Title: Protein-ligand simulations

Goal: The purpose of the course is to enable attendees to build a protein-ligand system to be simulated by molecular dynamics.

The initial system will be set up from both the free ligand and protein. The formation of the complex will be reached with Docking methodology.

If We have enough time, the free energy of solvation of the complex and its components will be determined.

Packages to install (previously):
Gromacs 5.1, autodock vina, pymol, plugin de autodock vina para pymol, autodock tools.

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