Data Files for Mapping the Conformational Free Energy of Aspartic Acid in the Gas Phase and in Aqueous Solution

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The data are divided in sub-projects where different systems were simulated with different force fields.

CHARMM_: simulations run with the CHARMM36 force field
AMBER_: simulations run with the AMBER FF99SB-ILDN force field
OPLS_: simulations run with the
OPLS-AA force field
Conformations_: ab initio (DFT-B3LYP & MP2) calculations on selected conformers

_NV.tar.gz: simulations of neutral Asp in vacuo
_ZW.tar.gz: simulations of zwitterionic Asp in water
_NW.tar.gz: simulations of neutral Asp in water
_ZV.tar.gz: simulations of zwitterionic Asp in vacuo

The simulations using force fields were run with the NAMD 2.9 molecular dynamics package and the metadynamics PLUMED 1.3 plug-in.

Ab initio geometry optimization and single point calculations were run with Gaussian 09

Types of input files:
- Configuration .conf: input files for NAMD 2.9; they can be read with any text editor.
- Amber topology .prmtop: topology files for the AMBER force field; they can be read with any text editor and modified with programs within the AmberTools Suite.
- CHARMM topology .psf: topology files for the CHARMM and OPLS force fields; they can be read with any text editor and modified with programs within the CHARMM Suite.
- Input coordinates .pdb:
PDB format files containing the initial coordinates; they can be read with any text editor and visualised with visualisation programs such as VMD and PyMol.
- Plumed input plumed*.dat: Input files for the PLUMED 1.3 plug-in; they can be read with any text editor.
-Gaussian input .in: input files for Gaussian 09; they can be read with any text editor

Types of output files:
- Coordinates .coor: coordinate files printed after every job; they can be read with any MD visualisation programs (e.g. VMD and PyMol) after loading the relative topology, they can also be used as checkpoint to restart the simulation.
- Velocity .vel: files containing the velocities after each simulation; they can be used as checkpoint to restart the simulation.
- Cell dimensions .xsc: files containing the dimensions of the PBC cell at each checkpoint; they can be used to restart the simulation.
- Cell trajectory .xst: sporadically, these files contain further information on the PBC cell and can be used to restart the simulation.
- Log file .log: output files containing the log of each simulation chunk; they can be read with any text editor.

- COLVAR & HILLS: text files containing information on the metadynamics CVs and the added bias during the simulation; they can be read with any text editor and can be used with any tool from the PLUMED suite to reconstruct the free energy.
-Projections .proj: where possible files containing the trajectories projected with Sketch-map have been added; they can be read with any text editor
- Checkpoint .chk: checkpoint coordinate files for Gaussian09, they can be used by Gaussian to restart a simulation
- Log files .log: log files produced by Gaussian09 containing the results of the ab initio calculations

The trajectories are in NAMD binary format .dcd and can be read with any MD visualisation program, such as VMD and PyMol after loading the appropriate topology file. They are divided according to the specific system simulated and they are numbered sequentially.