Protocol for generating RESP charges and AMBER parameters of a ligand

1. Create or obtain the structure of the ligand in `mol2` or `pdb` format
2. Create the Gaussian input from the structure file using `antechamber`:

   ```
   $ antechamber -i ligand.mol2 -fi mol2 -o ligand.com -fo gcrt -gv 1
   -ge ligand.gesp
   ```

   or

   ```
   $ antechamber -i ligand.pdb -fi pdb -o ligand.com -fo gcrt -gv 1 -
   ge ligand.gesp
   ```

   A Gaussian input file has been obtained with the proper keywords for the optimization of the structure and the calculation of RESP charges.

3. Check the keywords of the Gaussian input and change the method of calculation. Add keywords for calculation like %nproc. Check also the charge and multiplicity.
4. Once Gaussian calculation has finished, the calculated ESP charges (`gesp` file) have to be transformed using `espgen` in order to be readable by antechamber:

   ```
   $ espgen -i ligand.gesp -o ligand.esp
   ```

5. From Gaussian output and properly formatted RESP charges to antechamber file type using `antechamber`:

   ```
   $ antechamber -i ligand.log -fi gout -o ligand.ac -fo ac -c esp -
   cf ligand.esp
   ```

6. Generate `frcmod` file containing the parameters using `parmchk2`, so using GAFF2 forcefield:

   ```
   $ parmchk2 -i ligand.ac -f ac -o ligand.frcmod -a Y -w Y
   ```

7. Create `mol2` file containing the optimized coordinates of the ligand and the calculated RESP charges:

   ```
   $ antechamber -i ligand.ac -fi ac -o ligand.mol2 -fo mol2
   ```