

Open PHACTS

Deliverable 6.14

Organisation of prototype Training Event

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Approved by UNIVIE, USC, Janssen

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Project title: An open, integrated and sustainable chemistry, biology and pharmacology knowledge resource for drug discovery

Instrument: IMI JU

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Definitions

- Partners of the Open PHACTS Consortium are referred to herein according to the following codes:

Pfizer – Pfizer limited – **Coordinator**

UNIVIE – Universität Wien – **Managing entity of IMI JU funding**

DTU – Technical University of Denmark – DTU

UHAM – University of Hamburg, Center for Bioinformatics

BIT – BioSolveIT GmbH

PSMAR – Consorci Mar Parc de Salut de Barcelona

LUMC – Leiden University Medical Centre

RSC – Royal Society of Chemistry

VUA – Vrije Universiteit Amsterdam

CNIO – Spanish National Cancer Research Centre

UNIMAN – University of Manchester

UM – University of Maastricht

ACK – ACKnowledge

USC – University of Santiago de Compostela

UBO – Rheinische Friedrich-Wilhelms-Universität Bonn

AZ – AstraZeneca

GSK – GlaxoSmithKline

Esteve – Laboratorios del Dr. Esteve, S.A.

Novartis – Novartis

ME – Merck Serono

HLU – H. Lundbeck A/S

E.Lilly – Eli Lilly

NBIC – Stichting Netherlands Bioinformatics Centre

SIB – Swiss Institute of Bioinformatics

ConnDisc – Connected Discovery

EBI – European Bioinformatics Institute

Janssen – Janssen Pharmaceutica

OGI – OpenLink Software

- Grant Agreement:** The agreement signed between the beneficiaries and the IMI JU for the undertaking of the Open PHACTS project.
- Project:** The sum of all activities carried out in the framework of the Grant Agreement.
- Work plan:** Schedule of tasks, deliverables, efforts, dates and responsibilities corresponding to the work to be carried, out as specified in the Grant Agreement.
- Consortium:** The Open PHACTS Consortium composed of the above-mentioned legal entities.
- Project Agreement:** Agreement concluded amongst Open PHACTS participants for the implementation of the Grant Agreement. Such an agreement shall not affect the parties' obligations to the Community and/or to one another arising from the Grant Agreement.

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1 Introduction

A first prototype training event was organized on the occasion of the Vienna Summer School Drug Design 2013. Two days of the summer school (19th and 20th of September 2013) had lectures and workshops related to the Open PHACTS project.

Lectures connected to Open PHACTS were:

- G. Ecker: A novel platform for integrated data-driven drug discovery (This talk included a presentation of Explorer 2 by R. Ramgolam)
- G. Ecker: Open Data in Pharmacoinformatics - Do they improve our models?
- C. Batchelor: ChemSpider and drug discovery
- C. Lemmen: Surfing at the Interface of Chemistry and Biology
- B. Zdražil: How to deal with open access bioassay data?

The description of the workshop as sent out to the participants in advance was the following:

Open PHACTS workshop

Open PHACTS is building a generic semantic data integration infrastructure targeted on medicinal chemistry. Currently it integrates 10 different data sources, such as ChEMBL, Uniprot, Drugbank, and allows to look up answers to complex research questions, such as "give me all oxidoreductase inhibitors with an activity < 100 nM. Besides the Open PHACTs Explorer, which provides a basic user interface, several applications are available which allow sophisticated analysis of the data in the Open PHACTs Discovery Platform. These include e.g. ChemBioNavigator for intuitive navigation through the data, and PharmaTrek for polypharmacology browsing.

The workshop on Thursday will provide hands on training on the use of Open PHACTs Explorer, whereas the workshop on Friday will focus on the use of ChemBioNavigator and PharmaTrek.

2 Realisation of the workshops

2.1 Explorer

(Presented by Daniela Digles and Rishi Ramgolam)

The Explorer workshop started with the introduction of the Explorer landing page (<http://www.openphacts.org/explorer>), giving the users the possibility to register. Subsequently, the participants were led through the different options of the Explorer itself. This included the Compound and Target info pages, pharmacology pages including filtering possibilities, performing structural (similarity) searches, showing the provenance of the data and connections between these calls. The users could follow this directly on their computers. Afterwards, the participants were given time to independently try out their compounds and targets of interest.

For interested participants also the basics of the Open PHACTS API were shown.

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2.2 ChemBioNavigator / PharmaTrek

(Presented by Christian Lemmen and Lars Richter)

In the first part of the workshop the ChemBioNavigator (<http://www.chembionavigator.org/>) was introduced to the audience. Starting with a simple Aspirin query, subsequently enriched by compounds retrieved from chemical similarity search. Representation of the returned compound set in 2D plotting compound bioactivity against various physicochemical descriptors.

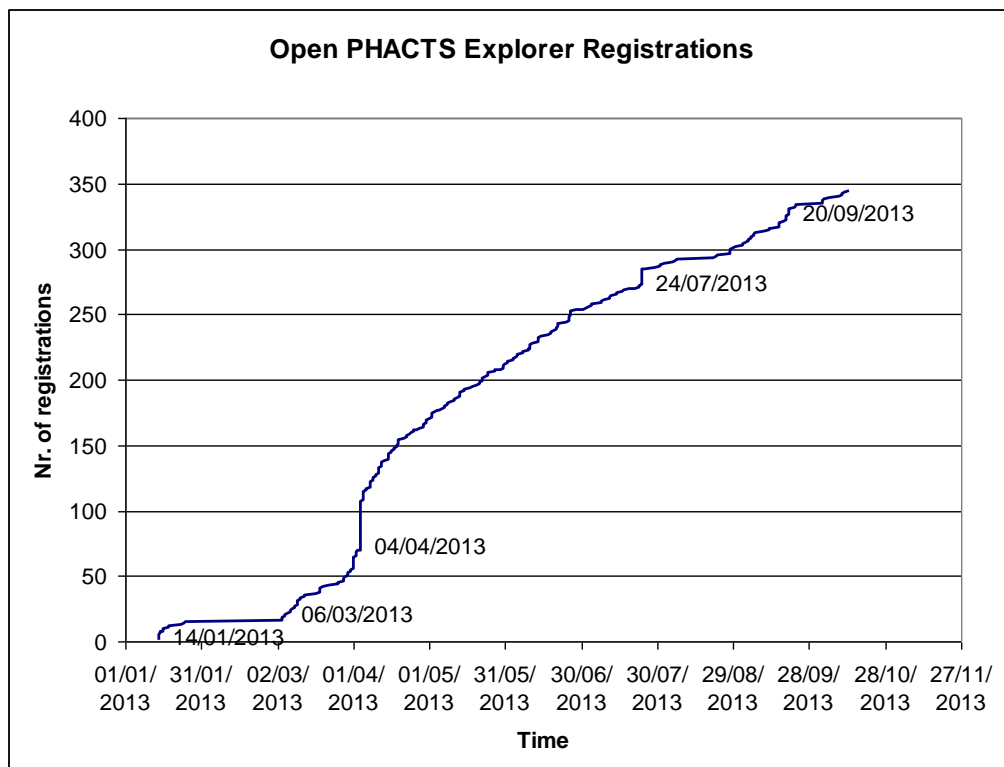
The subsequent part of the workshop was devoted to PharmaTrek (<http://www.pharmatrek.org/>). First the upcoming importance/ availability of polypharmacological data and its consequences to drug development was pointed out. Subsequently PharmaTrek was used to search for a highly potent SERT inhibitor with low activity against a list of antitargets (e.g. HERG). Finally the compounds 'Serotonin' and 'Dopamine' were queried in order to get a comparison of the bioactivity profile of these compounds.

In both workshops the interconnectivity between the various exemplars, enabled by implemented link-outs, was highlighted wherever possible.

3 Participants

The talks were visited by approx. 60 participants, mainly from academia.

The Explorer workshop on the 19th September was visited by 9 participants. As some people couldn't attend this workshop due to parallel courses, a second workshop was held on the 20th with 3 participants. The training event led to 10 new registrations to the Explorer in two days. The increase of registrations around the time of the Summerschool can be seen in the following diagram:



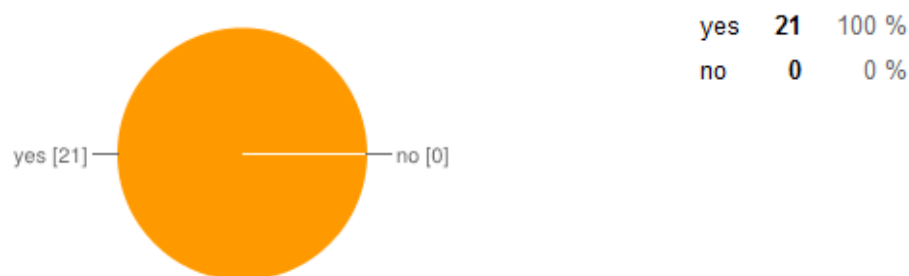
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The ChemBioNavigator / PharmaTrek workshop had 25 participants

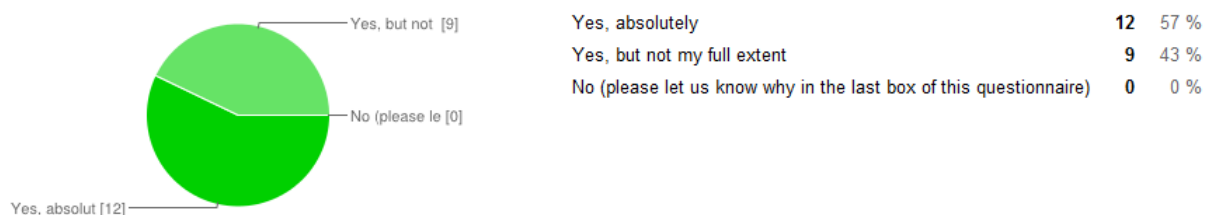
4 Feedback

Feedback for the lectures and workshops was generally very positive. Feedback gathered for the whole summer school is presented in the following diagrams:

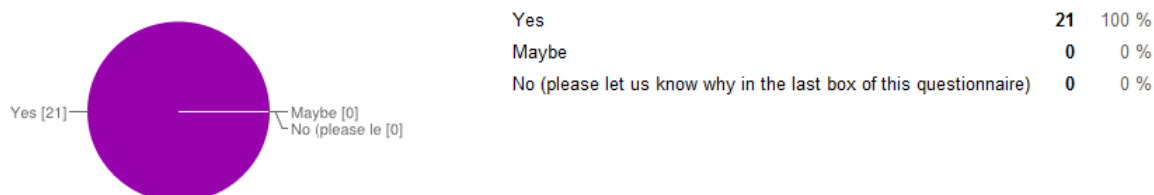
Was the content of the presentations helpful/interesting?



Did the conference fulfill your reason for attending?



Would you recommend this conference to others?



In the Explorer workshop, some known issues were found by the users (problems to query the protein of interest, performance of the Enzyme Pharmacology query). Additional questions and feature requests were the following:

- Which fingerprint is used for the similarity search?
- Request to perform a BLAST search for a given protein sequence.
- Request of a property filter for the similarity search (e.g. for molecular weight).
- Request to show the number of results for the Enzyme pharmacology call already in the hierarchy.
- Request to get compounds which are cocrystallized with a given protein.
- Request to zoom in to the structure of compounds.
- Request to search for a compound (which is a small peptide) by sequence instead of by SMILES.

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Feedback from the presenters:

R. Ramgolam: "After the Explorer 2 presentation I had lots of people asking questions about OPS and the Explorer. Some of them are going to try it and show it to other people upon their return, others were interested in using the API and had some more technical questions."

C. Lemmen: "The workshop about the ChemBioNavigator application went very well. The attendants could try what I demonstrated right away. The server had no problems at all handling the traffic of about 25 simultaneous visitors. A lot of questions came up indicating a high level of interest."