

Electronic Supplementary Information

How ABA Block Polymers Activate Cytochrome C in Toluene:

Molecular Dynamics Simulation and Experimental Observation

^aDepartment of Chemical Engineering, Tsinghua University, Beijing, 100084, China.

E-mail: ludiannan@tsinghua.edu.cn; liuzheng@mail.tsinghua.edu.cn.

Table S1. Summary of equilibrium simulation

	Protein number	Box length(nm)	Time(ns)	Considered Temperature(K)
Free Cyt c in benzene	1	15×15×15	1000	233 253 273 293 313
Cyt c-P85 in benzene	1	15×15×15	2000	233 253 273 293 313
Cyt c-P85 in benzene	2	17×17×17	1000×10	233 313
Cyt c-P85 in benzene	4	20×20×20	2000	233 313
Cyt c-F127 in benzene	1	18×18×18	1000	313

(simulated annealing)

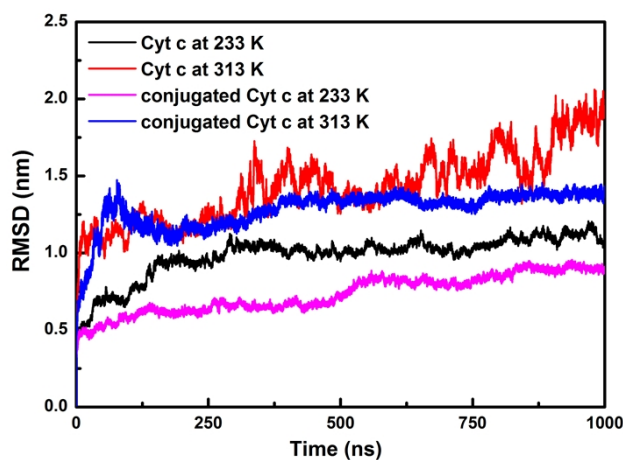


Fig S1. RMSD of free and conjugated CytC at different temperatures, this shows conjugated Cyt c is more stable

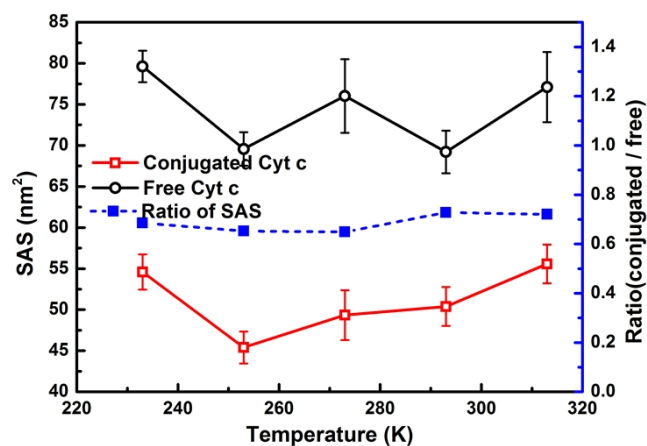


Fig S2. SAS of free and conjugated CytC at different temperatures and the ratio of SAS of conjugated one to free one.

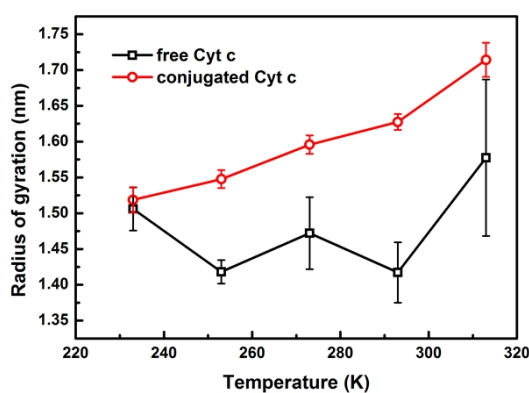


Fig S3. Radius of gyrate of free and conjugated CytC as a function of temperature

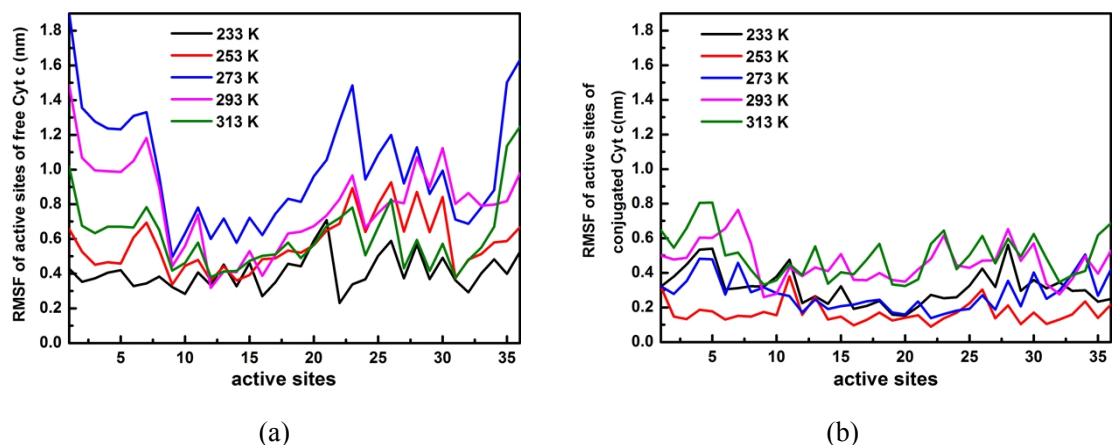


Fig S4. RMSF of active sites of (a)free CytC (b)conjugated CytC at different temperatures

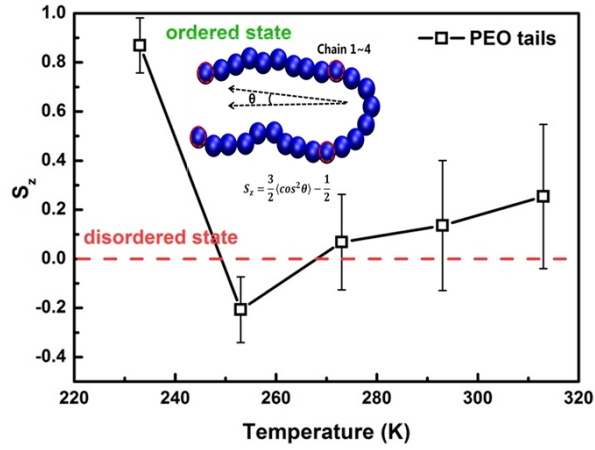


Fig S5. Order parameters of PEO tails as a function of temperature, this order parameter is obtained from lipid order parameter¹. And with $S_z=1$, the PEO chains form a perfect harpin structure, which corresponds to a fully ordered state, while $S_z=0$ represents a fully disordered state.

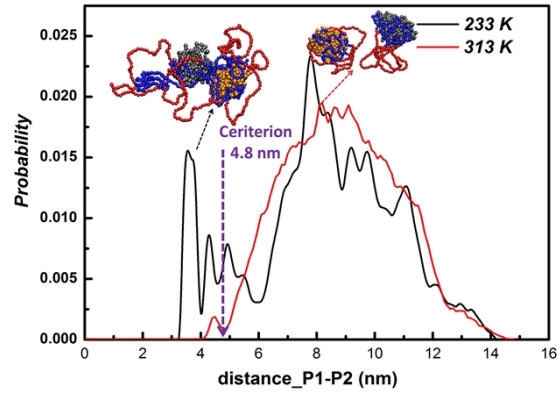


Fig S6. Distribution of the distance of COM of two conjugated CytC, it indicates that the distance criterion of forming aggregates is 4.8 nm.

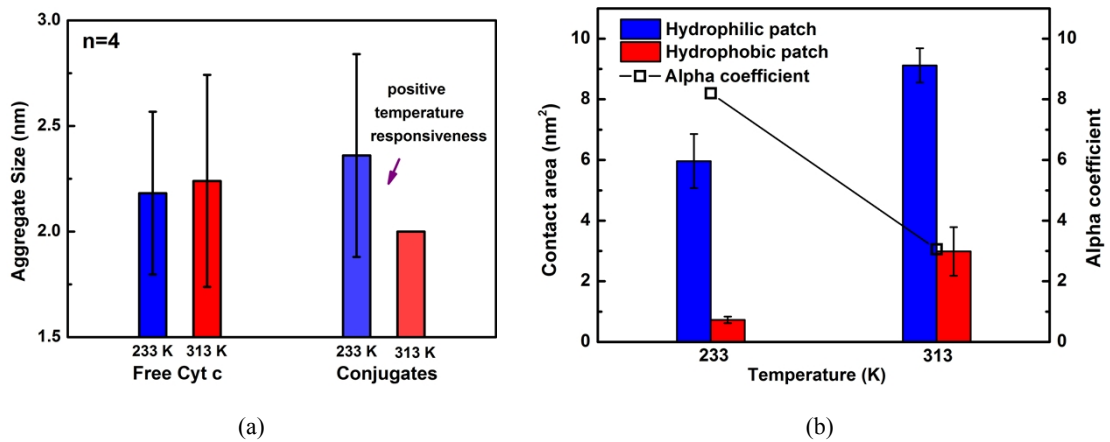


Fig S7. (a) Aggregate size for both conjugates and free CytC at different temperatures; (b) Contact area and alpha coefficient of conjugated CytC at 233 K and 313 K

As shown in Fig S7 (b), the contacting area of conjugated CytC is larger at high

temperature(313 K), which refers that CytC is more flexibility at higher temperature.

Notably, the average α is 8.32 at 233 K but only 3.15 at 313 K, indicating that the contact of conjugated CytC is tighter at lower temperature, and aggregate is more stable, which matches with the analysis of binding process using PMF methods.

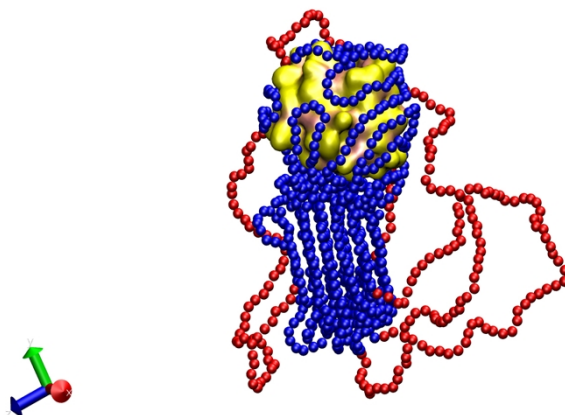


Fig S8. Entangled structure of Pluronic F127 chain around CytC at 313 K

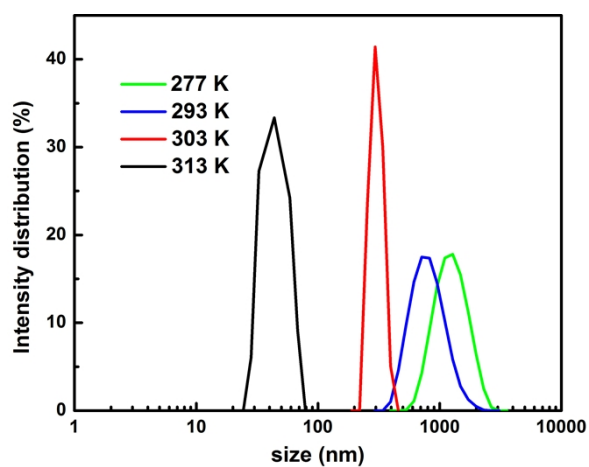


Fig S9. size distribution of conjugates in toluene at different temperatures detected by DLS.

reference

1. L. S. Vermeer, B. L. De Groot, V. Réat, A. Milon and J. Czaplicki, *European Biophysics Journal*, 2007, **36**, 919-931.