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# Removal of the rec. polar vect.: vdW radius probe
p15 1.83
# Coulombic fast energy: 1=distance dept diel / grid margin / grid spacing
p16 1 20.0 0.5
# van der Waals fast energy: grid margin / grid spacing
p17 20.0 0.3
# accurate energy: Coulombic cutoff for formal charges is automatically
# set to 1.3 x van_der_Waals_cutoff
# accurate energy (vdWaals): nonbonding cutoff / grid spacing
p18 12.0 1.0
# Multiplicative factor (k) for apolar docking to skip evaluation of
# electrostatics. The vdW energy cutoff is:
# k x Number of fragment atoms, including hydrogen atoms
p19 -0.333333
# Solvation grid: grid margin / grid spacing
p20 24.0 0.5
# Solvation: water radius / # points per sphere to generate SAS /
# solvent dielectric constant
p21 1.4 500 78.5
# Hydrophobicity maps: point densities (A^-2) on the SAS for apolar
# vectors on the receptor / on the fragment /
# probe radius to generate SAS for apolar vectors /
# scaling factor for desolvation and / vdW interactions
p22 1.0 1.0 1.4 1.0 1.0
# Scaling factors for fast and also accurate energy evaluation:
# van der Waals / electrostatic interaction / receptor desolvation /
# fragment desolvation
p23 1.0 1.0 1.0 1.0
# -----
# Clustering parameters
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# -----
# GSEAL : sim. weight factors (150 atom el.) 0 or # non-default + list
p24 4
6 6 2.0
7 7 10.0
8 8 10.0
16 16 10.0
# The clustering with GSEAL proceeds in two steps: the
# first clustering yields large clusters which contain almost
# overlapping as well as more distant fragments; the second
# clustering is done on each cluster found in the first clustering
# to eliminate fragments which are very close in space.
#
# First clustering: overall clustering
# GSEAL similarity exponential factor / cutoff factor
p25 0.9 0.4
#
# Second clustering: to discard redundant positions
# GSEAL similarity exponential factor / cutoff factor
p26 0.9 0.9
# Maximal number of positions to be clustered
p27 20
# Number of lines to be written in the output file for the sorted
# energies and the two clustering procedures /
# Printlevel (0=lean, 1=adds sorting before postprocessing, 2=adds 2nd
# clustering)
p28 100 1
# -----
# Forcefield parameters from now on
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# -----
# Parameters are CGenFF v4 (2016) and param36 (2012) with water and ions as per
# toppar_water_ions.str
#
# NB: if the user includes metal ions in the binding site, appropriate hydrogen bond
# distances with these ions should be provided in the "Hydrogen bond distances
# between donor and acceptor" section below

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