

Supplemental information

Molecular analysis of interactions between a PAMAM dendrimer-paclitaxel conjugate and a biomembrane

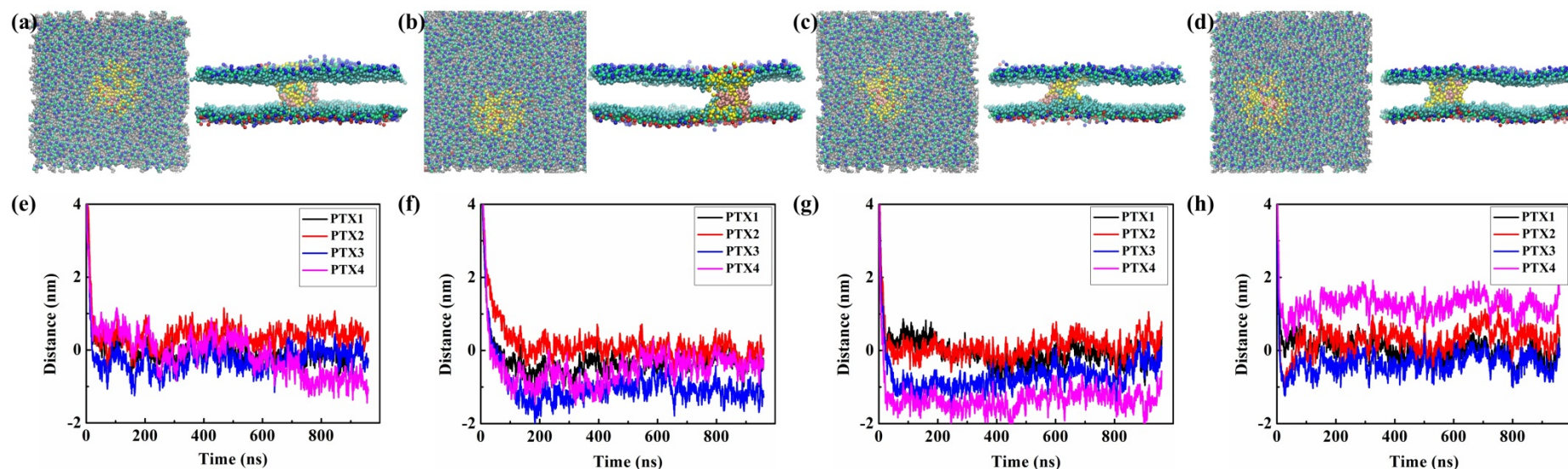
XiaoCong He ^{a,b}, Min Lin ^{b,c}, TianJian Lu^b, ZhiGuo Qu ^{a,b#}, Feng Xu ^{b,c#}

^a *Key Laboratory of Thermo-Fluid Science and Engineering of Ministry of Education, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an 710049, P.R. China*

^b *Bioinspired Engineering and Biomechanics Center (BEBC), Xi'an Jiaotong University, Xi'an 710049, P.R. China*

^c *The Key Laboratory of Biomedical Information Engineering of Ministry of Education, School of Life Science and Technology, Xi'an Jiaotong University, Xi'an 710049, P.R. China*

[#] *Corresponding authors: zgqu@mail.xjtu.edu.cn, fengxu@mail.xjtu.edu.cn*



Supplemental Figure 1. Repeated simulations of interactions between conjugates and asymmetric membranes (four PTX molecules, random distribution). (a-d) Snapshots of conjugates with random PTX molecules distributions interacting with asymmetric membranes in the equilibrated states. (e-h) Corresponding z-distances. The conjugate-asymmetric membrane interaction (four PTX molecules, random distribution) was repeated another four times. Within the four repeats, one of four PTX molecules penetrating through the membrane is observed in three repeats (**Fig. S1 a-c and e-f**). Only one repeat shows that one PTX molecule goes to the outer membrane leaflet (**Fig. S1 d and h**).