How the pockets were calculated

- Each PDB model was completed adding the hydrogens (ionizing the residues according to the physiological pH), charging the atoms (Gasteiger-Marsili approach), assigning the atom types (CHARMM 22) and was minimized by NAMD2 (conjugate gradients, 50 000 steps), keeping the protein backbone fixed. Ligands, waters, counterions were removed.
- The cavities were found by *fpocket* program setting the default parameters. For more detail about the method, see here:
  Peter Schmidtke, Axel Bidon-Chanal, Javier Luque, Xavier Barril, "MDpocket: Open Source Cavity Detection and Characterization on Molecular Dynamics Trajectories", Bioinformatics, 1;27(23):3276-85, 2011.
- For all cavities of each protein, at least one docking calculation was performed by *PLANTS* (ChemPLP scoring function, Speed1 exhaustiveness) with one or more ligands as probe known to be binders of the given protein or the protein class.
- Each pocket set was ranked according to a consensus function in which the total pocket score and the docking scores of each considered probe were taken into account.
- The results are saved to an Excel file in which could be present more than on sheet if the considered probes are known to be binders of a specific sub-pocket (e.g. othosteric and allosteric ligands).

About the files and the directories

For each protein, a zip archive is provided and named according the following rule:

Protein-name_pockets.zip

This file has the following structure:

Ligands	Directory of the ligand probes in Mol2 format.
Orthosteric	Directory of orthosteric ligands (optional).
Allosteric	Directory of allosteric ligands (optional).
RNA binding site	Directory of ligands of the RNA binding site (optional).
Model_1	Directory of the model #1. If it includes homology models, a sub-directory for each model is present with the same structure tree of the crystal ones.
Model_min_out	Directory of the pocket analysis.
pockets	Directory of the pocket files (two files for each pocket enumerated from 0).
pocket0_atm.pdb	Atoms defining the border of the pocket #0 in PDB format.
pocket0_vert.pqr	Spheres filling the pocket #0 in PQR format (PDB variant).
…	
poses_PROBEID	Directory the best poses for each pocket. If more than one probe was used for the analysis, this multiple copies of this directory could be present with different PROBEID.

pocket0_plants.mol2	Best pose for the pocket #0 in mol2 format.
…	
model_min.pml	Script to show the pockets whit PYMOL.
model_min.tcl	Script to show the pockets whit VMD.
model_min_out.pdb	PDB file including both input protein and the cavities.
model_min_out.xlsx	Excel file with the scores, volume, coordinates of the centre, radius, sizes along X, Y and Z axis, docking scores and consensus.
model_min_PROBEID_plants.csv	PLANTS output file with all docking scores in CSV format (one for each probe).
model_min_pockets.pqr	Spheres of all pockets in PQR format.
model_min_PYMOL.cmd	Batch file to run PYMOL.
model_min_VMD.cmd	Batch file to run VMD.
Model.pdb	Original PDB file.
Model_min.iff	Minimized structure in IFF format.
Model_min.pdb	Minimized structure in PDB format.