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Supplemental Information

Quantitative Studies of an RNA Duplex Electrostatics by Ion Counting

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Quantitative studies of an RNA duplex electrostatics by ion counting

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Overview of the Supplementary Information

In this supplementary information, we provide a table with preferential ion interaction coefficients Γ_i (e.g. the number of associated ions, i = Na^+ or Br^-), around 24-bp RNA, 24-bp and 23-bp DNA (Table S1) for NaBr; a table summarizing the fraction of charge neutralization from attraction of Na^+ measured by ASAX and BE-ICP-MS around dsRNA and dsDNA (Table S2); a table with preferential ion interaction coefficients from competition experiments between Na^+:Mg^{2+} and Cs^+:Mg^{2+} around 24-bp RNA. The results are consistent with observations in the main text and support the conclusions described therein.

Table S1: Experimentally determined preferential interaction coefficients (Γ_i) for NaBr around 24-bp RNA, 24-bp DNA, and 23-bp DNA

	24 bp RNA			**24 bp DNA**			**23 bp DNA**		
C [M]	Γ_{Na^+}	Γ_{Br^-}	**total**	Γ_{Na^+}	Γ_{Br^-}	**total**	Γ_{Na^+}	Γ_{Br^-}	**total**
0.01	39 ± 1.0	-6.0 ± 0.7	45.0 ± 1.2	37.0 ± 1.0	-9.0 ± 0.5	46.0 ± 1.0	36.0 ± 0.2	-8.0 ± 0.3	44.0 ± 0.3
0.02	39.5 ± 0.5	-6.5 ± 1.0	46.0 ± 1.0	37.0 ± 0.2	-8.75 ± 0.2	46.0 ± 0.3	35.0 ± 0.3	-8.6 ± 0.2	44.0 ± 0.3
0.10	37.0 ± 1.0	-8.0 ± 1.2	45.0 ± 1.6	34.0 ± 1.0	-11.5 ± 1.0	45.5 ± 1.4	32.0 ± 1.0	-12.0 ± 1.0	44.0 ± 1.0
0.12	36.0 ± 1.0	-10.0 ± 1.5	46.0 ± 1.8	-	-	-			
0.26	-	-	-	-	-	-	27.0 ± 1.5	-17.5 ± 1.0	44.5 ± 1.8
0.50	31.0 ± 1.5	-13 ± 2.0	44.0 ± 2.5	24.6 ± 1.0	-21.5 ± 1.5	46.0 ± 1.8			
0.65	-	-	-				18.0 ± 0.5	-26 ± 0.5	44.0 ± 0.5

Table S2. Interaction coefficients for NaBr around 24-bp DNA obtained previously in reference (3)

	NaBr		
C [M]	Γ_{Na^+}	Γ_{Br^-}	**total**
0.010	37.0 ± 0.9	-9.0 ± 0.9	46 ± 1.3
0.050	36.0 ± 0.7	-8.7 ± 0.7	44.7 ± 1.0
0.100	35.0 ± 1.0	-10 ± 1.0	45 ± 1.4
0.200	32.0 ± 1.5	-14.5 ± 1.5	46.5 ± 2.0
0.350	28.0 ± 1.5	-16.7 ± 1.2	44.7 ± 2.0
0.500	24.6 ± 1.0	-21.5 ± 1.5	46.1 ± 1.8

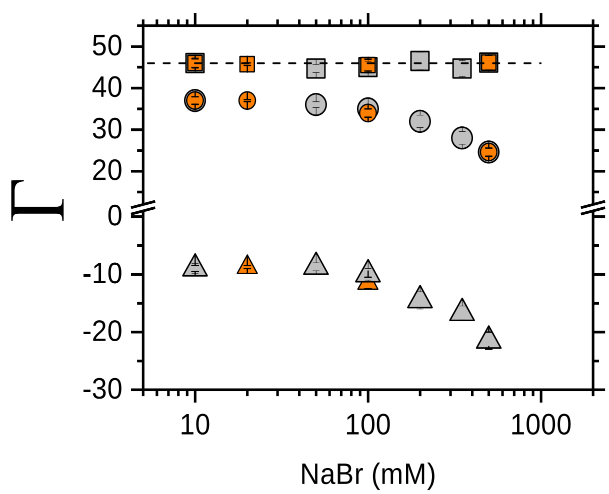

Figure S1. Comparison of current (orange symbols) and previous (grey symbols) ion counting results for association of NaBr around 24-bp DNA from BE-ICP-MS measurements. Data point in grey are from reference (3) and values are given in Table S2.

Table S3: Experimentally determined fraction of charge neutralization (Γ^*_{Na}) for Na^+ around dsRNA and dsDNA at 100 mM monovalent salt concentration.

	dsRNA		ds DNA	
C [M]	Γ^{*ASAXS}_{Na}	$\Gamma^{*BE-ICPMS}_{Na}$	Γ^{*ASAXS}_{Na}	$\Gamma^{*BE-ICPMS}_{Na}$
0.1	0.73 ± 0.06 [(a)]	0.80 ± 0.02	0.71 ± 0.06 [(b)]	0.74 ± 0.02

a) Data taken from reference 1
b) Data taken from reference 2

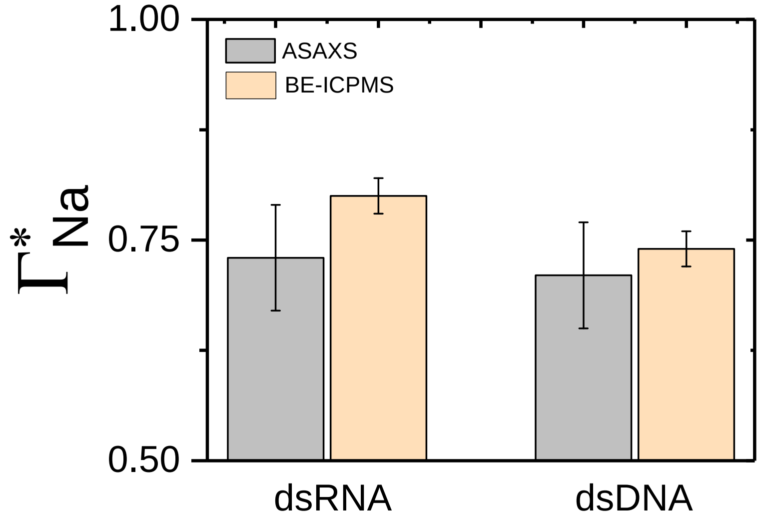

Figure S2. Comparison of experimentally determined fraction of charge neutralization (Γ^*_{Na}) for Na^+ around dsRNA and dsDNA from ASAXS and BE-ICP-MS. Data from Table S2.

Table S4: Experimentally determined preferential interaction coefficients and α value for **NaBr** and **CsBr** around 24-bp RNA in the presence of 6 mM $MgBr_2$.

NaBr	**24-bp RNA**				**CsBr**	**24-bp RNA**			
C [M]	Γ_{Na^+}	$\Gamma_{Mg^{2+}}$	Γ_{Br^-}	**total**	**C [M]**	Γ_{Cs^+}	$\Gamma_{Mg^{2+}}$	Γ_{Br^-}	**total**
0.00	0	21.0 ± 0.5	-3.0 ± 1.0	46.0 ± 1.0	0	0	21.0 ± 0.5	-4.0	46.0 ± 0.7
0.0015	0.6 ± 0.5	22.0 ± 0.5	-2.0 ± 0.5	46.8 ± 0.8	0.02	3.6 ± 1.0	19.0 ± 0.5	-5.4 ± 1.0	47.0 ± 1.5
0.01	2.9 ± 0.8	20.0 ± 0.4	-3.0 ± 1.6	45.6 ± 1.4	0.03	8.0 ± 1.0	16.0 ± 0.3	-5.0 ± 0.6	45.6 ± 1.2
0.02	3.9 ± 0.6	18.5 ± 0.4	-5.4 ± 1.4	46.5 ± 1.6	0.06	10.0 ± 0.5	16.0 ± 0.6	-4.0 ± 1.0	46.0 ± 1.2
0.03	6.5 ± 1.0	17.4 ± 0.4	-4.7 ± 1.8	46.0 ± 2.0	0.10	11.5 ± 1.0	13.5 ± 0.8	-7.0 ± 1.0	45.6 ± 1.6
0.05	9.3 ± 2.0	15.5 ± 1.4	-6.0 ± 1.2	46.3 ± 2.7	0.2	19.0 ± 0.9	8.1 ± 1.4	-10.0 ± 1.0	45.0 ± 1.7
0.08	10.0 ± 1.0	13.5 ± 1.0	-9.0 ± 1.0	46.0 ± 1.7		-	-	-	-
0.11	12.5 ± 2.0	11.0 ± 1.3	-11.0 ± 1.0	46.0 ± 2.7		-	-	-	-
0.20	19.8 ± 1.5	7.2 ± 0.4	-13.3 ± 1.3	47.5 ± 2.0		-	-	-	-
	α^*_{Na} = 17.0 ± 1.7					α^*_{Cs}= 18.3± 2.5			

*Defined in the main text

Table S5: Poisson Boltzmann calculations of preferential interaction coefficients and α value for monovalent salt (MX) around 24-bp DNA in the presence of 6 mM divalent salt (MX_2).

MX	24-bp DNA			
C [M]	Γ_{M^+}	$\Gamma_{M^{2+}}$	Γ_{X^-}	total
0.00	0	21.14	-3.7	46.0
0.005	2.5	19.5	-4.5	46.0
0.01	4.5	18.2	-5.1	46.0
0.02	7.53	16.16	-6.15	46.0
0.03	9.85	14.6	-6.95	46.0
0.04	11.73	13.32	-7.63	46.0
0.045	12.5	12.8	-7.95	46.0
0.05	13.23	12.26	-8.25	46.0
0.06	14.45	11.36	-8.83	46.0
0.08	16.45	9.85	-9.84	46.0
0.10	17.9	8.73	-10.7	46.0
0.15	20.0	6.68	-12.6	46.0
0.20	21.0	5.37	-14.26	46.0
0.30	21.27	3.79	-17.15	46.0
	$\alpha^*_{M^+} = 7.5$			

*Defined in the main text

Table S6: Poisson Boltzmann calculations of preferential interaction coefficients and α value for monovalent salt (MX) around 24-bp RNA in the presence of 6 mM divalent salt (MX_2).

MX	24-bp RNA			
C [M]	Γ_{M^+}	$\Gamma_{M^{2+}}$	Γ_{X^-}	total
0.00	0	21.45	-3.1	46.0
0.001	0.44	21.13	-3.3	46.0
0.01	3.5	19.1	-4.3	46.0
0.02	5.86	17.5	-5.14	46.0
0.03	7.62	16.32	-5.74	46.0
0.04	9.0	15.4	-6.2	46.0
0.05	10.24	14.5	-6.76	46.0
0.08	12.84	12.6	-7.96	46.0
0.10	14.13	11.62	-8.64	46.0
0.20	17.9	8.3	-11.5	46.0
0.3	19.5	6.3	-13.9	46.0
0.5	19.72	3.93	-18.43	46.0
	$\alpha^*_{M^+} = 13.3$			

*Defined in the main text

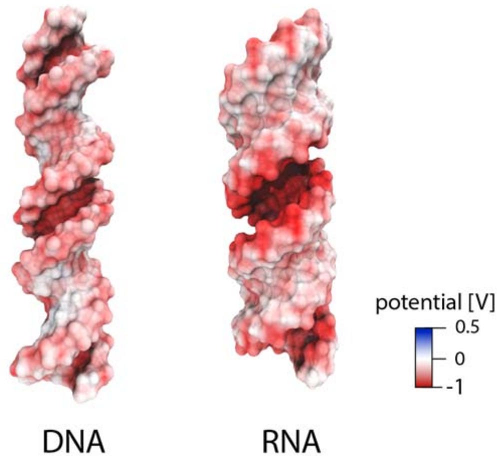

Figure S3. Poisson-Boltzmann calculations of electrostatic surface potential of the DNA and RNA duplexes. Calculations were carried out as described in the main text and Figure 3 in the main text.

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