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Pipeline Pilot Professional Client - [Calculate Interaction Energy*]

File Edit View Tools Window Help

Protocols

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SD Reader SD Writer HTML Molecular Table Viewer

Favorites Custom Manipulator (PilotScript) Custom Filter (PilotScript)

Top N Filter

1

DS Typed Structure Reader

CHARMm Interaction Energy

Mol2 Writer

Elapsed Time:

shikha Protocols Components All Calculate Inter...

Help

Calculates the interaction energy between sets of atoms across all conformations of a molecule

Uses CHARMM. The interaction energy is defined as the sum of the van der Waals and electrostatics energy.

The molecule must be typed with a supported forcefield.

Parameters

Input Typed Molecule	data\CHARMm\1crn_sdc.msv
Atom Selection 1	sele bynum 1:10 end
Atom Selection 2	sele bynum 10:20 end
Dielectric Model	None
Nonbond List Radius	14.0

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