AFITT- Working with Good Chemistry

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AFITT is a new molecular graphics program developed by OpenEye Scientific Software for protein crystallographers. It runs on most operating systems, reads almost all data formats, easily connects to databases and will generate good chemical structures from a SMILES string. It has the most up to date rotomer library and Ramachandran plot to easily check the protein structure for outlying residues. It will create refinement dictionaries (either REFMAC or XPLOR format) for ligands and other small molecules automatically. Because AFITT uses the OEChem chemical library and OMEGA conformer generator, good chemistry is preserved even when starting from a SMILES string. Rapid docking into electron density is provided by OpenEye's Shape technology. To enhance communication with chemists, it also provides a 2D graphics window and automatic SMILES naming. Scripting is easily accomplished using Python. AFITT should be particularly useful for those involved in modeling large numbers of structures with small molecules.

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