Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

A comparison of two classic Pb^{2+}-dependent RNA-cleaving DNAzymes

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Table S1. DNA sequences used in the paper.

A=Adenine; C=Cytosine; T=Thymine; G=Guanine; 2AP=2-AminoPurine; HX=Hypoxanthine

DNA	SEQUENCE (5′-3′)
Substrate	
WT	GTCACGAGTCACTAT**rAG**GAAGATGGCGAAA
rAA	GTCACGAGTCACTAT**rAA**GAAGATGGCGAAA
rA2AP	GTCACGAGTCACTAT**rA2AP**GAAGATGGCGAAA
rAHX	GTCACGAGTCACTAT**rAHX**GAAGATGGCGAAA
GR5 DNAzyme	
WT	TTTCGCCATCT--**GAAGTAGCGCCGCCG**TATAGTGACTCGTGAC
A6C	TTTCGCCATCT--**GAAGTCGCGCCGCCG**TATAGTGACTCGTGAC
A6T	TTTCGCCATCT--**GAAGTTGCGCCGCCG**TATAGTGACTCGTGAC
A6G	TTTCGCCATCT--**GAAGTGGCGCCGCCG**TATAGTGACTCGTGAC
G7A	TTTCGCCATCT--**GAAGTAACGCCGCCG**TATAGTGACTCGTGAC
G7C	TTTCGCCATCT--**GAAGTACCGCCGCCG**TATAGTGACTCGTGAC
G7T	TTTCGCCATCT--**GAAGTATCGCCGCCG**TATAGTGACTCGTGAC
C8A	TTTCGCCATCT--**GAAGTAGAGCCGCCG**TATAGTGACTCGTGAC
C5G	TTTCGCCATCT--**GAAGTAGGGCCGCCG**TATAGTGACTCGTGAC
C8T	TTTCGCCATCT--**GAAGTAGTGCCGCCG**TATAGTGACTCGTGAC
G9A	TTTCGCCATCT--**GAAGTAGCACCGCCG**TATAGTGACTCGTGAC
G9C	TTTCGCCATCT--**GAAGTAGCCCCGCCG**TATAGTGACTCGTGAC
G9T	TTTCGCCATCT--**GAAGTAGCTCCGCCG**TATAGTGACTCGTGAC
C14A	TTTCGCCATCT--**GAAGTAGCGCCGCAG**TATAGTGACTCGTGAC
C14G	TTTCGCCATCT--**GAAGTAGCGCCGCGG**TATAGTGACTCGTGAC
C14T	TTTCGCCATCT--**GAAGTAGCGCCGCTG**TATAGTGACTCGTGAC
G15A	TTTCGCCATCT--**GAAGTAGCGCCGCCA**TATAGTGACTCGTGAC
G15C	TTTCGCCATCT--**GAAGTAGCGCCGCCC**TATAGTGACTCGTGAC
G15T	TTTCGCCATCT--**GAAGTAGCGCCGCCT**TATAGTGACTCGTGAC
1=T	TTTCGCCATCTT-**GAAGTAGCGCCGCCG**TATAGTGACTCGTGAC
1=TC	TTTCGCCATCTTC**GAAGTAGCGCCGCCG**TATAGTGACTCGTGAC
2=AAG	TTTCGCCATCT---**AAGTAGCGCCGCCG**TATAGTGACTCGTGAC
2=AG	TTTCGCCATCT----**AGTAGCGCCGCCG**TATAGTGACTCGTGAC
2=G	TTTCGCCATCT------**GTAGCGCCGCCG**TATAGTGACTCGTGAC
2=none	TTTCGCCATCT--------**TAGCGCCGCCG**TATAGTGACTCGTGAC
3=A	TTTCGCCATCT--**GAAGAAGCGCCGCCG**TATAGTGACTCGTGAC
3=C	TTTCGCCATCT--**GAAGCAGCGCCGCCG**TATAGTGACTCGTGAC
3=G	TTTCGCCATCT--**GAAGGAGCGCCGCCG**TATAGTGACTCGTGAC
17E DNAzyme	
WT	TTTCGCCATCTTTC**TCCGAGCCGGTCGAAA**TAGTGACTCGTGAC
A6C	TTTCGCCATCTTTC**TCCGCGCCGGTCGAAA**TAGTGACTCGTGAC
A6G	TTTCGCCATCTTTC**TCCGGGCCGGTCGAAA**TAGTGACTCGTGAC
A6T	TTTCGCCATCTTTC**TCCGTGCCGGTCGAAA**TAGTGACTCGTGAC
G7A	TTTCGCCATCTTTC**TCCGAACCGGTCGAAA**TAGTGACTCGTGAC
G7C	TTTCGCCATCTTTC**TCCGACCCGGTCGAAA**TAGTGACTCGTGAC
G7T	TTTCGCCATCTTTC**TCCGATCCGGTCGAAA**TAGTGACTCGTGAC

C13A	TTTCGCCATCTTTC**TCCGAGCCGGTAGAAA**TAGTGACTCGTGAC
C13G	TTTCGCCATCTTTC**TCCGAGCCGGTGGAAA**TAGTGACTCGTGAC
C13T	TTTCGCCATCTTTC**TCCGAGCCGGTTGAAA**TAGTGACTCGTGAC
G14A	TTTCGCCATCTTTC**TCCGAGCCGGTCAAAA**TAGTGACTCGTGAC
G14C	TTTCGCCATCTTTC**TCCGAGCCGGTCCAAA**TAGTGACTCGTGAC
G14T	TTTCGCCATCTTTC**TCCGAGCCGGTCTAAA**TAGTGACTCGTGAC

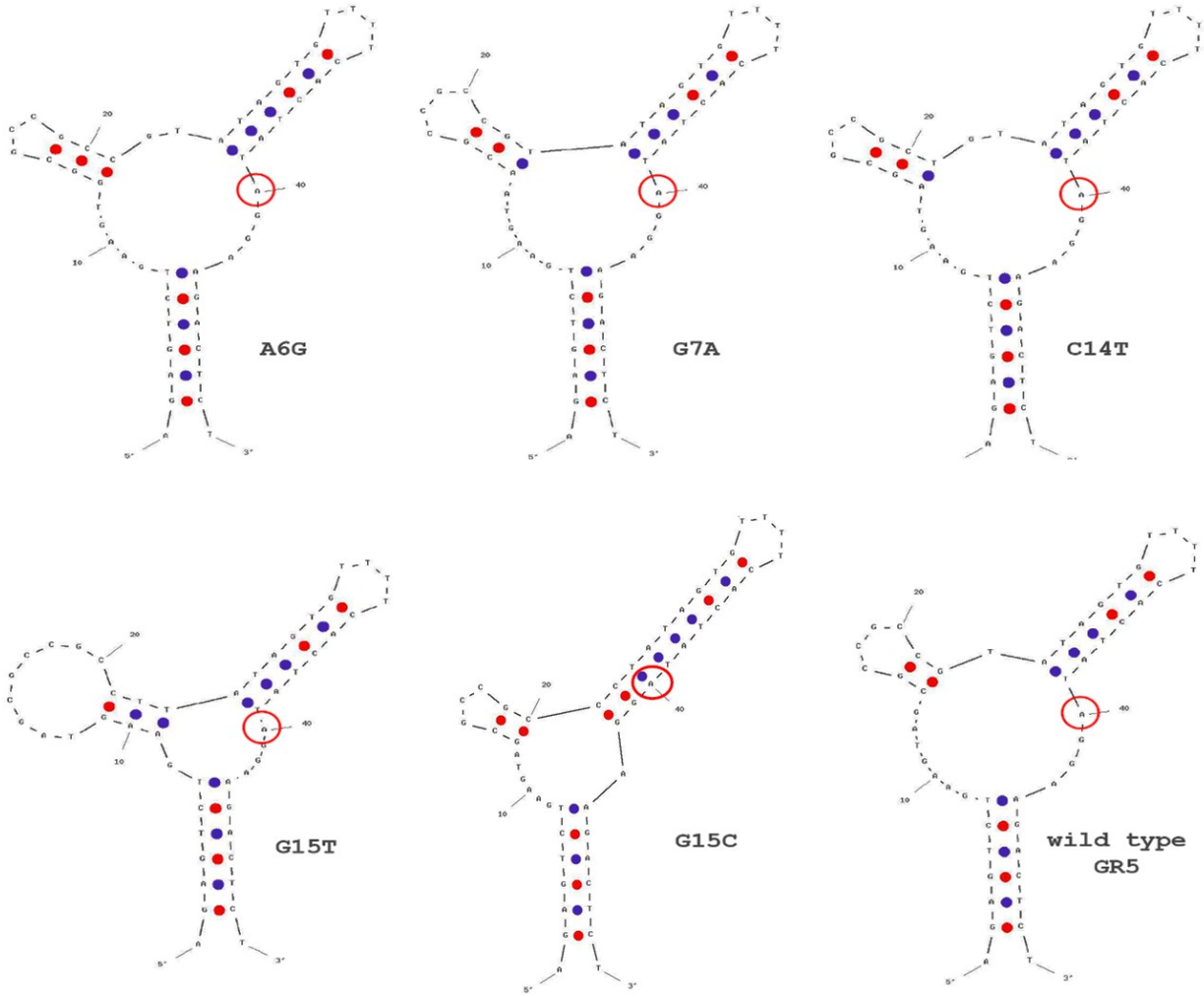

Figure S1. Mfold predicted secondary structures from a few GR5 mutants and the wild-type GR5. All the other mutants fold into a structure similar to that for the wild-type GR5 and are not listed here. The cleavage site adenine is marked by the red circle. The substrate and enzyme strands are linked by a TTTT loop. In the wild-type GR5 structure, two G-C base pairs are predicted in the enzyme loop. However, these nucleotides are highly conserved for catalysis and thus are unlikely

to be confined in such a hairpin structure. Therefore, we still used the simple loop structure in the original GR5 selection paper (Breaker, R. R.; Joyce, G. F. *Chem. Biol.* **1994**, *1*, 223) in this work. The mutants in this figure have three base pairs in the loop and their misfold (i.e. deviation from the simple loop structure) might also be a reason for their inhibited activity.