

Supplemental information for:

Recombinant production of rhesus θ -defensin-1 (RTD-1) using a bacterial expression system

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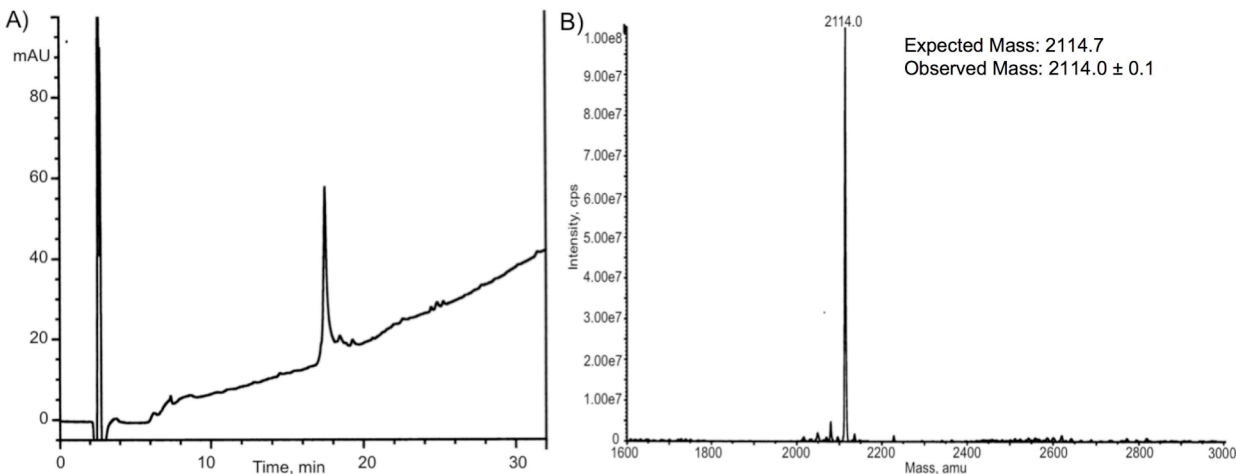


Figure S1. Characterization of ¹⁵N-labeled RTD-1. Reverse-phase HPLC analysis (A) and ES-MS analysis (B) of purified ¹⁵N-labeled RTD-1.

Table S1. Forward (p5) and reverse (p3) 5'-phosphorylated oligonucleotides used to clone the different RTD-intein linear precursors into the pTXB1 expression plasmid.

Precursor		Oligonucleotide sequence
RTD-C3	p5	5' -TATGTGCCGTTGCCTGTGCCGTCGTGGTGTGTTTGCCGTTGCATCTGCACCCGTGGTTTC-3'
	p3	5' - gcaGAAACCACGGGTGCAGATGCAACGGCAAACACCACGACGGCACAGGCAACGGCACA-3'
RTD-C7	p5	5' -TATGTGCCGTCGTGGTGTGTTTGCCGTTGCATCTGCACCCGTGGTTTCTGCCGTTGCCTG-3'
	p3	5' - GCACAGGCAACGGCAGAAACCACGGGTGCAGATGCAACGGCAAACACCACGACGGCACA-3'

Table S2. ¹H and ¹⁵N chemical shifts of cyclic RTD-1 at 298 K in 20 mM sodium phosphate buffer at pH 6.0, 90%/10% H₂O/D₂O.

Residue	H ^N (ppm)	H ^α (ppm)	¹⁵ N ^α (ppm)	δH ^N (ppm)*	δH ^α (ppm)*
G1	8.49	3.47/3.99	104.7	0.02	-0.21/-0.17
F2	7.82	4.77	121.0	-0.20	-0.24
C3	8.63	5.22	124.0	-0.01	-0.29
R4	8.49	4.49	123.1	-0.26	-0.24
C5	9.00	5.37	123.9	0.02	-0.27
L6	8.56	4.58	125.4	-0.29	-0.24
C7	9.01	5.45	123.6	-0.04	-0.26
R8	8.55	4.41	123.4	-0.23	-0.17
R9	9.58	3.70	125.2	0.07	-0.25
G10	8.60	3.48/4.06	104.3	0.03	-0.19/-0.18
V11	7.68	4.18	121.8	-0.17	-0.26
C12	8.98	5.36	126.5	0.06	-0.23
R13	8.56	4.57	123.5	-0.24	-0.25
C14	9.03	5.40	128.0	0.06	-0.30
I15	8.63	4.28	124.1	-0.28	-0.30
C16	9.00	5.48	124.8	-0.04	-0.23
T17	8.64	4.37	118.7	-0.22	-0.20
R18	9.35	3.77	125.2	-0.12	-0.21

*Difference between RTD-1 chemical shifts and that of previously reported by Trabi *et al.*⁶ The buffer used by Trabi et al was 20 mM sodium phosphate pH 4.5, 10% D₂O and 10% acetonitrile-d₃ at 310 K.