
SEED 3.3.5 Release November 22, 2013

The following is introduced after the SEED 3.3 release dated
August 8, 2004.

1. Various modifications to output and file handling

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Bugfix: enabled docking of water (line 112 ff)
Fixed: dynamic memory allocation to store fragment energies
Fixed: removal ofwrite/read cycles of temporary files from harddisk
Fixed: small speedup of 3D similarity calculation for clustering routine
Fixed: exception handling
Bugfix: reduction of the polar points routine when only one point was
created to begin with
Fixed: speed up of fast receptor desolvation routine
Fixed: removed output of fast algorithm-calculated energy values from seed.out

Files modified:
source/reduc_polvectre.c
source/solv_frag_fast.c
source/simila.c
source/main.c

2. Adaptions of .par files for CHARMM36, CGenFF and the MATCH atom typer

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Added: ligand atom types/parameters for CHARMM General Force Field (CGENFF)
Added: protein atom types/parameters for CHARMM36
Added: ligand atom types/parameters for MATCH atom types (CGENFF-derived)
Changed: seed.inp default parameter file now contains CHARMM36+CGENFF
Changed: MSI-CHARMM atom types now in seed_charmm-msi.par

Files created:
inputs/seed_charmm36-c37b2_cgenff-v2b8.par
inputs/seed_charmm36-c37b2_cgenff-v2b6_MATCH.par
inputs/seed_charmm-msi.par

Files changed:
inputs/seed.inp

New documentation:
doc_seed_3_3_5.pdf
