Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information for:

Collective Absorption of 2,4,6-Trinitrotoluene into Lipid Membranes and Its Effects on Bilayer Properties. A Computational Study

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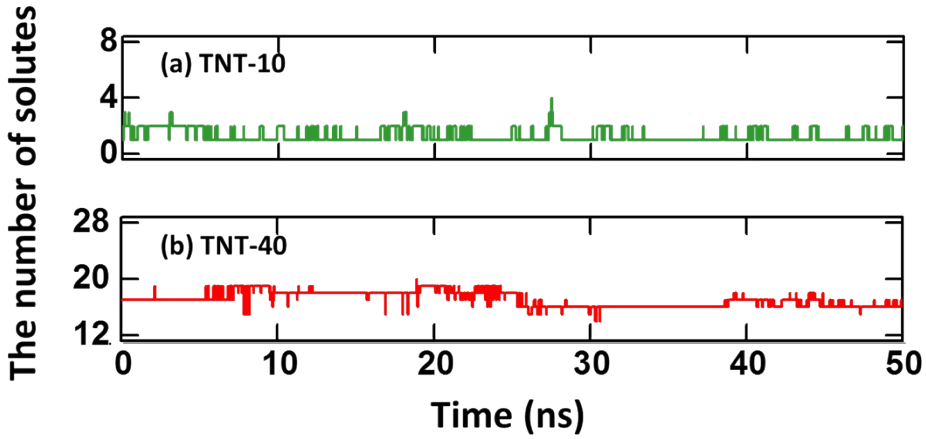

Figure S1. The number of TNT molecules contained in the largest aggregate with the simulation time for (a) TNT-10 system, and (b) TNT-40 system.

Table S1. The area per lipid and thickness of membrane in different systems.

System	Thickness [nm]	Area per lipid [Å^2]
Pure POPC membrane	3.89 (±0.06)	64.7 (±1.2)
TNT-10 system	3.88 (±0.07)	65.9 (±1.5)
TNT-40 system	3.84 (±0.06)	65.6 (±1.3)

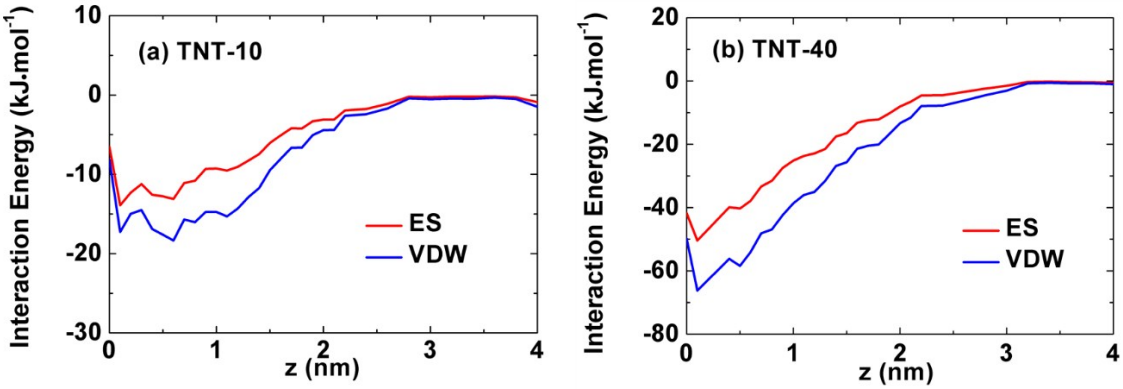

Figure S2. Interaction energy decomposition [electrostatic interaction (ES) and van der Waals interactions (VDW)] of the incoming TNT with the remaining TNT molecules in (a) TNT-10 system, and (b) TNT-40 system, as a function of the distance from the bilayer center.

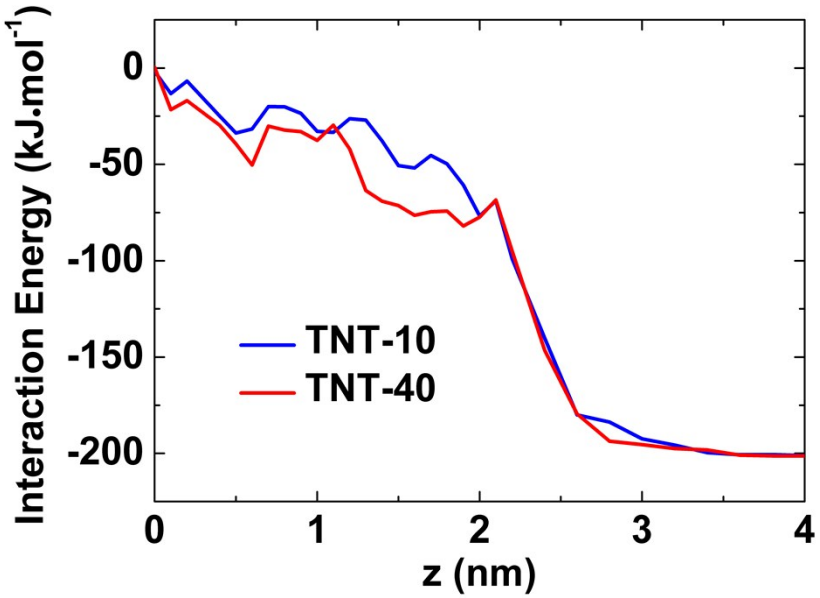

Figure S3. Interaction energy of the incoming TNT with solvent molecules in different systems, as a function of the distance from the bilayer center.

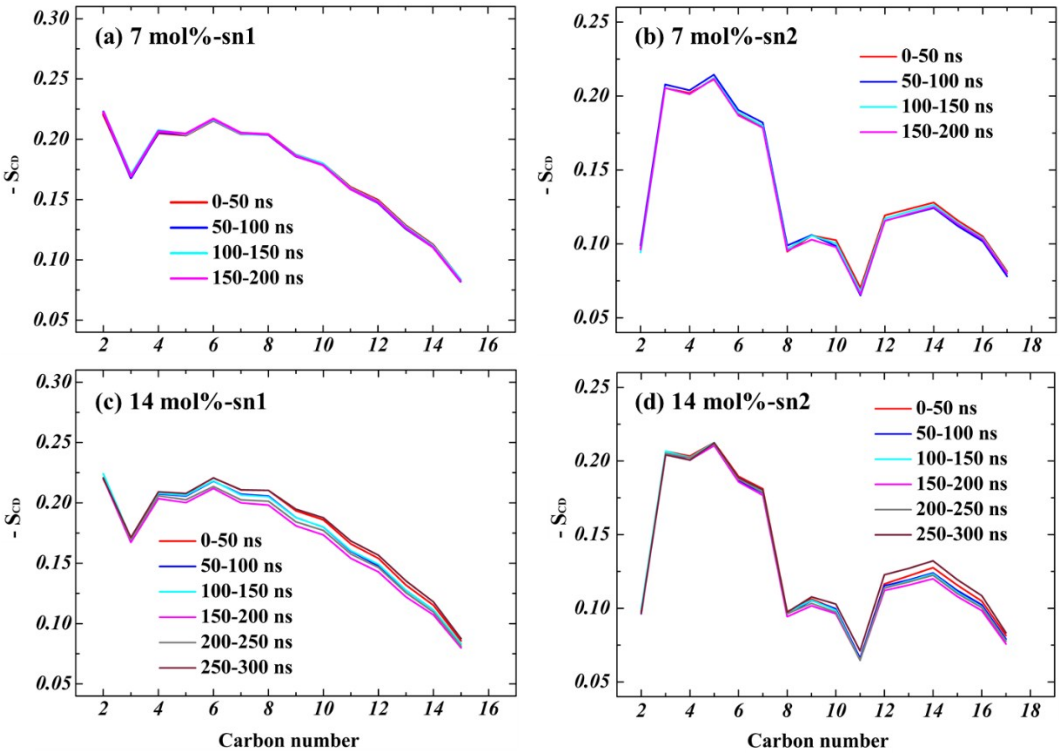

Figure S4. Deuterium order parameters ($-S_{CD}$) of POPC lipids with various TNT concentrations as a function of simulation time.