Electronic Supplementary Material (ESI) for RSC Advances.


# Supplementary Material to

# Molecular dynamics simulations of loading and unloading of drug molecule bortezomib on graphene nanosheet

## By

Songwei Zeng[a], Yu Ji[b], Yue Shen[b], Ruiyao Zhu[b], Xiaogang Wang[b], Liang Chen[b], Junlang Chen[a, b]

[a]*School of Information and Industry, Zhejiang A&F University, Lin'an 311300, China*

[b]*Department of Optical Engineering, Zhejiang A&F University, Lin'an 311300, China*

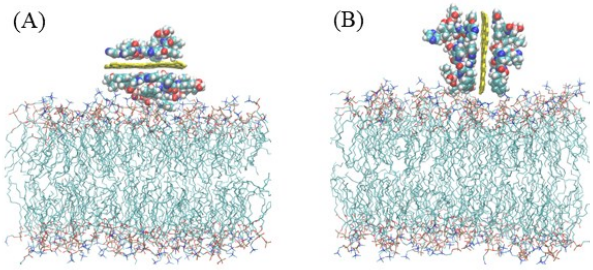


Figure S1. (A) Final snapshot of the complex lying flat out of the membrane, (B) Final snapshot of the complex standing vertically out of the membrane. Water molecules are not shown for clarity.

If the complex is positioned out of but close to the membrane (in detail, the PG sheet is restrained while BOR molecules are free to move), BOR molecules remain on the PG surface, as shown in Figure S1. The complex is highly stable in the water solution with a lipid bilayer.

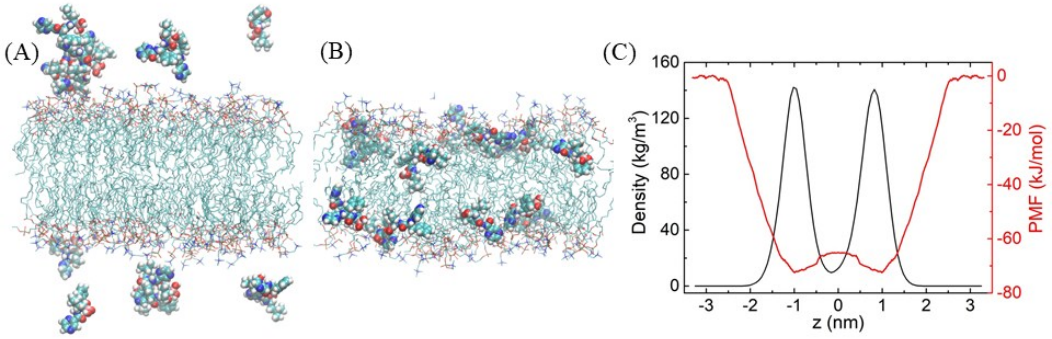


Figure S2. The distribution of BORT in the lipid bilayer. (A) Initial structure, (B) final snapshot, (C) mass density profile of BORT in the membrane and potential of mean force (PMF) of BORT across the membrane.

As shown in Figure S2, all the BORT molecules moved into the membrane and remained there (Figure S2B). Each BORT molecule presented the similar orientation with its polar groups interacting with the lipid headgroups and its aromatic rings immersed in the lipid tails. Mass density profile of BORT demonstrated that they were distributed almost evenly in the two leaflets (Figure S2C). The two symmetric peaks were at $z$=±1.0 nm, close to the lipid headgroups. The minimum of PMF was about -72.3 kJ/mol at the same positions (z = ± 1.0 nm) from the bilayer center, further confirming the energetically favorable locations of BORT in the lipid bilayer.

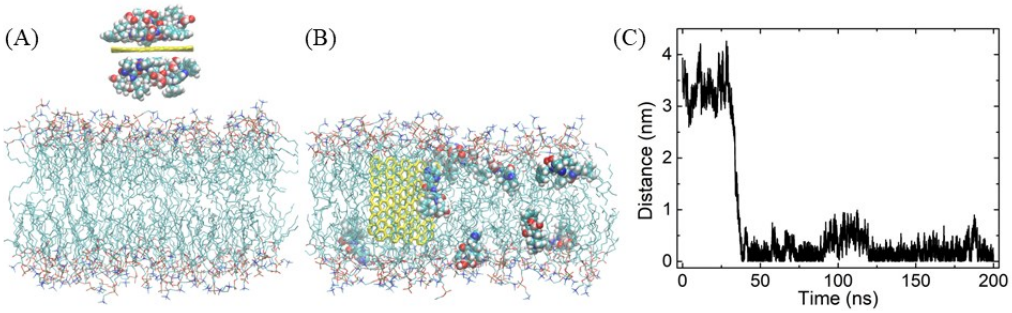


Figure S3. PG loading more BORT molecules. (A) Initial configuration, (B) final structure. (C) COM distance between the complex and lipid bilayer as functions of simulation time.

Similarly, the complex with PG loading 10 BORT molecules can readily enter the membrane. And after the insertion, BORT molecules leave the PG surface one by one and dissolve in the bilayer.