SUPPORTING INFORMATION

Circular DNA and DNA/RNA hybrid molecules as scaffolds for Ricin inhibitor design.

Matthew B. Sturm, Setu Roday and Vern L. Schramm

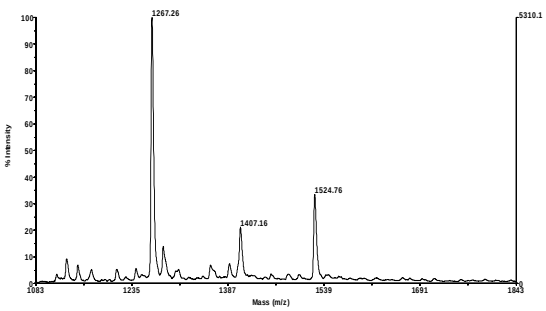
Department of Biochemistry, Albert Einstein College of Medicine, 1300 Morris Park Avenue, Bronx, NY 10461

MALDI data of cyclic molecules

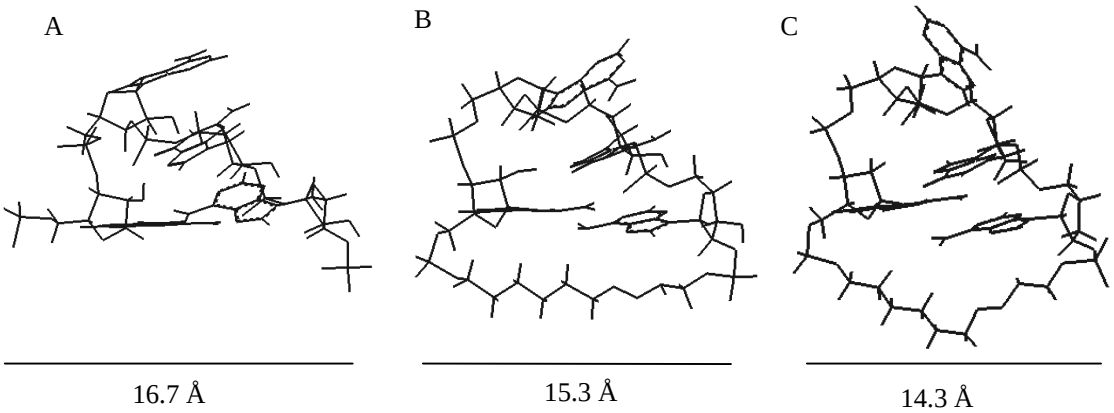
Circular construct	Calculated mass	Observed mass
Cyclic d(GAGA)	1521.3	1521.7
Cyclic GdAGA	1569.3	1570.2
Cyclic d[G(N-Bn)GA]	1477.3	1477.6
Cyclic G(N-Bn)GA	1525.3	1524.2
Cyclic d[G(N-Bn)G(N-Bn)]	1433.3	1433.6
Cyclic PS d(GAGA)	1300.2	1300.0
cyclic PS d(GA)	658.1	658.8
cyclic PS d[G(N-Bn)G(7deazaA)]	1255.2	1254.8

MALDI of fourth site depurination in cyclic d(GAGA)

MALDI-TOF analysis of catalyzed cyclic d(GAGA) showing mass fragments of starting material and 2 products with the largest signal observed for the di-abasic cyclic product (Mass : 1267). The mono-abasic peak is +Na at 1407 with masse errors from low peak resolution in spectrum.



Estimated phosphate distances of the 5- and 3- ends of the oxime linked tetraloop.



5’- to 3’-end phosphate distances for the truncated GAGA tetra-loop of A-12 (pdb 1ZIG) (A), cyclic GdAGA (B) and cyclic d(GAGA) (C). Structure B and C were obtained by manual modification of (A) followed by 2500 cycles of optimization in a periodic box of 1000 water molecules in Hyperchem using an Amber99 force field, 30 ps of molecular dynamics, 2500 cycles of re-optimization, and 30 ps of molecular dynamics.