

Computational Biology - 3/13/13 - Caly Allon

"Understanding the nano-bio interface through MD simulation of cytochrome c on phospholipid bilayer."

kind of
not that
impressed with
her...

- used "composed" instead of "comprised"
- "Understanding biophysicochemical interactions at the nano-bio interface" ⇒ Review article
- don't understand / cannot predict how these interfaces interact with biology.
- cytochrome c as a model membrane-binding protein

cytochrome
P50

is the
trans-membrane
one

- ↳ heme protein
- ↳ has another multidomain protein surrounding it.
- ↳ in mitochondria, target for the nano-bio things
- ↳ don't know how it binds to the bilayer
- cardiolipin mediates cytochrome c binding to the bilayer, though no structure of it bound to cytochrome c exists, so the mechanism of binding is unknown
- some experimental results, during which I quite frankly blacked out
- all-atom

↳ adaptin Poisson-Boltzmann electrostatic potential ← what is this??

↳ protein on the lipid bilayer
(~500k atoms, CHARMM27, NAMD, 200ns)

↳ four observables

1) COM-COM distance

2) # of H-bond contacts

3) distance of specific, chosen amino acids to bilayer

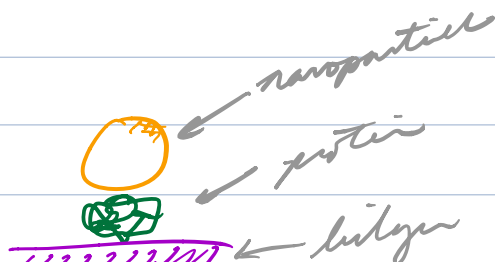
4) RMSD

- cytochrome c dissociates completely from zwitterionic lipid bilayer

- other bilayers exhibit behavior in which faces of the protein are rotating towards or away from the bilayer

↳ faces 1 and 2 are favoured in distance and H-bond contact information

- during the trajectories, the structure was fairly steady during all trajectories, in the RMSD and STRIDE data.



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