

Open PHACTS

D 4.5.3 Deliver second version of the LDC with all services released externally

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Approved by UNIMAN, Janssen, HLU, RSC, SIB

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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

OGL – 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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Introduction

The Open PHACTS Discovery Platform¹ is a suite of software components that allow users to answer scientific questions that require data to be connected across multiple biomedical and chemical databases. Users and application developers access these data through web services, known as the Open PHACTS Application Program Interface, API). This document describes the release of the second version of the API at the community workshop, held at the Royal Society Of Chemistry in London, UK on April 22nd 2013. We have chosen to publish this document a couple of months after the workshop as we wished to describe not just the event itself, but the **impact** of the workshop and the adoption of the API by the wider community

The Launch Workshop

The second version of the Open PHACTS Discovery Platform & API was released to the community in April 2013 at the Community Workshop. This was a very well attended meeting



with delegates from a wide range of organisations. Representatives from both business and technical areas of a number of scientific and informatics companies were present. At the workshop we provided basic access and usage details of the API. We also attempted to aid participants to quickly get up and running by walking through the creation of a simple drug discovery application using the API. The sessions were complemented by talks from

key example application developers such as PharmaTrek², Utopia³ and ChemBioNavigator⁴ that showed the API could power real-world advanced scientific applications. A full account of the workshop was reported in deliverable D8.3.4.

¹ <http://dev.openphacts.org>

² <http://pharmatrek.org>

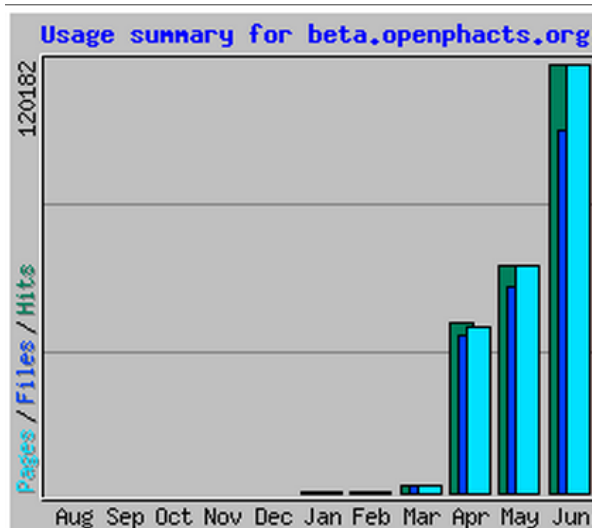
³ <http://getutopia.org>

⁴ <http://chembionavigator.org>

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Impact of the workshop, API signups

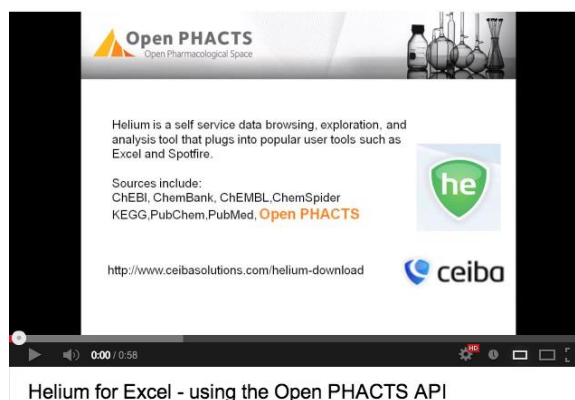
In the two month since the official launch of the Open PHACTS Discovery Platform there has been significant uptake by the scientific community. So far there have been over **750,000 calls** to the API and around **100 Organisations** have signed up to access the system. In June alone we served over **4GB of integrated data** to API consumers. The graph shows the rapid growth in usage since the workshop, and we will continue to track these statistics going forward. Furthermore, the diversity in new users has been notable with new accounts from both Industry (both large pharma not in the current project and many SMEs) and Academia (both European and beyond). A key factor in the uptake is the ease of use of the API. One SME was able to integrate with the software during one session of the Community Workshop itself.



We believe that this represents an excellent adoption rate at this early stage of the platform and a foundation on which to build with subsequent releases and workshops.

External Applications

Many application developers outside the consortium are still integration their applications with the API, however, we are beginning to see the first outcomes of integration with applications. For example, the Open PHACTS API has been integrated into the Helium Platform, a commercial (with free-community edition) platform for data analysis from Ceiba solutions⁵. This software provides an alternative mechanism for non-technical scientists to access Open PHACTS data via the API in a very familiar Microsoft Excel-based environment. A video demonstrating the utility of this platform for pharmacology analysis is available on YouTube⁶.



⁵ <http://www.ceibasolutions.com/helium-about>

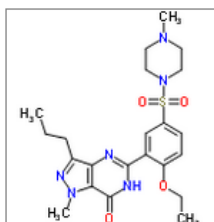
⁶ <http://www.youtube.com/watch?v=oqr4Og5M1Pw>

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About This Topic

Sildenafil

aka: sildenafil;
sildenafil oral spray;
sildenafil citrate;
uk92480; viagra;



Key Resources:

250 pharmacology data points @

Open PHACTS

The pharma intelligence news service, SciBite⁷ also integrates directly with the Open PHACTS API. Scientists use this site to stay on top of recent articles concerning biomedical topics. When a user visits a page on a drug or target (such as for sildenafil⁸) the site calls the API in the background and displays the number of pharmacological data points available (see figure on left). This tells the user that Open PHACTS has definitive pharmacology data on this entity, without the user needing to go to the platform. If data is found, the number of data points is displayed along with a link to the Open PHACTS explorer.

The release of the API has also facilitated development of tools such as Collector⁹ which provides mechanisms to create Quantitative Structure-Activity Relationship (QSAR) models. The Collector application uses the API to retrieve extensive pharmacology data and provides flexible filtering to tailor models to the experimental need. It is currently being used within the IMI eTox project¹⁰.



Workflow Tool Support

While the Open PHACTS API is a powerful tool for scientific discovery it is primarily an access point for software developers and not intended for direct consumption by most scientists. For the latter group, access to Open PHACTS data is made available by use-case focused applications (such as PharmaTrek, ChemBioNavigator or the Open PHACTS explorer). However, scientists may wish to further explore the data or perform other tasks not supported by an existing graphical application. Therefore it is critical to the project that we support the use of the API within scientific workflow tools. These bridge the gap between APIs and scientific users, allowing them to perform data-driven experiments without software development skills.

⁷ <http://scibite.com>

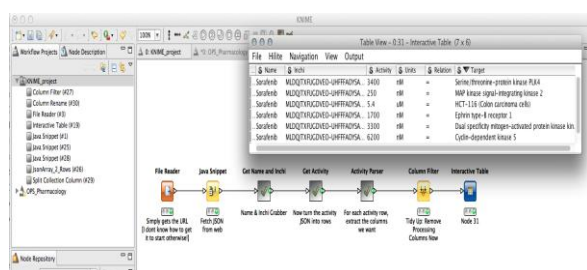
⁸ <http://scibite.com/site/topic/DRUG:CHEMBL192>

⁹ <http://phi.imim.es/collector/>

¹⁰ <http://www.etoxproject.eu/>

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One of the most important workflow tools to support is Pipeline Pilot¹¹, a commercial product from Accelrys. This tool is widely used across industry for many data-analysis tasks and had been identified as a critical platform to support if we wished to gain good adoption of the API within industry. Work on these components began in early 2013 through a group of project members, many from the industry participants in the project. Accelrys also provided much technical and logistic support and the together the group have successfully built a suite of Open PHACTS Pipeline Pilot components along with an active web-based community group¹² (shown in the image). The first version of these components was launched in early July¹³.



The Konstanz Information Miner (KNIME) is a second workflow tool that has high levels of adoption across industry and academia. As such, it was critical that Open PHACTS also provided a suite of components that would make it easy to work with out API using this platform. This work was led by the VU and was presented for the first time at the KNIME

User Day at the end of June 2013¹⁴. The image shows a screenshot from a real-life workflow using the KNIME nodes.

The Open PHACTS API has also been integrated into the Taverna Workbench¹⁵, a further data workflow tool extensively used within the life sciences. A protocol to perform some core API functions has been uploaded to the “MyExperiment” workflow sharing site¹⁶.(shown right). Both the Pipeline Pilot components and KNIME Nodes are made available from a workflow focused web page¹⁷. As the Taverna workflows are finalized they will make there way onto this site as well.



¹¹ <http://accelrys.com/products/pipeline-pilot/>

¹² <https://community.accelrys.com/groups/openphacts>

¹³ <https://community.accelrys.com/message/18054#18054>

¹⁴ <http://www.knime.org/user-day-london-2013>

¹⁵ <http://www.taverna.org.uk/>

¹⁶ <http://www.myexperiment.org/workflows/3628.html>

¹⁷ <https://dev.openphacts.org/workflow>

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Conclusions

Since its launch at the end of April 2013, use of the Open PHACTS Discovery platform has grown at a very encouraging rate. We have capitalized on the interest generated from the workshop by releasing a steady stream of additional access methods to broaden out the user base. We believe this represents a very positive start for the Open PHACTS platform.

Acknowledgements

The work described here covers a large number of individuals from many of the project partners. We acknowledge contribution across the entire Open PHACTS project to the delivery of this comprehensive set of technologies.