# Open PHACTS

# Exemplars

## Using the Open PHACTS platform API

## About

Open PHACTS is a 3-year project of the Innovative Medicines Initiative (IMI), aiming to reduce the barriers to drug discovery in industry, academia and for small businesses. The Open PHACTS consortium is building a freely available platform, integrating pharmacological data from a variety of information resources, and providing tools and services to question this integrated data to support pharmacological research.

### Why do we need Open PHACTS?

Currently, pharmaceutical companies expend significant and duplicated efforts aligning and integrating internal information with public data sources. This process is difficult and inefficient and the vast majority of drug discovery sources cannot easily interoperate. Open PHACTS is creating a precompetitive infrastructure to make these approaches available both to industry and to academia and smaller companies, who have historically not had access to large-scale integrated pharmacological data resources.

The public Beta of the Open PHACTS Explorer and Exemplars will be released in the 4Q 2012.

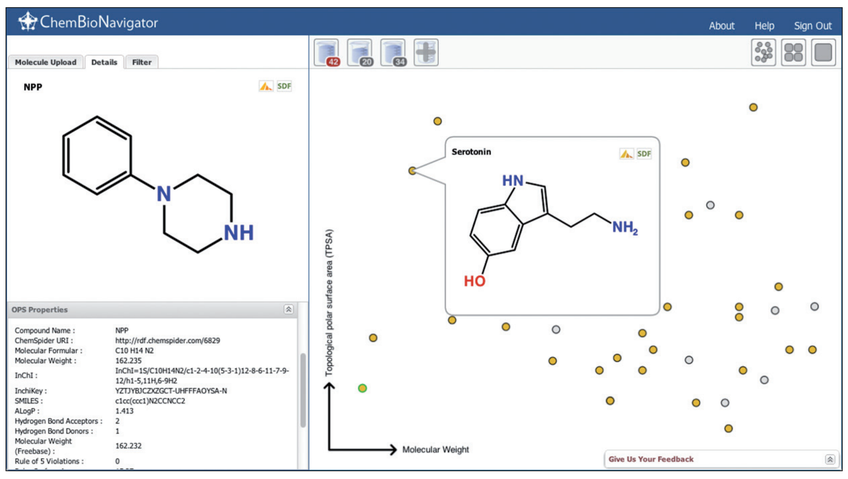
## Introduction

Further insight into the integrated information accessible through the Open PHACTS platform can be achieved by applications designed to extract and represent the data in specific ways.

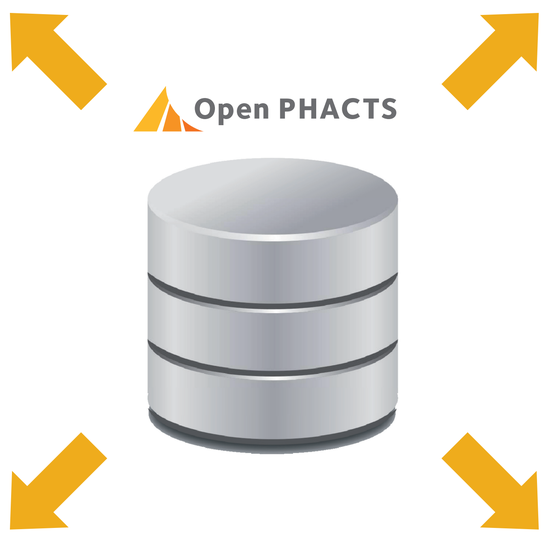
Here we show some Exemplars developed within the project: these applications illustrate how the Open PHACTS platform can be used to answer diverse research questions in the field of drug discovery.

Each application has been specifically tailored to address the needs of the end users in a different aspect of drug research. The data extracted from the Open PHACTS platform is used to build graphics, to run protocols, or to show compounds. The interfaces are highly interactive and allow the user to browse and to navigate the data for extract knowledge and support decisions.

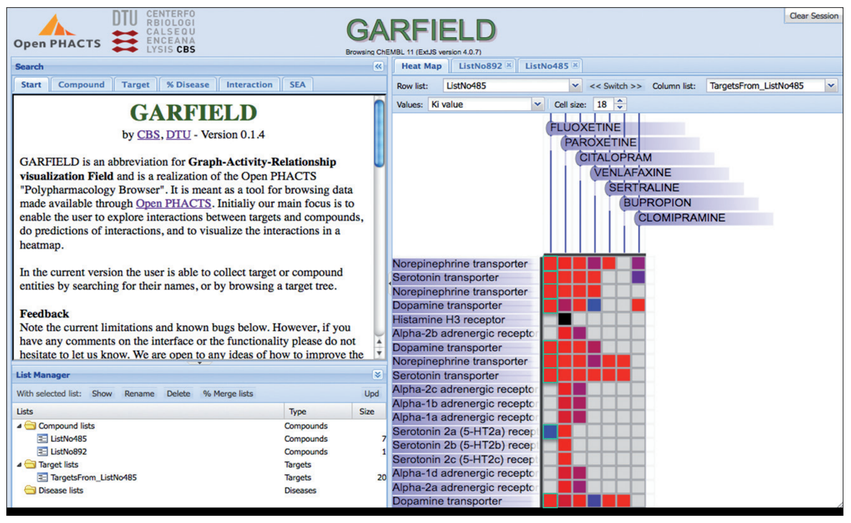
## ChemBio Navigator




The ChemBioNavigator (CBN) allows navigation of the interface of chemical and biological data, tailored for applications in pharmaceutical research. CBN lets you easily browse through sets of compounds: different sorting and plotting options offer a quick and intuitive overview of the physicochemical characteristics. An in-depth analysis of individual molecules uses the versatile data available from the Open PHACTS platform. Links into the original data sources, as well as into the Open PHACTS Explorer, allow for further investigation.

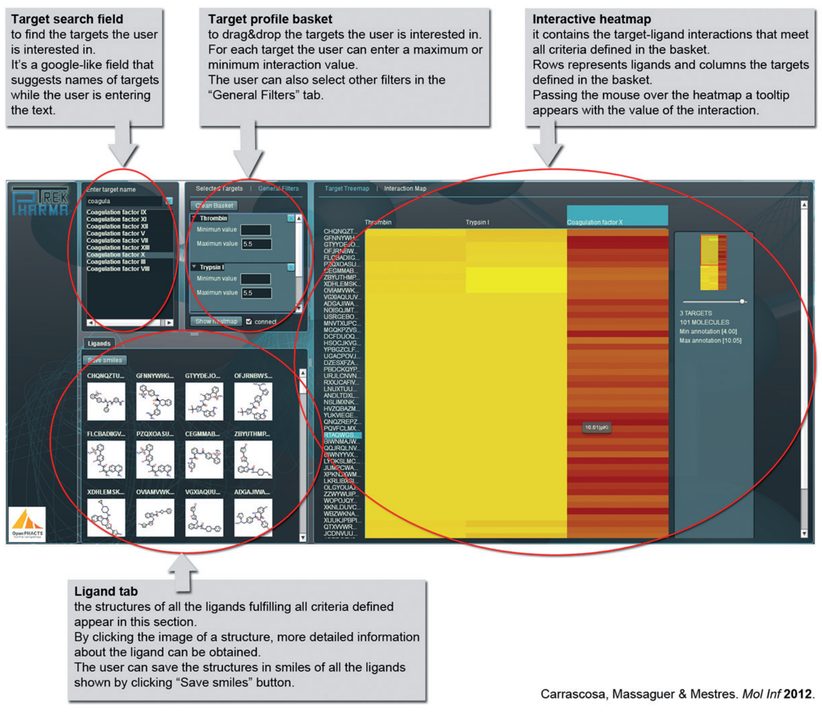



## Polypharmacology Browser: GARField




GARField is a tool for exploring the pharmacological space of small molecules. The user can search a compound from name, synonym, SMILES or structure drawing and retrieve target information associated with the compound query. Similarly, for a given protein, compounds with bioactivity data can be shown. With GARField it is possible to set a multiple query, filter the data by activity type ($K_i$, $IC_{50}$, $EC_{50}$…). The Similar Ensembl Approach (Keiser et al. *Nat. Biotechenol.*, 2007, **25,** 197) has been implemented, so the user can predict potential bioactive proteins based on their ligand similarity to a query compound.

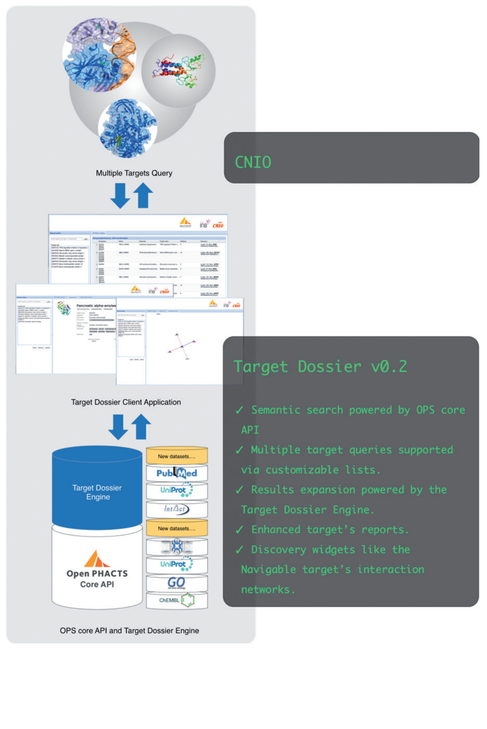
## Polypharmacology Browser: PharmaTrek




PharmaTrek proposes new mechanisms to navigate the pharmacological space in an interactive and flexible way. PharmaTrek is an integrative and interactive web application that will allow the scientist to extract new knowledge from the Open PHACTS platform. The main goal is to provide visual tools that allow the user to define custom questions around the biological activity between drugs and targets.

Carrascosa, Massaguer & Mestres. *Mol Inf* **2012**.

## Target Dossier




The Target Dossier uses the Open PHACTS platform to build comprehensive views of pharmacologically relevant targets, to answer questions regarding druggability, tissue expression profiles and implications in pathways, disease states and physiological mechanisms. The Target Dossier will provide a decision support platform for target selection and progression.

## Conclusions

These four project Exemplars demonstrate how the Open PHACTS platform and associated APIs can be exploited to address relevant problems/questions in the fields of drug development and biomedical research.

These Exemplars have been built using diverse languages and frameworks (ExtJS, Flash, etc), demonstrating the flexibility of the Open PHACTS platform API.

Other academic or commercial applications are encouraged, building on the Open PHACTS platform API, to cover other fields of pharmaceutical or biomedical research.

## More Information

Visit the Open PHACTS website (www.openphacts.org)

Follow our twitter account @Open_PHACTS

## Partners

This project has received support from the Innovative Medicines Initiative Joint Undertaking under grant agreement n° 115191, resources of which are composed of financial contribution from the European Union's Seventh Framework Programme (FP7/2007-2013) and EFPIA companies' in kind contribution. www.imi.europa.eu