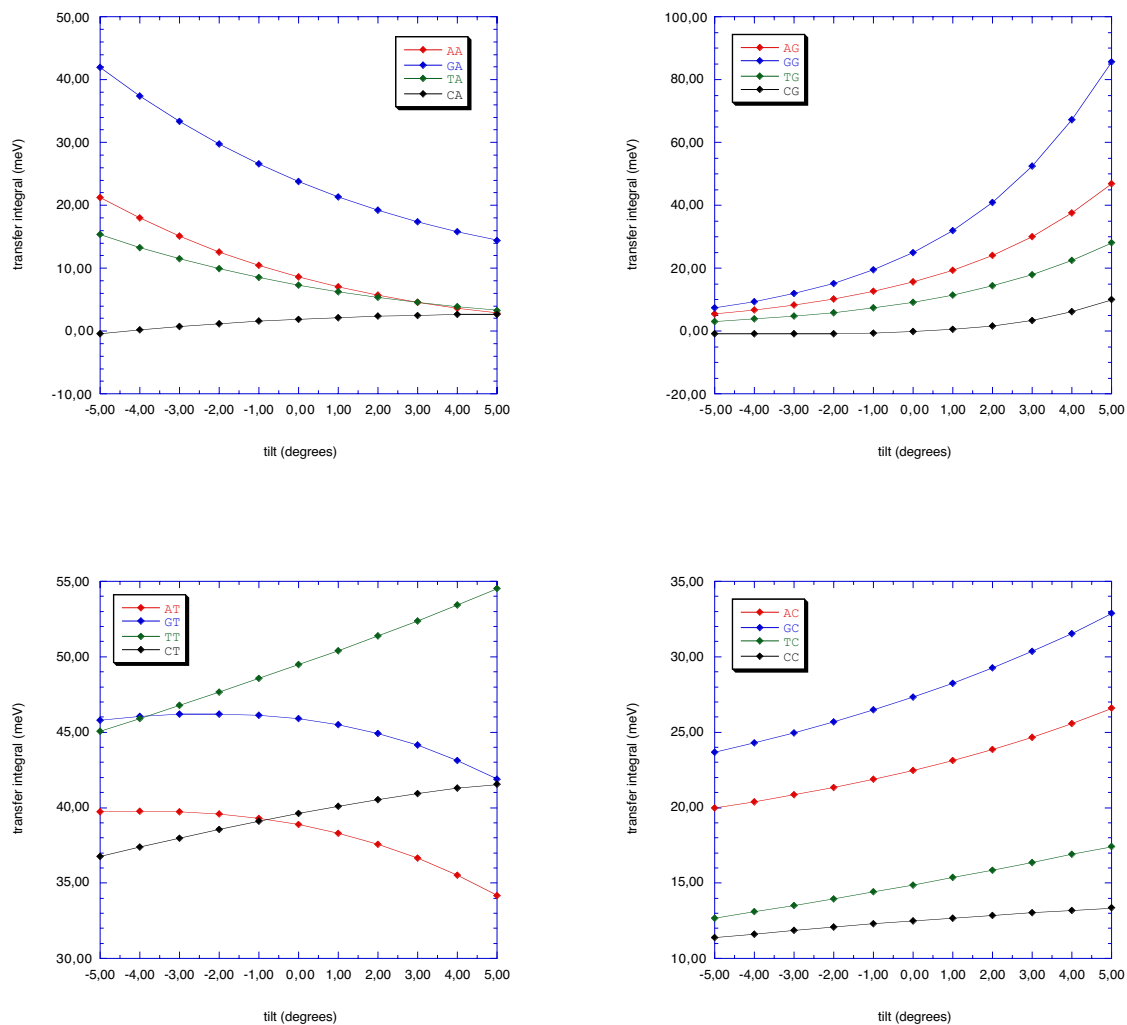
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Table S1 : Dependence of the Coulomb integrals (in eV) between first neighbour intrastrand nucleoside pairs on the translation parameters (Å).

XY	RISE		SLIDE		SHIFT	
	− 0.5	+ 0.5	− 1.0	+ 1.0	− 1.0	+ 1.0
AA	3.112	2.664	2.785	2.899	2.947	2.730
AC	3.040	2.627	2.639	2.955	2.892	2.692
AG	3.023	2.607	2.695	2.853	2.906	2.642
AT	3.028	2.623	2.614	2.972	2.827	2.739
CA	2.956	2.553	2.745	2.682	2.880	2.555
CC	3.074	2.637	2.733	2.875	2.971	2.660
CG	2.904	2.514	2.670	2.664	2.847	2.503
CT	3.155	2.694	2.763	2.982	2.976	2.779
GA	3.109	2.662	2.813	2.862	2.924	2.754
GC	3.107	2.670	2.700	2.987	2.928	2.764
GG	3.060	2.629	2.747	2.846	2.911	2.694
GT	3.089	2.661	2.666	3.003	2.862	2.799
TA	2.765	2.422	2.586	2.532	2.763	2.380
TC	2.880	2.501	2.588	2.704	2.845	2.475
TG	2.701	2.374	2.507	2.500	2.714	2.322
TT	3.004	2.587	2.653	2.842	2.898	2.613
Mean deviation	**7.7%**	**7.1%**	**3.7%**	**2.4%**	**3.4%**	**5.6%**

Table S2 : Dependence of the Coulomb integrals (in eV) between first neighbour intrastrand nucleoside pairs on the rotation parameters (degrees).

| XY	TWIST		ROLL		TILT	
	− 10.0	10.0	− 0.5	+ 0.5	− 0.5	+ 0.5
AA	2.926	2.817	2.840	2.913	2.943	2.812
AC	2.897	2.738	2.791	2.859	2.786	2.863
AG	2.868	2.734	2.699	2.918	2.618	3.014
AT	2.873	2.740	2.759	2.878	2.789	2.844
CA	2.811	2.666	2.710	2.779	2.818	2.675
CC	2.949	2.721	2.802	2.887	2.810	2.877
CG	2.785	2.602	2.593	2.811	2.537	2.880
CT	2.997	2.801	2.842	2.987	2.887	2.937
GA	2.909	2.828	2.842	2.905	2.945	2.805
GC	2.934	2.807	2.847	2.911	2.838	2.918
GG	2.887	2.770	2.728	2.943	2.642	3.048
GT	2.905	2.801	2.807	2.927	2.837	2.892
TA	2.668	2.498	2.555	2.616	2.648	2.528
TC	2.810	2.542	2.641	2.723	2.652	2.710
TG	2.631	2.425	2.439	2.625	2.394	2.680
TT	2.904	2.647	2.715	2.857	2.761	2.807
Mean deviation	**2.6%**	**3.3%**	**2.2%**	**2.15%**	**2.5%**	**3.0%**

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Table S3 : Dependence of the penetration integrals (in meV) between first neighbour intrastrand nucleoside pairs on the RISE parameter

XY	5'–XY–3'			3'–XY–5'		
	− 0.5	0.0	+ 0.5	− 0.5	0.0	+ 0.5
AA	134	125	112	92	79	66
AC	81	80	75	202	167	138
AG	256	224	195	9	8	5
AT	98	92	84	44	38	31
CA	108	98	86	72	60	48
CC	–1	10	14	185	155	128
CG	269	232	199	–4	–10	–14
CT	69	62	55	16	10	5
GA	159	143	127	84	75	63
GC	115	107	97	207	173	144
GG	261	227	196	–30	–24	–21
GT	108	99	89	36	31	25
TA	90	82	73	51	43	35
TC	–34	–20	–11	123	106	90
TG	274	236	203	8	3	–2
TT	79	69	59	–23	–20	–19

Table S4 : Dependence of the penetration integrals (in meV) between first neighbour intrastrand nucleoside pairs on the SHIFT parameter

XY	5'–XY–3'			3'–XY–5'		
	− 1.0	0.0	+ 1.0	− 1.0	0.0	+ 1.0
AA	156	125	94	64	79	92
AC	151	80	17	114	167	205
AG	192	224	243	47	8	–34
AT	99	92	88	12	38	60
CA	129	98	73	38	60	73
CC	75	10	–36	103	155	193
CG	229	232	226	9	–10	–35
CT	79	62	50	–24	10	39
GA	168	143	115	62	75	86
GC	167	107	50	124	173	208
GG	200	227	238	6	–24	–54
GT	109	99	88	2	31	59
TA	110	82	60	20	43	61
TC	33	–20	–54	53	106	156
TG	243	236	220	14	3	–17
TT	86	69	52	–51	–20	10

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Table S5 : Dependence of the penetration integrals (in meV) between first neighbour intrastrand nucleoside pairs on the SLIDE parameter

	5'–XY–3'			3'–XY–5'		
XY	– 0.5	0.0	+ 0.5	– 0.5	0.0	+ 0.5
AA	109	125	134	57	79	92
AC	80	80	76	153	167	165
AG	200	224	235	–13	8	28
AT	106	92	75	11	38	61
CA	93	98	90	20	60	91
CC	23	10	–7	109	155	185
CG	232	232	211	–42	–10	14
CT	86	62	30	–24	10	41
GA	121	143	157	51	75	91
GC	104	107	105	153	173	178
GG	198	227	240	–44	–24	–5
GT	113	99	85	9	31	49
TA	78	82	74	–7	43	83
TC	–6	–20	–36	58	106	143
TG	239	236	214	–47	3	44
TT	92	69	34	–62	–20	19

Table S6 : Dependence of the penetration integrals (in meV) between first neighbour intrastrand nucleoside pairs on the TWIST parameter

	5'–XY–3'			3'–XY–5'		
XY	– 10.0°	0.0	+ 10.0°	– 10.0°	0.0	+10.0°
AA	132	125	115	67	79	91
AC	100	80	62	140	167	191
AG	216	224	228	23	8	–7
AT	87	92	99	23	38	53
CA	110	98	86	44	60	70
CC	36	10	–9	117	155	183
CG	224	232	237	9	–10	–32
CT	55	62	72	–14	10	31
GA	149	143	134	64	75	87
GC	126	107	89	147	173	197
GG	210	227	237	–10	–24	–34
GT	92	99	108	14	31	51
TA	94	82	70	37	43	49
TC	–1	–20	–32	72	106	137
TG	231	236	238	30	3	–24
TT	57	69	79	–34	–20	–3

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Table S7 : Dependence of the penetration integrals (in meV) between first neighbour intrastrand nucleoside pairs on the ROLL parameter

XY	5'–XY–3'			3'–XY–5'		
	− 5.0	0.0	+ 5.0	− 5.0	0.0	+ 5.0
AA	131	125	118	78	79	81
AC	104	80	55	166	167	169
AG	193	224	262	3	8	13
AT	91	92	95	37	38	38
CA	104	98	93	59	60	60
CC	34	10	–15	157	155	´152
CG	202	232	267	–13	–10	–6
CT	62	62	64	14	10	6
GA	149	143	138	70	75	79
GC	132	107	81	162	173	187
GG	196	227	263	–29	–24	–19
GT	102	99	99	30	31	32
TA	87	82	77	43	43	41
TC	4	–20	–45	110	106	101
TG	205	236	273	0	3	4
TT	66	69	72	–13	–20	–28

Table S8 : Dependence of the penetration integrals (in meV) between first neighbour intrastrand nucleoside pairs on the TILT parameter

XY	5'–XY–3'			3'–XY–5'		
	− 5.0	0.0	+ 5.0	− 5.0	0.0	+ 5.0
AA	132.5	125	117	85	79	76
AC	75	80	84	180	167	156
AG	196	224	255	10	8	8
AT	80	92	105	40	38	36
CA	102	98	93	59	60	60
CC	7	10	11	152	155	158
CG	196	232	272	–10	–10	–9
CT	47	62	78	11	10	10
GA	155	143	133	63	75	85
GC	101	107	113	146	173	205
GG	200	227	255	–20	–24	–33
GT	88	99	112	24	31	38
TA	85	82	78	43	43	43
TC	–21	–20	–21	106	106	107
TG	199	236	279	2	3	3
TT	52	69	86	–18	–20	–21