IQmol HPCC Setup
IQmol interface can be used to submit jobs to different servers:

- It is preconfigured to submit jobs to Qchem server. This option is good for short small jobs.

- You can install Qchem on your laptop and configure IQmol to submit jobs to run on your laptop.

- You can configure IQmol to submit jobs to remote servers on which you have accounts. Below we show how to configure remote submission to USC HPCC cluster
IQmol: Server setup
This is a setup for USC HPCC cluster, but with small modifications it can be used for other clusters running pbs (such as fluffy).

**Username:** your USC account name used for the USC e-mail

**Password** (will be asked when you test connection): your password for the USC account.

Do not use `~/iqmol` for working directory! Spell the entire path explicitly. This is a recent ssh bug.
IQmol: Server setup

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!/bin/sh
#PBS -q ${QUEUE}
#PBS -l walltime=${WALLTIME}
#PBS -l ncpus=${NCPUS}

source /usr/usc/qchem/default/setup.sh
cd ${PBS_O_WORKDIR}
qchem -nt ${NCPUS} ${JOB_NAME}.inp ${JOB_NAME}.out