

Biophysical Journal, Volume 97

**Supporting Material**

**Coarse grained Brownian dynamics simulations of the 10-23 DNzyme**

Martin Kenward and Kevin Dorfman

# Coarse grained Brownian dynamics simulations of the 10-23 DNAzyme

Martin Kenward and Kevin D. Dorfman<sup>1</sup>  
Department of Chemical Engineering and Materials Science,  
University of Minnesota — Twin Cities, Minneapolis, MN

<sup>1</sup>Corresponding author. Address: Department of Chemical Engineering and Materials Science, University of Minnesota — Twin Cities, 421 Washington Ave. SE, Minneapolis, MN 55455, U.S.A., Tel.: (612)624-5560, Fax: (612)626-7246

## Supporting Material

Reduced activity (descending order)	Negligible activity (arbitrary order)
GGCTAG <b>C</b> GACAACGA	<b>C</b> GCTAGCTACAACGA
GGCTAG <b>C</b> AACAACGA	<b>A</b> GCTAGCTACAACGA
GGCTAGCT <b>T</b> CAACGA	<b>T</b> GCTAGCTACAACGA
GGCTAGCTAC <b>A</b> TCGA	<b>C</b> CCTAGCTACAACGA
GGCTAGCTACT <b>A</b> CGA	<b>G</b> ACTAGCTACAACGA
GGCTAGCTAC <b>A</b> CCGA	<b>G</b> TCTAGCTACAACGA
GGCTAG <b>C</b> CACAACGA	<b>G</b> G <b>G</b> TAGCTACAACGA
GGCTAG <b>A</b> TACAACGA	<b>G</b> G <b>C</b> AAGCTACAACGA
GGCTAGCT <b>A</b> AAACGA	<b>G</b> G <b>C</b> CAGCTACAACGA
GGCTAGCTACA <b>A</b> CG <b>G</b>	<b>G</b> G <b>C</b> GAGCTACAACGA
GG <b>A</b> TAGCTACAACGA	<b>G</b> GCT <b>T</b> GCTACAACGA
GGCTAG <b>T</b> TACAACGA	<b>G</b> GCT <b>G</b> GCTACAACGA
GGCTAGCT <b>A</b> TAAACGA	<b>G</b> GCT <b>A</b> CCTACAACGA
GGCTAGCTAC <b>G</b> ACGA	<b>G</b> GCT <b>A</b> ACTACAACGA
GGCT <b>C</b> GCTACAACGA	<b>G</b> GCT <b>A</b> TCTACAACGA
GGCTAGCTAG <b>A</b> ACGA	<b>G</b> GCTAGCT <b>C</b> CAACGA
GGCTAGCTACA <b>A</b> CG <b>T</b>	<b>G</b> GCTAGCTACA <b>A</b> GGA
GGCTAGCTACA <b>A</b> AGA	<b>G</b> GCTAGCTACA <b>A</b> TGA
GGCTAGCT <b>G</b> CAACGA	<b>G</b> GCTAGCTACA <b>A</b> CCA
GGCTAGCTAC <b>A</b> GCGA	<b>G</b> GCTAGCTACA <b>A</b> CAA
GGCTAGCTAC <b>C</b> ACGA	<b>G</b> GCTAGCTACA <b>A</b> CTA
GG <b>T</b> TAGCTACAACGA	<b>G</b> GCTAGCTACA <b>A</b> CGC
GGCTAG <b>G</b> TACAACGA	

Table S1. List of mutants from Ref. 28. Mutants with reduced activity (< 20% cleavage in Ref. 28) are listed in order of descending activity. Mutants with no activity are listed in an arbitrary order. The mutated base is indicated in bold. The data in Figs. (4) and (5) are listed according to the order appearing in this table. The 23 reduced activity mutants start from GGCTAG**C**GACAACGA and continue to GGCTAG**G**TACAACGA. The 22 negligible activity mutants start from **C**GCTAGCTACAACGA and end with GGCTAGCTACAAC**G**C.