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#seed.param v4.0
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#       PARAMETERS FORMERLY IN SEED.INP
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# -----
#       Dielectric constant of the solute (receptor and fragment)
p1 2.0
#       Ratio of kept vectors for docking : polar / apolar
p2 1.0 1.0
#       First value: write *_clus.mol2 file (y/n)
#       Second value: write *_best.mol2 file (y/n)
p3 n y
#       First value: write *_clus.dat summary table file (y/n)
#       Second value: write *_best.dat summary table file (y/n)
p4 y y
#       First value: maximum number of cluster members saved in *_clus*
#       output files. Note that this value determines the maximum number
#       of poses per cluster that go through slow energy evaluation.
#       Second value: maximum number of poses saved in *_best* output files.
p5 5 1
#       The docked fragments are saved in the dir ./outputs
#       Filename for output log file. This is the main SEED output file.
p6 ./outputs/seed.out
#       write (w) or read (r) Coulombic grid / grid filename
p7 w ./scratch/coulomb.grid
#       write (w) or read (r) van der Waals grid / grid filename
p8 w ./scratch/vanderwaals.grid
#       write (w) or read (r) receptor desolvation grid / grid filename
p9 w ./scratch/desolvation.grid
#
# -----
#       PARAMETERS FOR DOCKING
#       DEFINITIONS:
#       fast energy: used only to preprocess, i.e., as a filter
#                   [Majeux et al, PROTEINS 42, 256-268, 2001]
#       accurate (and slower) energy: used to postprocess and should
#                                   NOT be turned off
#                                   [Majeux et al, PROTEINS 37, 88-105, 1999]
# -----
#
#       Bump checking: used only if fast energy is switched off
#       n x atoms = maximum tolerated bumps /
#       scaling factor for interatomic distance /
#       severe overlap factor (beta factor in PROTEINS paper)
p10 2.0 0.89 0.6
#       van der Waals energy cutoff (kcal/mol):
#       used if fast energy is switched on
p11 1.0
#       Angle (deg) and number of points on the sphere around the HB vectors
p12 50.0 100
#       Number of fragment rotations around each axis
p13 72
#       Modification of February 2002:
#       Removal of rec. polar and apolar vectors using angle criterion
#       angle_rmin (deg)  angle_rmax  multipl_fact_rmin  multipl_fact_rmax
#       Method:
#       The minimal (minDist) and maximal (maxDist) distances
#       between the vectors and the points in the binding site
#       (as defined in the SEED input file) are evaluated.
#       A vector is discarded if the angle between the vector
#       and its closest point in the binding site is larger than
#       a cutoff angle value.
#       The cutoff angle value follows the following distribution:
#       - angle_rmin if distance <= (multipl_fact_rmin*minDist)
#       - angle_rmax if distance >= (multipl_fact_rmax*maxDist)
#       - linear dependence (range between angle_rmin and angle_rmax)
#       for other distances
p14 70.0 10.0 1.2 0.8

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