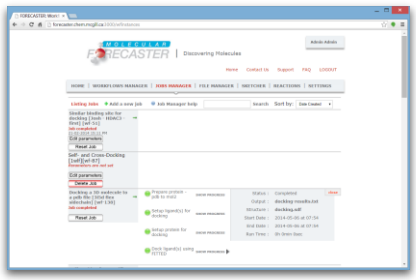
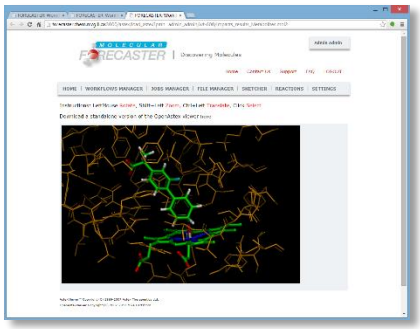
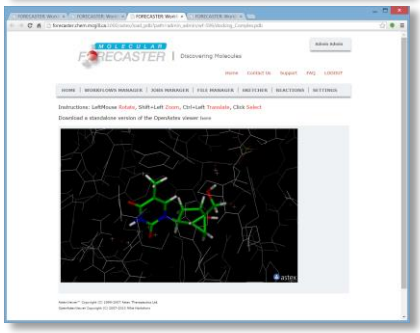
The FORECASTER Platform
Integrated Platform for Drug Design and Discovery

The FORECASTER Platform is a browser-based interface that integrates our highly specialized drug design and discovery computer programs.

All the programs are implemented for complete automation within different workflows: Virtual Screening, Lead Optimization, Combinatorial Chemistry, Docking, Protein Preparation, Library Selection and Extraction, etc…







Structure-based design:

- Docking flexible ligands to flexible macromolecules using **FITTED**
- Predicting sites of metabolism by cytochromes P450 using **IMPACTS**

Ligand-based design:

- Filtering by descriptors using **REDUCE**
- Searching for analogues using **SELECT**
- Extracting representative library through clustering using **SELECT**
- Pharmacophore identification and searching using **RESHAPES**
- Creating combinatorial libraries by combining fragments based on a defined chemical reaction using **REACT**
- Searching substructures from large databases of chemicals using **FINDERS**

Macromolecule:

- Superposing and making proteins similar using **MATCH-UP**
- Automated protein preparation and optimization from pdb files directly to mol2 using **PREPARE**
- Setup proteins for docking using **PROCESS**

Small molecule:

- Converting 2D small molecules to 3D using **CONVERT**
- Setup ligands for docking using **SMART**

MADE BY EXPERIMENTALISTS FOR EXPERIMENTALISTS

System Requirements

Server: Windows, Linux
Intel or AMD (32 and 64 bits)
4GB of RAM

Client: Windows, Linux, Mac OSX
Intel or AMD (32 and 64 bits)
1GB of RAM
Internet Explorer, Chrome, Safari (or any compatible browser)

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