GG only accepts files in the PDB file format. The results include the IDs of the oxygen atoms that possibly bind to calcium ions as well as the potential calcium locations. Three user-defined parameters in the GG program are explained as following:

1. O-O cutoff: the threshold distance between two oxygen atoms considered as ligands for one calcium-binding site.
2. Ca-O lower bound: the lower limit of the distances between calcium and ligand Oxygen atoms.
3. Ca-O upper bound: the upper limit of the distances between calcium and ligand Oxygen atoms.

##

Download the file gg.1.0.zip into a local folder; decompress gg.1.0.zip with WinZip or WinRAR to the following files:

gg.1.0.NET.1.0.exe: the executable file under windows with .NET Framework1.0;

sample1.pdb and sample2.pdb: two sample PDB files;

readme.html: user's guide.

Tutorial for GG execution

Double click the icon of gg.1.0.NET.1.0.exe (If you cannot run the program, please download .NET Framework 1.0 and install it. The blue parts below are program prompts, the green parts are the values that the user types in, and the values in the parenthesis are the suggested empirical values). The following information will be shown:

Please enter pdb file

sample1.pdb

Please enter O-O cutoff: (6.0)

6.0

Please enter Ca-O lower bound: (1.8)

1.8

Please enter Ca-O upper bound: (3.0)

3.0

Take oxygen atoms from non-water heteratoms as potential ligand? (y)

y or n

The program will run and finish in seconds. It creates 4 files:

psdCa.dat, psdCa_inc.pdb, psdCa_mrg.dat and psdCa_mrg_inc.pdb

Two dat files contain the oxygen ligand atom IDs (line 1 of each site), the residue information related to each oxygen ligand (line 2) the calcium coordinates (line 3), and the Ca-O distance (line 4). The psdCa.dat file contains the information for all of the predicted sites and the psdCa_mrg.dat only contains the sites after merging the closely located predictions.

Two corresponding output PDB files contain the pseudo-calcium information in addition to the original protein coordinates. The pseudo-calcium ions are shown in the end of the files in the form of "HETATM 0000 CAL NNN CAL XXX YYY ZZZ 1.0 DDD CA" (11 columns), where NNN indicates the serial number of the prediction, XXX, YYY and ZZZ are the coordinates, and DDD is the Ca-O distance in the predicted sites.

##

Reference:

[1] Hai Deng, Guantao Chen, Wei Yang and Jenny J. Yang, "Predicting Calcium Binding Sites in Proteins-A Graph Theory and Geometry Approach" submitted to Proteins in Oct. 2005.