CHL Lab
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Charmm Parametrization:

1. Making a new residue for charmm is a tricky business, but you always start from here: https://cgenff.paramchem.org/
   In upload molecules, you can upload a .mol2 file with the structure of the molecule you wish to parametrize.
   A .mol2 file can be created using the software IQmol: http://iqmol.org/downloads.html
2. The online platform will then generate a .str output file. Convert this file to a gmx .itp file using the program cgenff_charmm2gmx.py written by the Maryland people.
3. You might need to create novel bond/angle/dihedral parameters; in some cases, you might even need new LJ parameters. The partial atomic charges might need to be optimized. Ask Casey about this. My thesis has further information. Sorry I could not help further with this, but you should feel free to dig into my files for input files, Mathematica plots, etc. The optimization scripts can be found in scripts/optimization, and you should be able to know how to use them by reading my notebook entries.)
4. After you are done with step 3 — if you are adding a small molecule into the force field that is not bonded to the amino acid backbone, then you simply need to include the .itp file generated by cgenff_charmm2gmx.py in forcefields/charmm36MSCN.ff, and you are done.
5. However, if you are making a new aa residue: you need to follow these steps (MSCN used as an example):

— Created .rtp entry MSCN in **merged.rtp**
— Added new atoms types KS, KC, KN in **atomtypes.atp**
— Added new bond types in **ffbonded.itp**
— Added new angle types: CT1-CT2-KS from CT1-CT2-S in **ffbonded.itp**
— Added new dihedral types in **ffbonded.itp**
  HB1-CT1-CT2-KS <— HB1-CT1-CT2-S
  C-CT1-CT2-KS <— C-CT1-CT2-S
  NH1-CT1-CT2-KS <— NH1-CT1-CT2-S
  CT1-CT2-KS-KC <— EtSCN
  HA2-CT2-KS-KC <— MeSCN
— Added new .hdb entry for MSCN in **merged.hdb**
— Added MSCN to residuetypes.dat in **residuetypes.dat** (directly under forcefields)

*For all bonded interactions: used charmm standard function types (Harmonic for bonds, cosine functions for angles, multiple cosine functions for dihedrals) because the .rtp file only takes one function type per type of interaction! Refitted some of the potential energy surfaces (for all PESs, used only the 0-25 kJ/mol portion).
**For CA-CB-S-C dihedral: scanned from EtSCN and fitted with four cosine functions

6. Finally, you should do a test run of your small molecule / new residue in water. To solvate the small molecule is intuitive. To solvate a new aa residue, however, you need to cap both ends to make it charge-neutral (ACE-MSCN-NME, for example).