Vrms v1.0

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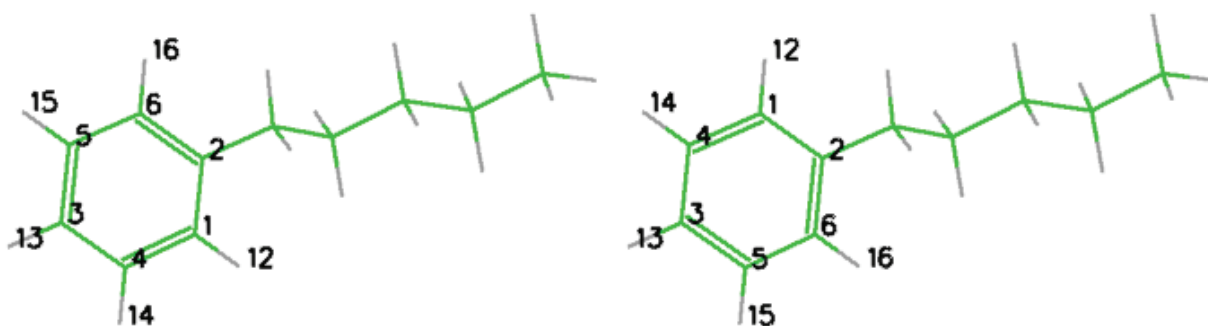
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OVERVIEW

Vrms provides the root-mean-square deviation (RMSD) between a series of test conformations of a molecule and a reference conformation. In one mode, each test conformation is superimposed on the reference conformation before the RMSD is computed; this mode is appropriate for comparing the conformations of a molecule free in solution. In a second mode, no superposition is performed; this mode is appropriate for comparing docked conformations of a ligand with the crystal conformation. Vrms can correct for global and local symmetries. For example, if the test conformation differs from the reference conformation only by a 180º rotation of a benzene ring (see Figure), the local symmetry of the benzene is detected and applied so that a low RMSD is obtained.

Figure: Two conformations that are identical except for a chemically irrelevant benzene flip.

The inputs are:
- a source SDfile file containing one or more conformations of the same molecule. (See www.mdli.com/downloads/literature/ctfile.pdf for a description of MOLfile and SDfile formats.)
- a file containing the coordinates of at least one reference conformation of the same molecule. If the reference structure contains all atoms, then their order does not need to match the order of the atoms in the source file. If the reference structure contains only non-hydrogen atoms, then the order of its must match the order of non-hydrogen atoms in the file of test conformations. The reference structure can be in any of the following formats:

  - Charmm coordinate file (.crd)
  - MDL MOLfile (.mol)
  - MDL SDfile (.sdf) containing one or more structures
  - PDB file containing one or more conformations

- command-line options

The outputs are:
- a log file containing a summary of the run information, the computed RMSDs (Angstroms) between each test conformation and the reference conformation, and, optionally, energy data if supplied in the source file.

- if superposition is requested, an SDfile containing the reference conformation followed by the optimally superimposed test conformations
- optionally, a file containing the symmetry-corrected correspondences and distances between the test and reference atoms for each test conformation. For example, in the Figure, Atom 1 would correspond to Atom 6, and their distance would be 0.000 since the conformations are identical.

COMMAND-LINE OPTIONS

Vrms is invoked via the following command line:

```
Vrms <source file(.sdf)> <reference file(.crd/.mol/.sdf/.pdb)> [-i
structNumber] [-all] [-nsup] [-ns] [-ts setupTimeLimit] [-rl limitRes] [-oe]
[-log logFile] [-out superFile] [-op] [-pf pairwiseFile]
```

(Items in square brackets are optional.)

Options:

-i   Reference structure index
      structNumber   Index of the structure in the reference file that is to be compared with the source conformations. This option is only valid with SDfile and PDB file formats.

      Default: 1

-all   Use all atoms
      Include hydrogen atoms in the RMSD comparison.

      Default: Use only heavy atoms.

-nsup   No superimposition
      Do not superimpose the source conformation and the reference conformation before calculating the RMSD. This option is useful when the source and reference conformations are in the same reference frame and deviations due to translations and rotations are of interest.

      Default: Superimpose test conformations on the reference conformation.

-ns   No symmetry
      Do not account for symmetry when computing the RMSD. The RMSD between two conformations in figure one would be non-zero if this option is used.

      Default: Include symmetry in the RMSD calculation.

-ts   Setup time limit
        `setupTimeLimit` Time limit for molecule setup, in seconds, where setup includes identification of alternate resonance forms and calculation of partial charges (used in symmetry calculation). Occcasionally a molecule will exceed this limit, usually due to an especially complex resonant system. A greater time limit may be used or the depth of the resonance search limited with (`-rl`). Another alternative, if it is acceptable, is to use the ignore symmetry option (`-ns`).

        Default: 120 seconds

-rl   Resonance generation limit
        `limitRes`   Stop resonance if any generation has more than specified number of states. Otherwise resonance will run until the setup time limit is reached.

        Default: 1000 generations

-oe   Output energy information
        Output the energy of each conformations with the calculated RMSD. This option is only valid when the source file contains the energy block "> <Energy>", as when the conformations are generated by VeraChem's conformational analysis program **Vconf**. Summary information is also output at the end of the file. This includes energies of the lowest and highest RMSD conformations and the index and RMSD of the lowest energy conformation.

        Default: Energy information is not written to the log file.

-log   Log file
        `logFile`   Name for the file containing the RMSD information.

        Default: `<input sdf filename>_vrms.log`.

-out   File of superimposed conformations
        `superFile`   Name for the file containing the superimposed conformations.

        Default: `<input sdf filename>_superimposed.sdf`.

-op   Output pairwise symmetry information
        Output an additional file specifying the symmetry-corrected atom-atom correspondence between each test conformation and the reference conformation, and the corresponding atom-atom distances, in Angstroms. (see `-pf` option).

        Default: Atom-atom correspondences not output.

`-pf`   Pairwise filename
        `pairFile`   Name for the log file containing the pairwise atom information from the `-op` option.

        Default: `<input sdf filename>_pairwise.log`.

Stopping a Run in Progress

A run in progress can be cleanly stopped by placing into the working directory an empty file with the name of the log file but with ".log" replaced by ".end". For example, if the log file is "diversity_Vrms.log", the run will be stopped by placing a file named "diversity_Vrms.end" in the same directory as the log file.

The Linux "touch" command provides an easy way to create this file; e.g., "`touch diversity_Vrms.end`".

The Files section of the log file includes a reminder of the name and location of the file required to stop the calculation; see the "Stop file:" line.

EXAMPLE

The **Vrms** distribution includes sample input and output files. The input file, `example.sdf`, contains conformations generated with **Vconf** (available separately).

The command:

```
../vrms.exe example.sdf example.sdf -i 1
```

generates the output files example_vrms.log, example_superimposed.sdf.