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#           Parameter filename
i1 ./seed4_cgenff4.par
#           Receptor coordinates (in mol2 format) filename
i2 receptor.mol2
#           Binding site residue list
#           First line:  number of residues
#           Following lines: residue numbers (one each line)
i3 1
    101
#           Modification of February 2002:
#           List of points (e.g. ligand heavy atoms of a known ligand-receptor
#           complex structure) in the binding site used to select polar and apolar
#           rec. vectors which satisfy the angle criterion (see parameters file)
#           First line:  number of points (0: no removal of vectors using the angle
#           criterion)
#           Following lines:  coordinates of the points
i4 6
    62.881  39.578  -4.449
    61.755  39.106  -4.248
    61.465  37.747  -3.723
    60.663  39.820  -4.501
    60.749  41.185  -5.002
    59.457  41.937  -4.647
#           Metals in the binding site
#           Make sure that the residue number of the metal is in the
#           binding site residue list.
#           First line:  total number of coordination points
#           Following lines:  atom number of metal / x y z of coordination point
i5 0
#           Spherical cutoff for docking (y,n / sphere center / sphere radius)
i6 n  2.133  1.359  25.539  10.00
#           Fragment library specifications
#           First line: Number of fragments / dock+energy (d), only energy (e)
#           Second line: Fragment library filename /
#           apolar docking (a), polar docking (p), or both (b) /
#           energy cutoff in kcal/mol / 2nd clustering cutoff in kcal/mol
i7 d
/home/ligands/library.mol2          b      2.0    2.0
end

```