

# Open PHACTS

## Milestone 5

**Demonstrated application/impact in experimental teams,  
active involvement of Associated Partners,  
growing community of users,  
sustainability/hosting resolved**

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Approved by UNIVIE, GSK, VUA, Novartis, LUMC, ACK, USC, Pfizer,  
CD, DTU

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Version 1.0

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

Instrument: IMI JU

Contract no: 115191

Start date: 01 March 2011

Duration: 42 months

<b>Nature of the Deliverable</b>	
Report	<b>x</b>
Prototype	
Other	
<b>Dissemination level</b>	
Public dissemination level	
For internal use only	<b>x</b>

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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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## 1 Demonstrated application / impact in experimental teams

The Open PHACTS Discovery Platform is used by a broad community, as the number of hits of the API (Figure 1), the number of developer accounts (Figure 2), the access statistics for the Open PHACTS Explorer (Figure 3), as well as the ecosystem of apps (Figure 4) built around the Open PHACTS API show.

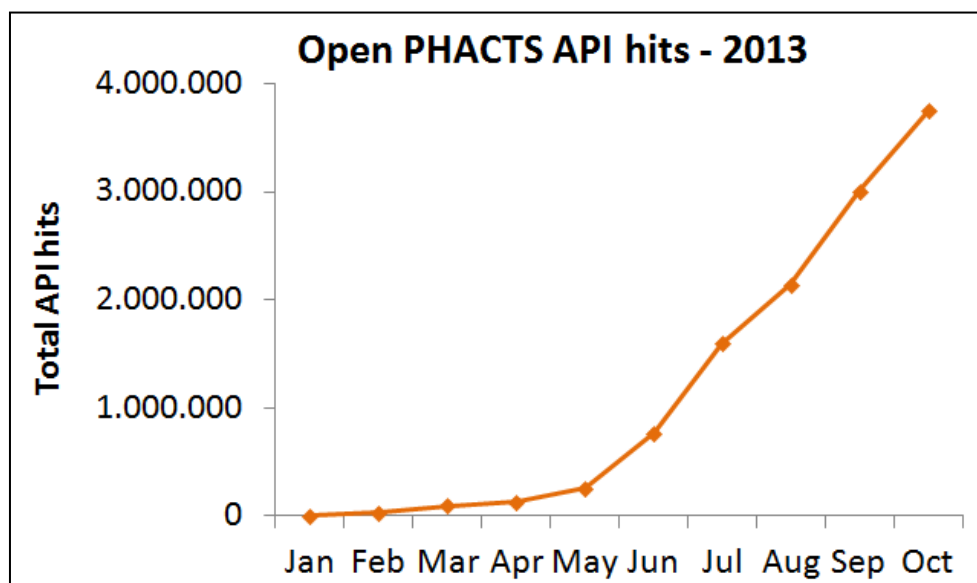


Figure 1: Total Open PHACTS API hits 2013

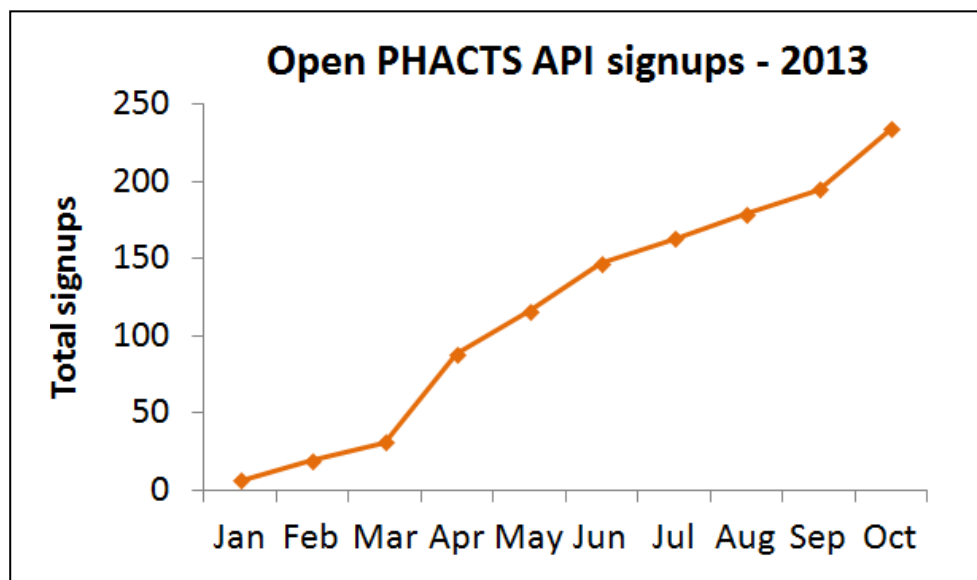


Figure 2: Total Open PHACTS API signups 2013

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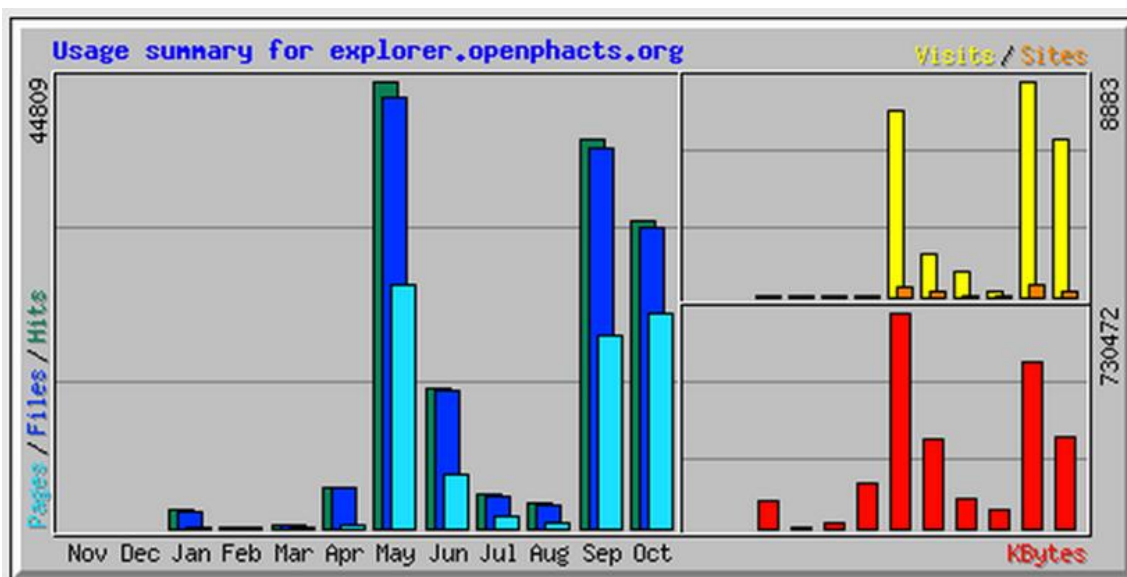


Figure 3: Summary of usage of the Open PHACTS Explorer



Figure 4: Ecosystem of apps

Furthermore, there are upcoming publications showing the use of the platform in experimental teams. One example is dealing with the development of a classification model for TRPV1 antagonists, which was published in Mol. Informatics<sup>1</sup>. This work also outlines the importance of a proper assay description, which prompted EBI to start working on a respective ontology (together with UNIVIE). This demonstrates, that the use of the Open PHACTS also feeds back to its further improvement.

<sup>1</sup> Daria A. Tsareva, Gerhard F. Ecker: How Far Could We Go with Open Data – A Case Study for TRPV1 Antagonists; Molecular Informatics, Volume 32, Issue 5-6, pages 555-562, June 2013, DOI: 10.1002/minf.201300019

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## 2 Active involvement of Associated Partners

The Waiting Room and Gatekeeper process for bringing Associated Partners on board is working very well. The Associate Partner programme has brought in a growing number of partners who wish to be aligned with the project, ranging across our targeted stakeholder groups with a healthy number in a position to support project sustainability. Open PHACTS now has more Associated Partners linked to the project than it has project partners – these cover a wide range of target stakeholders, from application builders (large and small), database publishers (public and commercial), semantic web experts, and medchem researchers.

See the list of all Associated Partners on our website:

<http://www.openphacts.org/partners/associated-partners>

Open PHACTS has a Memorandum of Understanding (MoU) ready to sign for mutual support and exchange of ideas, data or technology. The Associated Partner are the first to hear about the latest developments in the Open PHACTS project and also have the opportunity to present ideas and use cases to the core Open PHACTS team, e.g. at the Open PHACTS Community Workshops held twice a year in different locations.

In these regular community workshops Associated Partners have the possibility to:

- Learn more about Open PHACTS and the Open Pharmacological Space.
- Participate in new ideas and functions.
- Engage in development of new use cases.
- Contribute to development, and engage in plans for sustaining the Open Pharmacological Space.

Find summaries of all previous workshops on our website:

<http://www.openphacts.org/news-and-events/community-workshops/previous-community-workshops>

If an Associated Partner wants to do some more specific development work together with the Open PHACTS consortium (e.g. develop APIs, new data, algorithms etc), they have the possibility to enter a Development Partnership. This will give them greater access to the core of the project. Development Partnerships are focused on defined pieces of work of mutual interest and an agreed collaborative annex is added to the MoU.

As a major benefit, Associated Partners were privileged to get the first view of the beta of the Open PHACTS Discovery Platform and the Open PHACTS Explorer before we released it to the wider public. They were exclusively invited to test the system in January 2013 and to provide feedback, which was implemented before the wider public release in March 2013.

## 3 Growing community of users

The release of the Open PHACTS Development Platform happened in a staggered process:

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- After providing access to the EFPIA companies in the consortium, the Associated Partners were invited in January 2013 to test the Explorer and to provide feedback.
- Furthermore, on 6 March 2013 Gerhard Ecker personally invited 40 Med-Chem groups.
- On 4 May 2013 the participants of the EuroQSAR 2012 and ISMC conference 2012 were invited to use and test the Open PHACTS Discovery Platform and give feedback.
- V1.1 of the Open PHACTS Discovery Platform was finally publicly released on 22 April 2013 in the course of the [4<sup>th</sup> Open PHACTS Community Workshop](#) in London. Additionally to the Explorer, two of our Example Applications were released in London as well: ChemBioNavigator and PharmaTrek.

The following diagram shows the growth of number of registered users for the Open PHACTS Explorer:

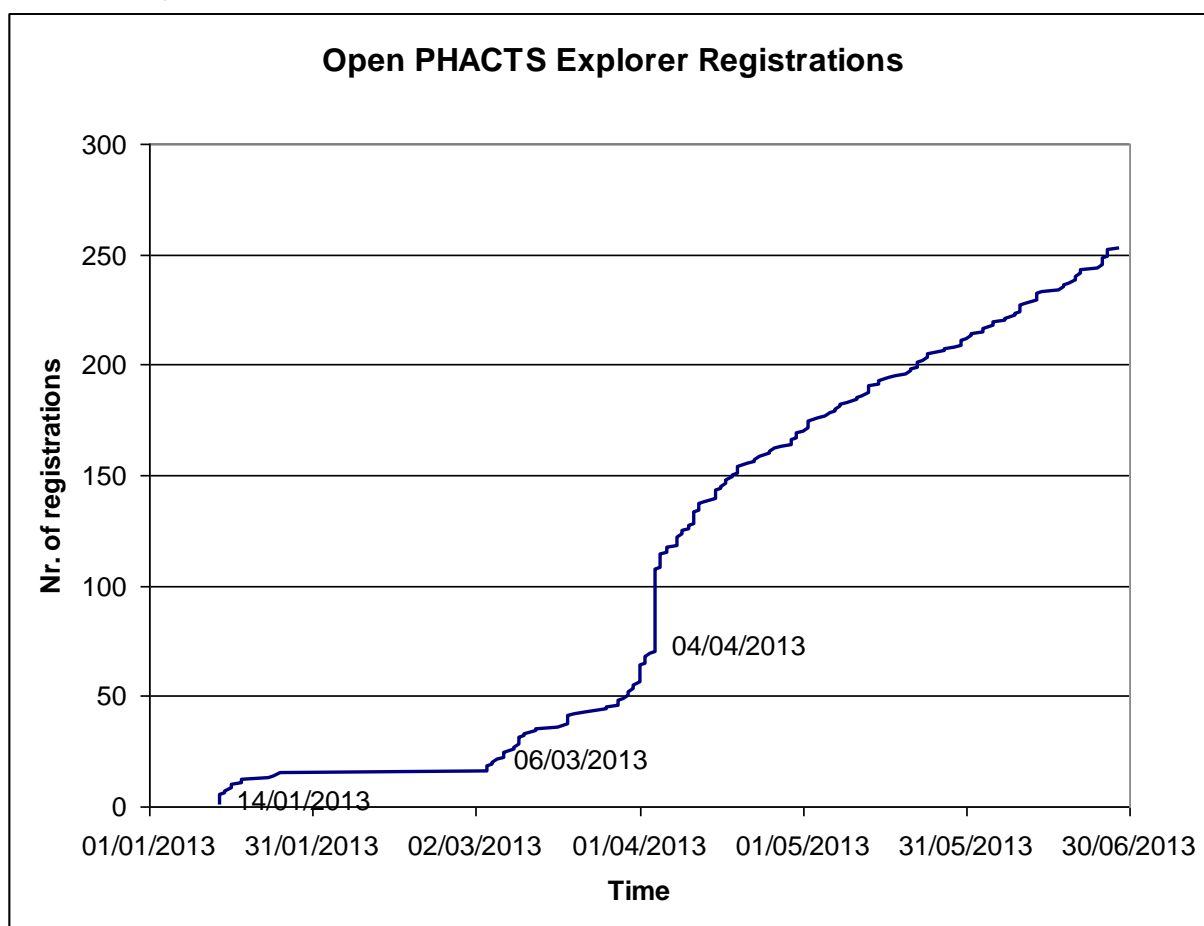


Figure 5: Open PHACTS Explorer registrations

The 3 shown dates mark the invitations to the Open PHACTS discovery Platform sent to different groups of users as described above. Especially the invitation of the EuroQSAR and ISMC participants (04/04/2013) led to a high increase of registrations. Currently, a steady increase of registrations can be observed.

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## 4 Community Feedback

Generally, the response from the Associated Partners as well as from the wider community regarding the application as well as the feedback mechanism was very positive. Main reported issues were (ordered by incidence):

- Why multiple entries for a compound name?
- Autocomplete behaviour / synonyms
- TSV Export
- SD Export
- Show synonyms in Explorer
- More supported activity types (Ki)
- Should I logout?
- Better provenance presentation
- Use Gene IDs
- Species independent search.
- Organism standardisation
- Connect explorer to Example Applications
- “null” values in rest of Structure Search Results table
- Save/Upload smiles/mol/acdraw

A detailed report on the community feedback can be found in Deliverable 6.15 „[Report on feedback received on version 1](#)”.

## 5 Hosting resolved

For hosting the Open PHACTS infrastructure a public call for adding a beneficiary was placed and successfully completed on 13 July 2012. OpenLink was added as new partner, the platform was transferred to them and since September 25, 2012 the system is running stable on the OpenLink infrastructure. Critically, OpenLink can now offer the possibility of providing security or privacy guarantees to EFPIA companies, services that were not central to the aims of the project. OpenLink’s inclusion allowed providing professional hosting and also bringing in expertise for project sustainability.

## 6 Sustainability resolved

In October 2012, a sustainability working group was set up to put in place a business plan to ensure post-project sustainability. The Consortium agreed to establish “The Open PHACTS Foundation”, a UK- based not-for-profit company with the aim to become an educational charity over time. It shall be a research based organisation, which can participate in global grant mechanisms (may developed mirrors/subsidiaries in other territories as necessary) and allows a greater breadth of partners/members/owners.

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A lot of interest for The Open PHACTS Foundation could already be generated at the CSHALS (Conference on Semantics in Healthcare and Life Science) conference in Boston end of February 2013, as well as at the 4<sup>th</sup> Community Workshop in London in April 2013. Active member recruitment was started with the [5<sup>th</sup> Open PHACTS Community Workshop](#) in Amsterdam on October 10-11, 2013.

The Open PHACTS Foundation was established in May 2013. For further information please visit the Open PHACTS Foundation website: [www.openphactsfoundation.org](http://www.openphactsfoundation.org).