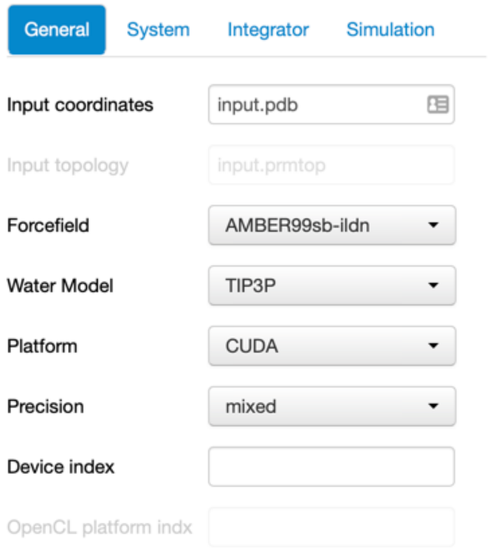
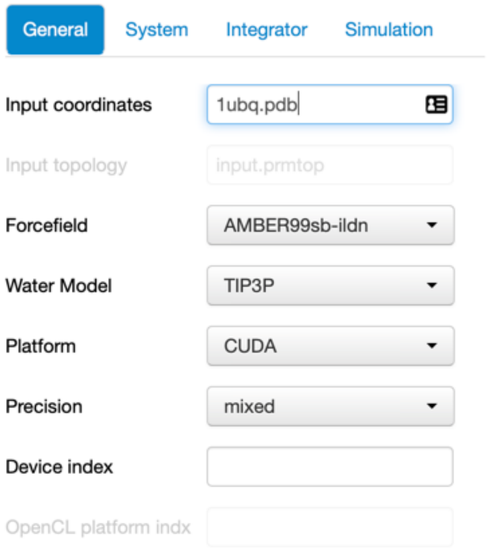
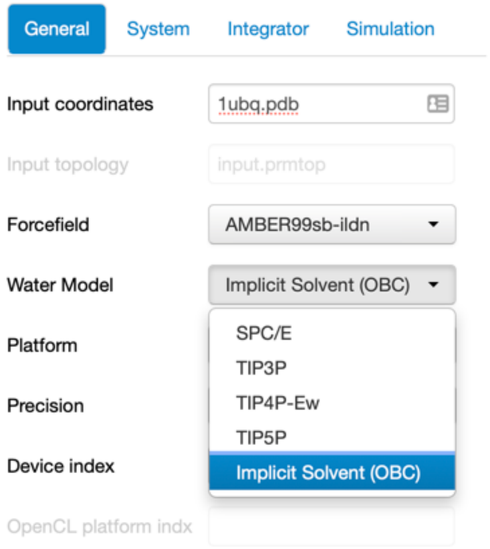
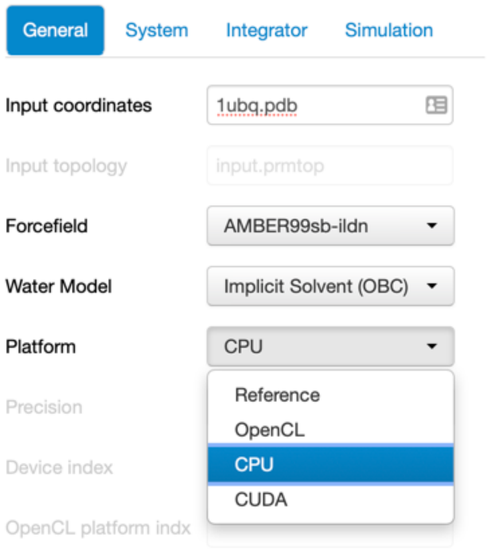
- For “Input coordinates”, enter 1ubq.pdb
- “Forcefield” is the set of parameters and functions that describes the energy of a system. Let’s keep “AMBER99sb-ildn”
- “Water Model” includes
  - descriptions that vary in the number of point charges
  - a description that doesn’t actually model water at all, but its effect on the electrostatic energy and a penalty for forming surfaces. For computational speed, let’s pick this “Implicit Solvent” version
- “Platform” describes the version of the code and the hardware it will run on
  - “Reference” is meant to be the most readable code
  - “CUDA” and “OpenCL” are meant for GPUs, which make MD simulations much faster. “CUDA” only works with Nvidia GPUs and “OpenCL” on others
  - “CPU” is a faster version of Reference.
  - Since the laboratory machines don’t have GPUs, let’s use “CPU”
- The other options are GPU-specific









- “Nonbonded method” describes how long-range interactions are treated. The more interactions that need to be computed, the slower an MD simulation will be.
  - Cutoffs don’t perform calculations if two particles are beyond a certain distance apart.
  - Ewald methods calculate long-range interaction energies between a system and its periodic images. It assumes the system repeats indefinitely.
  - Since we are using implicit solvent, we don’t need periodicity.
  - Let’s use “CutoffNonPeriodic”.
- “Constraints”
  - force a degree of freedom to be a certain value
  - allow a larger time step, giving you more bang (simulation time) for the buck (compute time)
- Let’s keep the other “System” parameters as is