

CHEMBIOBANK / ECBI PROJECTS:

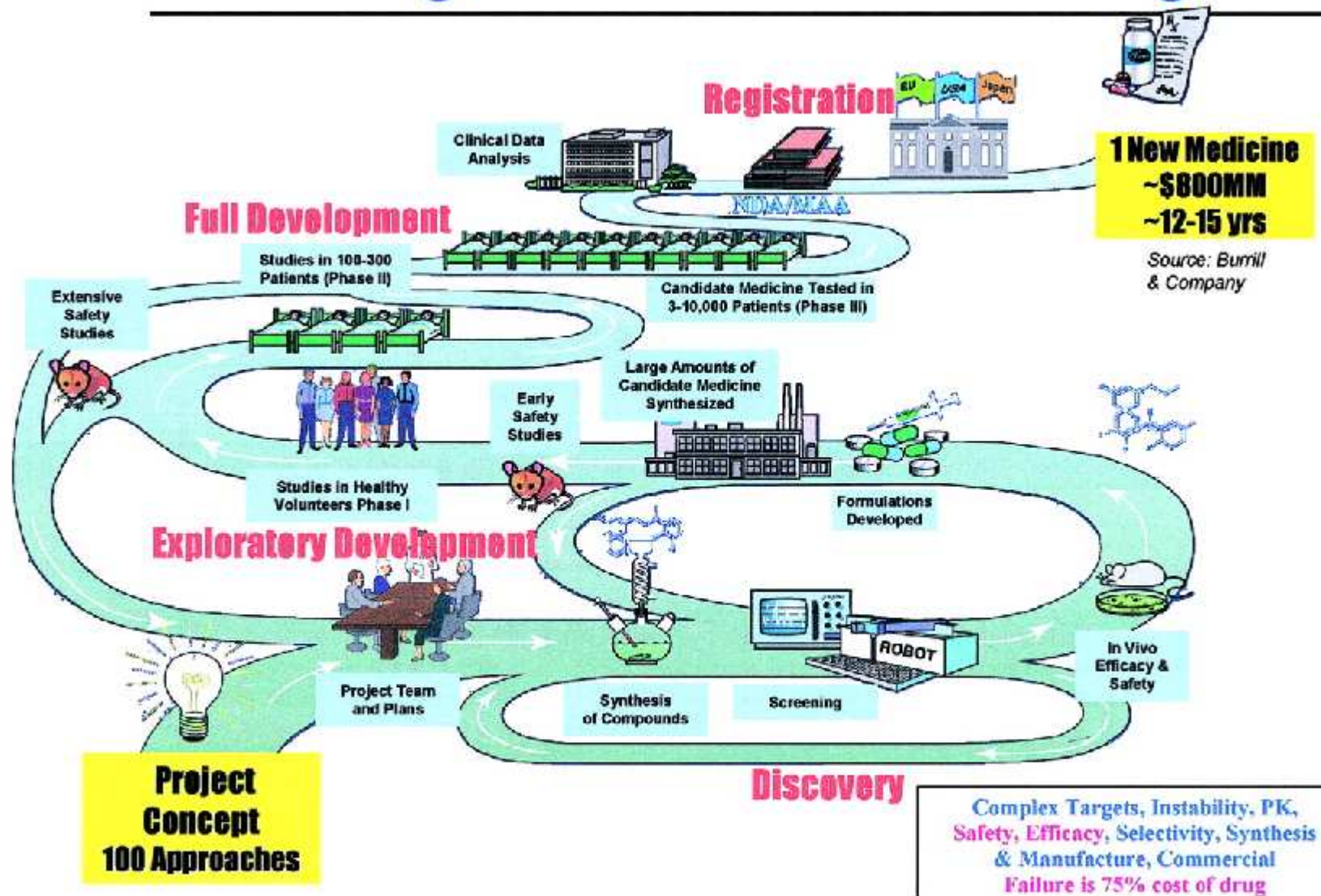
ANNOTATED MOLECULAR LIBRARIES



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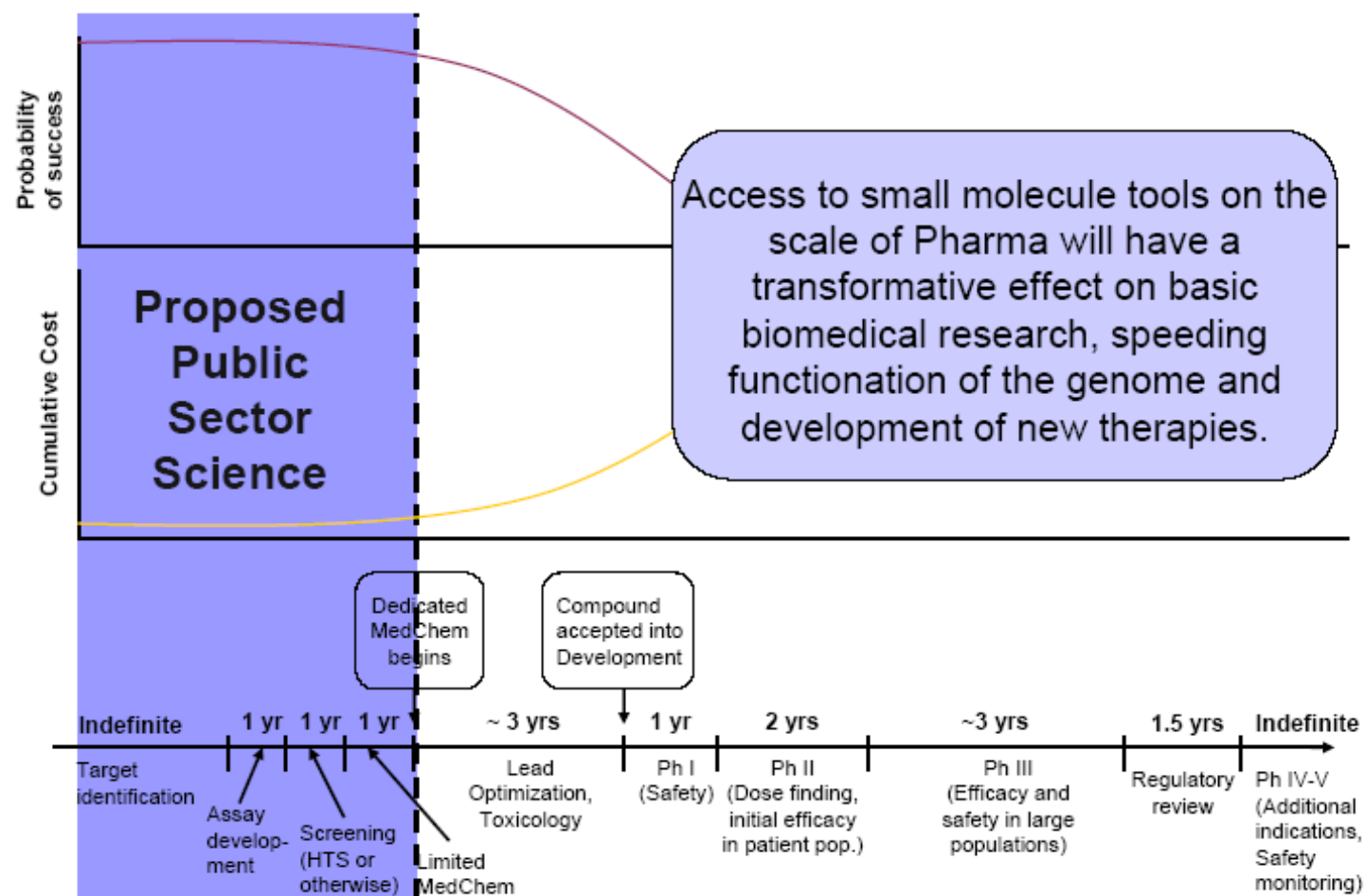
Univ. Santiago Compostela
22 Julio 2008

The Long Path from Idea to Drug



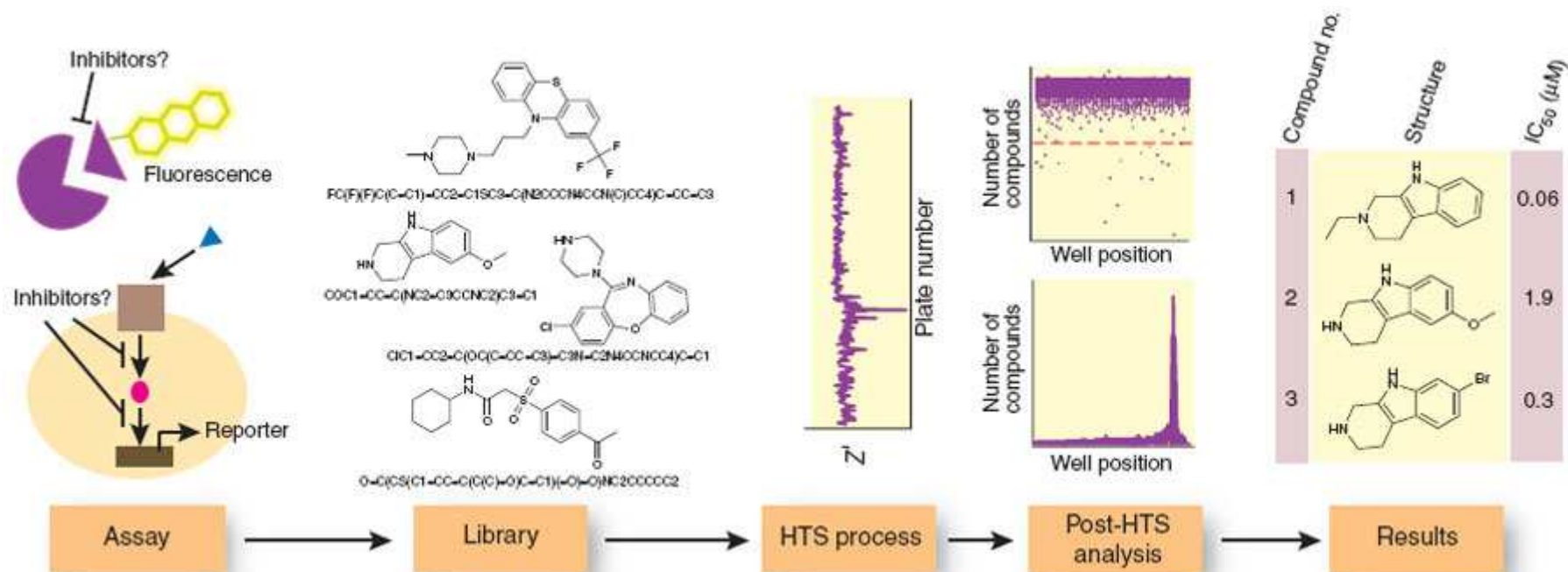
From: Scott P. Kennedy and B. J. Bormann, *Experimental Biology and Medicine* 231:1690-1694 (2006)

The Drug Development Pipeline



From: <http://www.mli.nih.gov/>

The flow of materials and data from assay to reported results in HTS



From: James Inglese, Caroline E Shamu & R Kiplin Guy
Nature Chemical Biology 3, 438-441 (2007)

CHEMBIOBANK PROJECT GOALS

- Build a chemical library with compounds provided mainly by academic laboratories in Spain (extended later to compounds from academic laboratories in Portugal and Latin America); selected commercially available compounds will also be included.
- Characterize the library compounds through virtual and experimental HTS screening procedures.
- Build a remotely accesible database, containing chemical structures of the library compounds, annotated with biological and bioinformatic data.



Chemistry, logistics,
project coordination

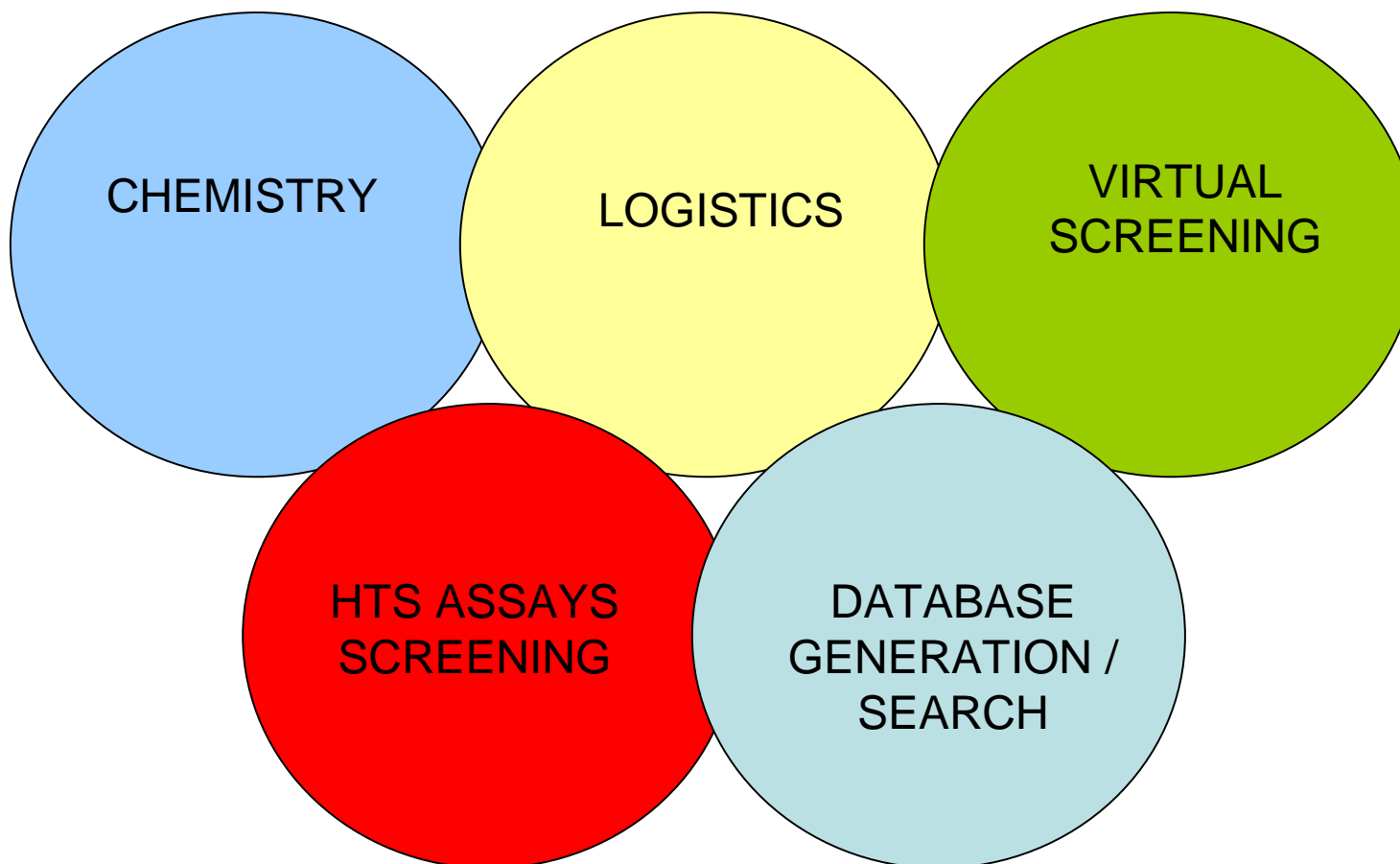


Pharmacological
screening

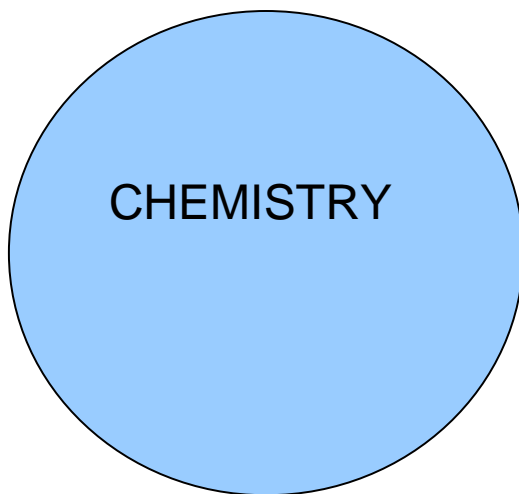


Virtual screening

CHEMBIOBANK COMPOUNDS AND DATA WORKFLOW

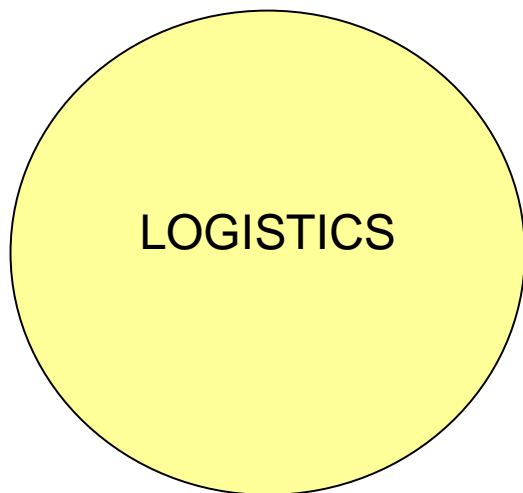


CHEMBIOBANK COMPOUNDS AND DATA WORKFLOW



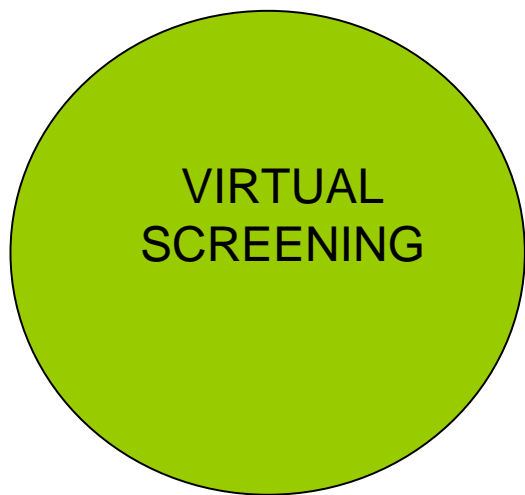
- Chemical compounds received at ChEMBioBank from academic partners with a signed material transfer agreement.
- Chemical compounds (natural and synthetic) properly characterized at ChEMBioBank with analytical methods (LC/MS).
- Compounds with adequate purity and confirmed structure registered in ChEMBioBank database.
- Chemical data (synthetic procedures reference, analytical chemistry, structure, codes) described in ChEMBioBank compound database entry.

CHEMBIOBANK COMPOUNDS AND DATA WORKFLOW



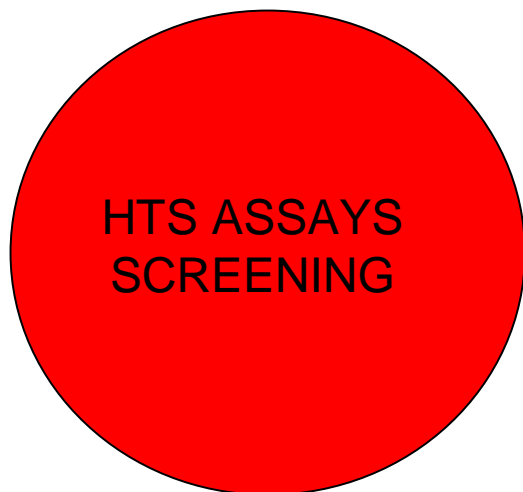
- Compound traceability of any compound deposited in the ChEMBioBank library assured through a logistic procedure covering proper handling and storage.
- Compounds stored as dry samples / DMSO solutions in mother plates.
- Daughter / copy plates with library compounds distributed to assay centers for HTS affinity / other pharmacological procedures.

CHEMBIOBANK COMPOUNDS AND DATA WORKFLOW



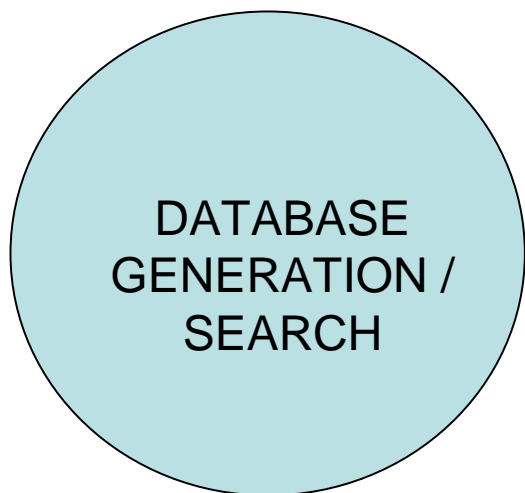
- Virtual screening (VS) of ChEMBioBank library compounds on a large variety of biological targets.
- VS results to guide the selection of targets for pharmacological affinity HTS screening.
- VS alternative procedures on ChEMBioBank compounds from other bioinformatics laboratories feasible.
- VS results may generate hypotheses for new compound derivatives.

CHEMBIOBANK COMPOUNDS AND DATA WORKFLOW



- Pharmacological characterization of compounds in HTS screens and other pharmacological assays.
- Compounds from ChEMBioBank library delivered to assay centers through a signed agreement.
- Requests for new assays from alternative screening centers feasible.
- Experimental Screening validated data results to be deposited in ChEMBioBank database

CHEMBIOBANK COMPOUNDS AND DATA WORKFLOW



- A secure database will contain the chemical structures, analytical data and associated informations for ChembioBank library compounds.
- The ChembioBank database will also contain the validated data results from virtual and experimental screening assays on library compounds.
- The database will be remotely and publically accessible.

CHEMBIOBANK: PROOF OF CONCEPT

- A library of nearly 500 compounds from academic origin was transferred from Universidade do Minho in Portugal to USC-USEF for pharmacological screening. 1000 additional compounds are currently being assayed.
- Chemogenomics lab (GRIB, IMIM-UPF, PRBB) carried out virtual screening on these compounds vs. a large array of targets.
- Hits have been virtually and experimentally discovered and confirmed; results are being analyzed for possible publication / patents.

CHEMBIOBANK: ACTION PLAN

- ***Phase I (October 2007 – September 2008)***
 - a) Building of Chembiobank laboratory in Parc Científic Barcelona (PCB) (LC/MS, liquid handling device, refrigerated and freezer rooms, logistics)
 - b) Definition of Material Transfer Agreements and Data Sharing / Intellectual Property Policies.
 - c) Gather academic / industrial laboratories interest on the Chembiobank project, create a list of Chembiobank partners.
 - d) Acquire selected commercially available compounds for workflow's *proof of concept* (i.e. Prestwick Chemical Library, <http://www.prestwickchemical.fr>)

- ***Phase II (September 2008 – September 2009)***
 - a) Start Chembiobank operations at laboratory in Parc Científic Barcelona (PCB)
 - b) Proof of concept for Chembiobank's workflow: delivery of a remotely accessible database with experimental and virtual results on acquired commercially available compounds.
 - c) Establishment of database access for academic and industrial partners, in agreement with Material Transfer and Data Sharing / Intellectual Property approved policies.

- ***Phase III (September 2009 - ...)***
 - a) Expansion of Chembiobank library and Chembiobank annotated database with academic / commercial compounds.
 - b) Design and synthesis of chemical libraries derived from chemical hits
 - c) Use Chembiobank compounds for target identification and validation projects with biologists.
 - d) Analyze viability of user-fee based access maintenance of Chembiobank database.

CHEMBIOBANK: ORGANIZATION

- **Chembiobank Steering Committee (CBB-SC)**

Mabel Loza, Director (USC-USEF)

Fernando Albericio, Director (PCB)

Ferran Sanz, Director, GRIB (IMIM-UPF)

Jordi Quintana, Coordinator Chembiobank Project (PCB)

- **Chembiobank Project Team (CBB-PT)**

Analytical Chemistry / Logistics (PCB)

Virtual Screening, Chemogenomics Lab, GRIB (IMIM-UPF)

Pharmacological HTS / Assay Screening (USC-USEF)

Database / Web, PCB & GRIB (IMIM-UPF)

Coordinator Chembiobank Project (PCB)

Projects in European countries: France (Chimiothèque Nationale)



Chimiothèque Nationale



Registered users access

Your email :

Your password :

OK

Forgotten password ?
Please enter your identifier :

OK

Registration

Information

- [Welcome](#)
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Intranet

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22nd 2007 : 33.415 compounds registered

Latest news

The "**Chimiothèque Nationale (CN)**" - French National Chemical Library - is a service-oriented division of the French National Centre for Scientific Research (CNRS) and was created in July 2003. It results from an **agreement** between the **CNRS** and **17 higher education and research organizations**.

The **principal mission** of the Chimiothèque Nationale is to **federate collections of synthesis products and natural extracts** available in French academic laboratories and to **promote their scientific and industrial valorisation**.

Information concerning **available molecules and extracts** are contained in two national databases (synthesis products and natural extracts), **accessible through this portal**. These products are conditioned either in bulk or into 96-wells microplates, in order to allow either a **targeted or a systematic biological evaluation** respectively. Registration to the Chimiothèque Nationale is **free** but submitted to approval. It gives access to both databases.

The following actions are currently available to registered users:

- downloading an SD File containing all the structures present in the **synthesis product database**.
- searching through the **natural extracts** databases.
- searching through the **synthesis products** databases and ordering specific compounds.

You are working in a **biology or a pharmacology laboratory**, either public or private, and you would like to **get access to the chemicals or the extracts available in the CN ?**
[click here](#)

You are working in a **chemistry laboratory** and you wish to **become a member** of the Chimiothèque Nationale ?
[click here](#)

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Phone : +33 (0)2 31 93 41 69

Secretaryship : **Françoise HERTH**
Phone : +33 (0)3 90 24 42 20
Fax : +33 (0)3 90 24 43 10

Powered by : Action Presence Net, IDBS , Molinspiration Cheminformatics , and Chemaxon.

[Legal information](#)

<http://chimiotheque-nationale.enscm.fr/>; Project proposal:

European Chemical Libraries (ECL)

Projects in European countries: Germany (Chembionet)



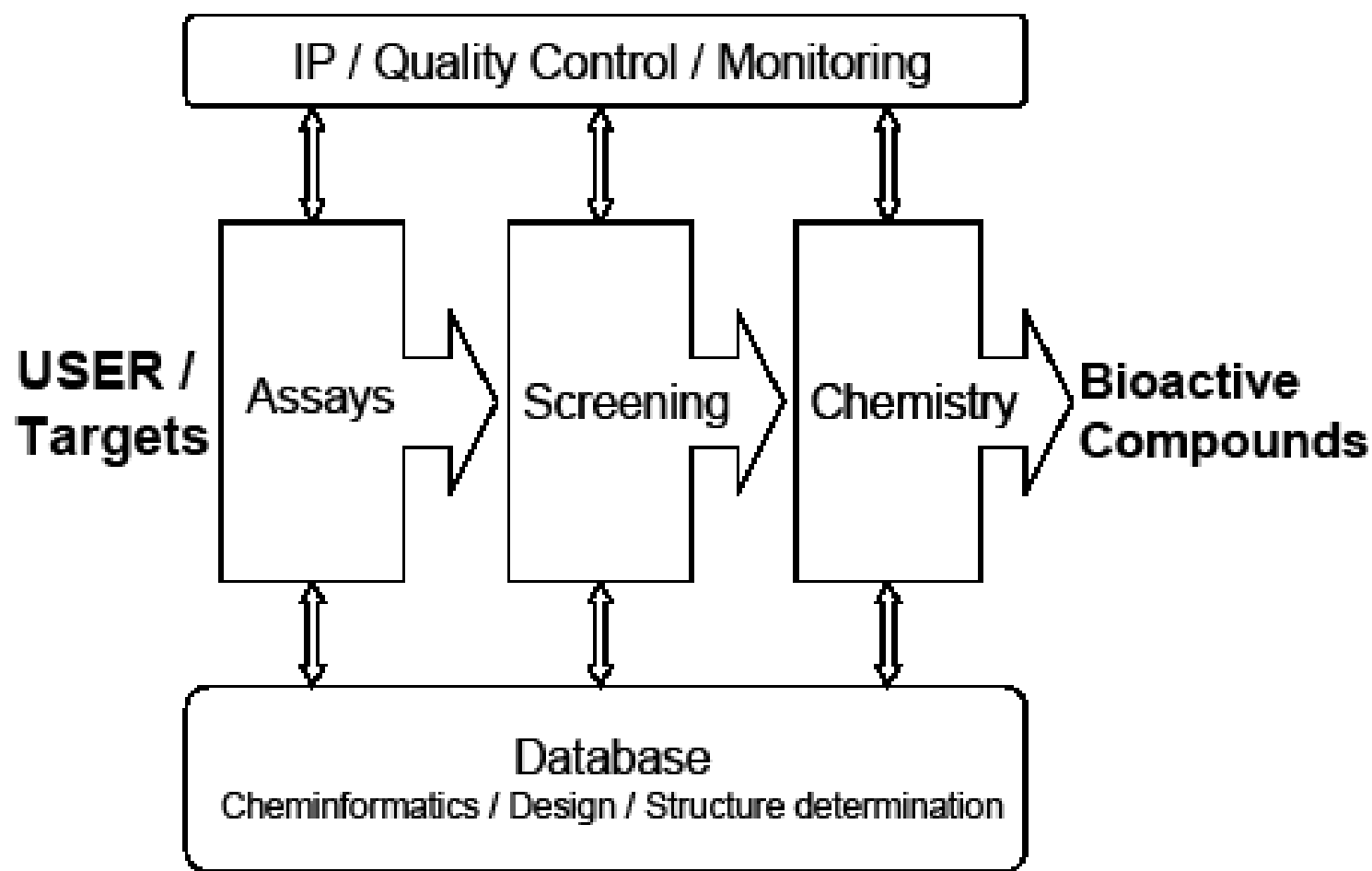
<http://chembionet.de/>; Project proposal:

European Chemical Biology Infrastructure (ECBI) (<http://www.ecbi.eu>)

European Chemical Biology Infrastructure

ECBI

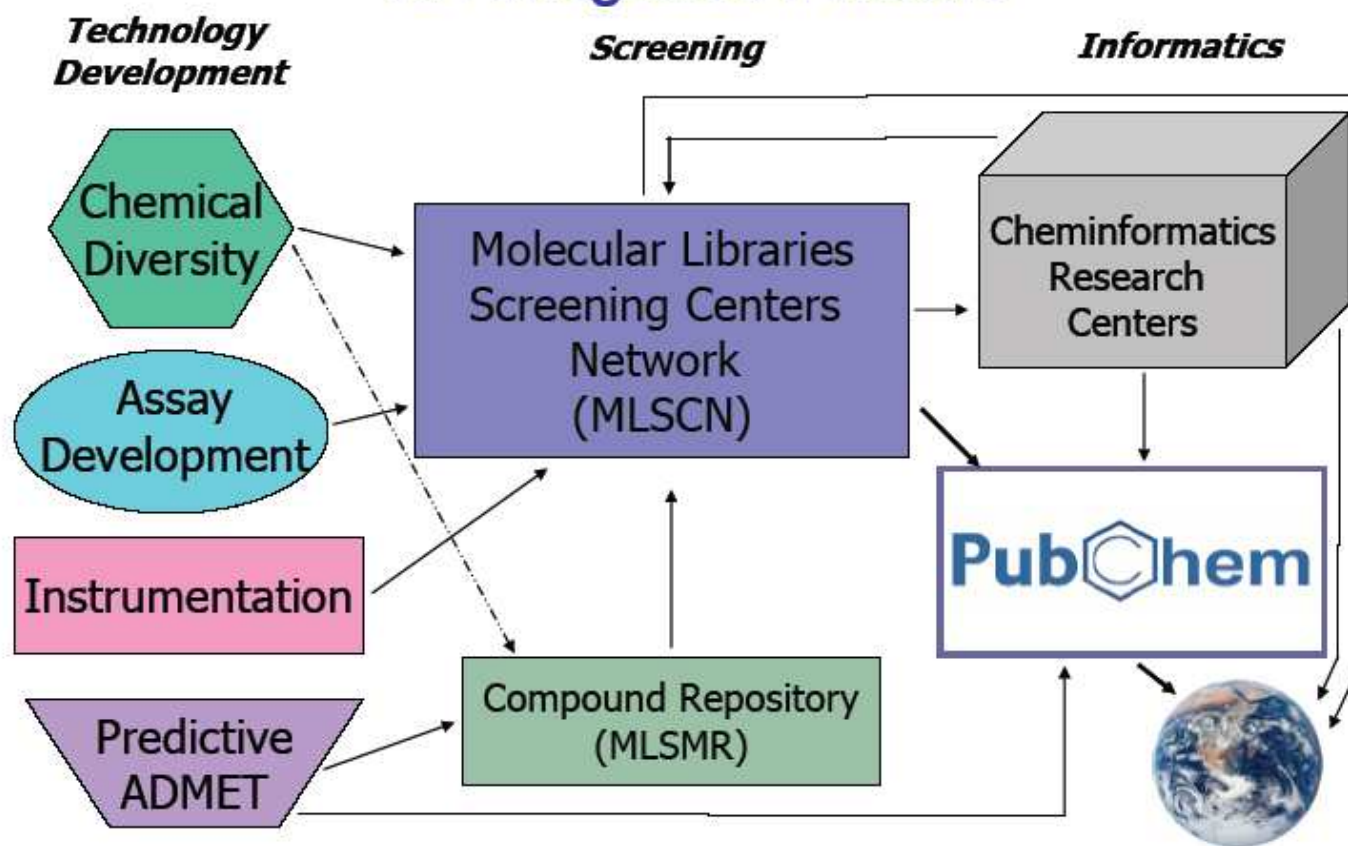
- www.ecbi.eu
- Chembionet (Germany), Chimiothèque Nationale (France), Dundee (Scotland), Chembiobank (Spain), Scandinavian Chemical Biology Initiative (Norway, Sweden), EPFL (Switzerland), Univ. Milano (Italy)...
- Network existing isolated Screening and Hit Development Infrastructures by: a) Sharing compound libraries and screening methodology; b) providing chemistry and cheminformatics/bioinformatics resources: c) creating a common European Chemical Biology Database; d) creating a European Compound library Inventory.
- Offer Access to Screening Technology and Hit Optimization or European Researchers.



Schematic representation of the European Chemical Biology Infrastructure (ECBI).

Projects in the USA: NIH Roadmap / Molecular Libraries Initiative

The Molecular Libraries Roadmap: An Integrated Initiative



<http://www.mli.nih.gov/>, <https://www.mli.nih.gov/mlscn/index.php>,
http://mlsmr.glp.gov/MLSMR_HomePage/project.html,
<http://pubchem.ncbi.nlm.nih.gov/>

CONCLUSIONS

- The ChEMBioBank project goals and compounds / assays and data workflows have been defined.
- The ChEMBioBank project may be of interest to the chemical and biological research community in academia and in industry.
- The ChEMBioBank annotated molecular library may be an important new tool in drug discovery projects.
- The ChEMBioBank project will be coordinated with similar projects across Europe (ECL, ECBI) and the USA (NIH Roadmap).

ACKNOWLEDGEMENTS

- Miriam Royo, Gloria Sanclimens,
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(<http://www.pcb.ub.cat>)
- Jordi Mestres, Ferran Sanz @ GRIB
(<http://www.imim.es/grib>)
- Mabel Loza, José Manuel Brea @ USEF
(<http://imaisd.usc.es/riaidt/usef/index.asp>)

<http://www.pcb.ub.cat/ECBS2008>

European Chemical Biology Symposium (ECBS 2008)

Barcelona, 10 – 11 July, 2008

Parc Científic Barcelona (PCB) &

Institut Municipal Investigacions Mèdiques (IMIM)

CHEMBIOBANK CONTACT DETAILS

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