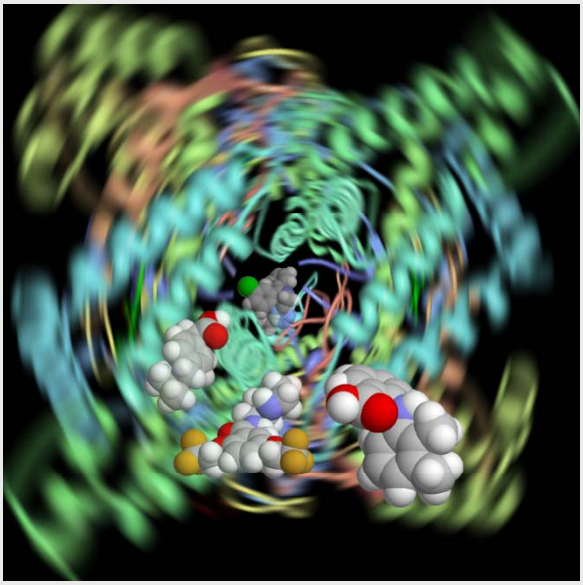
isoCYP

Prediction of Isoform Specificity of P450 Substrates

Oxidation reactions mediated by cytochrome P450 isoforms play a crucial role in phase I of the human metabolism of xenobiotics. **isoCYP** provides a powerful and fast method to predict the predominant human cytochrome P450 isoform by which a given chemical compound is metabolized in phase I.



The underlying model includes the isoform specificities for cytochrome P450 3A4, 2D6 and 2C9 substrates and has been specifically designed for drug-like molecules.

isoCYP is intended to be used in the early ADMET assessment in the drug discovery process and assists medicinal scientists in analyzing the pharmacological properties of novel lead structures and in optimizing their metabolic profile.

The robust and reliable model was thoroughly validated and performs with an excellent predictivity in cross-validation experiments and with external validation data sets.

Key Features

- Visualization of chemical structures, predicted cytochrome P450 isoform specificity and read-in information
- Highly interactive and intuitive, wizard-driven graphical user interface
- Sorting and filtering of compounds
- Structure input via file or by a molecule editor
- Applicable to a broad range of organic chemistry (typically drug-like molecules)

Areas of Application

- Drug discovery and design
- Lead optimization
- Pharmacokinetic profiling, *e.g.*, in ADME/Tox studies
- Risk assessment of chemicals

Molecular Networks
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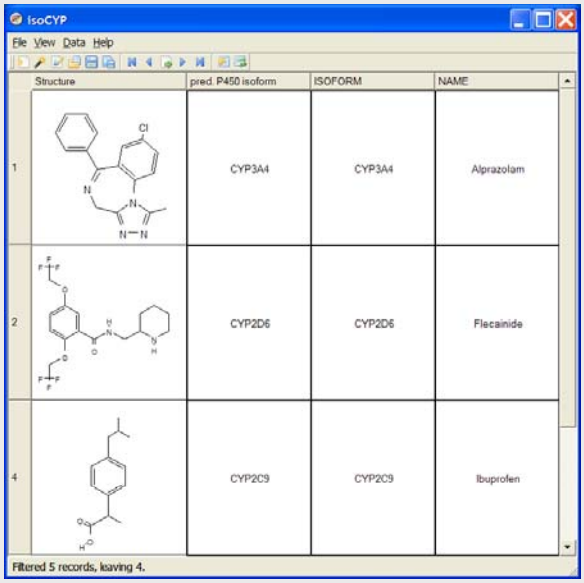
isoCYP reads in chemical structures and predicts their human cytochrome P450 isoform specificity purely on their constitutional information. Therefore, **isoCYP** is rapid enough to handle massive volumes of structures such as in those in databases or large virtual compound libraries.



Technical Features

- Graphical user interface, optional batch mode execution and web service
- Interface for integration into internal IT environments and workflows
- Also available as component for SciTegic® Pipeline Pilot®

Reference

L. Terfloth, B. Bienfait, J. Gasteiger
J. Chem. Inf. Model. **2007**, *47*, 1688-1701.

System Requirements

isoCYP is available for Microsoft® Windows® platforms and x86 Linux systems (32 and 64 bit).

Test Version

isoCYP can be tested free of charge online on the web server of Molecular Networks at www.molecular-networks.com/online_demos.

A 30 days evaluation copy of **isoCYP** is available free of charge in the Download Area of the web server of Molecular Networks at www.molecular-networks.com.

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