Supplementary Information

2'-Deoxy-2'-fluoro-arabinonucleic acid: A valid alternative to DNA for biotechnological applications using charge transport

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Table S1. Electronic coupling values (in meV) obtained using the method in ref 1 for the indicated nucleobase pairs in the DNA and 2'F-ANA snapshots at the times t_i of their MD simulations. The electronic coupling values at intermediate times, starting from 10 ns, were calculated in ref 2.

	DNA				2'F-ANA			
t_i (ns)	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.5	6.6	205.1	52.8	16.7	1.6	45.5	2.3	4.6
11.5	16.0	99.2	71.0	1.6	5.1	3.8	44.3	1.2
12.5	68.4	68.3	4.9	64.2	48.4	49.8	22.1	4.5
13.5	12.3	6.2	10.4	23.1	15.4	46.4	9.5	25.8
14.5	0.4	34.2	- [a]	76.4	36.6	21.1	24.8	11.3
15.5	3.2	136.1	66.0	4.0	1.1	4.9	7.2	9.6
16.5	2.2	65.6	15.9	4.7	0.4	41.6	44.4	12.5
17.5	11.4	262.5	110.5	14.5	6.0	46.9	13.6	6.8
18.5	6.8	161.2	109.3	10.7	36.6	21.1	24.8	11.3
19.5	6.2	110.7	18.8	138.7	0.6	53.6	14.3	5.0
20.5	5.8	92.1	43.1	33.4	18.6	52.6	47.7	121.1
21.5	3.9	68.5	58.0	37.1	9.5	33.2	12.5	0.3
22.5	0.1	120.8	53.4	23.9	10.4	39.1	12.8	3.8×10^{-2}
23.5	4.4	14.6	17.2	10.7	12.7	13.6	32.9	14.6
24.5	7.2	8.9	109.2	40.1	4.8	48.7	30.4	6.3
25.5	1.2	5.0	60.6	27.6	10.2	40.3	6.7	95.6
26.5	7.9	16.9	32.0	23.1	3.4	83.0	77.8	0.3
27.5	26.1	52.6	37.1	54.8	18.9	44.7	5.4	1.3×10^{-2}
28.5	6.6	22.1	58.0	17.0	1.2	12.5	22.9	2.8
29.5	9.8	54.0	37.3	11.7	0.5	37.4	52.0	1.5
30.5	5.0	37.1	3.0	4.4	15.4	25.3	4.6	3.2
31.5	14.0	118.0	49.6	35.7	1.6	42.5	32.0	7.5
32.5	7.6	76.1	63.4	14.7	3.3	7.0	5.2	5.7
33.5	1.8	57.0	39.9	3.2	6.6	28.0	2.6	83.2
34.5	6.2	10.9	17.5	4.5	3.0	15.9	24.4	167.1
35.5	21.9	65.4	13.7	309.4	3.3	66.0	2.4	27.2
36.5	4.9	184.4	83.4	22.5	60.2	0.5	37.4	105.7
37.5	4.1	233.0	20.1	12.2	2.5	73.2	0.2	1.1
38.5	0.7	126.7	14.9	2.6	15.3	71.8	80.8	2.4
39.5	19.4	67.9	29.7	12.0	18.0	26.3	8.6	15.8
40.5	0.3	109.3	269.3	7.4	5.2	0.5	56.9	12.8
41.5	18.9	4.2	68.2	13.5	0.3	53.5	36.3	33.4
42.5	11.2	34.4	103.2	146.6	12.9	21.1	33.9	9.0
43.5	9.5	191.7	47.7	18.1	4.7	45.9	8.6	0.2
44.5	33.7	31.0	12.2	7.1	1.8	33.9	54.0	17.8
45.5	37.1	12.6	19.3	2.8	22.0	24.9	20.6	15.3
46.5	28.5	11.3	30.6	0.6	0.8	18.5	63.9	5.6
47.5	15.2	67.1	205.0	9.7	4.1	53.0	0.2	13.5
48.5	9.3	12.8	12.1	4.0	4.6	9.2	51.3	149.9
49.5	0.5	94.4	3.9	39.3	35.0	31.2	17.3	4.6

[a] DFT convergence was not obtained for this electronic coupling calculation.

Table S2. Norm of the ground-state vector expansion on the diabatic electronic states required to calculate the electronic couplings using the method of ref 1. The norm proximity to unity measures the quality of the two-state approximation.[1]

t_i (ns)	DNA				2'F-ANA			
	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.5	0.999	0.998	0.996	0.992	0.998	0.999	0.998	0.998
11.5	0.997	0.999	0.995	0.986	0.999	1.000	0.997	0.999
12.5	0.992	0.999	0.998	0.994	0.997	0.999	0.998	0.994
13.5	0.998	0.999	0.999	0.984	0.998	1.000	0.998	0.990
14.5	0.998	0.999	-	0.994	0.996	1.000	0.995	0.968
15.5	0.997	0.998	0.996	0.968	0.998	1.000	0.998	0.996
16.5	0.998	1.000	0.998	0.996	0.998	0.999	0.992	0.999
17.5	0.998	0.997	0.995	0.990	1.000	1.000	0.997	0.964
18.5	0.998	0.999	0.993	0.998	0.996	1.000	0.995	0.968
19.5	0.999	0.999	0.995	0.988	0.998	1.000	1.000	0.986
20.5	0.998	0.999	0.996	0.996	0.999	0.998	0.993	0.976
21.5	0.997	0.999	0.996	0.990	0.999	0.998	0.994	0.968
22.5	0.998	1.000	0.997	0.991	1.000	0.998	0.997	0.967
23.5	0.997	0.999	0.993	0.998	0.998	1.000	0.995	0.999
24.5	0.997	0.999	0.998	0.991	0.998	1.000	0.995	0.983
25.5	0.998	1.000	0.995	0.998	0.998	1.000	0.998	0.988
26.5	0.997	1.000	0.993	0.997	0.998	0.998	0.997	0.996
27.5	0.998	0.998	0.997	0.993	0.998	0.999	0.995	0.999
28.5	1.000	0.999	0.998	0.995	0.999	0.999	0.996	0.996
29.5	0.998	0.999	0.996	0.997	1.000	0.998	0.993	0.986
30.5	0.999	1.000	0.994	0.999	0.997	0.998	0.991	0.989
31.5	0.998	0.999	0.997	0.980	0.998	0.998	0.998	0.982
32.5	0.998	1.000	0.996	0.969	0.998	0.999	0.995	0.998
33.5	0.999	0.999	0.999	0.996	0.998	0.999	0.997	0.993
34.5	0.998	1.000	0.998	0.984	0.999	0.999	0.996	0.993
35.5	0.997	0.999	0.995	0.991	0.999	0.995	0.997	0.977
36.5	0.998	0.999	0.994	0.997	0.987	0.999	0.996	0.994
37.5	0.998	0.998	0.998	0.999	0.999	0.999	0.999	0.998
38.5	0.999	0.999	0.998	0.985	0.998	0.998	0.993	0.975
39.5	0.997	1.000	0.999	0.992	0.997	0.999	0.999	0.997
40.5	0.999	0.999	0.990	0.999	0.999	1.000	0.995	0.998
41.5	0.998	0.999	0.997	0.991	0.998	0.999	0.999	0.991
42.5	0.999	0.998	0.997	0.992	0.998	0.999	1.000	0.998
43.5	0.997	0.998	0.996	0.985	0.998	0.998	0.997	0.988
44.5	0.998	1.000	0.998	0.995	0.998	0.999	0.997	0.998
45.5	0.998	0.999	0.999	0.994	0.999	0.999	0.999	0.989
46.5	0.997	1.000	0.995	0.994	0.998	1.000	0.994	0.989
47.5	0.997	0.998	0.994	0.989	0.998	1.000	0.998	0.990
48.5	0.999	0.999	0.999	0.998	0.999	0.999	0.997	0.989
49.5	0.997	1.000	0.981	0.992	0.997	0.999	0.997	0.987

Table S3. Atomic coordinates and Löwdin charges (in units of electron elementary charge) of the G nucleobase in the DNA CG base pair used to calculate the effective radius R_G and the center of charge position vector $\mathbf{r}_c$ at 10 ns. The partial atomic charges were obtained from DFT calculations at the M11/6-311g** level of computational accuracy.

atom	x	y	z	q
N	39.3200	35.0240	21.4930	-0.0357
C	38.7180	35.6110	22.5750	0.2098
N	37.7610	34.9520	23.1000	-0.0263
C	37.5160	33.9330	22.1530	0.3549
C	36.4360	32.9690	22.0140	-0.0597
O	35.4850	32.7430	22.7560	0.1896
N	36.3710	32.3920	20.7380	-0.0111
C	37.3920	32.4800	19.8560	0.0239
N	37.2560	31.6820	18.8370	0.0760
N	38.4950	33.1960	20.0150	0.2131
C	38.4170	34.0500	21.0840	0.0639
H	40.0343	35.4373	20.9031	-0.0012
H	39.0150	36.4590	23.1020	0.0012
H	35.7400	31.6330	20.4850	-0.0009
H	36.5470	31.0000	18.6380	0.0020
H	38.0310	31.6200	18.1540	0.0007

Table S4. Atomic coordinates and Löwdin charges of the G nucleobase in the DNA GC base pair at 10 ns.

atom	*x*	*y*	*z*	*q*
N	37.5250	28.0100	20.0440	-0.0182
C	36.4860	27.2560	20.3600	0.2085
N	36.0120	27.4700	21.5720	0.0195
C	36.8230	28.4990	22.0860	0.2598
C	36.8390	29.1880	23.3760	-0.0451
O	36.1850	29.0180	24.4080	0.1454
N	37.7310	30.2560	23.3270	-0.0087
C	38.7340	30.3430	22.4760	0.0276
N	39.6470	31.2240	22.7850	0.0887
N	38.7570	29.7030	21.3070	0.2519
C	37.7650	28.7830	21.1600	0.0710
H	38.0712	28.0172	19.1902	-0.0008
H	36.0210	26.5540	19.6560	-0.0013
H	37.7380	30.7960	24.2030	-0.0009
H	39.5250	31.8530	23.5700	0.0020
H	40.4560	31.2920	22.1210	0.0006

Table S5. Atomic coordinates and Löwdin charges of the A nucleobase in the DNA A_1T base pair at 10 ns.

atom	x	y	z	q
N	42.4550	28.2340	21.4650	0.0016
C	41.5780	27.2090	21.2230	0.1025
N	40.7620	26.9100	22.2190	0.0298
C	40.9910	27.9980	23.1010	0.1832
C	40.5150	28.4090	24.4000	0.0122
N	39.7150	27.7780	25.1820	0.2817
N	41.1280	29.3920	25.0450	0.1130
C	42.0900	30.0500	24.5190	-0.0238
N	42.6600	29.9020	23.3030	0.3467
C	42.0260	28.7940	22.6220	-0.0551
H	43.1457	28.6203	20.8317	-0.0006
H	41.5750	26.5140	20.4380	0.0004
H	39.4140	28.2200	26.0380	0.0042
H	39.5370	26.7850	25.0510	0.0048
H	42.4510	30.7210	25.1350	-0.0006

Table S6. Atomic coordinates and Löwdin charges of the A nucleobase in the DNA A_2T base pair at 10 ns.

atom	x	y	z	q
N	44.7160	28.0420	24.9380	-0.0118
C	44.4820	26.8260	24.2690	0.1415
N	43.6830	26.0180	24.9340	0.0146
C	43.2780	26.8220	26.0320	0.2254
C	42.3120	26.6730	27.0690	0.0141
N	41.4500	25.6730	27.1120	0.3124
N	42.1410	27.6020	28.0050	0.0804
C	42.9440	28.6760	27.9910	0.0018
N	43.8870	28.8940	27.1090	0.2197
C	43.9720	27.9990	26.1000	-0.0070
H	45.3474	28.7822	24.6546	-0.0007
H	44.9560	26.6160	23.3070	-0.0007
H	40.7470	25.6440	27.8300	0.0051
H	41.5010	24.8910	26.4760	0.0053
H	42.8280	29.3380	28.8470	-0.0001

Table S7. Atomic coordinates and Löwdin charges of the A nucleobase in the DNA TA base pair at 10 ns.

atom	*x*	*y*	*z*	*q*
N	40.4440	24.2390	33.8170	-0.0055
C	39.9780	23.2770	32.9750	0.1234
N	40.4460	23.2790	31.7570	0.0318
C	41.4430	24.2620	31.8300	0.2104
C	42.3950	24.7100	30.9290	0.0177
N	42.3460	24.2520	29.7460	0.2558
N	43.2710	25.5910	31.2770	0.0634
C	43.1060	26.2230	32.3900	0.0236
N	42.2350	25.9520	33.3870	0.2897
C	41.4680	24.8070	33.0700	-0.0179
H	40.2333	24.3898	34.7955	-0.0006
H	39.1840	22.5660	33.2130	-0.0005
H	43.0600	24.6670	29.1360	0.0032
H	41.6970	23.5670	29.4910	0.0058
H	43.7730	27.0200	32.5650	-0.0002

Table S8. Atomic coordinates and Löwdin charges of the G nucleobase in the 2'F-ANA CG base pair at 10 ns.

atom	*x*	*y*	*z*	*q*
H	18.0411	15.8493	14.6907	-0.0011
N	18.7960	16.4900	14.4750	-0.0311
C	20.0700	16.5210	15.0200	0.2243
H	20.4340	15.7600	15.6760	-0.0005
N	20.7980	17.5420	14.6100	-0.0060
C	19.9000	18.2720	13.8110	0.2926
C	20.0390	19.4800	13.0150	-0.0524
O	21.0010	20.2120	12.7730	0.1772
N	18.9510	19.8980	12.4520	-0.0139
H	19.0070	20.7800	11.9750	-0.0012
C	17.7220	19.2400	12.4950	0.0226
N	16.7640	19.6900	11.7420	0.0866
H	16.9240	20.4910	11.1410	0.0018
H	15.9040	19.1400	11.6360	0.0011
N	17.5450	18.0690	13.1130	0.2261
C	18.6820	17.6840	13.7530	0.0737

Table S9. Atomic coordinates and Löwdin charges of the G nucleobase in the 2'F-ANA GC base pair at 10 ns.

atom	*x*	*y*	*z*	*q*
N	14.7560	24.1400	12.3850	-0.0361
C	15.4770	25.1440	11.8490	0.2287
N	16.7210	25.2280	12.1940	-0.0309
C	16.8380	24.0480	12.9550	0.3620
C	17.9200	23.5500	13.7390	-0.0481
O	19.0700	23.9080	13.8090	0.1698
N	17.5570	22.4210	14.4550	-0.0151
C	16.3150	21.8010	14.4140	0.0224
N	16.1360	20.8540	15.2580	0.0824
N	15.2250	22.3080	13.8300	0.1993
C	15.5860	23.4130	13.1150	0.0675
H	13.7732	23.9489	12.2250	-0.0013
H	15.0650	25.9140	11.1250	-0.0024
H	18.2390	22.0770	15.1280	-0.0010
H	16.8750	20.4220	15.8300	0.0017
H	15.2460	20.3480	15.1960	0.0010

Table S10. Atomic coordinates and Löwdin charges of the A nucleobase in the 2'F-ANA A_1T base pair at 10 ns.

atom	x	y	z	q
N	13.9720	24.1590	16.6750	-0.0008
C	14.0150	25.2750	15.8510	0.1605
N	15.2590	25.8040	15.8180	0.0477
C	16.0780	24.8980	16.5370	0.1971
C	17.4730	24.7270	16.8400	0.0172
N	18.4400	25.5680	16.5010	0.2790
N	17.8770	23.6260	17.4670	0.0527
C	16.9640	22.6760	17.9290	0.0304
N	15.6290	22.8180	17.7840	0.1938
C	15.2790	23.9080	17.0640	0.0177
H	13.1834	23.5518	16.8669	-0.0005
H	13.1640	25.7440	15.3260	-0.0009
H	19.3860	25.3110	16.7750	0.0040
H	18.1830	26.4020	15.9070	0.0026
H	17.2390	21.7510	18.4590	-0.0003

Table S11. Atomic coordinates and Löwdin charges of the A nucleobase in the 2'F-ANA A_2T base pair at 10 ns.

atom	x	y	z	q
N	14.9630	24.3300	20.8030	0.0071
C	14.1360	25.2140	20.1760	0.1038
N	14.7720	26.1350	19.5290	0.0380
C	16.1340	25.8770	19.8030	0.1774
C	17.3370	26.6090	19.5740	0.0022
N	17.5090	27.7250	18.8600	0.3203
N	18.4880	26.1400	20.0800	0.1106
C	18.4290	25.0370	20.7560	-0.0163
N	17.4200	24.3100	21.0860	0.2778
C	16.2470	24.7690	20.5440	-0.0272
H	14.7137	23.5241	21.3636	-0.0004
H	13.1120	25.0850	20.1280	0.0002
H	18.4700	28.1260	18.8840	0.0031
H	16.7280	28.0950	18.2740	0.0035
H	19.3370	24.7270	21.1130	-0.0001

Table S12. Atomic coordinates and Löwdin charges of the A nucleobase in the 2'F-ANA TA base pair at 10 ns.

atom	*x*	*y*	*z*	*q*
N	23.3100	31.6740	20.8790	0.0000
C	22.6580	32.3480	19.7740	0.1050
N	21.4150	32.0850	19.6670	0.0237
C	21.1760	31.1050	20.6510	0.2016
C	20.0560	30.3490	20.9690	0.0071
N	18.8570	30.4580	20.3410	0.3544
N	20.0310	29.6150	22.0990	0.1004
C	21.1760	29.5420	22.8230	-0.0169
N	22.3510	30.0370	22.4740	0.2436
C	22.2560	30.8710	21.4200	-0.0309
H	24.2699	31.7283	21.1924	-0.0005
H	23.1950	33.1460	19.2330	-0.0010
H	18.0780	29.9500	20.6550	0.0070
H	18.8220	30.9630	19.4870	0.0065
H	21.2050	28.7850	23.5870	0.0000

Table S13. Center-to-center distance R_{D-A} (in Å) for the indicated charge-donor (*D*) and acceptor (*A*) DNA nucleobase pairs in the selected MD snapshots at the indicated simulation times t_i. R_{D-A} is obtained as the distance between the *D* and *A* centers of charge (see Methods section).

t_i (ns)	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.0	4.84	4.18	3.61	5.78
10.5	6.16	3.54	3.31	6.01
11.0	5.36	4.01	3.50	5.88
11.5	6.22	4.28	3.33	6.16
12.0	6.62	3.71	3.60	5.60
12.5	5.98	3.55	3.75	5.77
13.0	5.90	3.38	3.57	5.86
13.5	5.14	4.11	3.77	6.46
14.0	6.67	3.86	3.81	5.96
14.5	6.62	4.00	3.80	5.87
15.0	6.10	3.75	3.56	5.32
15.5	5.78	3.89	3.55	6.55
16.0	5.35	3.60	3.76	6.33
16.5	5.48	3.62	3.76	5.86
17.0	6.12	3.37	3.93	6.58
17.5	5.22	3.56	3.78	5.99
18.0	5.64	3.47	3.66	5.61
18.5	6.35	3.78	3.43	6.43
19.0	6.03	3.79	3.82	6.55
19.5	5.64	3.59	3.43	6.52
20.0	6.47	3.98	3.42	6.04
20.5	5.88	3.92	3.49	5.78
21.0	6.18	3.91	3.68	5.92
21.5	5.62	3.79	3.57	5.89
22.0	6.14	4.04	3.49	6.07
22.5	6.16	3.70	3.54	6.16
23.0	5.90	3.48	3.94	5.52
23.5	5.05	3.55	3.60	6.06
24.0	5.57	3.88	3.84	6.20
24.5	5.67	3.49	3.62	6.58
25.0	5.22	3.82	3.76	6.31
25.5	5.49	3.73	3.52	6.12
26.0	5.88	3.91	3.66	6.65
26.5	5.50	3.86	3.61	6.13
27.0	6.21	3.74	3.70	6.19
27.5	6.27	3.65	3.87	6.03
28.0	5.60	3.73	3.40	6.28
28.5	5.38	3.95	3.63	5.91

29.0	6.04	3.75	3.76	6.40
29.5	5.69	4.35	3.72	6.11
30.0	6.04	4.00	3.81	5.95
30.5	6.07	3.79	3.52	6.51
31.0	5.11	4.23	3.93	6.16
31.5	6.09	3.83	3.51	5.63
32.0	5.97	4.13	3.60	5.95
32.5	6.07	3.80	3.45	6.47
33.0	5.66	3.91	3.90	6.32
33.5	6.64	3.54	3.95	6.22
34.0	4.61	3.59	3.55	6.13
34.5	5.63	3.62	3.89	6.32
35.0	6.56	4.07	3.94	5.90
35.5	5.42	3.95	3.61	6.10
36.0	5.77	4.12	3.69	6.21
36.5	5.53	3.60	3.43	5.82
37.0	5.78	4.05	4.06	5.53
37.5	6.11	3.65	3.64	6.23
38.0	6.28	4.05	3.48	5.86
38.5	6.50	3.62	3.73	5.83
39.0	5.64	3.77	4.26	6.22
39.5	6.15	3.69	3.88	5.81
40.0	5.75	3.74	4.08	6.04
40.5	5.79	4.15	3.53	6.14
41.0	5.72	3.45	3.64	6.14
41.5	6.31	3.68	3.67	5.71
42.0	5.70	3.66	3.88	5.75
42.5	5.79	3.58	3.83	6.08
43.0	6.08	3.91	3.33	6.28
43.5	5.69	3.72	3.69	6.42
44.0	6.21	3.73	3.69	6.90
44.5	6.50	3.49	3.64	6.07
45.0	5.37	3.70	3.84	6.50
45.5	6.00	3.87	3.80	6.21
46.0	5.16	3.82	4.27	6.33
46.5	5.37	3.97	4.01	6.82
47.0	5.28	3.63	3.90	6.47
47.5	5.46	4.11	3.68	6.35
48.0	5.10	4.09	3.62	6.36
48.5	6.04	3.57	4.08	6.29
49.0	5.48	3.76	3.60	6.18
49.5	5.49	4.01	3.62	6.65
50.0	6.00	3.83	4.12	6.40

Table S14. Center-to-center distance R_{D-A} (in Å) for the indicated 2'F-ANA nucleobase pairs in the selected MD snapshots at the indicated simulation times t_i.

t_i (ns)	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.0	6.00	3.64	3.48	5.99
10.5	4.44	3.97	4.18	6.77
11.0	5.12	3.68	3.47	6.24
11.5	4.97	4.33	3.86	7.24
12.0	5.31	4.04	3.32	6.79
12.5	5.47	4.05	3.86	6.82
13.0	5.49	4.42	3.70	5.67
13.5	4.32	4.12	4.11	6.18
14.0	3.88	4.34	3.90	6.22
14.5	4.51	3.90	3.51	6.13
15.0	5.30	3.68	3.73	6.45
15.5	5.03	4.52	4.03	6.36
16.0	5.12	4.02	3.92	6.63
16.5	5.30	4.35	3.99	6.22
17.0	5.06	3.56	4.01	7.59
17.5	5.08	3.90	3.66	5.83
18.0	4.36	3.96	3.74	5.94
18.5	4.51	3.90	3.51	6.13
19.0	4.79	3.73	4.03	6.73
19.5	4.89	3.90	3.92	6.81
20.0	5.63	3.80	3.70	6.65
20.5	4.43	4.06	3.86	6.96
21.0	4.95	4.53	4.72	7.26
21.5	5.37	3.97	4.12	7.70
22.0	5.03	3.88	3.64	6.98
22.5	4.92	4.24	3.91	7.24
23.0	4.78	3.85	3.75	6.11
23.5	5.40	3.84	3.50	6.13
24.0	4.80	3.68	3.66	6.06
24.5	5.25	4.11	3.89	6.77
25.0	4.98	4.11	3.83	6.14
25.5	4.62	4.31	3.67	6.92
26.0	5.46	3.69	3.70	6.26
26.5	4.88	4.07	3.90	7.22
27.0	5.24	4.19	3.97	7.76
27.5	5.02	3.98	3.61	7.89
28.0	5.36	3.43	4.09	6.28
28.5	4.86	3.86	3.88	5.62
29.0	5.11	4.03	3.69	7.67
29.5	5.01	3.86	3.97	6.67

30.0	5.40	3.94	3.64	6.79
30.5	5.36	4.01	3.83	6.75
31.0	4.41	4.14	3.71	6.47
31.5	4.63	3.62	3.62	6.21
32.0	4.84	3.88	3.77	6.51
32.5	5.05	3.53	3.60	7.04
33.0	4.99	4.21	3.58	6.31
33.5	5.08	3.90	4.04	6.93
34.0	5.52	3.74	3.58	6.63
34.5	5.74	3.66	3.67	6.05
35.0	5.53	4.04	3.63	5.97
35.5	5.42	4.21	4.24	6.34
36.0	4.18	4.15	3.85	7.07
36.5	5.31	3.77	3.77	6.94
37.0	4.92	3.84	3.96	6.31
37.5	4.95	3.47	3.98	7.20
38.0	4.99	3.77	3.74	6.47
38.5	5.47	4.05	3.78	7.87
39.0	5.55	4.17	3.94	7.84
39.5	5.53	3.91	3.95	6.66
40.0	5.02	4.01	3.91	6.65
40.5	4.73	3.81	3.52	6.34
41.0	5.25	3.85	3.69	6.79
41.5	5.18	4.27	3.60	6.34
42.0	4.80	4.24	4.40	6.05
42.5	5.46	3.82	3.80	6.54
43.0	5.36	4.05	3.56	6.78
43.5	5.32	3.80	3.80	7.59
44.0	5.48	3.88	4.07	7.49
44.5	4.81	3.98	3.64	6.34
45.0	5.91	3.44	4.05	7.06
45.5	4.86	3.57	3.78	6.27
46.0	5.64	3.63	3.67	6.61
46.5	5.24	3.96	3.43	6.92
47.0	5.40	3.68	3.41	6.44
47.5	4.53	4.03	4.19	6.30
48.0	5.00	3.94	3.90	6.73
48.5	5.62	3.83	3.41	6.55
49.0	4.43	3.88	3.76	7.72
49.5	5.15	4.26	3.83	6.76
50.0	5.30	4.08	3.57	6.89

Table S15. Purine nucleobase effective radius, $R_{\text{purine}}(\text{base pair})$, for the different DNA base pairs at the indicated MD simulation times t_i. These radii (in Å) are used in eq 4b.

t_i (ns)	R_G (CG)	R_G (GC)	R_A (A_1T)	R_A (A_2T)	R_A (TA)
10.0	2.45	2.43	2.32	2.33	2.26
10.5	2.42	2.43	2.33	2.35	2.29
11.0	2.41	2.43	2.28	2.31	2.29
11.5	2.43	2.44	2.31	2.33	2.29
12.0	2.42	2.43	2.33	2.33	2.30
12.5	2.45	2.43	2.30	2.30	2.33
13.0	2.42	2.43	2.28	2.30	2.30
13.5	2.45	2.45	2.32	2.32	2.29
14.0	2.44	2.46	2.34	2.31	2.33
14.5	2.48	2.44	2.33	2.33	2.30
15.0	2.42	2.43	2.29	2.34	2.34
15.5	2.45	2.42	2.32	2.29	2.29
16.0	2.43	2.45	2.31	2.31	2.28
16.5	2.42	2.41	2.30	2.31	2.30
17.0	2.42	2.44	2.31	2.27	2.32
17.5	2.42	2.44	2.33	2.30	2.30
18.0	2.43	2.42	2.33	2.39	2.36
18.5	2.43	2.43	2.27	2.27	2.27
19.0	2.42	2.43	2.29	2.30	2.33
19.5	2.45	2.43	2.35	2.30	2.33
20.0	2.42	2.42	2.31	2.29	2.32
20.5	2.41	2.44	2.30	2.32	2.31
21.0	2.40	2.46	2.32	2.34	2.28
21.5	2.45	2.43	2.32	2.33	2.29
22.0	2.46	2.43	2.29	2.33	2.30
22.5	2.46	2.44	2.30	2.31	2.30
23.0	2.41	2.44	2.33	2.32	2.30
23.5	2.43	2.44	2.30	2.32	2.29
24.0	2.45	2.46	2.33	2.41	2.32
24.5	2.45	2.42	2.30	2.31	2.32
25.0	2.45	2.44	2.31	2.31	2.33
25.5	2.46	2.45	2.31	2.29	2.32
26.0	2.46	2.46	2.33	2.28	2.30
26.5	2.45	2.46	2.37	2.32	2.31
27.0	2.40	2.43	2.33	2.31	2.29
27.5	2.46	2.42	2.31	2.30	2.35
28.0	2.47	2.44	2.29	2.31	2.31
28.5	2.44	2.48	2.28	2.34	2.32
29.0	2.43	2.44	2.33	2.28	2.30
29.5	2.44	2.40	2.31	2.32	2.30

30.0	2.43	2.42	2.32	2.36	2.32
30.5	2.43	2.39	2.28	2.31	2.30
31.0	2.42	2.44	2.28	2.30	2.31
31.5	2.44	2.44	2.31	2.28	2.32
32.0	2.44	2.43	2.30	2.34	2.34
32.5	2.44	2.41	2.34	2.29	2.34
33.0	2.41	2.42	2.30	2.32	2.28
33.5	2.43	2.42	2.32	2.30	2.29
34.0	2.44	2.41	2.32	2.30	2.32
34.5	2.44	2.43	2.37	2.29	2.28
35.0	2.46	2.44	2.31	2.33	2.31
35.5	2.45	2.41	2.34	2.33	2.28
36.0	2.45	2.45	2.30	2.29	2.30
36.5	2.43	2.43	2.33	2.31	2.32
37.0	2.43	2.43	2.30	2.35	2.31
37.5	2.43	2.40	2.33	2.32	2.26
38.0	2.43	2.46	2.30	2.32	2.31
38.5	2.44	2.43	2.38	2.35	2.31
39.0	2.46	2.43	2.29	2.32	2.33
39.5	2.47	2.41	2.27	2.32	2.32
40.0	2.42	2.43	2.28	2.30	2.28
40.5	2.43	2.44	2.29	2.30	2.30
41.0	2.43	2.46	2.31	2.35	2.31
41.5	2.42	2.44	2.30	2.32	2.38
42.0	2.41	2.46	2.28	2.38	2.35
42.5	2.45	2.44	2.27	2.31	2.33
43.0	2.43	2.47	2.29	2.31	2.30
43.5	2.41	2.43	2.34	2.28	2.31
44.0	2.41	2.41	2.33	2.30	2.29
44.5	2.46	2.42	2.31	2.32	2.30
45.0	2.45	2.43	2.32	2.31	2.27
45.5	2.44	2.42	2.29	2.31	2.33
46.0	2.45	2.41	2.31	2.28	2.29
46.5	2.43	2.43	2.31	2.28	2.32
47.0	2.43	2.45	2.29	2.32	2.30
47.5	2.45	2.42	2.31	2.32	2.36
48.0	2.40	2.44	2.30	2.31	2.29
48.5	2.44	2.40	2.31	2.28	2.35
49.0	2.44	2.45	2.29	2.31	2.34
49.5	2.41	2.42	2.31	2.29	2.32
50.0	2.44	2.42	2.31	2.31	2.29

Table S16. Effective radius (Å) of the purine nucleobase in each 2'F-ANA base pair indicated, at the MD simulation time t_i.

t_i (ns)	R_G (CG)	R_G (GC)	R_A (A_1T)	R_A (A_2T)	R_A (TA)
10.0	2.43	2.43	2.33	2.32	2.35
10.5	2.44	2.43	2.27	2.28	2.31
11.0	2.43	2.44	2.32	2.31	2.32
11.5	2.43	2.50	2.28	2.27	2.35
12.0	2.45	2.43	2.31	2.29	2.29
12.5	2.43	2.41	2.31	2.30	2.33
13.0	2.44	2.46	2.31	2.33	2.32
13.5	2.43	2.45	2.29	2.33	2.32
14.0	2.44	2.45	2.32	2.34	2.32
14.5	2.43	2.42	2.31	2.30	2.37
15.0	2.41	2.46	2.30	2.30	2.31
15.5	2.44	2.42	2.33	2.31	2.29
16.0	2.45	2.46	2.34	2.27	2.30
16.5	2.42	2.43	2.35	2.29	2.31
17.0	2.42	2.44	2.48	2.31	2.29
17.5	2.41	2.42	2.29	2.30	2.32
18.0	2.43	2.42	2.28	2.30	2.26
18.5	2.43	2.42	2.31	2.30	2.37
19.0	2.43	2.43	2.30	2.31	2.29
19.5	2.44	2.44	2.29	2.29	2.26
20.0	2.44	2.46	2.33	2.30	2.29
20.5	2.45	2.43	2.33	2.30	2.30
21.0	2.45	2.43	2.30	2.30	2.34
21.5	2.40	2.44	2.31	2.31	2.30
22.0	2.44	2.41	2.33	2.30	2.32
22.5	2.42	2.43	2.29	2.31	2.33
23.0	2.42	2.42	2.34	2.32	2.27
23.5	2.42	2.43	2.34	2.31	2.32
24.0	2.42	2.44	2.32	2.32	2.31
24.5	2.42	2.45	2.34	2.32	2.33
25.0	2.41	2.43	2.29	2.29	2.32
25.5	2.44	2.43	2.30	2.31	2.30
26.0	2.45	2.45	2.29	2.27	2.32
26.5	2.46	2.42	2.32	2.29	2.33
27.0	2.45	2.43	2.34	2.32	2.30
27.5	2.42	2.43	2.32	2.31	2.32
28.0	2.43	2.42	2.29	2.31	2.32
28.5	2.42	2.43	2.31	2.32	2.34
29.0	2.41	2.43	2.33	2.31	2.31
29.5	2.42	2.45	2.33	2.32	2.31

30.0	2.42	2.48	2.28	2.33	2.34
30.5	2.44	2.43	2.31	2.30	2.31
31.0	2.42	2.44	2.32	2.29	2.29
31.5	2.42	2.44	2.30	2.33	2.31
32.0	2.42	2.43	2.30	2.32	2.31
32.5	2.45	2.44	2.30	2.29	2.32
33.0	2.45	2.44	2.34	2.26	2.33
33.5	2.42	2.41	2.29	2.32	2.39
34.0	2.43	2.42	2.31	2.33	2.29
34.5	2.43	2.43	2.33	2.36	2.28
35.0	2.44	2.40	2.33	2.29	2.33
35.5	2.43	2.44	2.32	2.26	2.31
36.0	2.43	2.43	2.30	2.29	2.34
36.5	2.43	2.43	2.32	2.31	2.31
37.0	2.41	2.42	2.30	2.32	2.32
37.5	2.42	2.45	2.26	2.32	2.31
38.0	2.42	2.41	2.29	2.31	2.31
38.5	2.46	2.42	2.34	2.30	2.31
39.0	2.45	2.44	2.31	2.30	2.29
39.5	2.45	2.43	2.31	2.32	2.32
40.0	2.42	2.44	2.29	2.33	2.32
40.5	2.45	2.44	2.32	2.29	2.32
41.0	2.45	2.43	2.26	2.27	2.32
41.5	2.45	2.43	2.31	2.31	2.31
42.0	2.40	2.44	2.35	2.31	2.35
42.5	2.43	2.41	2.31	2.28	2.32
43.0	2.46	2.42	2.29	2.33	2.32
43.5	2.42	2.44	2.31	2.31	2.29
44.0	2.48	2.43	2.28	2.32	2.31
44.5	2.46	2.37	2.31	2.29	2.26
45.0	2.43	2.46	2.31	2.34	2.31
45.5	2.44	2.40	2.32	2.30	2.31
46.0	2.43	2.43	2.32	2.28	2.29
46.5	2.41	2.45	2.31	2.33	2.33
47.0	2.44	2.44	2.30	2.36	2.35
47.5	2.42	2.43	2.30	2.31	2.31
48.0	2.44	2.46	2.30	2.33	2.32
48.5	2.46	2.46	2.31	2.32	2.30
49.0	2.44	2.44	2.29	2.32	2.32
49.5	2.39	2.41	2.29	2.33	2.29
50.0	2.46	2.43	2.36	2.30	2.32

Table S17. $\lambda^{i}_{D-A} + \lambda^{o}_{D-A}(t_i)$ (see eq 4a), in eV, for the indicated DNA base pairs, using the dielectric constant set $S_1 = \{\varepsilon_o = 2.27, \varepsilon_s = 12.4\}$.

t_i (ns)	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.0	1.67	1.46	1.21	1.78
10.5	1.91	1.23	1.06	1.79
11.0	1.79	1.43	1.19	1.78
11.5	1.91	1.49	1.10	1.82
12.0	1.98	1.30	1.20	1.73
12.5	1.88	1.25	1.28	1.76
13.0	1.88	1.18	1.23	1.78
13.5	1.73	1.43	1.27	1.86
14.0	1.95	1.33	1.29	1.78
14.5	1.94	1.39	1.27	1.77
15.0	1.91	1.33	1.19	1.65
15.5	1.85	1.37	1.20	1.89
16.0	1.77	1.25	1.28	1.85
16.5	1.82	1.29	1.29	1.78
17.0	1.90	1.16	1.36	1.89
17.5	1.76	1.24	1.28	1.80
18.0	1.84	1.20	1.19	1.67
18.5	1.94	1.35	1.19	1.89
19.0	1.89	1.35	1.32	1.86
19.5	1.83	1.25	1.13	1.86
20.0	1.96	1.40	1.15	1.80
20.5	1.87	1.38	1.17	1.75
21.0	1.91	1.36	1.23	1.78
21.5	1.82	1.33	1.19	1.78
22.0	1.90	1.43	1.18	1.80
22.5	1.89	1.30	1.20	1.82
23.0	1.87	1.20	1.33	1.72
23.5	1.72	1.24	1.22	1.81
24.0	1.80	1.35	1.25	1.77
24.5	1.83	1.23	1.23	1.86
25.0	1.74	1.34	1.28	1.83
25.5	1.79	1.31	1.19	1.81
26.0	1.84	1.36	1.25	1.90
26.5	1.79	1.32	1.19	1.81
27.0	1.93	1.31	1.25	1.83
27.5	1.92	1.29	1.32	1.78
28.0	1.81	1.32	1.14	1.83
28.5	1.76	1.39	1.23	1.76
29.0	1.89	1.31	1.28	1.87
29.5	1.85	1.53	1.26	1.81

30.0	1.90	1.41	1.27	1.76
30.5	1.92	1.37	1.20	1.86
31.0	1.74	1.49	1.36	1.82
31.5	1.89	1.35	1.20	1.75
32.0	1.88	1.45	1.21	1.76
32.5	1.90	1.33	1.15	1.85
33.0	1.85	1.39	1.33	1.85
33.5	1.97	1.24	1.35	1.84
34.0	1.63	1.26	1.20	1.81
34.5	1.82	1.25	1.31	1.86
35.0	1.94	1.43	1.33	1.77
35.5	1.79	1.38	1.20	1.81
36.0	1.84	1.44	1.27	1.84
36.5	1.81	1.25	1.13	1.76
37.0	1.86	1.43	1.37	1.70
37.5	1.91	1.29	1.22	1.85
38.0	1.91	1.42	1.17	1.77
38.5	1.95	1.24	1.22	1.75
39.0	1.82	1.34	1.45	1.81
39.5	1.90	1.33	1.34	1.76
40.0	1.86	1.33	1.41	1.82
40.5	1.85	1.46	1.20	1.82
41.0	1.83	1.19	1.21	1.79
41.5	1.93	1.30	1.25	1.71
42.0	1.84	1.29	1.30	1.71
42.5	1.84	1.27	1.32	1.80
43.0	1.88	1.37	1.11	1.84
43.5	1.85	1.29	1.25	1.86
44.0	1.93	1.31	1.24	1.92
44.5	1.95	1.22	1.23	1.81
45.0	1.77	1.30	1.31	1.88
45.5	1.89	1.37	1.30	1.81
46.0	1.75	1.36	1.46	1.86
46.5	1.79	1.40	1.38	1.91
47.0	1.76	1.28	1.33	1.85
47.5	1.80	1.45	1.24	1.81
48.0	1.75	1.44	1.23	1.85
48.5	1.90	1.27	1.40	1.83
49.0	1.79	1.33	1.22	1.80
49.5	1.82	1.42	1.23	1.88
50.0	1.88	1.36	1.40	1.86

Table S18. $\lambda^{i}_{D-A} + \lambda^{o}_{D-A}(t_i)$, in eV, for the 2'F-ANA base pairs, using $S_1 = \{\varepsilon_o = 2.27, \varepsilon_s = 12.4\}$.

t_i (ns)	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.0	1.89	1.27	1.15	1.77
10.5	1.58	1.42	1.45	1.90
11.0	1.73	1.29	1.16	1.82
11.5	1.68	1.49	1.35	1.94
12.0	1.77	1.42	1.10	1.91
12.5	1.82	1.43	1.32	1.90
13.0	1.79	1.52	1.25	1.73
13.5	1.54	1.45	1.40	1.81
14.0	1.40	1.50	1.31	1.81
14.5	1.60	1.38	1.19	1.79
15.0	1.77	1.28	1.28	1.86
15.5	1.72	1.55	1.37	1.85
16.0	1.72	1.39	1.34	1.90
16.5	1.78	1.49	1.35	1.83
17.0	1.73	1.17	1.29	1.98
17.5	1.74	1.39	1.26	1.76
18.0	1.56	1.41	1.29	1.82
18.5	1.60	1.38	1.19	1.79
19.0	1.67	1.32	1.38	1.90
19.5	1.68	1.38	1.36	1.93
20.0	1.81	1.32	1.25	1.89
20.5	1.57	1.42	1.31	1.92
21.0	1.70	1.57	1.57	1.94
21.5	1.79	1.39	1.40	1.99
22.0	1.72	1.37	1.22	1.91
22.5	1.70	1.49	1.34	1.93
23.0	1.68	1.35	1.26	1.83
23.5	1.79	1.34	1.16	1.80
24.0	1.67	1.29	1.24	1.80
24.5	1.76	1.42	1.31	1.88
25.0	1.72	1.45	1.32	1.82
25.5	1.63	1.51	1.25	1.91
26.0	1.78	1.30	1.28	1.84
26.5	1.68	1.43	1.33	1.94
27.0	1.75	1.45	1.33	1.99
27.5	1.72	1.40	1.22	2.00
28.0	1.79	1.21	1.40	1.83
28.5	1.69	1.37	1.32	1.72
29.0	1.74	1.41	1.24	1.98
29.5	1.71	1.34	1.34	1.88

30.0	1.77	1.38	1.24	1.87
30.5	1.78	1.41	1.31	1.90
31.0	1.57	1.44	1.27	1.87
31.5	1.63	1.27	1.22	1.81
32.0	1.69	1.37	1.28	1.86
32.5	1.72	1.24	1.23	1.93
33.0	1.70	1.45	1.22	1.85
33.5	1.74	1.39	1.38	1.87
34.0	1.82	1.32	1.20	1.87
34.5	1.85	1.28	1.21	1.79
35.0	1.82	1.42	1.23	1.79
35.5	1.79	1.47	1.46	1.87
36.0	1.51	1.46	1.33	1.92
36.5	1.78	1.33	1.28	1.91
37.0	1.71	1.36	1.35	1.83
37.5	1.70	1.23	1.38	1.93
38.0	1.73	1.35	1.28	1.86
38.5	1.80	1.42	1.27	2.00
39.0	1.80	1.46	1.35	2.01
39.5	1.80	1.38	1.34	1.87
40.0	1.72	1.42	1.33	1.86
40.5	1.64	1.33	1.19	1.84
41.0	1.75	1.38	1.29	1.91
41.5	1.74	1.49	1.22	1.84
42.0	1.68	1.46	1.46	1.78
42.5	1.81	1.36	1.31	1.88
43.0	1.77	1.44	1.20	1.88
43.5	1.77	1.33	1.29	1.98
44.0	1.79	1.39	1.40	1.96
44.5	1.69	1.43	1.24	1.87
45.0	1.86	1.19	1.36	1.91
45.5	1.69	1.26	1.29	1.84
46.0	1.83	1.27	1.25	1.90
46.5	1.76	1.39	1.14	1.89
47.0	1.78	1.30	1.12	1.81
47.5	1.61	1.42	1.43	1.84
48.0	1.70	1.38	1.32	1.87
48.5	1.80	1.33	1.13	1.87
49.0	1.57	1.37	1.28	1.98
49.5	1.77	1.50	1.30	1.89
50.0	1.76	1.41	1.19	1.90

Table S19. $\lambda^{i}_{D-A} + \lambda^{o}_{D-A}(t_i)$, in eV, for the DNA base pairs, using $\mathcal{S}_2 = \{\varepsilon_o = 1.8, \varepsilon_s = 80\}$.

t_i (ns)	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.0	2.21	1.95	1.62	2.47
10.5	2.57	1.60	1.39	2.49
11.0	2.39	1.90	1.59	2.48
11.5	2.57	1.99	1.44	2.53
12.0	2.67	1.70	1.60	2.40
12.5	2.52	1.62	1.73	2.44
13.0	2.52	1.52	1.64	2.48
13.5	2.29	1.90	1.71	2.60
14.0	2.63	1.75	1.73	2.47
14.5	2.61	1.84	1.71	2.46
15.0	2.56	1.75	1.59	2.28
15.5	2.48	1.81	1.60	2.64
16.0	2.36	1.63	1.72	2.58
16.5	2.43	1.68	1.73	2.47
17.0	2.56	1.49	1.84	2.64
17.5	2.34	1.60	1.73	2.50
18.0	2.46	1.55	1.59	2.31
18.5	2.61	1.78	1.58	2.64
19.0	2.54	1.77	1.78	2.60
19.5	2.44	1.62	1.50	2.59
20.0	2.64	1.86	1.53	2.51
20.5	2.51	1.82	1.55	2.43
21.0	2.57	1.79	1.64	2.47
21.5	2.43	1.75	1.59	2.47
22.0	2.55	1.90	1.56	2.51
22.5	2.54	1.71	1.60	2.53
23.0	2.51	1.54	1.79	2.38
23.5	2.28	1.62	1.63	2.51
24.0	2.40	1.77	1.68	2.46
24.5	2.45	1.59	1.64	2.60
25.0	2.31	1.76	1.72	2.54
25.5	2.38	1.71	1.59	2.53
26.0	2.47	1.79	1.67	2.65
26.5	2.38	1.73	1.58	2.52
27.0	2.59	1.71	1.67	2.55
27.5	2.58	1.68	1.78	2.48
28.0	2.41	1.73	1.51	2.55
28.5	2.35	1.83	1.65	2.45
29.0	2.54	1.71	1.73	2.60
29.5	2.47	2.04	1.69	2.52
30.0	2.55	1.86	1.70	2.45
30.5	2.58	1.81	1.61	2.60

31.0	2.31	1.99	1.84	2.54
31.5	2.54	1.77	1.60	2.43
32.0	2.52	1.93	1.62	2.44
32.5	2.55	1.75	1.52	2.58
33.0	2.48	1.83	1.79	2.58
33.5	2.66	1.61	1.82	2.56
34.0	2.14	1.64	1.59	2.52
34.5	2.44	1.62	1.76	2.60
35.0	2.61	1.89	1.80	2.46
35.5	2.39	1.83	1.60	2.53
36.0	2.46	1.92	1.70	2.56
36.5	2.42	1.63	1.50	2.45
37.0	2.49	1.90	1.85	2.36
37.5	2.57	1.68	1.64	2.58
38.0	2.57	1.88	1.56	2.46
38.5	2.63	1.60	1.63	2.43
39.0	2.43	1.76	1.97	2.52
39.5	2.55	1.74	1.80	2.44
40.0	2.49	1.75	1.92	2.53
40.5	2.47	1.94	1.60	2.54
41.0	2.45	1.53	1.62	2.50
41.5	2.60	1.70	1.67	2.37
42.0	2.46	1.69	1.75	2.37
42.5	2.47	1.65	1.79	2.50
43.0	2.52	1.81	1.47	2.56
43.5	2.47	1.69	1.68	2.60
44.0	2.60	1.71	1.67	2.69
44.5	2.63	1.59	1.64	2.51
45.0	2.36	1.70	1.76	2.63
45.5	2.53	1.81	1.76	2.52
46.0	2.32	1.79	1.99	2.60
46.5	2.39	1.85	1.87	2.67
47.0	2.35	1.67	1.80	2.59
47.5	2.40	1.92	1.67	2.53
48.0	2.32	1.91	1.64	2.59
48.5	2.55	1.65	1.91	2.55
49.0	2.39	1.74	1.64	2.51
49.5	2.43	1.87	1.65	2.63
50.0	2.53	1.79	1.91	2.59

Table S20. $\lambda^{i}_{D-A} + \lambda^{o}_{D-A}(t_i)$, in eV, for the 2'F-NA base pairs, using $S_2 = \{\varepsilon_o = 1.8, \varepsilon_s = 80\}$.

t_i (ns)	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.0	2.53	1.65	1.53	2.46
10.5	2.07	1.88	1.98	2.66
11.0	2.30	1.68	1.54	2.54
11.5	2.22	1.99	1.83	2.72
12.0	2.35	1.88	1.45	2.67
12.5	2.42	1.90	1.78	2.65
13.0	2.39	2.03	1.67	2.40
13.5	2.01	1.92	1.90	2.52
14.0	1.80	2.00	1.77	2.51
14.5	2.11	1.82	1.58	2.49
15.0	2.35	1.67	1.72	2.59
15.5	2.28	2.08	1.85	2.58
16.0	2.28	1.84	1.81	2.65
16.5	2.37	1.99	1.82	2.56
17.0	2.30	1.50	1.73	2.78
17.5	2.32	1.84	1.68	2.45
18.0	2.05	1.87	1.74	2.53
18.5	2.11	1.82	1.58	2.49
19.0	2.20	1.73	1.87	2.65
19.5	2.23	1.82	1.84	2.70
20.0	2.42	1.73	1.68	2.65
20.5	2.06	1.88	1.77	2.69
21.0	2.25	2.10	2.16	2.71
21.5	2.39	1.84	1.90	2.79
22.0	2.29	1.80	1.64	2.68
22.5	2.26	1.99	1.81	2.70
23.0	2.22	1.77	1.69	2.54
23.5	2.39	1.75	1.54	2.51
24.0	2.21	1.68	1.65	2.50
24.5	2.34	1.88	1.76	2.63
25.0	2.28	1.93	1.79	2.53
25.5	2.14	2.01	1.67	2.68
26.0	2.37	1.70	1.73	2.57
26.5	2.22	1.90	1.80	2.71
27.0	2.33	1.93	1.79	2.79
27.5	2.28	1.84	1.63	2.81
28.0	2.38	1.56	1.90	2.54
28.5	2.23	1.80	1.78	2.38
29.0	2.32	1.86	1.66	2.78
29.5	2.27	1.77	1.81	2.62
30.0	2.36	1.82	1.66	2.61
30.5	2.37	1.87	1.77	2.65

31.0	2.06	1.92	1.70	2.62
31.5	2.15	1.65	1.63	2.52
32.0	2.23	1.81	1.73	2.60
32.5	2.27	1.60	1.65	2.70
33.0	2.25	1.93	1.63	2.58
33.5	2.31	1.84	1.87	2.61
34.0	2.43	1.73	1.60	2.62
34.5	2.48	1.66	1.61	2.49
35.0	2.44	1.89	1.64	2.49
35.5	2.39	1.95	1.99	2.60
36.0	1.97	1.94	1.80	2.69
36.5	2.37	1.74	1.72	2.67
37.0	2.26	1.80	1.82	2.55
37.5	2.25	1.59	1.86	2.70
38.0	2.29	1.77	1.72	2.59
38.5	2.40	1.87	1.71	2.81
39.0	2.41	1.94	1.83	2.82
39.5	2.41	1.81	1.81	2.61
40.0	2.28	1.87	1.80	2.60
40.5	2.16	1.75	1.58	2.57
41.0	2.33	1.82	1.74	2.67
41.5	2.31	1.98	1.62	2.56
42.0	2.22	1.94	2.00	2.48
42.5	2.42	1.79	1.77	2.62
43.0	2.36	1.90	1.60	2.62
43.5	2.36	1.75	1.74	2.78
44.0	2.38	1.83	1.90	2.75
44.5	2.23	1.89	1.66	2.61
45.0	2.50	1.53	1.85	2.67
45.5	2.24	1.63	1.73	2.56
46.0	2.45	1.65	1.68	2.65
46.5	2.35	1.83	1.50	2.64
47.0	2.37	1.70	1.48	2.52
47.5	2.11	1.88	1.94	2.56
48.0	2.25	1.82	1.78	2.62
48.5	2.41	1.75	1.50	2.60
49.0	2.06	1.81	1.72	2.77
49.5	2.35	2.00	1.76	2.64
50.0	2.34	1.87	1.58	2.66

Table S21. $\lambda^{i}_{D-A} + \lambda^{o}_{D-A}(t_i)$, in eV, for the DNA base pairs, using $\mathcal{S}_3 = \{\varepsilon_o = 2, \varepsilon_s = 8\}$.

t_i (ns)	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.0	1.72	1.50	1.24	1.83
10.5	1.97	1.26	1.09	1.84
11.0	1.84	1.47	1.22	1.84
11.5	1.97	1.53	1.12	1.88
12.0	2.03	1.33	1.24	1.78
12.5	1.93	1.28	1.32	1.81
13.0	1.93	1.21	1.26	1.84
13.5	1.77	1.47	1.31	1.92
14.0	2.01	1.37	1.32	1.84
14.5	2.00	1.43	1.31	1.83
15.0	1.96	1.36	1.23	1.71
15.5	1.91	1.41	1.24	1.95
16.0	1.82	1.28	1.31	1.91
16.5	1.87	1.32	1.32	1.84
17.0	1.96	1.19	1.40	1.95
17.5	1.81	1.27	1.32	1.86
18.0	1.89	1.23	1.22	1.72
18.5	1.99	1.39	1.22	1.95
19.0	1.95	1.38	1.36	1.92
19.5	1.88	1.28	1.16	1.92
20.0	2.02	1.44	1.18	1.86
20.5	1.92	1.42	1.20	1.81
21.0	1.97	1.39	1.26	1.84
21.5	1.87	1.37	1.23	1.84
22.0	1.95	1.47	1.21	1.86
22.5	1.95	1.34	1.23	1.88
23.0	1.93	1.23	1.37	1.77
23.5	1.76	1.28	1.25	1.86
24.0	1.85	1.38	1.29	1.83
24.5	1.88	1.25	1.26	1.93
25.0	1.79	1.38	1.31	1.89
25.5	1.84	1.34	1.22	1.87
26.0	1.90	1.39	1.28	1.96
26.5	1.84	1.35	1.22	1.87
27.0	1.98	1.34	1.28	1.89
27.5	1.97	1.32	1.36	1.84
28.0	1.86	1.35	1.17	1.89
28.5	1.81	1.43	1.27	1.82
29.0	1.94	1.34	1.32	1.93
29.5	1.90	1.57	1.30	1.87
30.0	1.95	1.44	1.30	1.82
30.5	1.97	1.41	1.24	1.92

31.0	1.79	1.53	1.40	1.88
31.5	1.95	1.38	1.23	1.81
32.0	1.93	1.49	1.24	1.82
32.5	1.95	1.37	1.18	1.91
33.0	1.90	1.43	1.37	1.91
33.5	2.03	1.27	1.39	1.90
34.0	1.67	1.30	1.23	1.87
34.5	1.88	1.28	1.35	1.93
35.0	2.00	1.47	1.37	1.83
35.5	1.84	1.42	1.23	1.87
36.0	1.89	1.48	1.30	1.90
36.5	1.86	1.28	1.17	1.82
37.0	1.91	1.47	1.41	1.76
37.5	1.97	1.32	1.26	1.91
38.0	1.97	1.46	1.20	1.83
38.5	2.01	1.27	1.25	1.81
39.0	1.87	1.38	1.49	1.87
39.5	1.95	1.36	1.37	1.81
40.0	1.91	1.37	1.45	1.88
40.5	1.90	1.50	1.23	1.88
41.0	1.88	1.22	1.25	1.85
41.5	1.99	1.33	1.28	1.76
42.0	1.89	1.32	1.34	1.76
42.5	1.90	1.30	1.36	1.85
43.0	1.93	1.41	1.14	1.90
43.5	1.90	1.33	1.29	1.93
44.0	1.99	1.34	1.28	1.98
44.5	2.00	1.25	1.26	1.86
45.0	1.82	1.33	1.34	1.94
45.5	1.94	1.41	1.34	1.87
46.0	1.80	1.39	1.50	1.92
46.5	1.84	1.43	1.42	1.97
47.0	1.81	1.31	1.37	1.92
47.5	1.85	1.49	1.28	1.87
48.0	1.79	1.48	1.26	1.92
48.5	1.96	1.30	1.45	1.89
49.0	1.84	1.36	1.26	1.86
49.5	1.87	1.45	1.27	1.94
50.0	1.94	1.39	1.45	1.92

Table S22. $\lambda^{i}_{D-A} + \lambda^{o}_{D-A}(t_i)$, in eV, for the 2'F-NA base pairs, using $\mathcal{S}_3 = \{\varepsilon_o = 2, \varepsilon_s = 8\}$.

t_i (ns)	CG-GC	GC-A_1T	A_1T-A_2T	A_2T-TA
10.0	1.94	1.30	1.18	1.82
10.5	1.62	1.46	1.49	1.97
11.0	1.78	1.32	1.19	1.88
11.5	1.72	1.53	1.39	2.00
12.0	1.82	1.46	1.13	1.97
12.5	1.87	1.47	1.36	1.96
13.0	1.84	1.56	1.28	1.78
13.5	1.58	1.49	1.44	1.87
14.0	1.44	1.54	1.35	1.86
14.5	1.65	1.41	1.22	1.85
15.0	1.81	1.32	1.31	1.92
15.5	1.77	1.60	1.41	1.91
16.0	1.77	1.43	1.38	1.96
16.5	1.83	1.54	1.38	1.89
17.0	1.78	1.20	1.32	2.05
17.5	1.79	1.43	1.29	1.82
18.0	1.60	1.45	1.33	1.88
18.5	1.65	1.41	1.22	1.85
19.0	1.71	1.35	1.42	1.96
19.5	1.73	1.42	1.40	2.00
20.0	1.86	1.35	1.29	1.96
20.5	1.61	1.46	1.35	1.99
21.0	1.74	1.61	1.62	2.00
21.5	1.84	1.43	1.44	2.05
22.0	1.77	1.40	1.26	1.98
22.5	1.75	1.53	1.38	1.99
23.0	1.72	1.38	1.30	1.88
23.5	1.84	1.37	1.19	1.86
24.0	1.72	1.32	1.27	1.86
24.5	1.81	1.46	1.34	1.94
25.0	1.77	1.49	1.36	1.88
25.5	1.67	1.55	1.28	1.98
26.0	1.83	1.33	1.32	1.90
26.5	1.73	1.47	1.37	2.00
27.0	1.80	1.49	1.37	2.06
27.5	1.77	1.43	1.25	2.07
28.0	1.84	1.24	1.44	1.88
28.5	1.73	1.40	1.36	1.77
29.0	1.79	1.44	1.28	2.05
29.5	1.76	1.38	1.38	1.94
30.0	1.82	1.42	1.27	1.93
30.5	1.83	1.45	1.35	1.96

31.0	1.61	1.48	1.30	1.93
31.5	1.67	1.30	1.25	1.87
32.0	1.73	1.41	1.32	1.92
32.5	1.76	1.27	1.27	1.99
33.0	1.74	1.49	1.26	1.91
33.5	1.79	1.43	1.42	1.93
34.0	1.87	1.35	1.23	1.94
34.5	1.90	1.31	1.24	1.85
35.0	1.87	1.46	1.26	1.85
35.5	1.84	1.51	1.50	1.93
36.0	1.55	1.50	1.37	1.99
36.5	1.83	1.36	1.32	1.97
37.0	1.75	1.40	1.39	1.89
37.5	1.74	1.26	1.42	2.00
38.0	1.77	1.38	1.32	1.92
38.5	1.85	1.45	1.31	2.07
39.0	1.85	1.50	1.39	2.08
39.5	1.85	1.41	1.38	1.93
40.0	1.77	1.45	1.37	1.92
40.5	1.68	1.37	1.22	1.90
41.0	1.80	1.42	1.33	1.97
41.5	1.79	1.53	1.25	1.90
42.0	1.72	1.50	1.51	1.84
42.5	1.86	1.39	1.35	1.94
43.0	1.82	1.47	1.24	1.94
43.5	1.82	1.37	1.33	2.05
44.0	1.84	1.42	1.44	2.03
44.5	1.73	1.47	1.27	1.93
45.0	1.91	1.21	1.40	1.97
45.5	1.74	1.29	1.32	1.90
46.0	1.88	1.30	1.29	1.96
46.5	1.81	1.42	1.17	1.95
47.0	1.83	1.33	1.15	1.87
47.5	1.65	1.46	1.47	1.90
48.0	1.74	1.41	1.36	1.93
48.5	1.85	1.37	1.16	1.93
49.0	1.61	1.41	1.32	2.04
49.5	1.82	1.54	1.34	1.95
50.0	1.81	1.45	1.22	1.97

Table S23. $\lambda^{o}_{D-A} \equiv < \lambda^{o}_{D-A}(t) >$ (see eq 4), in eV, for the indicated systems and choices of dielectric constants.

	DNA			2'F-ANA		
base pair	S_1	S_2	S_3	S_1	S_2	S_3
CG-GC	1.23	1.86	1.28	1.10	1.66	1.15
GC-A_1T	0.82	1.23	0.85	0.87	1.31	0.90
A_1T-A_2T	0.84	1.26	0.87	0.88	1.32	0.91
A_2T-TA	1.39	2.10	1.45	1.46	2.20	1.52

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