Supplementary Information

Insights into DNA catalysis from structural and functional studies of the 8-17 DNAzyme

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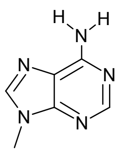
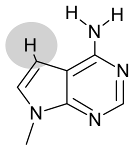
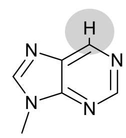
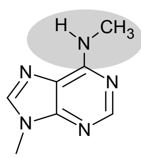
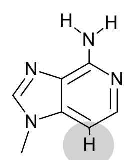
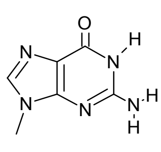
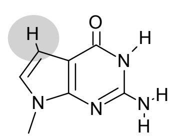
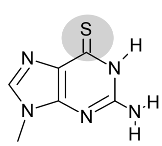
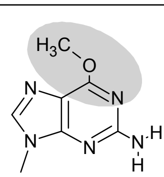
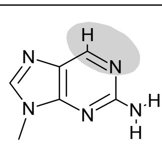
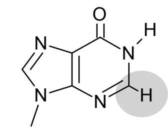
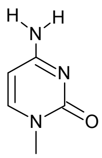
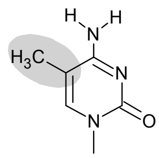
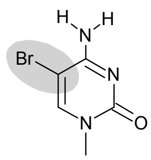
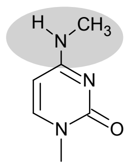
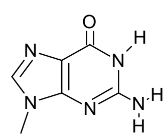
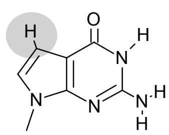
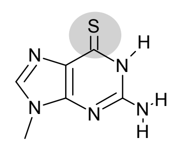
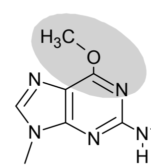
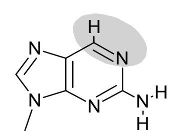
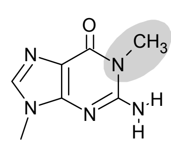
Supplementary Table 1.

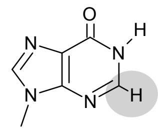
Comparison of different numbering systems for the 8-17 residues.

Numbering adopted in most of the functional literature [1]	Numbering adopted in the structural paper in Liu et al. [2]	Residues numbering in the PDB file (5XM8)	Notes
G18	**G-1**	**dG12 (chain F)**	**Subtrate residues flanking the cleavable phosphodiester**
G1.1	**G+1**	**dG13 (chain F)**	
T2.1	**T1**	**dT11 (chain E)**	
G3	**G2**	**dG12 (chain E)**	**Residues involved in the core stem (P3)**
C4	**C3**	**dC13 (chain E)**	
C5	**C4**	**dC14 (chain E)**	
A6	**A5**	**dA15 (chain E)**	
G7	**G6**	**dG16 (chain E)**	
C8	**C7**	**dC17 (chain E)**	
G9	**G8**	**dG18 (chain E)**	**Residues involved in the core stem (P3)**
G10	**G9**	**dG19 (chain E)**	
C11	**C10**	**dC20 (chain E)**	
T12	**T11**	**dT21 (chain E)**	
C13	**C12**	**dC22 (chain E)**	
G14	**G13**	**dG23 (chain E)**	**General acid-base catalyst**
A15	**A14**	**dA24 (chain E)**	
A15.0	**A15**	**dA25 (chain E)**	

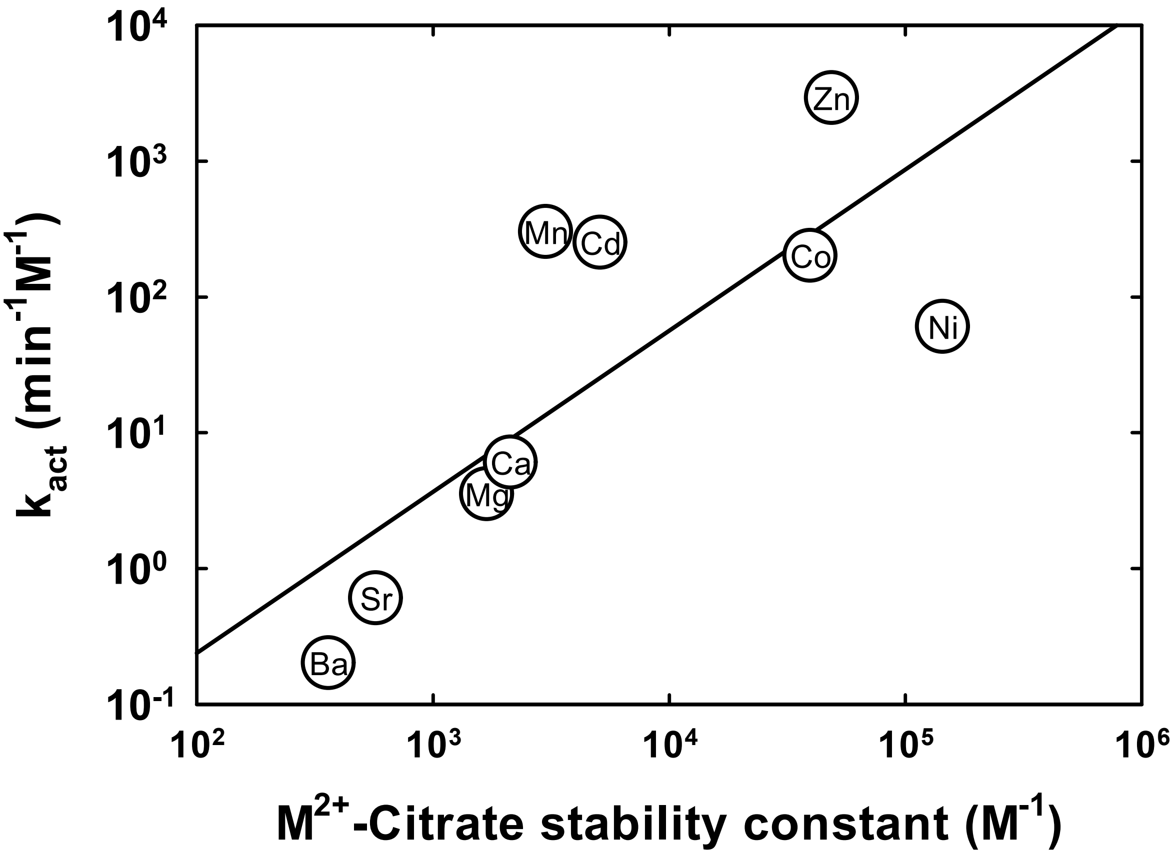
Supplementary Table 2.
Functional effects arising from substitution of selected functional groups in the 8-17 core.

		k_{rel}				
Original residue	**Modification**	**Mg (3 mM)**	**Mg (10 or 20 mM)**	**Mn (30 mM)**	**Pb (0.5 mM)**	**Reference**
 **A6**		**0.007**		**0.011**		3
		**0.12**		**0.13**		3
		**0.013**		**0.022**		3
			**1.4**			4
 **G7**		**0.04**	**0.4**	**0.17**		3, 5
		**0.0004**		**0.0007**		3
					**0.036**	2
		**0.001**		**0.002**		3

		**0.06**		**0.03**		3
 **C13**		**0.6**		**0.8**		3
		**0.25**		**0.2**		3
		**0.03**		**0.02**		3
 **G14**		**0.3**	**0.3**	**0.3**		3, 5
		**0.5**		**0.1**		3
					**0.025**	2
		**≤0.0005**		**0.0002**		3
					**≤0.0001**	2

		**0.003**		**0.003**		3

Legend of Supplementary Table 2.
k_{rel} is defined as k_{mutant}/k_{wt}, where k_{mutant} and k_{wt} are the first-order rate constants for cleavage measured, respectively, for the mutant and for the “wild-type” 8-17 construct.
Data from different studies were obtained not only in the presence of different metal ions but also at different temperatures, pH, buffers and using different constructs.



Supplementary Figure 1 – Apparent correlation between the activating ability of nine different divalent metal ions and their affinity for trianionic citrate. k_{act} values are taken from)[6]: in that publication the metals' activating effciencies were correlated to the affinities for AMP, which however can coordinate metals through both oxygen and nitrogen groups; these latter are biased towards binding of 'soft' metal ions. Citrate, on the other hand, contains only oxygen liganding groups. Stabilities for the complexes between trianionic citrate and the metals (at 0.1 M ionic strength, 25°C) were taken from.[7-10] The solid line is the linear best fit of the data, with a slope of 1.19 and r^2=0.59.

References

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