



Equipe de Bioinformatique du Médicament

Institut Gilbert Laustiat

Département Pharmacochimie de la Communication cellulaire

CNRS UMR-ULP 7175-LC1

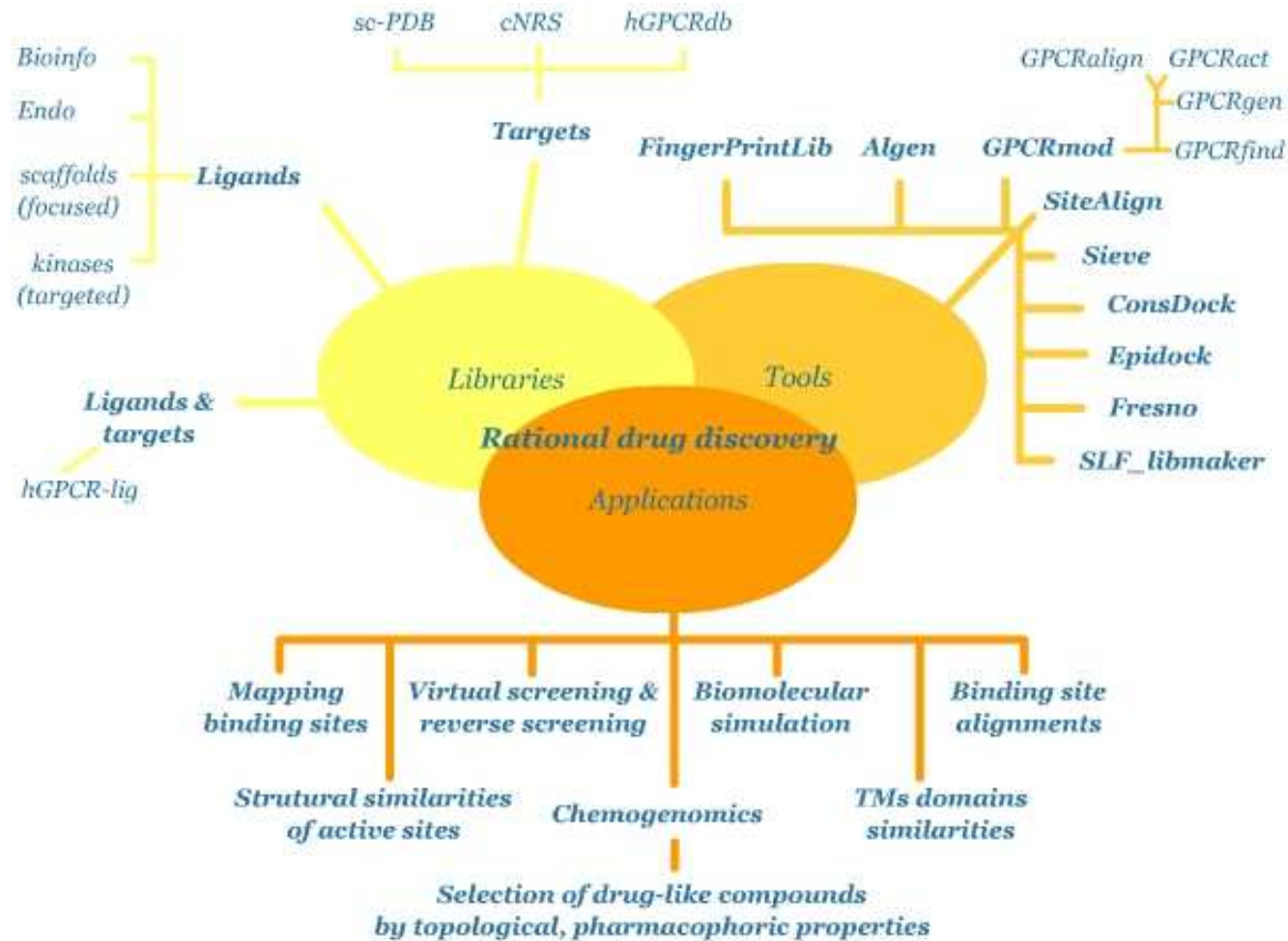
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<http://bioinfo-pharma.u-strasbg.fr>

Equipe crée en Octobre 2000

Didier ROGNAN	DR CNRS
Esther KELLENBERGER	MC ULP
Chris DE GRAAF	Post-doc
Bernard COUPEZ	Post-doc
Caterina BARILLARI	Post-doc
Claire SCHALON	Ph.D.
Nathanael WEILL	Ph.D
Nicolas FOATA	I.R

## Developpement de bases de données et de nouveaux outils en chémogénomique structurale



- A l'interface de nombreuses disciplines

Chimie Médicinale:

Biologie Moléculaire:

Biologie structurale:

Pharmacologie:

Informatique:

Developpement méthodologique

- . Conception de chimiothèques
- . Conception de ciblothèques
- . Conception de fingerprints

- **Pluridisciplinarité** dans l'Equipe (Mathématiciens, Physiciens, Chimistes, Biochimistes, Biologistes structuraux, Pharmaciens)

- **Nécessité de collaborations fortes** (UMR7175, IFR85, Genopôle, UE, privé)

Enseignement en modélisation moléculaire, bio/chemoinformatique  
et drug design

- ✓ Masters de  
Cheminformatique (M2)  
Génomique structurale et bio-informatique (M2)  
Chimie et Biologie (M2)  
Sciences du Médicament (M1)



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Introduction



Medicinal Chemistry has just entered a new era with the complete sequencing of a human genome. The number of potentially interesting drug targets will no doubt dramatically increase in the incoming years. To just give an idea of the revolution to come, about 500 targets are currently used by the modern pharmacopoeia, but between 5,000 and 10,000 are foreseen in a near future. A significant number of these new targets will probably be orphan targets for which no or very few information on endogenous ligands will be available. To get first insights into the molecular structures of such ligands, virtual screening of chemical databases against a protein active site or a pharmacophore is an emerging technique that allow to enrich a reduced dataset in true hits.

Libraries

- Bioinfo**  
2007, release 4  
Private access >>  
more info
- sc-PDB**  
2007, release 4  
>> more info
- hGPCR-lig**  
2006, release 1  
>> more info
- sc-PDB**  
2006, release 3  
>> more info
- SBI**  
2005, release 1  
>> more info
- GPCR-db**  
2005, release 1  
>> more info

