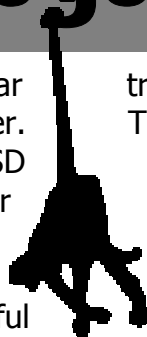


SCUT Monkeys

The jobs of modelers are filled with tasks that appear to be surprisingly difficult to carry out in a robust manner. These tasks include, among others, file format conversion, passing SD tag data to Excel spreadsheets, determining RMSD between similar structures, and cleaning up structures pulled from a database. OEChem includes a suite of Python scripts that address Some Common Unfinished Tasks (SCUT). Each of these scripts is useful as is, but can easily be customized to any working environment.

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These tasks
tag data to
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OEChem
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Over 60 simple programs are provided with the OEChem Toolkit, including:

- AdjustCharge – adjusts formal charges on specified atoms
- BitVecTest – manipulates fingerprints, calculates Tanimoto
- ❖ Babel2 – converts data between file formats
- CanSMI – writes canonical SMILES
- Clique – enumerates common substructures
- ❖ Flipper – enumerates unspecified stereocenters of SMILES input
- Frag – SMARTS based molecular fragmentation for R-group analysis
- LibGen – generates product library from SMIRKS and reactant list
- MCSS – determines maximum common substructure
- MolCount – counts molecules and conformers
- ❖ MolGrep – searches flat files for molecules containing specified substructures
- ❖ PDB2Lig – ligand extraction from PDB files
- ❖ RMSD – determines minimum RMS distance between two molecules, with proper recognition of automorphism
- SimpleMolCount – reports average number of atoms, bonds and conformers
- ❖ Sdf2csv – writes SD tag values into comma separated format suitable for spreadsheets
- TPSA – 2D topology based polar surface area



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