

Open PHACTS API Use Example: Accelrys Hackathon

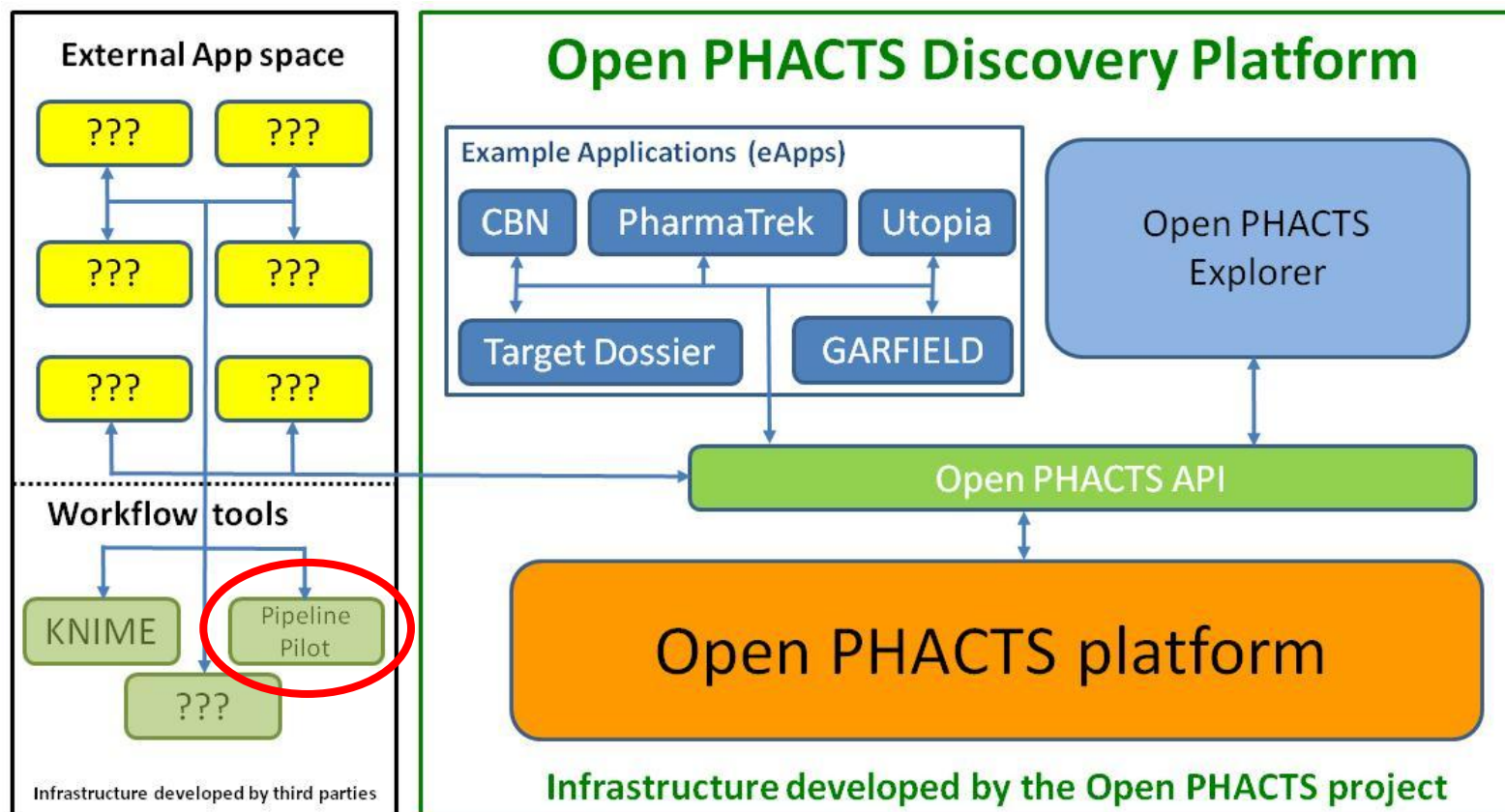
Stefan Senger

Using the Power of Open PHACTS

Open PHACTS 4th Community Workshop, London, 22-23 April 2013



The Open PHACTS ecosystem





Using the Power of Open PHACTS, London, 22-23 April 2013

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Create!

Build with the Open PHACTS discovery platform. The platform provides a convenient API to query across multiple pharmacology datasets.

You'll find complete documentation for the API in our [documentation](#) section. You'll need an API key to use the platform. [Sign-up](#) is free.

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Agenda Pipeline Pilot Hackathon

February 20, 2013

Accelrys European Headquarter

334 Cambridge Science Park,
Cambridge CB4 0WN
United Kingdom

Aim of the hackathon

Provide a brief introduction to the Open PHACTS API and develop some prototype Pipeline Pilot components and/or workflows showing how the API might be used. Participants can choose if they want to spend their time developing core Pipeline Pilot modules/components that map to specific API calls, or creating workflows that consume the API, perhaps combining it with other data.

09:00 – 09:30	Welcome & Introduction
09:30 – 10:00	Overview of the Open PHACTS API
10:00 – 10:30	Walk through of a sample Open PHACTS workflow
10:30 – 11:00	Tea/coffee break and setting up
11:00 – 12:30	Coding
12:30 – 13:15	Lunch
13:15 – 15:30	Coding (with tea/coffee breaks as required)
15:30 – 16:45	Presentation of components/workflows
16:45 – 17:00	Closing

**14 participants from workflow
tools novices to experts**



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OpenPHACTS

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ANNOUNCEMENT: Open PHACTS API will officially be launched in April [Show Details](#)

Group Overview



The OpenPHACTS group page on Accelrys Community

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[Stefan Senger](#)
[nmalcolm](#)
[Adrian Stevens](#)
[Veronica Wilson](#)

Tags: [pipeline](#), [pilot](#), [accelrys](#), [openphacts](#)

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Open PHACTS

Scientific competency questions
Guiding the technical development

About

Open PHACTS is a joint project from several leading research centres (MRC) aiming to reduce the barriers to drug discovery, industry, academia and from the life sciences. The Open PHACTS consortium is building a framework to support the development of the next generation of drug discovery, by providing a common infrastructure for the life sciences, industry, academia and from the life sciences. The Open PHACTS consortium is building a framework to support the development of the next generation of drug discovery, by providing a common infrastructure for the life sciences, industry, academia and from the life sciences.

Why do we need Open PHACTS?

Currently, the pharmaceutical companies spend a significant amount of time and effort in integrating and integrating internal information with public data sources. This process is often a slow and costly one, and the lack of integration of drug discovery across the entire life sciences is a major barrier to the development of new drugs. Open PHACTS is a joint project from several leading research centres (MRC) aiming to reduce the barriers to drug discovery, industry, academia and from the life sciences. The Open PHACTS consortium is building a framework to support the development of the next generation of drug discovery, by providing a common infrastructure for the life sciences, industry, academia and from the life sciences.

The public beta of the Open PHACTS 2.0 database will be released in Q4 2012.

Introduction

We have the collection of data with a representative set of the compounds with a view to use the data in the Open PHACTS 2.0 database.

The Open PHACTS 2.0 database is a joint project from several leading research centres (MRC) aiming to reduce the barriers to drug discovery, industry, academia and from the life sciences. The Open PHACTS consortium is building a framework to support the development of the next generation of drug discovery, by providing a common infrastructure for the life sciences, industry, academia and from the life sciences.

Results and Discussion

Open PHACTS 2.0 is a joint project from several leading research centres (MRC) aiming to reduce the barriers to drug discovery, industry, academia and from the life sciences. The Open PHACTS consortium is building a framework to support the development of the next generation of drug discovery, by providing a common infrastructure for the life sciences, industry, academia and from the life sciences.

Conclusions

Open PHACTS 2.0 is a joint project from several leading research centres (MRC) aiming to reduce the barriers to drug discovery, industry, academia and from the life sciences. The Open PHACTS consortium is building a framework to support the development of the next generation of drug discovery, by providing a common infrastructure for the life sciences, industry, academia and from the life sciences.

More Information

Visit the Open PHACTS website:
www.openphacts.org

Follow our twitter account: @Open_PHACTS

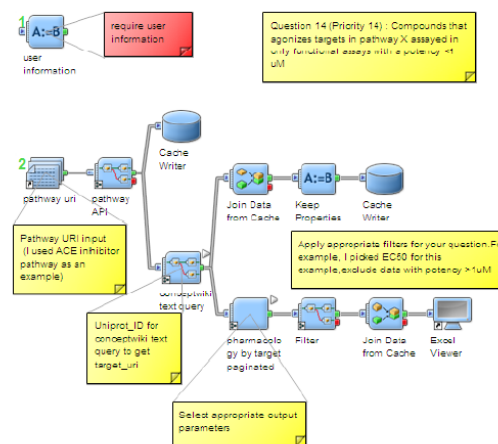
Partners

Open PHACTS Scientific Competency Questions – Guiding the technical development (EuroQSAR 2012 in Vienna, 30.08.2012)

<http://www.openphacts.org/posters>

Compounds that agonizes targets in pathway X assayed in only functional assays with a potency <1 μ M.

How long does it take to answer this research question?



1. Select EC50 bioactivity data entry
2. Relation not equal to >
3. Convert activity unit from nM/-LogEC50 to uM
4. Assay with potency <1uM

output columns
target_uri
target_title
activity_ID
pmid
activity_type
relation
standardValue
standardUnits
chembl_assay_id
description
assay_organism
chembl_target_id
target_organism
chembl_compound_id
chemspider_uri
compound_uri
prefLabel
inchi
inchikey
full_mwt
smiles
ro5_violations
uM
pathway_title
citesAsDataSource



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... and another one

Hackathon PLP protocol

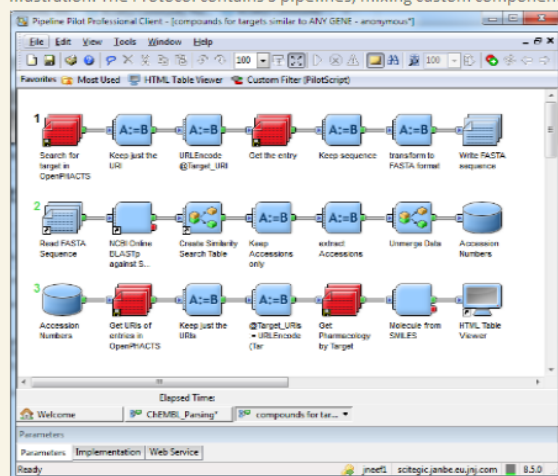
VERSION 1

Created on: Mar 15, 2013 8:28 AM by [Jean-Marc Neefs](#) - Last Modified: Mar 15, 2013 8:45 AM by [Jean-Marc Neefs](#)

This would be my contribution to PLP protocols:

It answers a business question: "if we have a new target without known or effective drugs, find if there are drugs available for similar targets."


Illustration: The Protocol contains 3 pipelines, mixing custom components to call the OpenPHACTS API (red), and existing Pipeline Pilot components (blue).



Steps:

1. Enter target information -- gene symbols would be nice but they are not accepted in this protocol. The protocol will fetch the requested entry from OpenPHACTS, keep its protein sequence and save it in FASTA format.
2. The FASTA formatted sequence is sent to NCBI BLAST to search for similar sequences, in this case limited to SwissProt and human entries. The UniProt Accession numbers of the top 20 hits are kept.
3. Each Accession number is used to search for its corresponding entry in OpenPHACTS, and the URI of each entry is used to fetch Pharmacology information by Target in OpenPHACTS. A structure image is calculated from Smiles codes and the resulting table can be viewed in HTML.

Attachments:

 [Hackathon.xml](#) (440.9 K)



In a nutshell...

Combining the Open PHACTS API with a workflow tool enables scientists to answer relevant research questions quicker.