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:

* ULV = 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
* savepdb ULV ULV.pdb
* quit

Run ULV 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 ULV.pdb \

 -o ULV.prepi \

 -c bcc \

 -s 2 \

 -nc -1

parmchk2 -f prepi \

 -i ULV.prepi \

 -o ULV.frcmod

* xleap
* load force fields (.gaff, .protein.ff14SB, .water.tip3p)
* loadamberparams ULVfrcmod
* Loadamberprep ULV.prepi
* edit cat

saveoff cat ULV.lib

savepdb cat ULV.pdb

saveamberparm cat ULV.prmtop ULV.inpcrd