

Potential Setup

Title: CHARMM22

File: /usr/local/moe/lib/charmm22.ff

Load:	AMBER89	AMBER94	CHARMM22	MMFF94	MMFF94s
	Engl-Huber	OPLS-AA	PEF95SAC	TAFF	Rule

Term	Weight
<input checked="" type="checkbox"/> Bond Stretch	1
<input checked="" type="checkbox"/> Angle Bend	1
<input checked="" type="checkbox"/> Stretch-Bend	1
<input checked="" type="checkbox"/> Torsion	1
<input checked="" type="checkbox"/> Out of Plane	1
<input checked="" type="checkbox"/> Electrostatics	1
<input checked="" type="checkbox"/> Van der Waals	1
<input type="checkbox"/> Solvation	0

Van der Waals

1-4 Scale: 1

Buffer 1: 0

Buffer 2: 0

Electrostatics

Dielectric: 1

Solvent Dielectric: 1

Dielectric Offset: -0.09

1-4 Scale: 1

Buffer: 0

Distance Dependent

Nonbonded Cutoff

On: 6.5

Off: 7

State Scale

Like: 1

Unlike: 0

Wild: 1

Apply

Default

Close