Laboratoire d'Infochimie,

Institut de Chimie de Strasbourg (UMR 7177)
Université Louis Pasteur
http://infochim.u-strasbg.fr

Directeur - **Alexandre VARNEK**

Composition de l'équipe :

Alexandre Varnek – professeur,
Gilles Marcou –maître de conférences,
Olga Klimchuk _ chercheuse contractuelle,
Denis Fourches – doctorant,
Frank Hoonakker– doctorant,
Cédric Gaudin – doctorant,
Natalia Kireeva– doctorante,
Thomas Fleurentdidier – doctorant.

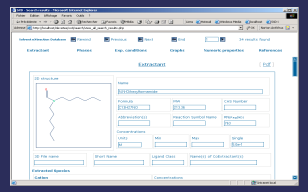
Professeurs invités en 2004-2007 :

J. Gasteiger, A. Tropsha, C. Steinbeck, I. Baskin, V. Solovev, I. Tetko

Projets de recherche

- *développement des outils en chemoinformatique (projet ISIDA) ;*
- *plate forme du criblage virtuel ADME/Tox ;*
- *outils de recherche de réactions chimiques par similarité,*
- *prédicteur de constantes de complexation des métaux (projet COMET),*

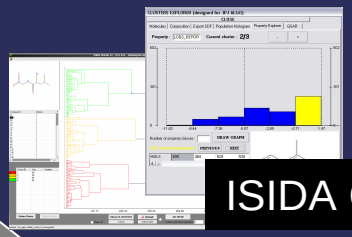
In Silico Design and Data Analysis



EdiSDF EdChemS
SXD

Database

1



2

Data analysis :
Clustering, Filtering, …

ISIDA Cluster

3

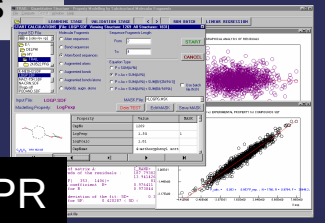
Similarity Search

ISIDA Similarity

4

QSAR models

Applicability domains

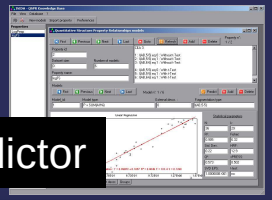


ISIDA/QSPR

5

QSAR models

Assessment of properties
of virtual compounds



ISIDA/Predictor

6

Hits selection

7

**Synthesis and
experimental tests**

ISIDA

QSPR / ISIDA modelling using fragment descriptors

Complexation of metals and neutral guests in solution by organic molecules

- **Metals:** alkali, alkaline-earth, transition, lanthanides, actinides
- stability constants of 1:1 and 1:2 complexes
- in aqueous and non- aqueous solvents

Solvent Extraction of metals

- Extraction constants
- Distribution coefficients
- Separation factors

H-bond complexes

- ΔH and ΔG

QSPR / ISIDA modelling using fragment descriptors

Models for ADME/Tox screening

- **Liquid/ Water and Liquid / Air partition coefficients**
  Liquid: octanol, chloroform, hexadecane
- **Aqueous solubility**
- **Skin Permeation Rate**
- **Brest Milk / Blood Partition Coefficients**
- **Blood / Air and Tissue / Air Partition Coefficients**
- **Blood / Brain Barrier Permeation**
- **Tetrahymena toxicity**

Biological activity

- **anti-HIV;**
- **antimicrobial,**
- **….**

Tools for chemical reactions

- **reaction similarity search;**
- **reaction databases classifications;**
- **QSRR – “structure – reactivity” approach**

Enseignement

- Master en Chemoinformatique (depuis 2001) ;

- Cours d'initiation à a chemoinformatique en Licence de Chimie et Chimie Physique

Visit our website : **http://infochim.u-strasbg.fr**