

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