

Supporting Information

The role of Na⁺ in Catalysis by the 8-17 DNAzyme

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Table S1. k_{obs} values measured in presence of 100 $\mu\text{M Pb}^{2+}$ and 25 $\mu\text{M Pb}^{2+}$ at pH 5.5 and 20 mM Mg^{2+} at pH 7.0 as a function of the concentration of Na^+ . The activity with each divalent cofactor was measured under different pH conditions considering the ability of each cation to activate de 8-17 DNAzyme. Data plotted in Figure 3 and Figures S1.

$[\text{Na}^+]$ (mM)	k_{obs} 100 $\mu\text{M Pb}^{2+}$ (min^{-1})	$[\text{Na}^+]$ (mM)	k_{obs} 25 $\mu\text{M Pb}^{2+}$ (min^{-1})	$[\text{Na}^+]$ (mM)	k_{obs} 20 mM Mg^{2+} (min^{-1})
12.7	0.207	9.8	0.009	20.3	0.249
24.5	0.403	15.3	0.048	24.7	0.200
26.5	0.592	21.7	0.246	34.6	0.274
32.3	1.479	31.4	0.374	39.1	0.228
32.7	1.014	32.8	1.013	48.1	0.219
34.1	1.102	43.2	1.157	58.5	0.214
38.9	1.639	48.8	1.309	78.3	0.261
44.6	2.479	55.4	2.293	92.7	0.340
48.6	2.800	62.3	1.964	105.3	0.238
52.1	3.628	63.8	1.985	123.0	0.209
56.7	4.091	72.7	2.331	135.3	0.189
66.2	4.447	83.8	2.116		
74.6	5.673	88.6	2.556		
83.3	6.181	93.1	2.139		
99.6	5.886	99.6	1.617		
103.1	5.613	103.4	1.690		
110.4	5.048	108.0	1.202		
123.4	5.984	110.4	1.747		
128.7	5.179	128.7	1.287		
142.9	5.2834	139.7	1.371		
149.9	4.77149	148.4	1.029		
151.2	5.00921	156.0	1.083		
156.9	4.71546				
pH 5.5				pH 7.0	

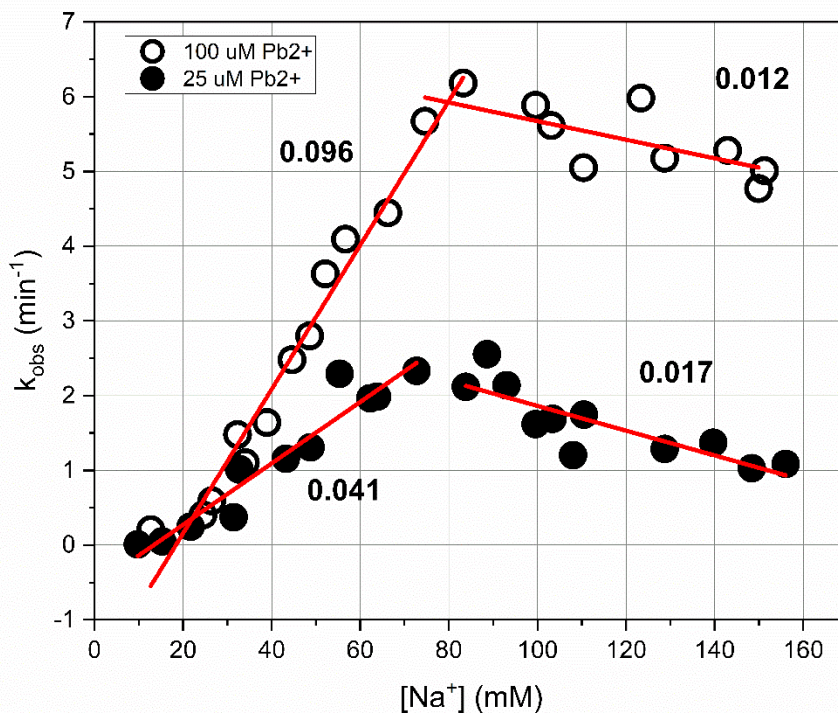


Figure S1. Influence of Na^+ concentration on the activity of the 8-17 DNAzyme with $100 \mu\text{M}$ (open circles) and $25 \mu\text{M}$ Pb^{2+} (black circles) at pH 5.5. Linear fittings are shown in red lines. Slopes are indicated in bold in each portion of the graph. Linear trend analysis of each portion are shown from Table S2-S5.

Table S2. Linear trend analysis of the 8-17 activity measured in presence of $100 \mu\text{M}$ Pb^{2+} . The fitting covers the region of Na^+ concentrations lower than 80 mM displayed in Figure S1. Data are informed as presented by Origin 8.5 software.

Equation	$y = a + b \cdot x$
Intercept	-1.77425 ± 0.23777
Slope	0.09649 ± 0.00487
Residual Sum of Squares	1.49607
Pearson's r	0.98508
R-Square (COD)	0.97037
Adj. R-Square	0.9679

Table S3. Linear trend analysis of the 8-17 activity measured in presence of 100 μM Pb^{2+} . The fitting covers de region of Na^+ concentrations higher than 80 mM displayed in Figure S1. Data are informed as presented by Origin 8.5 software.

Equation	$y = a + b*x$
Intercept	6.91751 ± 0.5893
Slope	-0.01244 ± 0.00511
Residual Sum of Squares	0.95844
Pearson's r	-0.67754
R-Square (COD)	0.45906
Adj. R-Square	0.38178

Table S4. Linear trend analysis of the 8-17 activity measured in presence of 25 μM Pb^{2+} . The fitting covers de region of Na^+ concentrations lower than 80 mM displayed in Figure S1. Data are informed as presented by Origin 8.5 software.

Equation	$y = a + b*x$
Intercept	-0.55076 ± 0.17695
Slope	0.0411 ± 0.00384
Residual Sum of Squares	0.58449
Pearson's r	0.96297
R-Square (COD)	0.9273
Adj. R-Square	0.91923

Table S5. Linear trend analysis of the 8-17 activity measured in presence of 25 μM Pb^{2+} . The fitting covers de region of Na^+ concentrations higher than 80 mM displayed in Figure S1. Data are informed as presented by Origin 8.5 software.

Equation	$y = a + b*x$
Intercept	3.51909 ± 0.41488
Slope	-0.01657 ± 0.00355
Residual Sum of Squares	0.70042
Pearson's r	-0.84139
R-Square (COD)	0.70794
Adj. R-Square	0.67548

Table S6. k_{obs} values of the 8-17 G14-AP variant measured at different pHs in presence of 100 μM Pb^{2+} . Data at 100 mM Na^+ were extracted from reference 18. The results were fitted to equations 2.

pH	k_{obs}	
	100 mM Na^+	25 mM Na^+
5.0	0.0775	0.0223
5.5	0.1728	0.0839
6.0	0.1835	0.1251
6.5	0.2340	0.1327
7.0	0.1439	0.0726
7.5	0.0569	0.0425
8	0.0298	0.0088
100 μM Pb^{2+}		

Table S7. Fitting parameters obtained from the pH-rate profile of the 8-17 G14AP variant measured in presence of 100 μM Pb^{2+} and 25 mM Na^+ . Data are informed as displayed by Origin 8.5 software.

Equation	$k/(1+10^{(A1-x)}+10^{(x-A2)})$
A1	5.79737 ± 0.14854
A2	6.72515 ± 0.14233
k	0.2328 ± 0.04005
Reduced Chi-Sqr	7.42434E-5
R-Square (COD)	0.97869
Adj. R-Square	0.96804

Table S8. Fitting parameters obtained from the pH-rate profile of the 8-17 G14AP variant measured in presence of 100 μM Pb^{2+} and 100 mM Na^+ . Data are informed as displayed by Origin 8.5 software.

Equation	$k/(1+10^{(A1-x)}+10^{(x-A2)})$
A1	5.41746 ± 0.19391
A2	7.00626 ± 0.18191
k	0.2912 ± 0.04693
Reduced Chi-Sqr	5.09052E-4
R-Square (COD)	0.93982
Adj. R-Square	0.90973