Supplementary Data

From general base to general acid catalysis in a sodium-specific DNAzyme by a guanine-to-adenine mutation

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Table S1. DNA sequences used in this work. FAM = carboxyfluorescein; rA = adenine ribonucleotide; /2AP/ = 2-aminopurine; /2,6-diAP/ = 2,6-diaminopurine; /I/ = hypoxanthine. The asterisk denotes for a PS modification. The individual mutants are not listed here and they can be obtained based on Figure 2B and Figure 3A.

DNA Names	**Sequences and modifications**
FAM-PO-Sub	GTCACGAGTCACTAT**rA**GGAAGATGGCGAAA-**FAM**
NaH1	TTTCGCCATAGGTCAAAGGTGGGTGGGAGTTTTTACTCCGCATTAGTGACTCGTGAC
NaA43T	TTTCGCCATCCAGGTCAAAGGTGGGTGAGGAGTTTTTACTCCGCGGTTAGTGACTCGTGAC
NaH1-G	TTTCGCCATAGGTCAAAGGTGGGTGGGAGTTTTTACTCCGCGTTAGTGACTCGTGAC
NaH1-2AP	TTTCGCCATAGGTCAAAGGTGGGTGGGAGTTTTTACTCCGC/**2AP**/TTAGTGACTCGTGAC
NaH1-2,6diAP	TTTCGCCATAGGTCAAAGGTGGGTGGGAGTTTTTACTCCGC/**2,6-diAP**/TTAGTGACTCGTGAC
NaA43T-A	TTTCGCCATCCAGGTCAAAGGTGGGTGAGGAGTTTTTACTCCGCGATTAGTGACTCGTGAC
NaA43T-I	TTTCGCCATCCAGGTCAAAGGTGGGTGAGGAGTTTTTACTCCGCG/**I**/TTAGTGACTCGTGAC
Sub	GTCACGAGTCACTAT**rA**GGAAGATGGCGAAA
Sub-dA	GTCACGAGTCACTATAGGAAGATGGCGAAA
FAM-PS-Sub	GTCACGAGTCACTAT**rA***GGAAGATGGCGAAA-FAM

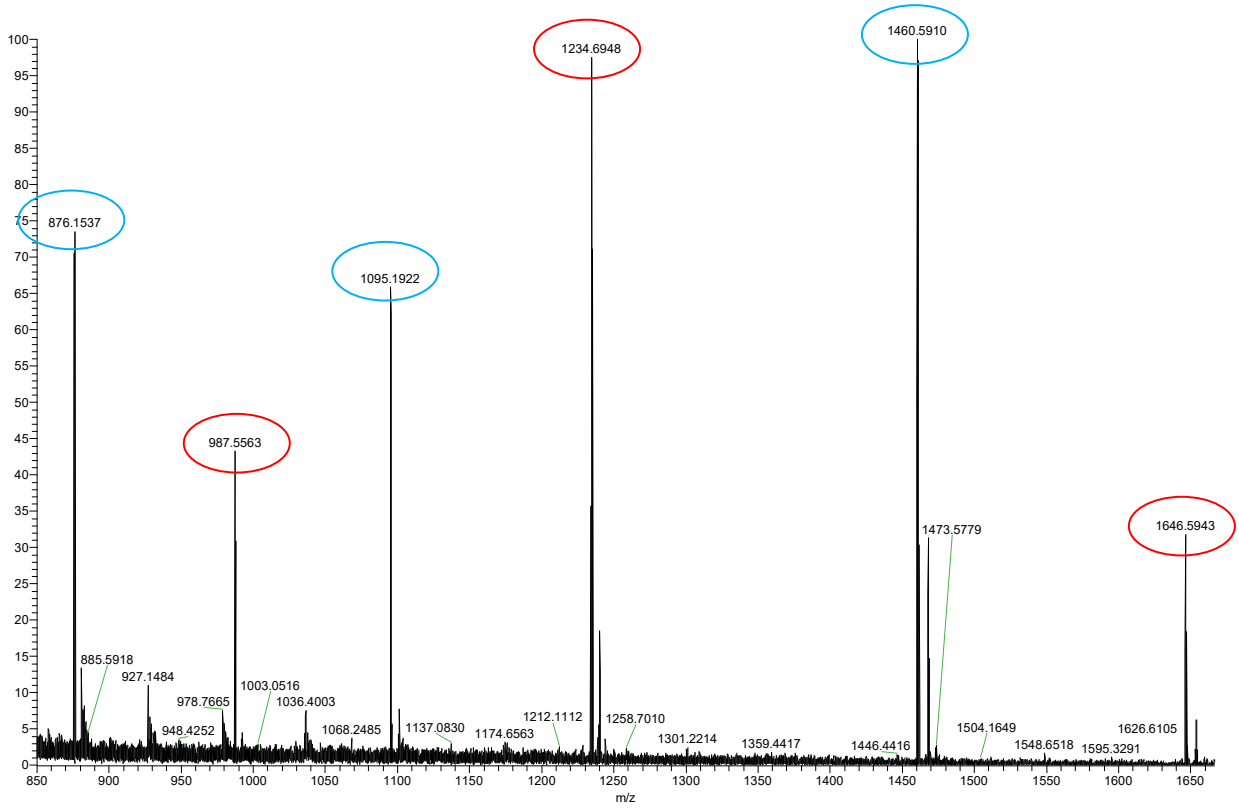

Figure S1. Mass spectrometry characterization of the NaH1 cleavage product. The red peaks represent the 5′-fragment of the cleaved-substrate containing a 2′, 3′-cyclic phosphate group (MW=4942.7 Da, 3, 4 and 5 charges for three marked peaks). The blue peaks represent the 3′-fragment of the cleaved-substrate (MW=4384.7 Da. 3, 4 and 5 charges for the three marked peaks). The sample was prepared by reacting non-labeled substrates (**Table S1**) with NaH1 DNAzymes (in 1:1.5 ratio) in 50 mM MES buffer (pH 6, 25 mM LiCl, 100 mM NaCl) for overnight. A Sep-Pak column was further used to desalt the sample. After dried, the sample was re-suspended in 20 µL Milli-Q water with a final substrate concentration of ~50 µM and analyzed with an ESI mass spectrometer.