Supporting Information for

SCX-tip aided LC-MS detection of active ricin via oligonucleotide substrate for depurination kinetics

Zhifang Yang,[#a] Chenyu Wang ,[#ab] Lan Xiao,[ab] Chuang Wang, [ab] Li Tang[b], Lei Guo,*[a] and Jianwei Xie [a]

[a] State Key Laboratory of Toxicology and Medical Countermeasures, and Laboratory of Toxicant Analysis, Institute of Pharmacology and Toxicology, Academy of Military Medical Sciences, Beijing, 100850, China.

[b] Key Laboratory of Ethnomedicine Ministry of Education (Minzu University of China), School of Pharmacy, Minzu University of China

† Electronic Supplementary Information (ESI) is available.

[#] These authors contributed equally to this work.

*To whom correspondence should be addressed.

Prof. Li Tang

E-mail: tangli6972@muc.edu.cn

Prof. Lei Guo

E-mail: guolei@bmi.ac.cn

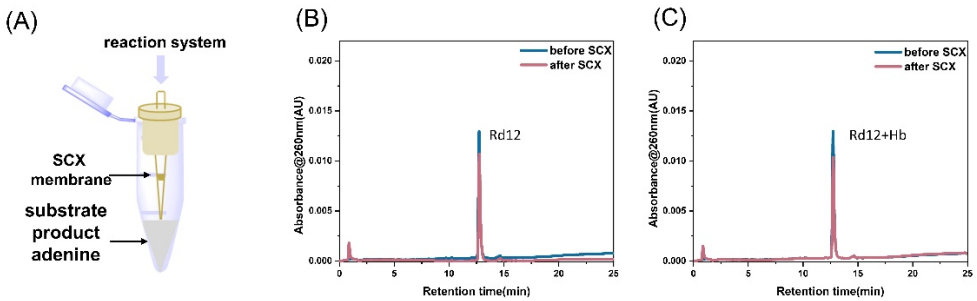

Fig. S1 (A) Diagram of SCX membrane device (A), the effect of pretreatment and pretreatment on peak area and retention time of Rd12 (B) alone, or Rd12 and hemoglobin (Hb)(C).

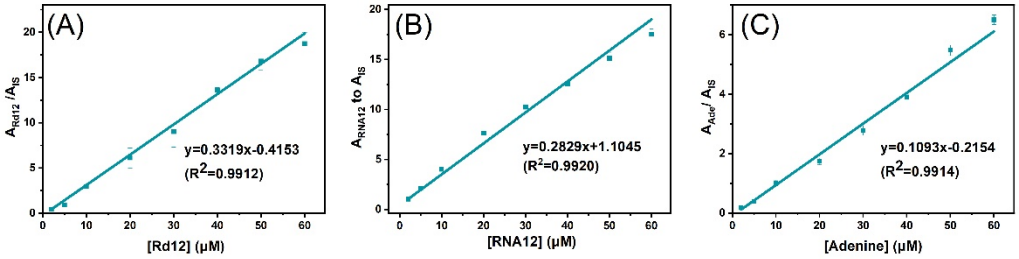

Fig. S2 Linear curves of Rd12, RNA12, and adenine in LC-TUV-QDa detection. The peak area of the analyte or IS (r(GCGCGGGCGC)) was collected from the QDa channel. The MW of IS was 3229.992, and the employed concentration was 2 μM.

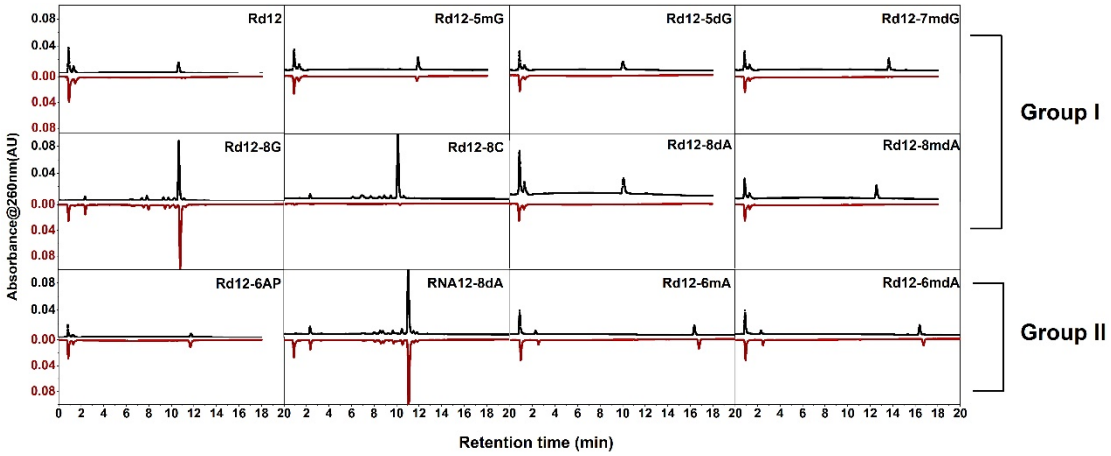

Fig. S3 The chromatograms of Rd-based oligos before and after reaction with ricin in LC-TUV-QDa, where the TUV channel was shown, and Rd12 was used as the positive control.

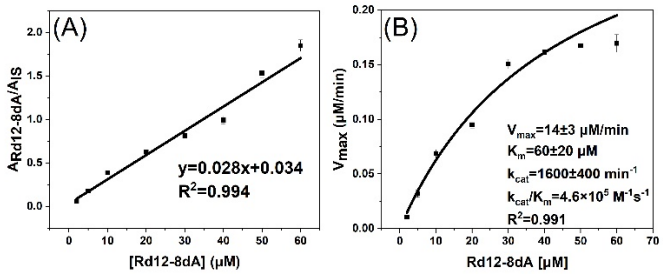

Fig. S4 (A) The linear curve of Rd12-8dA; (B) the enzymatic kinetic curve of Rd12-8dA with ricin at pH 4.0.

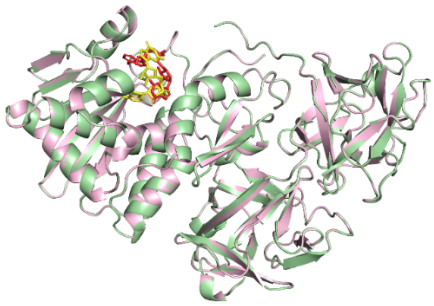

Fig. S5 The alignment between the crystal structure of ricin with dinucleotide ApG (PDB: 3RTJ) and molecular docking of ricin (the model in our work) with a dinucleotide ApG.

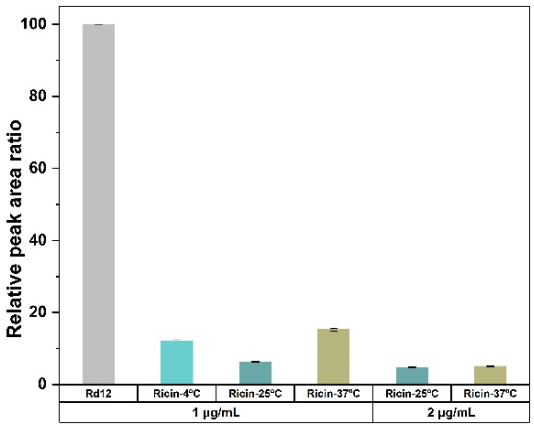

Fig. S6 The relative peak area ratio of Rd12 substrate before and after reaction with ricin in LC-TUV. Conditions: 20 μM Rd12, 1 μg/mL (16 nM) or 2 μg/mL ricin in PBS at pH 7.4.

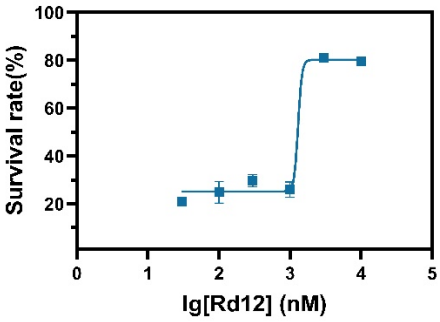

Fig. S7 The cell survival rate curve with the increase of Rd12 concentration at pH 7.4.

Table S1. The molecular docking of modified oligos and ricin at pH 4.0

Oligo	Modified sites	Docking score (kcal/mol)	RMSD (Å)	Align RMSD(Å)
Rd12-5mG	-mGdAGA	-181.8	99.8	0
Rd12-5dG	-dGdAGA	-207.9	99.8	0
Rd12-7mdG	-GdAmdGA	-180.2	99.3	0
Rd12-8G	-GdAGG	-210.2	99.2	0
Rd12-8C	-GdAGC	-237.5	98.4	0
RNA12-8dA	-GAGdA	-183.1	100.6	0
Rd12-8mdA	-GdAGmdA	-194.8	99.4	0
Rd12-6AP	-GdAPGA	-209.9	99.4	0
RNA12-6mA	-GmAGA	-200.5	99.5	0
Rd12-6mdA	-GmdAGA	-195.9	99.6	0
Rd12-8dA	-GdAGdA	-177.0	100.8	0