New directory (ULV):

* xleap

Load force fields:

* source /home/ebill/amber18/dat/leap/cmd/leaprc.gaff
* source /home/ebill/amber18/dat/leap/cmd/leaprc.protein.ff14SB

Build undecyl (undecanal) group:

* edit und

click ‘draw’ and select “c” in elements. Draw 11 carbon chain with a C=O group on the end. Select Unit > Add H and build



savepdb undecyl undecyl.pdb

saveoff undecyl undecyl.lib

quit

Run the undecyl group in antechamber to get the .prepi and .frcmod for that particular molecule using the pdb that was generated previously.

antechamber -fi pdb \

 -fo prepi \

 -i undecyl.pdb \

 -o undecyl.prepi \

 -c bcc \

 -s 2 \

 -nc 0

parmchk2 -f prepi \

 -i undecyl.prepi \

 -o undecyl.frcmod

xleap

load .gaff and .protein.ff14SB force fields again

loadamberprep undecyl.prepi

loadamberparams undecyl.frcmod

edit und

remove the H adjacent to the carbonyl

set und head null

set und tail und.1.C11

Now we are creating the ULV monomer unit using the following command:

* ULVm = sequence {und LEU CVAL}
* edit ULV

click on the 2 terminal carboxyl groups and make the overall charge of the molecule -1

* check overall charge
* check unit
* savemol2 ULVm ULVm.mol2 0
* quit

gedit the .mol2 file and delete all of the weird symbols (KýÞ#) hat may appear. Be sure that all of the columns line up well.

Run through parmck2 to get the frcmod file

parmchk2 -f mol2 \

 -i ULVm.mol2 \

 -o ULVm.frcmod

* xleap
* load force fields (.gaff, .protein.ff14SB, .water.tip3p)
* loadamberparams ULVm.frcmod
* cat = loadmol2 ULVm.mol2
* edit cat

saveoff cat ULVm.lib

savepdb cat ULVm.pdb

saveamberparm cat ULVm.prmtop ULVm.inpcrd