Electronic Supplementary Information

TBA loop mapping with 3'-inverted-deoxythymidine for a fine-tuning of the binding affinity for α-thrombin

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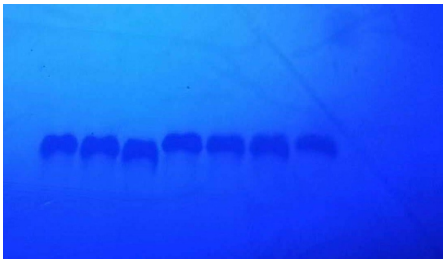
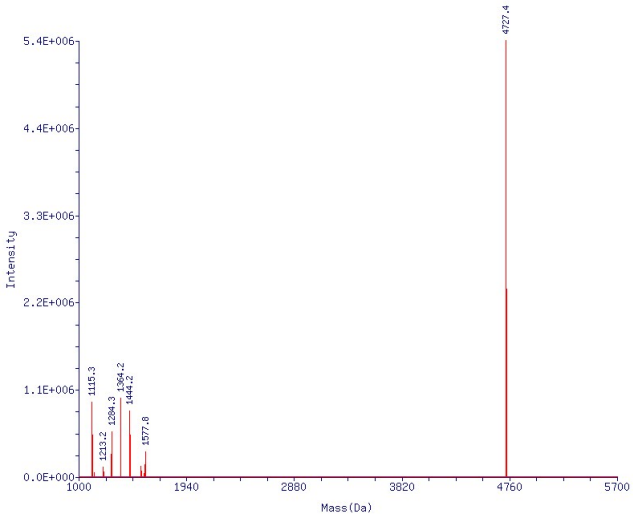
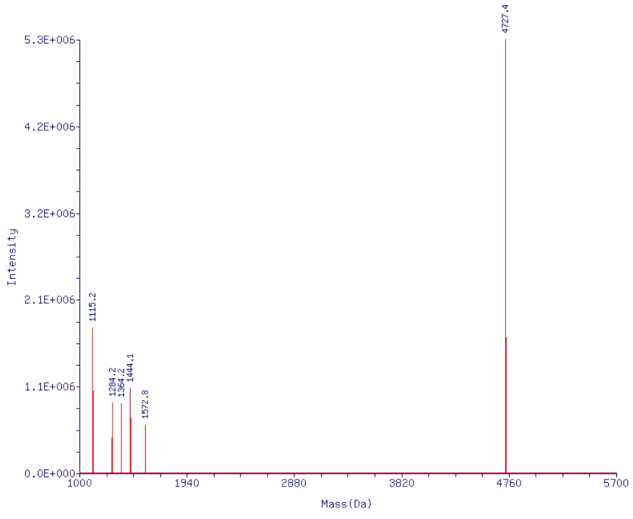


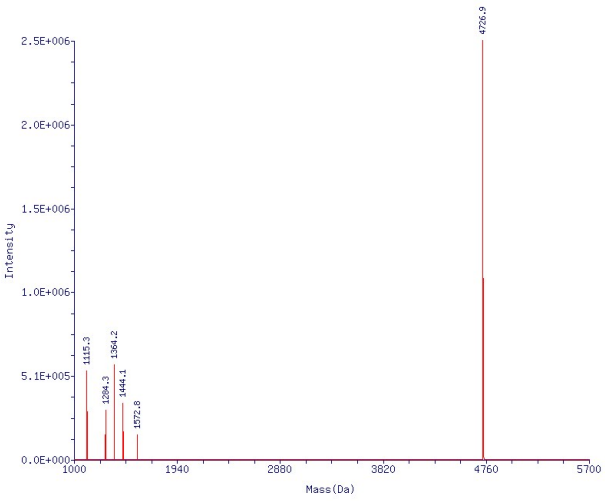
Fig. S1 The purity of TBA analogues by denaturing PAGE (20%, 8 M urea). The bands were shown under UV (λ = 254 nm), TBA-^{i}T3, TBA-^{i}T4, TBA-^{i}T7, TBA-G8-^{i}T8, TBA-^{i}T9, TBA-^{i}T12, and TBA-^{i}T13 were presented, respectively from left to right.



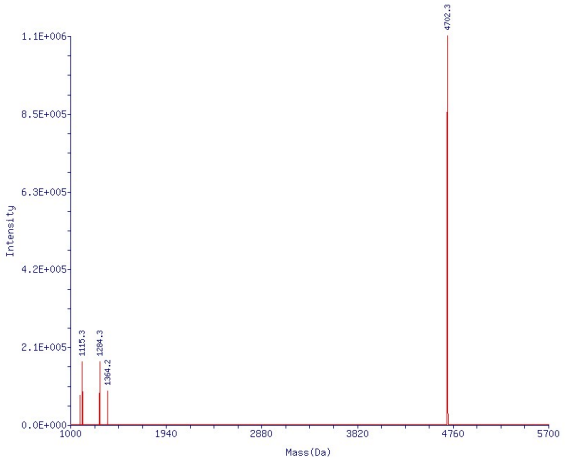
TBA-^{i}T3



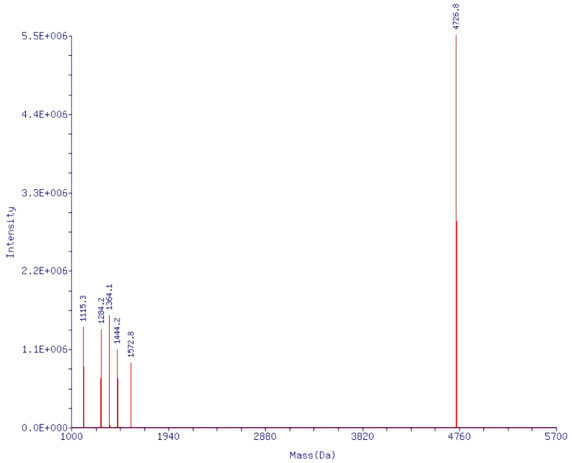
TBA-^{i}T4



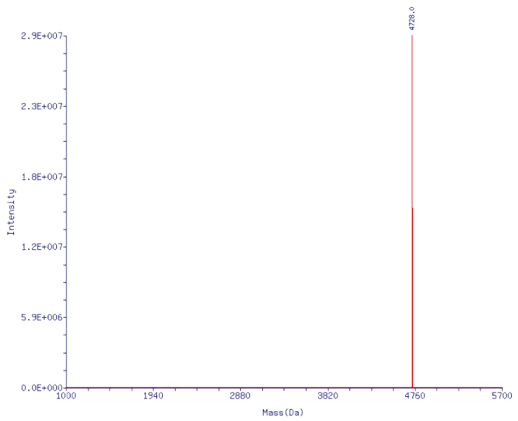
TBA-^{i}T7



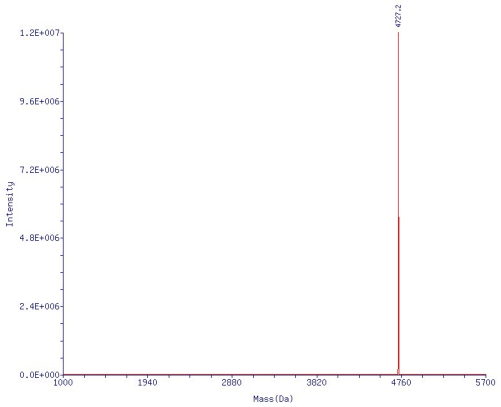
TBA-G8-^{i}T8



TBA-^{i}T9



TBA-^{i}T12



TBA-^{i}T13

Fig. S2 Mass spectra of TBA and its modified analogues. ESI-MS was measured with on a HTCS Oligo LC/MS system (Thermo Finnigan, Somerset, NJ, USA).

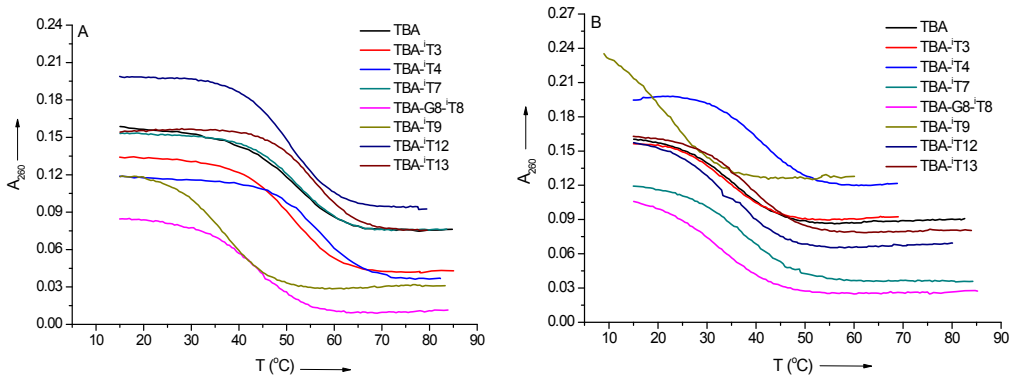


Fig. S3 Melting curves of TBA and its modified analogues. A, TBA analogues in K^{+}-buffer (100 mM KCl); B, TBA analogues in Na^{+}-buffer (138 mM NaCl, 2.7 mM KCl, 10 mM Na_2HPO_4, and 1.76 mM KH_2PO_4, pH 7.4)

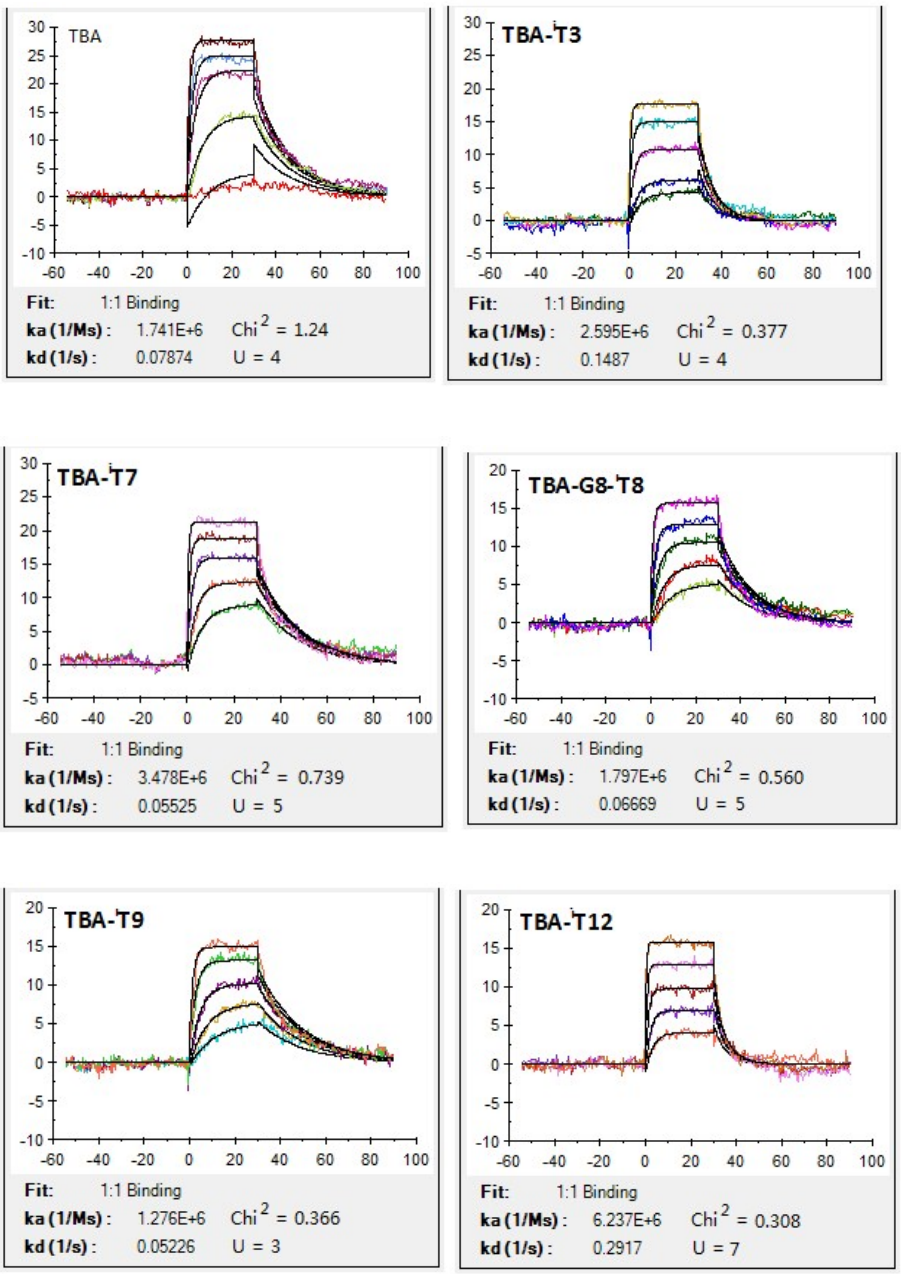


Fig. S4 MCK curves of TBA analogues in Na^+-buffer (138 mM NaCl, 2.7 mM KCl, 10 mM Na_2HPO_4, and 1.76 mM KH_2PO_4, pH 7.4).

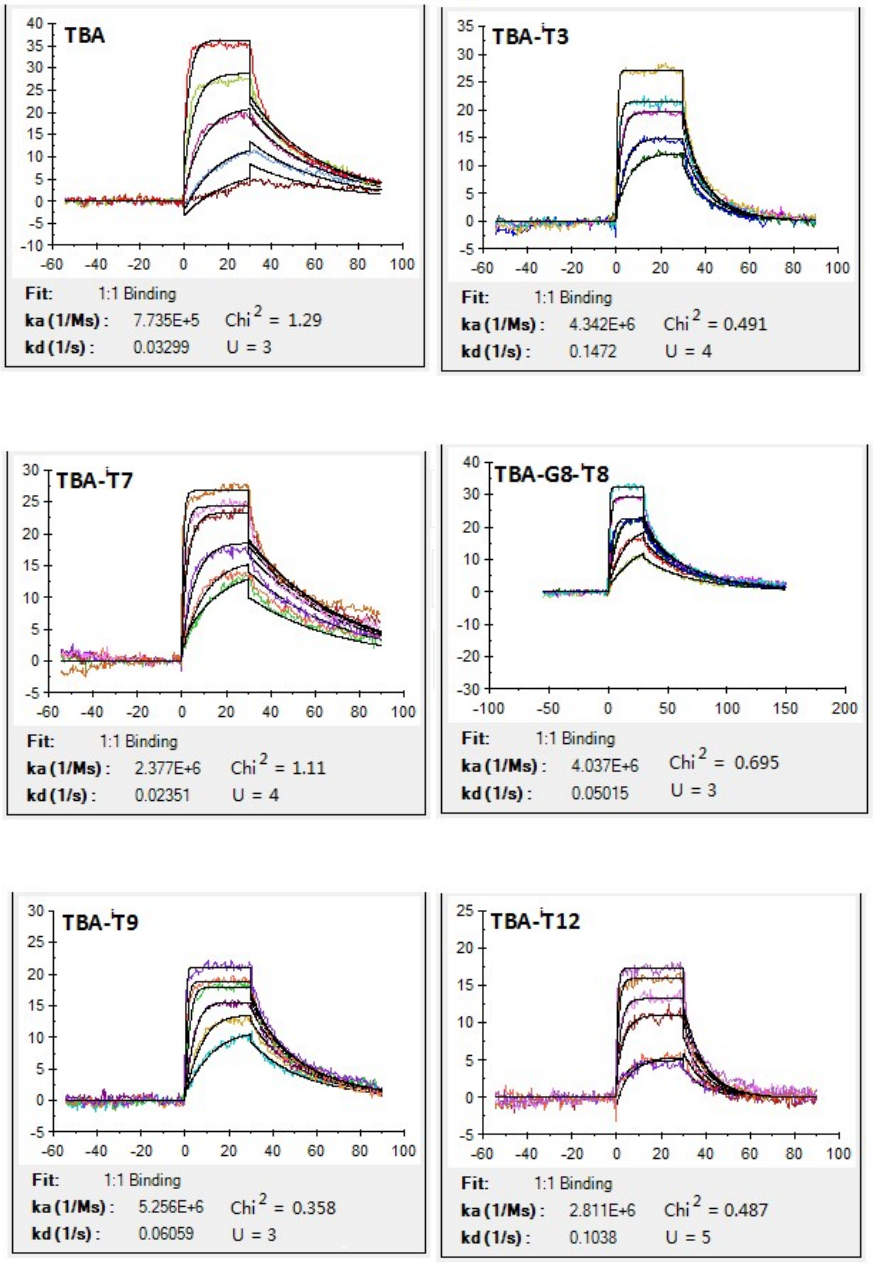


Fig. S5 MCK curves of TBA analogues in K+-buffer (100 mM KCl).

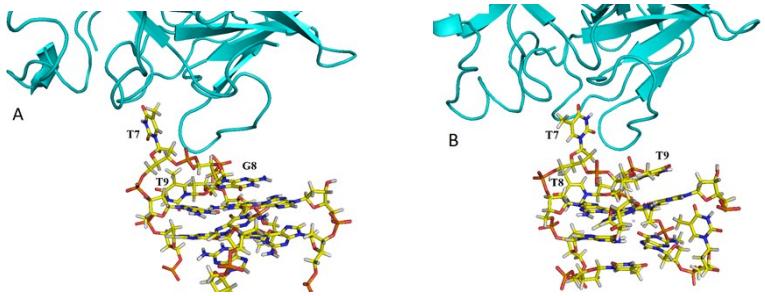


Fig. S6 Moleular dynamics simulation results of aptamer-thrombin complexes. TBA-thrombin (A) and TBA-G8-iT9-thrombin (B) complexes were calculated on the base of 1HAP. Thrombin molecule is presented as cartoon, and aptamer molecule is presents as sticks.

Table S1 Interactions between aptamer-thrombin exosite I by molecular dynamic simulation

interactions	TBA-thrombin		TBA-G8-^{i}T8-thrombin	
	TBA	thrombin	TBA-G8-^{i}T9	thrombin
H-bond	T7	GLY38		
H-bond	T9	ASN103		
H-bond	T9	ARG102	T9	ARG102
H-bond			T7	GLU101
H-bond			^{i}T8	ARG99
H-bond			G10	ARG102
Electrostatic	G8	ARG99	^{i}T8	ARG99
Electrostatic			G10	ASN103
Hydrophobic	T7	ILE37	T7	ILE37