Supplementary Material

Similarities and differences in interaction of K^+ and Na^+ with condensed ordered DNA. A molecular dynamics simulation study.

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Table 1S. General properties of the simulated systems.

System	Cell dimension, Å	Density, g/cm^3	Box volume, nm^3	Species concentration, M	Diffusion parameters: $D\cdot10^{10}$, m^2/s (<R>, Å)*
K/20	43.4×37.6×33.0	1.318	53.85	37.52 (H_2O) 2.001 (K^+) 0.125 (Cl^-)	7.0 (20.6) H_2O 3.52 (14.6) K^+ 3.0 (13.5) Cl^-
K/15	39.5×34.2×33.2	1.375	44.7	33.21 (H_2O) 2.214 (K^+)	4.35 (16.2) H_2O 1.76 (10.3) K^+
Na/20	42.8×37.1×32.9	1.326	52.2	38.39 (H_2O) 2.048 (Na^+) 0.128 (Cl^-)	5.5 (18.2) H_2O 1.33 (8.9) Na^+ 3.22 (10.3) Cl^-
Na/15	39.1×33.8×32.8	1.382	43.9	34.82 (H_2O) 2.321 (Na^+)	2.82 (13.0) H_2O 0.58 (5.93) Na^+
K/20-22¶	45.9×39.8×29.4	1.320	53.72	37.11 (H_2O) 1.979 (K^+) 0.124 (Cl^-)	6.9 (20.4) H_2O 3.30 (14.1) K^+ 3.08 (13.6) Cl^-
K/15-22¶	43.3×37.5×27.7	1.371	44.8	33.30 (H_2O) 2.220 (K^+)	4.30 (16.1) H_2O 1.90 (10.7) K^+
Na/20-22¶	44.2×38.3×30.85	1.328	51.9	38.40 (H_2O) 2.045 (Na^+) 0.128 (Cl^-)	4.75 (17.0) H_2O 1.40 (9.2) Na^+ 2.05 (11.2) Cl^-
Na/15-22¶	43.3×34.3×32.0	1.380	43.3	34.55 (H_2O) 2.303 (Na^+)	2.85 (13.1) H_2O 0.56 (5.8) Na^+

* D is diffusion coefficient; <R> is root mean square displacement calculated for 1 ns. ¶ 10 ns MD simulations with CHARMM22 force field, other conditions are similar to these of corresponding system simulated with the use of the CHARMM27 force field.

Experimental and MD simulation data for comparison

I. Low water content

1. Ref. (1); Experimental data on Na-DNA oriented fibers, NMR relaxation method: 85% relative humidity (RH), 13 H_2O/nucleotide, D_{wat}=2.1·10^{-10} m^2/s; 95% RH, 22 H_2O/nucleotide, D_{wat}=5.3·10^{-10} m^2/s.
2. Ref. (1); MD simulation data; CHARMM22 force field, water model SPC, Ref. (2). Na^+, model Ref. (3), *15 H_2O/phosphate:* D_{Na}=0.55·10^{-10} m^2/s, D_{wat}=2.5·10^{-10} m^2/s; *20 H_2O/phosphate:* D_{Na}=1.3·10^{-10} m^2/s, D_{wat}=4.6·10^{-10} m^2/s.

II. Water solutions.

3. Ref. (4); experimental data for simple salt solution at infinite dilution,: D_{Na}=13.3·10^{-10} m^2/s; D_K=19.6·10^{-10} m^2/s; D_{wat}=23·10^{-10} m^2/s.
4. Ref. (5); MD simulations of water: water model, SPC, Ref. (2), D_{wat}= (42.0±0.8)·10^{-10} m^2/s; water model SPC/E, Ref. (6), D_{wat}= (27-28)·10^{-10} m^2/s; water model TIP3P original Ref. (7), D_{wat}= (54-56)·10^{-10} m^2/s; water model TIP3P modified Ref. (8), D_{wat}= (59.0±0.8)·10^{-10} m^2/s.
5. Ref. (9); MD simulation data for simple salt solution at infinite dilution (water model, SPC/E, Ref. (6), Na^+, K^+, Ref. (3)): D_{Na}=(12.8±0.5)·10^{-10} m^2/s; D_K=(18.3±1.3)·10^{-10} m^2/s.
6. Ref. (10), MD simulation of the DNA solution, (227 H_2O/DNA phosphate; Amber, parm99; water model, TIP3P; Na^+ and K^+ models, Ref. (11)): D_{Na}=17·10^{-10} m^2/s, D_K=28·10^{-10} m^2/s.
7. Ref. (12), MD simulation of the DNA solution, (180 H_2O/DNA phosphate; Amber, parm94, water model TIP3P; Na^+, Ref. (11)): D_{Na}~10·10^{-10} m^2/s.

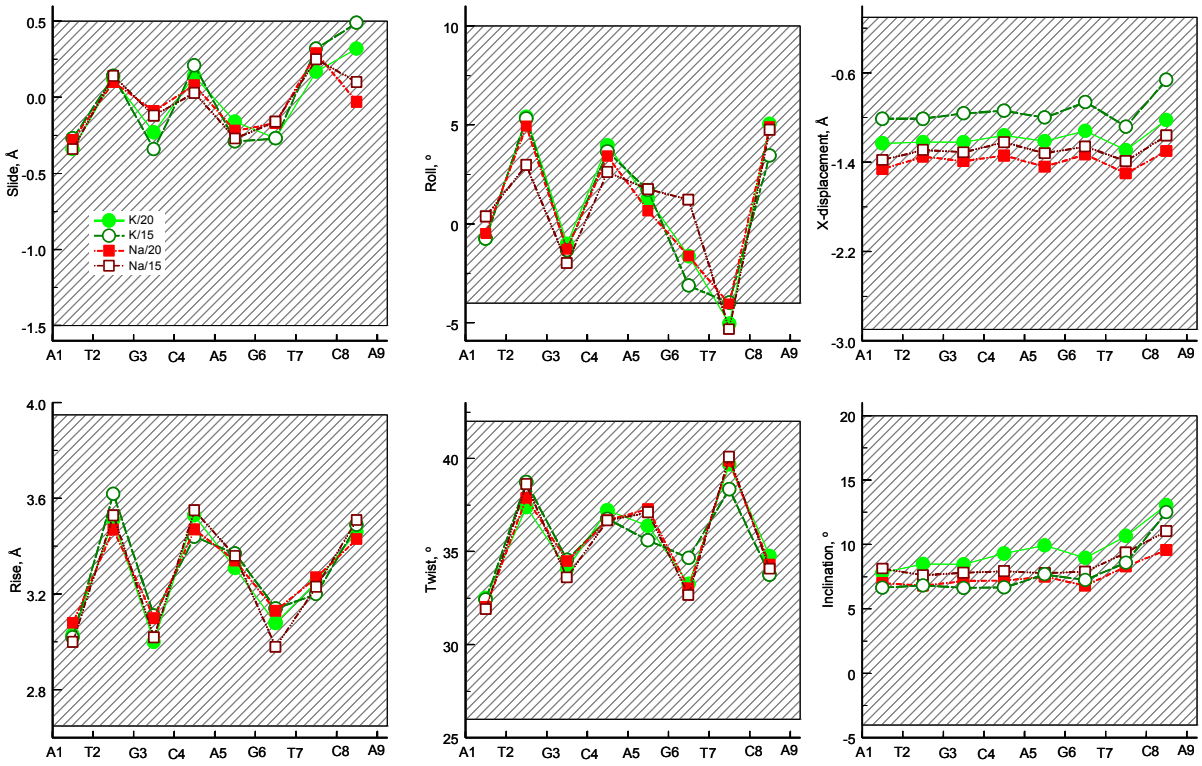

Figure 1S. Structural parameters (slide, roll, x-displacement, rise, twist, and inclination) of DNA base pair steps calculated by Curve5.2 (13) from averaged (over 20 ns and 3 decamers in the simulation cell) DNA structures of the four systems studied in the present work. The graphs show variation of the parameters in dependence of the DNA sequence. Shaded area shows regions typical for the B-DNA family found from analysis of X-ray crystallography data. The values of these six parameters are grouped in pairs (slide/rise, roll/twist, x-displacement/inclination) and displayed in Fig. 1 of the main text.

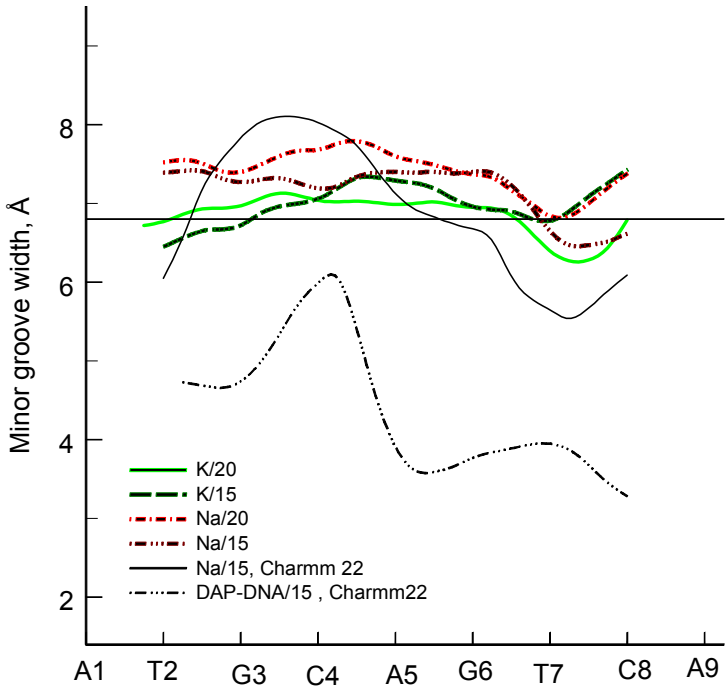

Figure 2S. Average minor groove width of the DNA sequence (*x*-axis) studied in the present work. For comparison, data is given form our earlier work (14) using Charmm22 force field calculated from a 6 ns simulation for the same DNA sequence and 15 H_2O/nucleotide with Na^+ (thin black line) and the synthetic polyamine (diaminopropane^{2+}, DAP, thin dot-dashed black line) as the DNA counterions. The DAP-DNA system shows an example of strong influence of the ligand binding on the DNA structure. Horizontal bar shows the value of the minor groove width of the "ideal" B-DNA.

Table 2S. Averaged occupancies and residence times (in ps) for water (Ow) and K^+/Na^+. Numbers separated by slash are average and longest residence time respectively.

DNA site		Ow				K^+ or Na^+			
		K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
Phosphate oxygen									
O1P	Occupancy	2.59	2.82	2.61	2.68	0.24	0.17	0.35	0.22
	Res. time	6.99/1278	5.56/1188	6.00/2520	5.95/2028	7.84/1566	5.88/510	58.3/11880	41.4/4752
O2P	Occupancy	2.67	2.65	2.58	2.75	0.14	0.09	0.14	0.08
	Res. time	7.54/1158	7.29/876	8.48/1482	7.35/1020	5.77/684	5.02/414	24.3/3744	18.8/1506
O3*	Occupancy	1.05	1.06	1.18	1.15	0.08	0.06	0.04	0.02
	Res. time	3.36/648	3.09/372	3.99/1878	3.58/744	5.45/702	4.73/288	5.62/1392	3.58/894
O5*	Occupancy	0.29	0.32	0.38	0.36	0.03	0.02	0.01	0.01
	Res. time	2.05/342	1.58/288	2.08/3612	1.81/732	3.55/678	3.54/2682	1.78/270	3.57/2328
Sugar									
O4*	Occupancy	1.00	1.14	1.32	1.19	0.24	0.17	0.05	0.05
	Res. time	4.90/1404	4.64/888	5.76/5628	5.63/2742	14.0/3702	13.1/1722	16.2/7240	17.9/2328
Minor groove									
TO2	Occupancy	0.87	1.05	1.54	1.61	0.47	0.31	0.10	0.14
	Res. time	3.49/1098	3.74/498	5.23/2046	5.14/1518	16.5/2532	15.2/1278	28.0/2868	27.9/2484
CO2	Occupancy	1.09	1.11	1.22	1.22	0.21	0.16	0.04	0.04
	Res. time	5.57/714	5.00/1380	6.41/4734	6.44/1938	8.78/2004	8.56/1440	9.60/768	9.86/990
AN3	Occupancy	0.89	0.94	1.08	1.08	0.30	0.20	0.03	0.05
	Res. time	5.05/834	6.11/672	9.27/5196	8.23/3396	32.8/4194	25.5/1884	10.0/696	23.6/1896
GN3	Occupancy	1.04	1.07	1.13	1.15	0.15	0.12	0.03	0.03
	Res. time	6.91/858	6.89/1188	7.75/2994	7.94/1500	12.07/1770	7.82/774	27.1/2160	13.9/1356

Continuation of Table 2S

DNA site		Ow				K^+ or Na^+			
		K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
Major groove									
AN7	Occupancy	0.95	0.95	1.09	1.09	0.22	0.19	0.09	0.09
	Res. time	5.28/438	5.46/438	5.29/852	5.12/618	22.5/2700	16.8/1080	38.3/2406	44.6/1452
GN7	Occupancy	0.98	1.11	1.27	1.31	0.28	0.26	0.05	0.06
	Res. time	4.02/696	3.67/444	4.72/840	4.61/576	23.5/1038	25.1/1398	22.1/708	19.5/1020
GO6	Occupancy	0.95	0.95	1.40	1.43	0.30	0.27	0.05	0.05
	Res. time	3.97/252	3.95/270	5.49/948	5.46/1278	32.65/2946	32.75/2856	16.0/654	12.0/588
TO4	Occupancy	1.05	1.00	1.38	1.26	0.14	0.17	0.01	0.01
	Res. time	3.76/228	3.73/240	4.31/612	4.24/582	8.44/996	9.15/1110	5.15/174	5.87/258

K^+/Na^+	Occupancy	7.28	7.56	5.295	5.47
	Res. time	7.06/3120	5.98/1280	19.9/5820	18.3/2920

MD simulation results on K^+/Na^+ – Ow coordination number and residence time:

Data for comparison: Ref. (9); MD simulation data for simple salt solution at infinite dilution (water model, SPC/E, Ref. (6), Na^+, K^+, Ref. (3)): K^+ - Ow occupancy 7.1, RT_{av} = 14.3 ps; Na^+ - Ow occupancy 5.8, RT_{av} = 22.4 ps. (In the cited work, values of RT_{av} were calculated assuming 2 ps delay time; delay time used in the present work was 1 ps).

Table 3S. Occupancies and average and longest (in parentheses) residence times (in ps) of K^+/Na^+ and water (Ow) near electronegative sites of the DNA bases.

TO2

DNA site	K^+ or Na^+				Ow			
	K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
T2 Occupancy	0.65	0.39	0.10	0.14	0.90	1.13	1.57	1.60
Res. time	11.2 (1566)	11.5 (804)	23.7 (942)	26.0 (1806)	3.45 (444)	3.59 (348)	5.18 (1188)	5.13 (1224)
T7 Occupancy	0.50	0.34	0.23	0.13	0.84	1.02	1.67	1.49
Res. time	31.5 (2532)	20.9 (1074)	92.0 (3180)	29.4 (1434)	3.08 (288)	3.59 (498)	4.98 (2046)	4.99 (1086)
T11 Occupancy	0.48	0.31	0.05	0.04	0.78	0.99	1.37	1.35
Res. time	31.6 (2130)	28.7 (1278)	17.0 (1182)	17.4 (1074)	3.05 (942)	3.23 (330)	5.31 (1428)	4.71 (846)
T15 Occupancy	0.40	0.18	0.06	0.20	0.90	1.16	1.41	1.37
Res. time	22.6 (2502)	20.6 (852)	26.4 (816)	36.5 (2496)	3.54 (720)	4.12 (390)	5.74 (870)	5.15 (972)
T19 Occupancy	0.33	0.33	0.12	0.18	1.17	1.19	1.81	1.46
Res. time	10.0 (1788)	11.6 (960)	15.9 (1146)	22.9 (1806)	4.46 (1098)	4.28 (396)	5.16 (918)	4.66 (600)

CO2

DNA site	K^+ or Na^+				Ow			
	K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
C4 Occupancy	0.08	0.06	0.00	0.01	0.94	0.98	0.92	1.09
Res.time	10.80(474)	8.79(252)	5.68(78)	6.78(96)	5.14(348)	5.22(414)	5.82(1476)	6.36(1572)
C8 Occupancy	0.38	0.32	0.09	0.07	0.97	0.98	1.37	1.55
Res.time	8.87(942)	9.60(1440)	7.34(702)	9.27(750)	4.56(480)	3.89(246)	6.87(4734)	6.90(2010)
C14 Occupancy	0.21	0.18	0.03	0.09	1.17	1.17	1.33	1.23
Res.time	7.29(1998)	8.90(810)	14.33(570)	25.71(990)	6.65(360)	5.74(402)	6.11(1974)	6.55(1284)
C17 Occupancy	0.10	0.09	0.03	0.01	0.95	1.01	0.96	1.07
Res.time	22.67(678)	16.49(516)	19.17(768)	4.55(72)	5.35(318)	5.24(318)	5.94(624)	6.40(678)
C20 Occupancy	0.31	0.20	0.02	0.04	1.02	1.28	1.48	1.28
Res.time	7.38(744)	6.65(474)	14.10(294)	8.26(210)	4.36(468)	5.01(1380)	6.94(3966)	6.27(1056)

AN3

DNA site	K^+ or Na^+				Ow			
	K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
A1 Occupancy	0.41	0.21	0.02	0.04	0.73	0.97	1.11	1.13
Res.time	43.8 (4194)	30.5 (1884)	27.7 (468)	25.0 (564)	6.04 (774)	6.61 (678)	9.60 (5196)	8.19 (2628)
A5 Occupancy	0.21	0.19	0.06	0.01	0.88	0.88	1.01	1.05
Res.time	26.5 (1242)	30.9 (750)	28.0 (696)	19.3 (402)	5.82 (564)	6.07 (534)	8.96 (2484)	9.74 (1428)
A9 Occupancy	0.16	0.26	0.05	0.12	1.18	0.97	1.15	0.97
Res.time	12.8 (816)	20.4 (1338)	8.12 (576)	32.9 (1896)	5.03 (834)	4.63 (606)	7.26 (3528)	7.37 (1368)
A13 Occupancy	0.54	0.14	0.01	0.06	0.62	1.02	1.11	1.08
Res.time	59.0 (1920)	16.6 (1434)	5.78 (228)	20.7 (1380)	3.67 (486)	6.01 (606)	8.16 (4416)	7.43 (2448)
A18 Occupancy	0.20	0.20	0.01	0.06	0.96	0.93	1.10	1.12
Res.time	29.1 (1254)	32.8 (1038)	29.5 (408)	37.2 (870)	6.75 (660)	7.21 (660)	10.4 (2022)	9.39 (3396)

GN3

DNA site	K^+ or Na^+				Ow			
	K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
G3 Occupancy	0.12	0.09	0.01	0.01	1.04	1.12	1.23	1.20
Res.time	10.4 (1152)	6.91 (426)	16.5 (288)	10.4 (168)	7.52 (858)	7.08 (516)	8.30 (1512)	7.51 (1500)
G6 Occupancy	0.15	0.10	0.02	0.02	1.03	1.08	1.26	1.26
Res.time	10.9 (1770)	9.93 (372)	22.3 (360)	34.1 (774)	8.34 (696)	8.55 (582)	8.42 (2994)	10.4 (1926)
G10 Occupancy	0.07	0.16	0.06	0.04	1.09	0.95	1.14	1.08
Res.time	12.5 (870)	14.3 (600)	63.9 (2160)	21.5 (1356)	6.58 (780)	6.56 (984)	5.98 (1536)	8.18 (1170)
G12 Occupancy	0.30	0.10	0.01	0.02	0.83	1.05	1.07	1.15
Res.time	16.0 (924)	10.3 (444)	9.25 (84)	13.7 (222)	6.20 (732)	6.02 (1188)	7.51 (1710)	6.74 (768)
G16 Occupancy	0.11	0.11	0.07	0.05	1.23	1.12	1.13	1.17
Res.time	7.10 (504)	8.06 (738)	43.8 (1458)	25.9 (726)	6.82 (810)	6.63 (582)	7.76 (1740)	7.69 (852)

GN7

DNA site	K^+ or Na^+				Ow			
	K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
G3 Occupancy	0.06	0.06	0.00	0.03	1.16	1.13	1.19	1.23
Res.time	14.2 (300)	18.5 (792)	8.70 (24)	23.0 (618)	4.72 (456)	4.78 (444)	5.53 (840)	4.96 (546)
G6 Occupancy	0.46	0.41	0.15	0.05	0.99	0.97	1.30	1.38
Res.time	20.9 (1014)	22.8 (636)	29.8 (1212)	15.1 (486)	3.64 (276)	3.78 (384)	5.50 (738)	5.43 (378)
G10 Occupancy	0.61	0.56	0.08	0.17	0.61	0.80	1.16	1.21
Res.time	48.4 (1998)	45.2 (1398)	24.6 (708)	23.3 (1200)	2.64 (216)	2.46 (156)	4.08 (330)	3.69 (234)
G12 Occupancy	0.21	0.15	0.03	0.02	1.33	1.28	1.40	1.41
Res.time	20.5 (618)	23.6 (402)	16.6 (204)	10.4 (510)	3.36 (264)	3.45 (222)	4.29 (534)	4.32 (576)
G16 Occupancy	0.08	0.06	0.02	0.03	1.15	1.14	1.22	1.23
Res.time	14.1 (294)	15.2 (342)	26.0 (420)	33.6 (936)	4.63 (696)	4.87 (324)	5.20 (456)	5.35 (498)

GO6

DNA site	K^+ or Na^+				Ow			
	K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
G3 Occupancy	0.12	0.11	0.00	0.02	1.60	1.46	1.38	1.66
Res.time	20.5 (786)	14.9 456)	7.46 (144)	9.15 (216)	6.01 (414)	5.71 (294)	5.80 (402)	6.42 (636)
G6 Occupancy	0.51	0.45	0.17	0.10	0.58	0.73	1.34	1.43
Res.time	37.6 (1326)	40.8 (1296)	18.6 (654)	23.0 (528)	2.82 (180)	2.68 (150)	4.87 (816)	4.66 (1092)
G10 Occupancy	0.61	0.57	0.05	0.12	0.54	0.58	1.36	1.60
Res.time	105 (2946)	89.5 (2856)	12.5 (342)	10.8 (588)	2.58 (150)	2.66 (108)	5.37 (696)	5.38 (456)
G12 Occupancy	0.12	0.10	0.01	0.01	1.18	1.05	1.32	1.29
Res.time	11.7 (774)	15.1 (732)	7.09 (96)	14.4 (168)	5.38 (252)	5.48 (270)	5.84 (444)	5.84 (540)
G16 Occupancy	0.11	0.11	0.01	0.01	1.36	1.43	1.71	1.51
Res.time	14.2 (414)	13.8 (414)	14.5 (138)	5.64 (132)	5.64 (306)	5.68 (360)	5.95 (498)	5.83 (768)

AN7

DNA site	K^+ or Na^+				Ow			
	K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
A1 Occupancy	0.02	0.03	0.06	0.01	1.10	1.05	1.11	1.10
Res.time	20.4 (318)	26.5 (330)	107 (654)	84.3 (558)	6.21 (372)	6.82 (480)	6.67 (672)	6.83 (426)
A5 Occupancy	0.46	0.36	0.21	0.15	0.88	0.92	1.18	1.19
Res.time	22.3 (780)	16.9 (900)	29.4 (2406)	45.9 (1242)	3.48 (234)	3.58 (252)	3.83 (852)	3.90 (372)
A9 Occupancy	0.57	0.49	0.13	0.22	0.77	0.84	1.19	0.93
Res.time	23.4 (2058)	15.9 (972)	50.7 (2010)	35.6 (936)	2.90 (240)	3.19 (234)	3.47 (540)	3.66 (228)
A13 Occupancy	0.01	n.a.	0.03	0.05	1.13	1.13	1.04	1.05
Res.time	26.0 (282)	n.a.	129 (1500)	101 (1452)	4.94 (438)	5.04 (402)	6.95 (570)	6.25 (618)
A18 Occupancy	0.03	0.07	0.03	0.02	1.07	1.01	1.07	1.09
Res.time	22.9 (486)	55.4 (1080)	109 (1368)	71.0 (492)	7.27 (444)	6.81 (438)	8.35 (546)	6.78 (516)

TO4

DNA site	K^+ or Na^+				Ow			
	K/15	K/20	Na/15	Na/20	K/15	K/20	Na/15	Na/20
T2 Occupancy	0.03	0.05	0.01	0.01	1.06	1.25	1.25	1.28
Res.time	5.24 (126)	5.70 (168)	4.65 (60)	6.31 (198)	3.38 (162)	3.43 (150)	3.76 (414)	3.81 (264)
T7 Occupancy	0.24	0.27	0.06	0.03	1.55	1.66	1.87	1.88
Res.time	7.66 (300)	8.88 (240)	8.97 (870)	6.44 (258)	5.33 (240)	5.31 (342)	5.70 (774)	5.70 (552)
T11 Occupancy	0.00	0.00	n.a.	0.00	0.61	0.78	0.94	0.96
Res.time	4.00 (156)	1.84 (30)	n.a.	8.50 (138)	3.28 (156)	3.16 (144)	3.39 (288)	3.35 (306)
T15 Occupancy	0.00	0.01	0.00	n.a.	0.87	0.85	1.01	0.95
Res.time	1.59 (42)	2.49 (72)	6.93 (84)	n.a.	3.85 (174)	4.22 (240)	4.53 (372)	4.15 (288)
T19 Occupancy	0.47	0.48	0.01	0.02	1.03	0.98	1.93	1.58
Res.time	12.4 (1008)	13.7 (1110)	3.88 (90)	4.89 (132)	3.52 (168)	3.11 (222)	5.09 (528)	4.50 (582)

References

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