**Supplemental information**

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

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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).