

source/geomcent.c

New documentation:
doc.ps

SEED 3.3 Release August 9, 2004

The following is introduced after the SEED 3.2 release dated
June 24, 2004.

1. Enhancement of input/output and energy evaluation mode

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The keyword RESN in fragment files is not mandatory any more. If RESN
is not found a fragment name is automatically assigned.

The maximal number of geometrical centers to write in *_geomcent.mol2
files is set in the parameter file.

In the postprocess mode the writing of *_pproc* files can be
activated or deactivated in the parameter file.

In the energy evaluation mode energies are not evaluated if the
ligand does not lie completely in the grids. Moreover a warning
message is written in the output log file.

Files modified:
source/refrfi_mol2.c
source/funct.h
source/reinfi.c
source/checkresn.c
source/geomcent.c
source/main.c
inputs/seed.par

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