

Toolkits: what do you want to do?

A summary of toolkit projects

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Abstract

OpenEye is changing support for toolkits by making it easier for customers to get custom code to solve their problems. But OpenEye has always had a policy of working to produce solutions. Summarized here are some of the many projects involving toolkits. Let us know about your own problems, we may already have a solution.

Example projects

- Multi-conformer substructure search (see **Figure 1**)
- Visual substructure ROCS
- Custom SiteHopper
 - Similar sizes (see **Figure 7**)
 - Custom binding sites
 - Data integration
- Fast random molecule sampling
- Water-water correlation
- Chemically relevant FastROCS
- Custom molecular property filter (PAINS)
- Macrocycle conformers
- Binding pocket analysis
- Library construction
- Library deconstruction
- Covalent docking (see **Figure 3**)
- Shape fragment cocktailing
- Py2exe
- Matched pair reporting (see **Figure 6**)
- Daylight replacement
- 3rd party software integration
- Automated Brood queries
- Custom fingerprints
- Custom python extensions
- Report generation
- SQL integration

Substructure searching

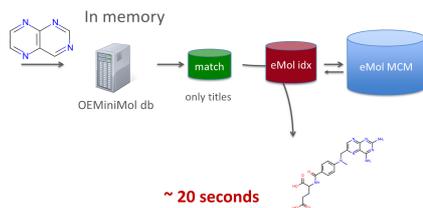


Figure 1: Improved workflow for substructure recovery from a 55Gb (7M molecule) database.

Custom web interface

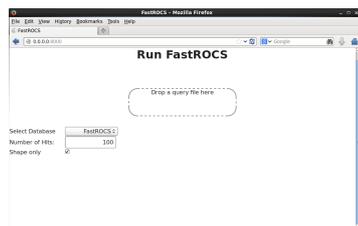


Figure 2: Custom FlaskROCS interface for searching multiple molecule databases.

Covalent docking

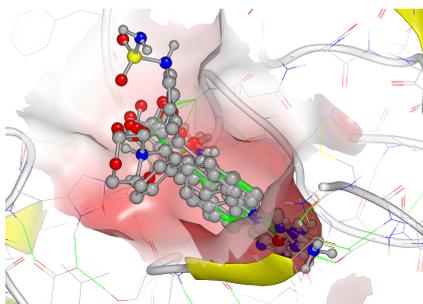


Figure 3: Combining OEChem TK, Szybki TK and OEDocking TK for covalent docking.

Pictorial GUI

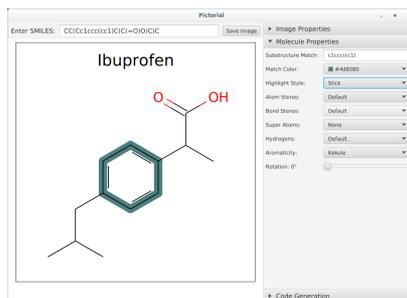


Figure 4: GUI for generation of OEDepict source code.

More example projects

- Compound normalization
- Scaffold analysis
 - Rgroups
 - Reagents
 - Patents
- Matched pairs
- Clustering
- Structured water detection
- ROCS query construction
- Custom conformers
- Web services
 - Depictions
 - Naming
 - FlaskROCS (see **Figure 2**)
- Hardware benchmarking
- Code optimization
- Retrosynthesis
- Debugging
- Parallelization
- Multi-conformer FastROCS (see **Figure 5**)
- Custom data management
- Vida extensions
- Stand alone GUIs (see **Figure 4**)
- iPython notebooks
- Custom file formats
- Database preparation

FastROCS customization

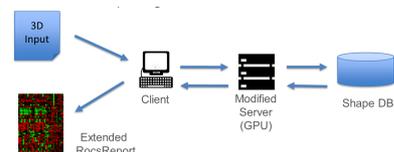


Figure 5: Customization of FastROCS to provide N by N shape comparisons.

Matched Pair report

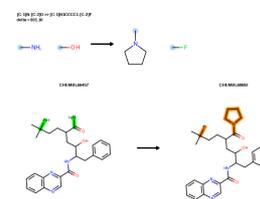


Figure 6: Display of MMP output.

SiteHopper modification

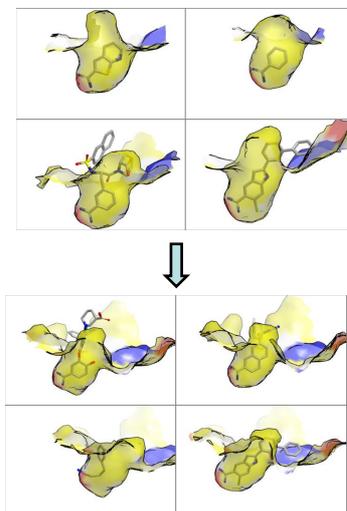


Figure 7: Modification of SiteHopper results to normalize the binding pocket across a series of results.

Acknowledgments

Thanks to the many OpenEye employees who contributed to these projects. Special thanks to Jose Batista, Brian Cole, Bob Tolbert, Burt Leland, Greg Warren and Justin Scheiber for the examples shown.

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