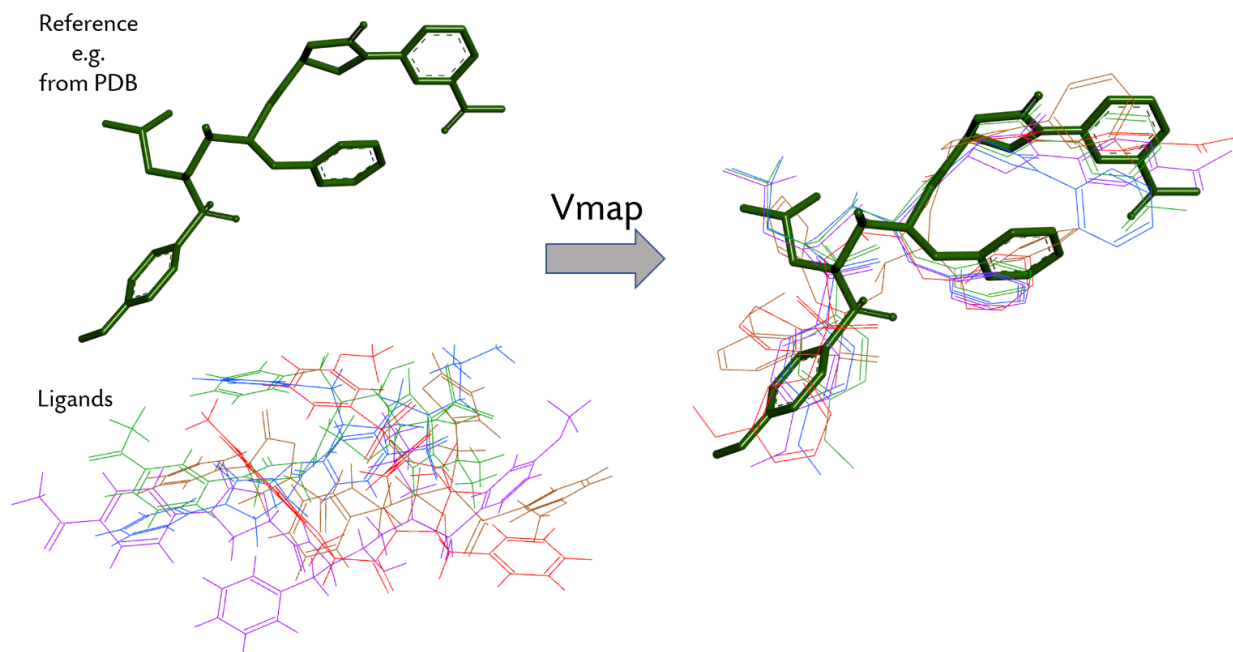
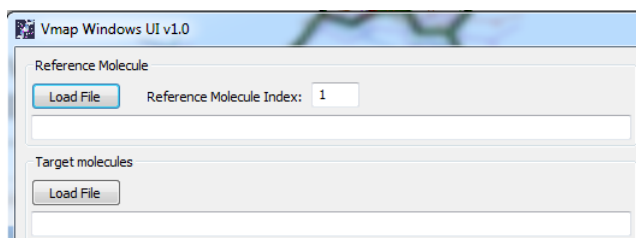


Vmap GUI Beta 0.9 Quick Start

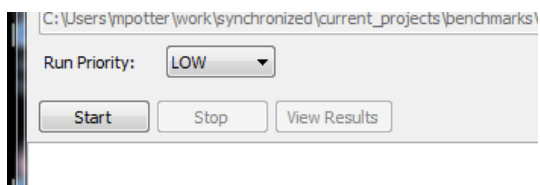
Vmap is used to superimpose a series of structurally related ligands on a reference molecule. This can provide excellent starting structures for use in docking, VM2, or any other task that benefits from having a reasonable guess at a starting conformation.



For example, a co-crystallized ligand from a PDB structure can be used as a reference to generate VM2 starting conformations for a related series of ligands.



At the top left, use the Load File button to select the reference molecule (PDB, MOL, SDF, and CRD formats supported). Then select the ligands to superimpose using the Load File button in the Target Molecules section (only SDF format supported). Then select Start.



For more details see the following pages.

Vmap identifies the maximum common substructure (MCS) shared by the reference molecule and each of a series of ligands. This information is then used to superimpose each ligand in the series on the reference molecule. Atom number pairs describing the MCS correspondences between the reference and ligands are output for use with other applications. For example, VM2 can use the atom pair mappings to 'snap' an input ligand conformation to that of a reference molecule while optimizing atoms not shared between the two in the context of the binding site. Several options allow the details of this process to be controlled. These include which atoms are considered for determination of the MCS, which are used to calculate the RMSD of the resulting superimposition, and the method of superimposition itself, rigid, or including optimization of dihedrals. It is possible to disable superimposition entirely with 'Docking Mode' which will output atom pair mappings and RMSD relative to the reference molecule without superimposition. This can be useful when evaluating docking results. Select View Results to see the resulting coordinates for the reference and the ligand series in 3D using Vdisplay.

