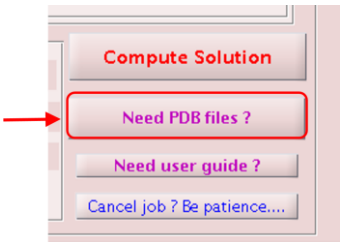
Welcome to the beginners user guide. You can run MPBEC to perform biomolecular electrostatic calculations in three simple steps:

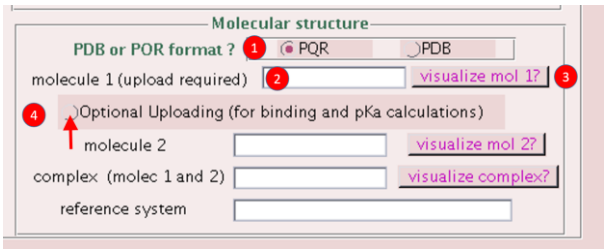
Step 1: Upload molecular structure files



If you do not have the molecular structure file(s) of the biomolecule(s) of interest, you can click the button ***Need PDB files?*** to get them from the Protein Data Bank (PDB) website.

Once you have the molecular structure files,

1. Select either PQR or PDB to choose the format of the molecular structures files. If you upload a PDB file, MPBEC will convert it automatically to PQR file.



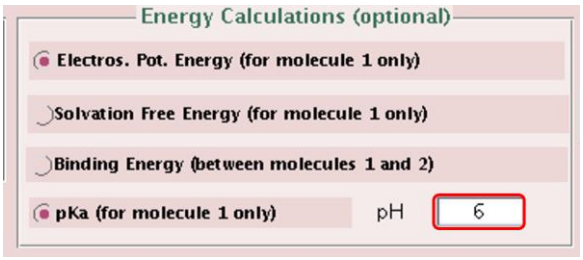
2. Click on ***molecule 1*** box and press enter to search and select your file.
3. If you want to visualize the 3D molecular structure of your molecule press ***visualize mol 1.***
4. For calculations involving two molecules select ***Optional Uploading*** and enter the required files as explained in 2. In the ***reference system*** file enter the file (molecule 1, molecule 2, or complex) that will be used for calculation of the center of coordinate system.

Step 2: Write a name for the Input file/output folder

Click on the box ***Input file name*** and write the desired name for your input file, for instance, *proteinX.inm*. This name will be used to create the name of the Output folder that MPBEC will generate after completion. Note that the name must end with the extension *.inm*. The output folder will be located in the following directory ~/MPBEC/program/src/examples/solutions/.

Step 3: Select energy calculations

By default, MPBEC will always perform the calculation of the mean electrostatic potential. In addition, you may select energy calculations. Click the option corresponding to the energy calculation you want to obtain. Options ***Electros. Pot. Energy*** (electrostatic potential energy) and ***Solvation free energy*** can be chosen to perform these calculations on ***molecule 1.*** These calculations are perfomed at nuetral pH. To perform energetic calculations for acid or alkaline electrolyte solutions, you have to select the ***pKa*** option (for ***molecule 1***) and type in the pH box the value of the pH you want. If you upload files corresponding to ***molecule 2*** and ***complex,*** you may select ***Binding energy*** option.



Finally, run the simulation by pressing the button!!