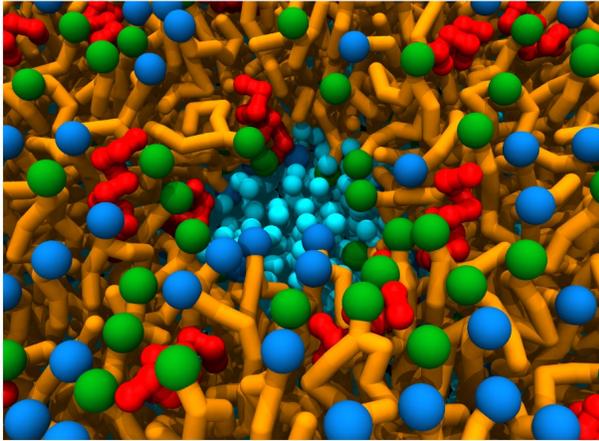
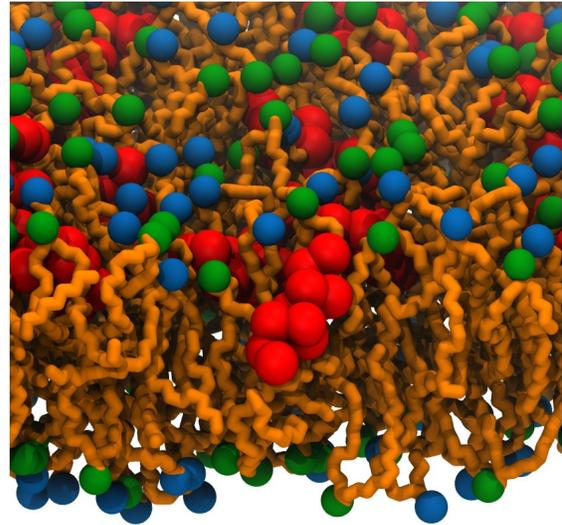
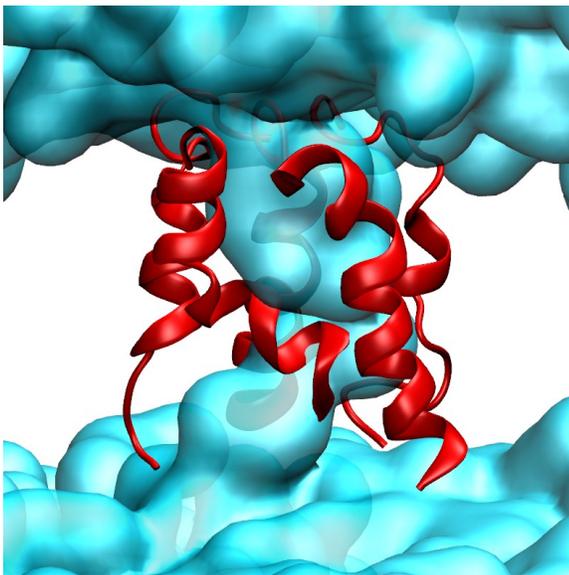
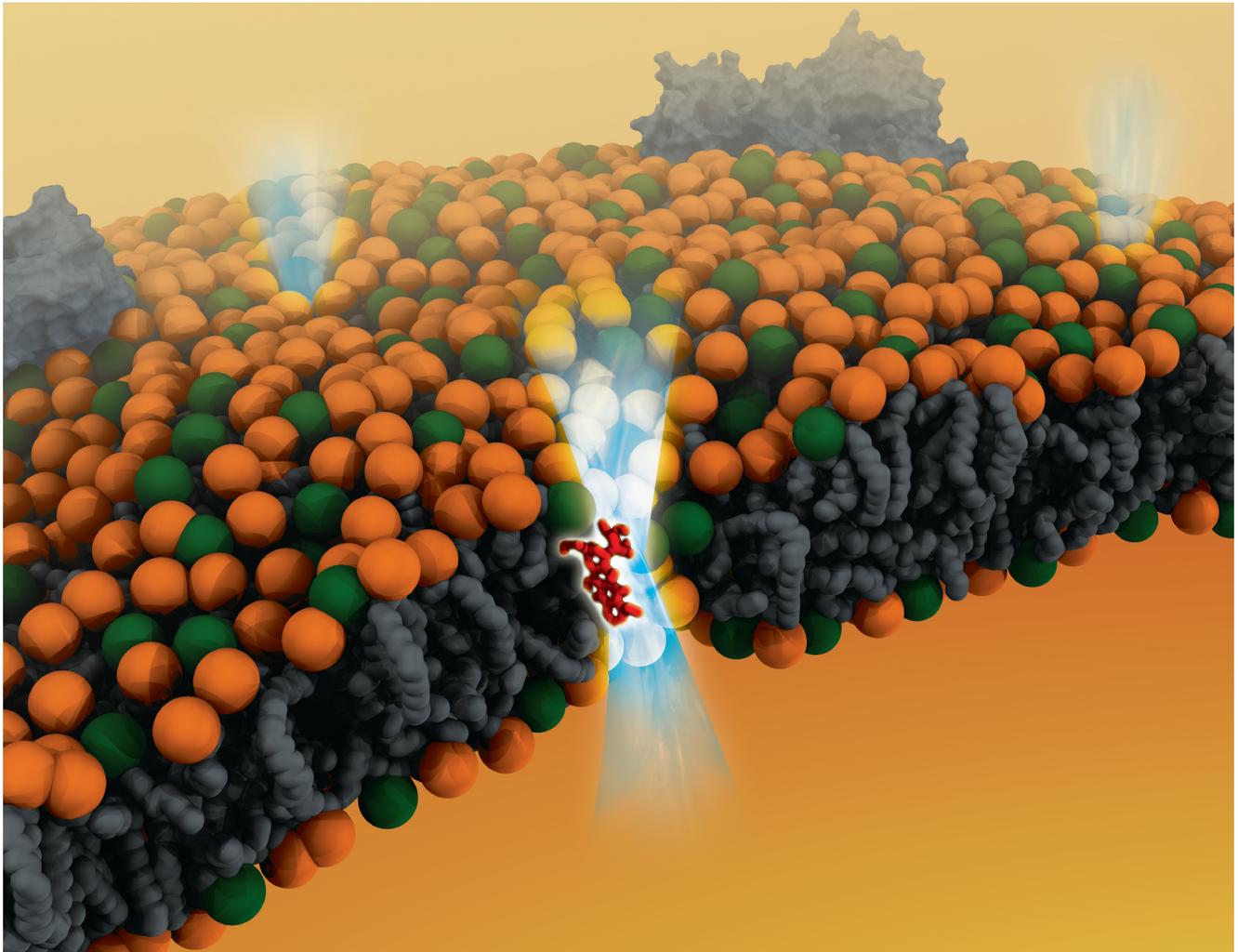


**A****B**

**Figure 1 - A:** BP100 interacting with a mixed anionic and zwitterionic lipid membrane, at a coarse-grain level of description. A disordered toroidal pore is formed in the  $10^2$  ns timescale. Peptide backbones are in shown in red, anionic headgroups in blue and zwitterionic ones in green, acyl tails in orange and water in cyan. For clarity, the waters above the membrane are not shown and the phospholipid headgroups are represented by a single bead instead of four. **B:** improvement of the detail of the system by using a multiscale approach: coarse grained peptides interact with atomistic detail membranes. Color legend is the same as in **A**, except that water is not shown, and that the phospholipid headgroups now represent the phosphate-choline/glycerol moieties.



**Figure 2 -** Alamethicin pore observed in a multiscale system. The peptide was simulated at a full atomistic description, whereas the lipids and the water were described at the coarse grain level. Peptides are in red, water occupancy as a translucent blue surface; lipids were omitted for clarity.



**Figure 3** - Artist's view of the process of doxorubicin (in red) translocation, enhanced by short-tail phospholipids. Figure adapted from actual simulation data on doxorubicin interaction with membranes