Notes about mds related to cco

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**MEMBRANE -> tutorial from NAMD** [**tutorial**](http://www.ks.uiuc.edu/Training/Tutorials/science/membrane/mem-tutorial.pdf)

*/media/88bc6e86-bfdd-41a3-b3f0-9921ae91f5b7/awoelke/awoelke/md\_cco/membrane/*

* *CHARMM\_scripts/*
* SCRIPTS TO DO IN ORDER: 1. rename POPC/water

2. read files read\_cco.inp

3. delete\_overlap with everything else

* *solvate\_smaller/*
* also solvate is all right but sometimes it puts water around membrane which is not ok

\*\*\* run long membrane equilibration run about 40ns or more (equilibration is done for membrane and waterbox)

* *md\_lipids\_water\_const\_ratio/*
* this folder contains equlibration script for membrane/waterbox together

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**old files to recycle and re-use also for rhodobacter**

**/media/88bc6e86-bfdd-41a3-b3f0-9921ae91f5b7/awoelke/awoelke/md\_glu101b/deprot\_protlys\_cbt4/Petra/**