SFSXplorer Adaptative Force Field

The Lennard-Jones potential (V LJ) has the following expression,

where VLJ is the Lennard-Jones potential used to model the van der Waals’ interactions involving two dipoles;

m and n are the Lennard Jones parameters (n=12, m=6) used to model the van der Waals’ interactions;

ri,j is the interatomic distance;

reqm,I,j is the equilibrium separation between the nuclei of two atoms i an j;

εI,j is the pairwise potential energy or well depth, and

the summation is taken over all pair of atoms, being i from the ligand and j from the macromolecule.

We approximate the hydrogen bond potential using similar equation. Originally, for hydrogen bond potential, literature used m = 10 and n = 12. Here we vary this terms.

where VHB is the hydrogen-bond potential used to model the intermolecular hydrogen bond interactions;

m and n are the parameters (n=12, m=10) used to model the hydrogem-bond interactions;

ri,j is the interatomic distance;

Reqm,i,i is the equilibrium separation between the nuclei of two atoms i and j;

εI,j is the pairwise potential energy or well depth, and

the summation is taken over all pair of atoms, being i from the ligand and j from the macromolecule