Change-log file

SEED 1.0 Release 1999

Version of SEED corresponding to

N Majeux, M Scarsi, J Apostolakis, C Ehrhardt, A Caflisch,
Proteins: Structure, Function and Genetics, 37, pp. 88-105, 1999

SEED 2.0 Release September 25, 2000

Version of SEED corresponding to

N Majeux, M Scarsi, A Caflisch,
Proteins: Structure, Function and Genetics, 42, pp. 256-268, 2001

SEED 2.1 Release February 25, 2002

The following is introduced after the SEED 2.0 release dated
September 25, 2000.

1. Enhancement of the receptor vector selection
   Name : Nicolas Majeux
   Email address : majeux@bioc.unizh.ch
   Institution : Department of Biochemistry
   University of Zurich
   Date : February 25, 2002

To discard polar and apolar receptor vectors that point outside of
the binding site a selection using an angle criterion can be
activated (page 10 of the corresponding SEED documentation).

Files modified:
source/funct.h
source/main.c
source/reduc_polvectre.c
source/reinfi.c
source/solv_lookup.c
inputs/seed.inp
inputs/seed.par

New documentation:
doc.ps

SEED 3.0 Release March 5, 2003

The following is introduced after the SEED 2.1 release dated
February 25, 2002.

1. Enhancement of the generalized Born model
   Name : Nicolas Majeux
   Email address : majeux@bioc.unizh.ch
   Institution : Department of Biochemistry
   University of Zurich
   Date : March 5, 2003

Empirical correction term to the Coulomb field approximation
[MS Lee, FR Salsbury Jr, CL Brooks III,
Journal of Chemical Physics, 116 (24), 10606, 2002]

for the accurate screened interaction and fragment desolvation
energies.

Files modified:
source/main.c
source/solv_frag.c
source/solv_lookup.c
source/funct.h
source/reinfi.c
inputs/seed.par

New documentation:
doc.ps

SEED 3.1 Release May 26, 2004

The following is introduced after the SEED 3.0 release dated
March 5, 2003.

1. Reduction of the number of output files
   Name : Nicolas Majeux
   Email address : majeux@bioc.unizh.ch
   Institution : Department of Biochemistry
   University of Zurich
   Date : May 26, 2004

The following files are not written out any more if the
"postprocess scheme" is selected: FragmentName_xxx.mol2,
FragmentName.chm, FragmentName_clus.chm, FragmentName_clus_reduc.chm .

File modified:
source/main.c

New documentation:
doc.ps

SEED 3.2 Release June 24, 2004

The following is introduced after the SEED 3.1 release dated
May 26, 2004.

1. Calculation of geometrical centers for FFLD
   Name : Nicolas Majeux
   Email address : majeux@bioc.unizh.ch
   Institution : Department of Biochemistry
   University of Zurich
   Date : June 24, 2004

The geometrical centers for FFLD are written out in
FragmentName_geomcent.mol2 files. The method is described
on page 413 of
M Cecchini, P Kolb, N Majeux, A Caflisch, Journal of Computational
Chemistry, 25, pp. 412–422, 2004.
Also on page 24 of the corresponding SEED documentation.

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

File added:

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
   Name   : Nicolas Majeux
   Email address : majeux@bioc.unizh.ch
   Institution   : Department of Biochemistry
                   University of Zurich
   Date   : August 9, 2004

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

New documentation:
doc.ps
