

Supplementary Information

Rational design of ratiometric fluorescent aptasensor for patulin in traditional Chinese medicine through the studies of interaction mechanism between DNA aptamer and target molecule†

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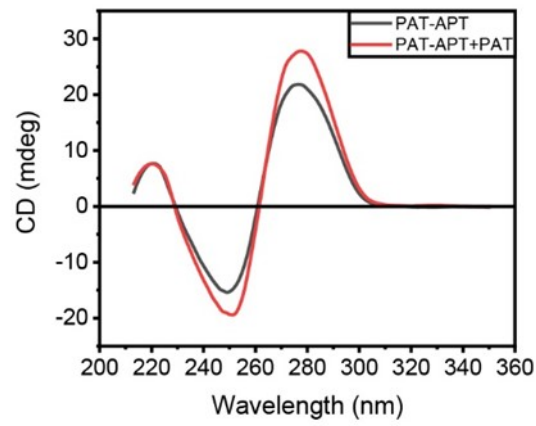


Fig. S1. CD Spectra of PAT-APT before and after binding with PAT.

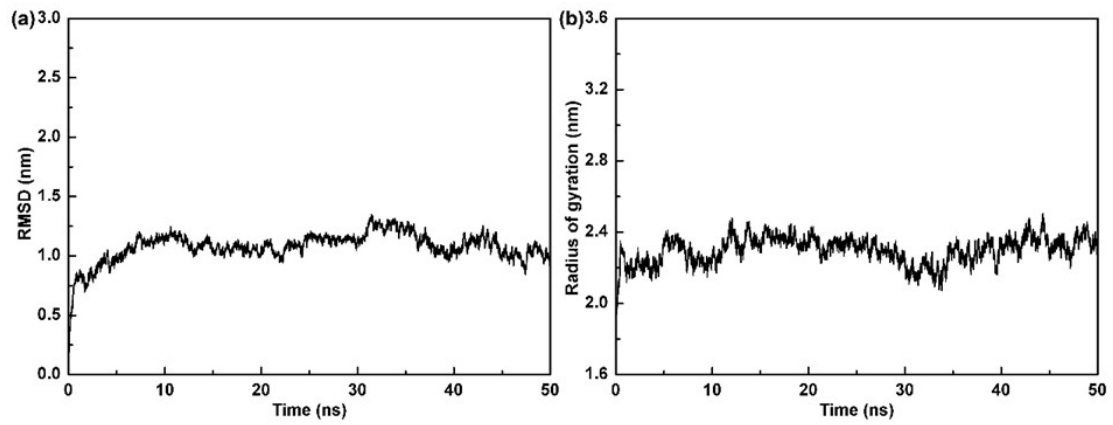


Fig. S2. The RMSD value (a) and Rg value(b) of PAT-APT in the system as the simulation time change

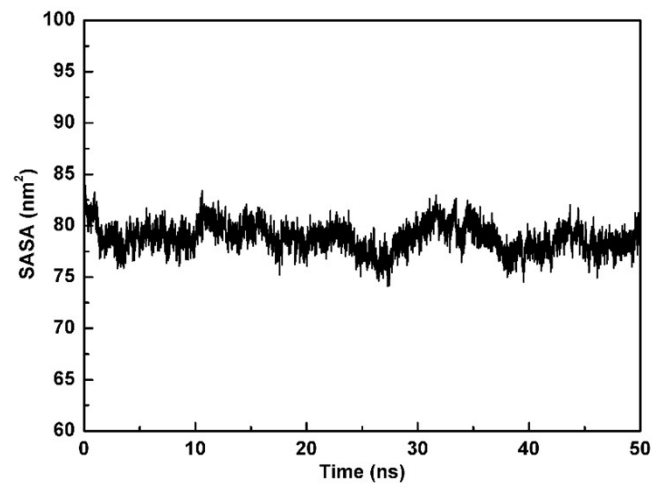


Fig. S3. The SASA of PAT-APT system as the simulation time change

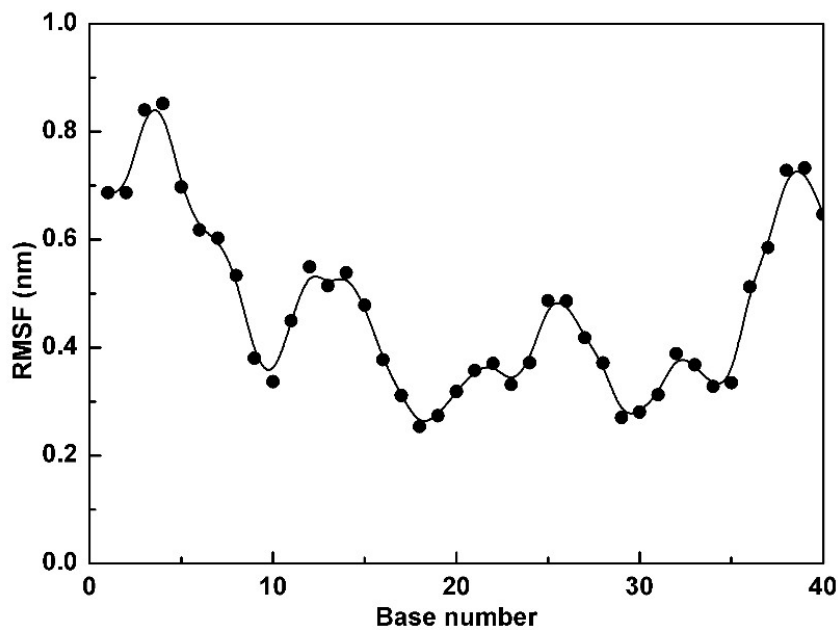


Fig. S4. RMSF distribution of the PAT-APT system

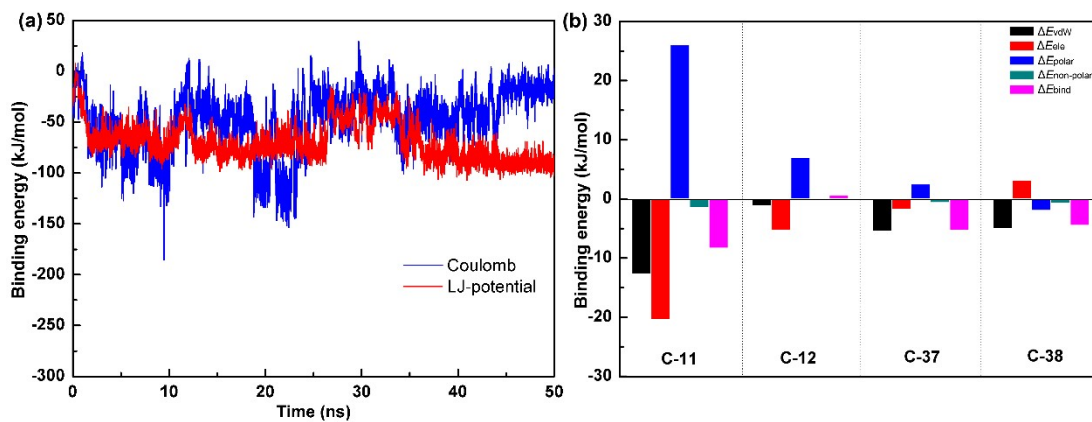


Fig. S5. Binding energy of PAT and aptamer PAT-APT. (a) the comparing of LJ potential and Coulombic force; (b) contribution of the bases in aptamer to binding energy.

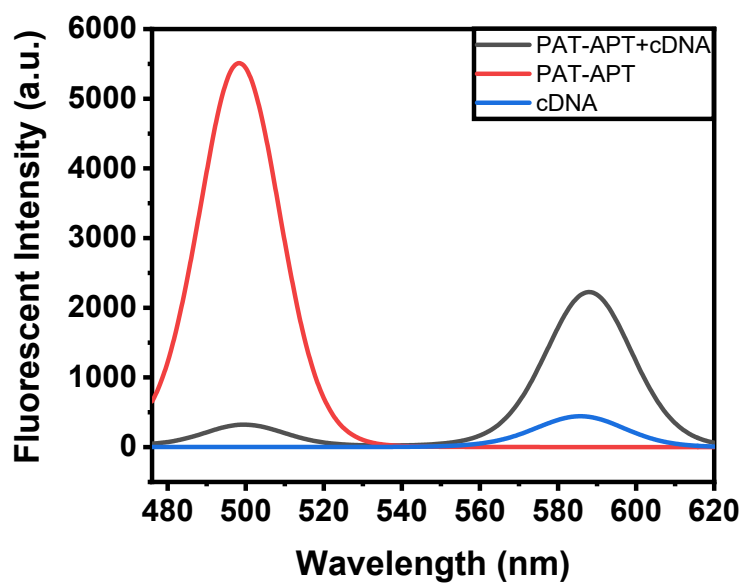


Fig. S6. Fluorescence characterization of PAT-APT, cDNA and FRET detection system

Tab. S1 cDNA sequences designed for the optimization of the length

cDNAs	Sequence (from 5' to 3')
L6-PAT-C	CGGGCC-ROX
L8-PAT-C	GGCGGGCC-ROX
L10-PAT-C	TTGGCGGGCC-ROX
L12-PAT-C	GGTTGGCGGGCC-ROX
L15-PAT-C	GCGGGTTGGCGGGCC-ROX

Tab. S2 Optimization of hybridization position in cDNA combination

cDNAs	Sequence (from 5' to 3')
PL-PAT-C	TTGGCGGGCC-ROX
PM1-PAT-C	ATGATGCGGG-ROX
PM2-PAT-C	ATCAGTGTAG-ROX
PR-PAT-C	AAGGTAAAAT-ROX