

Streamline your pharmacophore modeling and analyses.

Access cutting-edge 3D pharmacophore modeling and 3D database management tools.

Perform conformer generation, 3D database creation, pharmacophore hypothesis generation, virtual screening and more.

Catalyst Component Collection

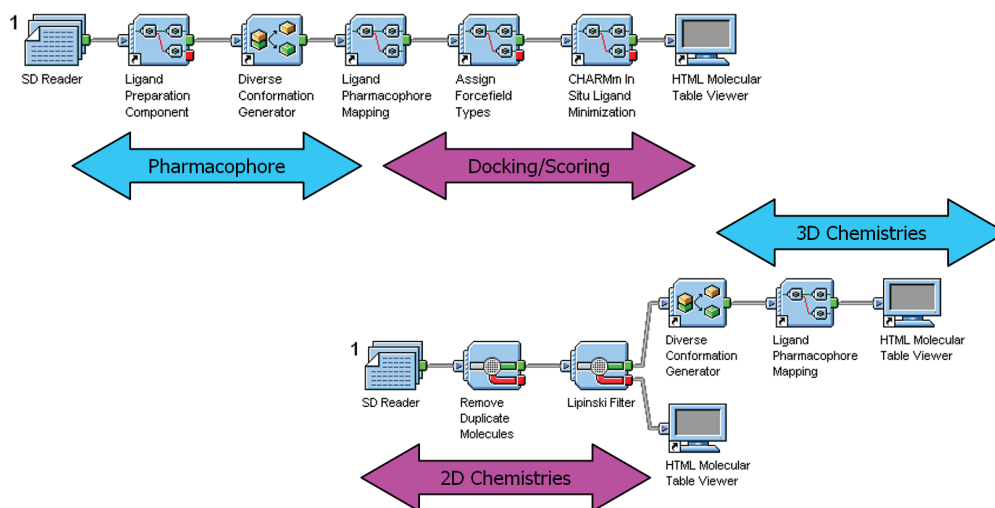
The Catalyst® Component Collection is a comprehensive solution for pharmacophore modeling and 3D database management. The renowned technologies of Catalyst, the most cited tool of its kind in peer-reviewed publications, are packaged into the Pipeline Pilot™ platform for creating automated, easy-to-use workflows that streamline your pharmacophore modeling and analyses. Simply drag-and-drop Catalyst 3D chemistries tasks into the Pipeline Pilot workflow scheme and deploy Catalyst's sophisticated algorithms to perform conformer generation, 3D database creation, pharmacophore hypothesis generation, virtual screening, and much more. All of these tasks are available at the convenience of your desktop using Windows or Linux. With the integration of Pipeline Pilot, the well-validated Catalyst algorithms are more convenient and accessible than ever before.

Increase Your Ability to Collaborate With Others Anywhere in the World

In conjunction with Pipeline Pilot Web Port, Catalyst can be configured to be accessible via a web interface. With web interface access, you can conveniently carry out research remotely, communicate your results with colleagues in other locations, and/or customize the modeling tasks that you would like to make accessible for others. Accessing Catalyst tools via the web-based interface allows you to effectively integrate your research processes and increase overall productivity.

Benefits of the Catalyst Component Collection

- Optimized algorithmic and code level refinements enhance performance.
- 2D and 3D chemistries are seamlessly integrated in Pipeline Pilot.
- Analysis and reports can be derived directly from modeling results.
- The integration of new science provides users with cutting edge tools to carry out such tasks as rapid conformer generation (CAESAR), library creation with a *de novo* fragment linker, and much more.



Examples of Included Protocols and Components

3D QSAR Pharmacophore Generation Identify likely active compounds with automated 3D hypothesis generation. Given only 2D structures and known biological activity, you can create an interaction hypothesis to explain and predict the variation in activity across a set of molecules.

Build 3D Database Create an extensive 3D compound database from your own corporate/project/vendor data, which can be queried in terms of pharmacophore model, molecular shape, and/or substructures.

Common Feature Pharmacophore Generation Generate pharmacophore models from a feature-based alignment of a collection of compounds and use them to iteratively search chemical databases.

Diverse Conformer Generation Calculate coverage-based conformational models to provide a comprehensive and diverse representation of a compound's conformational space. Use these models to create hypotheses, fit molecules to hypotheses, and create multi-conformational 3D databases.

Feature Mapping Examine molecules in terms of all the possible pharmacophore features that can be mapped; easily identify important protein-ligand interactions.

Interaction Generation Generate interaction (Ludi) maps directly from features in a receptor active site. These active site maps can be edited and clustered using proprietary knowledge to retain only essential information before virtual screening of 3D compound databases.

Ligand Pharmacophore Mapping Reliably compare and fit molecules onto hypotheses and calculate interaction fit scores.

Pharmacophore Comparison Compare and fit two pharmacophore hypotheses onto one another and calculate the best RMSD value.

Screen Library Screen a collection of compounds in a library while varying the different permutations of the pharmacophore model. Based on the size of your hit list, expand or contract your results by specifying the required number of chemical features each molecule must satisfy.

Search 3D Database Perform rapid searches of extensive 3D databases in terms of pharmacophore models, molecular shape, and/or required substructures.

Search by Shape Use a 3D topological representation of a molecule, generated from a specified conformation, to perform database searches based on shape to identify compounds that more accurately emulate the 3D shape of an active site.

Steric Refinement with Excluded Volume Automatically generate exclusion volumes for pharmacophore model optimization with information gleaned from inactive molecules, which allow your model to account for steric constraints, and thereby, improve its accuracy and selectivity.

Prerequisites

- Catalyst Discovery Studio® 1.7 licenses
- Pipeline Pilot Client 6.0 license with Chemistry Collection (Reporting Collection and Integration Collection are strongly recommended).