

# Open PHACTS

## Milestone 6

**Long term funding implemented with permanent beta developer team; Open PHACTS Discovery Platform hosted and running; secure access implemented**

**Also covers:**

**D 3.2.5 Open PHACTS Discovery Platform version 3.0 developed and 'signed off' by TTF and EC on criteria formulated in WP1-6**

**D 4.5.5 Final version of LDC and services as sustainable production type**

Prepared by Lee Harland (SciBite), Anika Robl (UNIVIE)

Approved by UNIMAN, Janssen, CD, VUA, RSC, SIB

August 2014

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: 60 months

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

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| <b>Open PHACTS</b> | Milestone: Long term funding implemented with permanent beta developer team; Open PHACTS Discovery Platform hosted and running; secure access implemented | Milestone 6<br>D 3.2.5 & 4.5.5 |       |
| IMI - 115191       | Authors: Lee Harland (SciBite), Anika Robl (UNIVIE)   | Version: 1.0                   | 2 / 8 |

## Definitions

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

- 1 - **GSK** – GlaxoSmithKline – **Coordinator**
- 2 - **UNIVIE** – Universität Wien – **Managing Entity of IMI JU funding**
- 3 - **DTU** – Technical University of Denmark
- 4 - **UHAM** – University of Hamburg, Center for Bioinformatics
- 5 - **BIT** – BioSolveIT GmbH
- 6 - **PSMAR** – Consorci Mar Parc de Salut de Barcelona
- 601 - **FIMIM** – Fundacio Institut Mar d'Investigacions Mediques
- 602 - **UPF** – Universitat Pompeu Fabra
- 7 - **LUMC** – Leiden University Medical Centre
- 8 - **RSC** – Royal Society of Chemistry
- 801 - **RSCWW** – RSC World Wide Ltd
- 9 - **VUA** – Stichting VU-VUMC
- 10 - **CNIO** – Centro Nacional de Investigaciones Oncológicas
- 11 - **UNIMAN** – University of Manchester
- 12 - **UM** – Universiteit Maastricht
- 13 - **ACK** – ACKnowledge
- 14 - **USC** – Universidade de Santiago de Compostela
- 15 - **UBO** – Rheinische Friedrich-Wilhelms-Universität Bonn
- 16 - **AZ** – AstraZeneca AB
- 17 - **Pfizer** – Pfizer Limited
- 18 - **Esteve** – Laboratorios del Dr. Esteve, S.A.
- 19 - **Novartis** – Novartis Pharma AG
- 20 - **ME** – Merck
- 21 - **HLU** – H. Lundbeck A/S
- 22 - **Lilly** – Eli Lilly and Company Limited
- 23 - **NBIC** – Stichting Netherlands Bioinformatics Centre
- 24 - **SIB** – Swiss Institute of Bioinformatics
- 25 - **CD** – ConnectedDiscovery
- 26 - **EMBL-EBI** – European Molecular Biology Laboratory
- 27 - **Janssen** – Janssen Pharmaceutica NV
- 28 - **OGI** – OpenLink Group Ltd
- 29 - **OPF** – The Open PHACTS Foundation
- 30 - **ALM** – Laboratorios Almirall S.A.
- 31 - **SciBite** – SciBite Limited

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## 1 Introduction

This Milestone 6 also covers the following deliverables:

- **D 3.2.5** Open PHACTS Discovery Platform version 3.0 developed and ‘signed off’ by TTF and EC on criteria formulated in WP1-6 (Prototype)
- **D 4.5.5** Final version of LDC and services as sustainable production type (Prototype)

## 2 Open PHACTS Discovery Platform hosted and running

A key goal for the project is to host the Open PHACTS Discovery Platform on a professional hosting environment. The first phase of this work was the recruitment of the hosting partner through a competitive tender process. The successful applicant was OpenLink, and work was then undertaken to install the system on their servers. This was a considerable undertaking, and required:

- Purchase and configuration of the correct hardware
- Packing and testing of Open PHACTS software and data for transition to OpenLink
- Install of the core platform on the OpenLink servers
- Connection of the hosted core to the additional Open PHACTS services (ConceptWiki, IMS, ChemSpider)
- Installation of the GUI (Explorer) on the OpenLink servers
- Configuration of access, security (SSL certificates)
- Installation and configuration of logging and system monitoring (see D 4.6.3)

This complex procedure was carried out jointly by the core platform developers and OpenLink and required many hours of testing and validation. However, due to the design principles behind the system, the installation proceeded in good time and resulted in a fully working on the OpenLink servers.

The Open PHACTS Discovery Platform is now running 24/7 and is used by Academia as well as EFPIA. As shown in Appendix 1, the Open PHACTS API is gaining significant usage from a wide variety of organisations. The appendix shows a weekly usage report from three selected weeks – demonstrating that while the “top users” each week will obviously vary, there is a good mix of different organisations, including pharma and academia.

The Open PHACTS Explorer is running on the OpenLink server at [explorer.openphacts.org](http://explorer.openphacts.org) and the Open PHACTS API at [dev.openphacts.org](http://dev.openphacts.org). Feedback from users is gathered via the support portal available at [support.openphacts.org](http://support.openphacts.org) (tickets and forum) or alternatively via email to [support@openphacts.org](mailto:support@openphacts.org).

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#### Related publications:

Harland L (2012) Open PHACTS: A semantic knowledge infrastructure for public and commercial drug discovery research. Springer, Lecture Notes in Computer Science, Volume 7603, 1-7.

[http://link.springer.com/chapter/10.1007/978-3-642-33876-2\\_1?LI=true](http://link.springer.com/chapter/10.1007/978-3-642-33876-2_1?LI=true)

Special Issue: Open Innovation in Drug Discovery. Molecular Informatics, Volume 31, Issue 8, 517-609, August 2012

<http://onlinelibrary.wiley.com/doi/10.1002/minf.v31.8/issuetoc>

Gray AJ, Groth P, Loizou A, Askjaer S, Brenninkmeijer C, Burger K, Chichester C, Evelo CT, Goble C, Harland L, Pettifer S, Thompson M, Waagmeester A, Williams AJ (2012) Applying Linked Data Approaches to Pharmacology: Architectural Decisions and Implementation. Semantic Web Journal.

<http://www.semantic-web-journal.net/content/applying-linked-data-approaches-pharmacology-architectural-decisions-and-implementation>

Williams AJ, Harland L, Groth P, Pettifer S, Chichester C, Willighagen EL, Evelo CT, Blomberg N, Ecker GF, Goble C, Mons B (2012) Open PHACTS: semantic interoperability for drug discovery. Drug Discovery Today, Volume 17, Issues 21-22, 1188-1198.

<http://www.sciencedirect.com/science/article/pii/S1359644612001936>

Further publications can be found on our website:

<http://www.openphacts.org/news-and-events/publications>

### 3 Long term funding implemented with permanent beta developer team

A major milestone towards sustainability has been reached in August 2013, when the Open PHACTS Foundation, a not-for-profit membership organisation, was established. The aim of the Open PHACTS Foundation is to start to build a membership to continue the work of the project, ensuring the infrastructure is sustained and extended, and the needs of the scientific community served. In December 2013, the Open PHACTS Foundation joined the Open PHACTS project as a partner.

In June 2014, the Open PHACTS Foundation proudly announced its first three members – GlaxoSmithKline, Janssen and Roche – who will steer the future of the successor organisation to the Open PHACTS project.. The commitment by these global pharmaceutical industry members signifies a major step in ensuring the sustainability of infrastructure developed during the Open PHACTS project. The Open PHACTS community covering academia, industry, application developers and semantic web experts has delivered a powerful cloud-based data platform, demonstrating the effectiveness of robust data integration in answering real scientific questions.

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As a leading IMI project, the Open PHACTS project has built a sustainable succession plan through the Foundation to both continue provision of the Open PHACTS Discovery Platform and to extend the coverage of data and functionality. Collaboration with existing and future consortia will engage the scientific community and involve relevant applied life science R&D.

A core developer team is now responsible for maintaining and enhancing the Open PHACTS API. This core group consists of staff from the RSC, VU, UNIMAN and SIB. Routine teleconferences and skype discussions are held and the git system is used to provide extensive issue tracking and discussion (see appendix 2).

#### **4 Secure access implemented**

The Open PHACTS API is accessible via [dev.openphacts.org](http://dev.openphacts.org), which is secured with a SSL certificate. The system is now fully secured and private, according to a detailed specification worked out between the Open PHACTS team, Open Link and EFPIA. The full document is available at

<http://support.openphacts.org/support/solutions/articles/156157-what-is-your-security-privacy>

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## Appendix 1: Selection of usage reports



2014-08-31 - 2014-08-25

### Weekly Report (dev.openphacts.org - API)

Traffic



#### Top Users

| Name                                     | Hits   |
|--|--------|
| Newcastle University                     | 202978 |
| VU university Amsterdam, The Netherlands | 152650 |
| OpenPHACTS Explorer                      | 39333  |
| BioSolveIT/CBN                           | 34390  |
| GlaxoSmithKline                          | 24268  |

#### Users

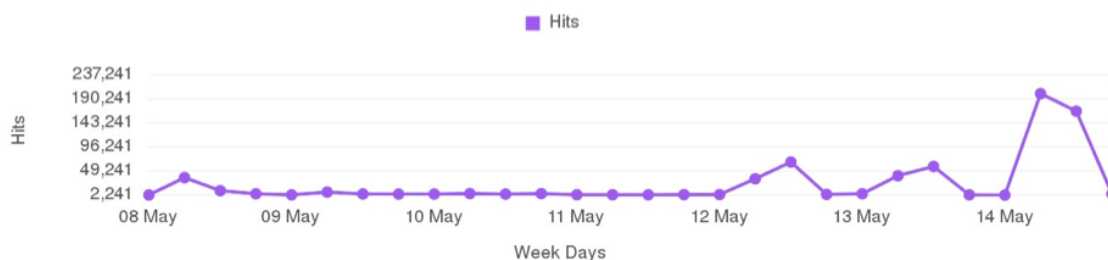
| Plan                  | Users |
|-----------------------|-------|
| Default               | 432   |
| Commercial Data Demo  | 1     |
| OpenPHACTS Developers | 0     |



2014-05-14 - 2014-05-08

### Weekly Report (dev.openphacts.org)

Traffic



#### Top Users

| Name                | Hits  |
|---------------------|-------|
| LASIGE              | 81284 |
| OpenPHACTS Explorer | 54638 |
| J&J                 | 40786 |
| GlaxoSmithKline     | 24256 |
| GSK                 | 16456 |

#### Users

| Plan                  | Users |
|-----------------------|-------|
| Default               | 368   |
| Commercial Data Demo  | 1     |
| OpenPHACTS Developers | 0     |

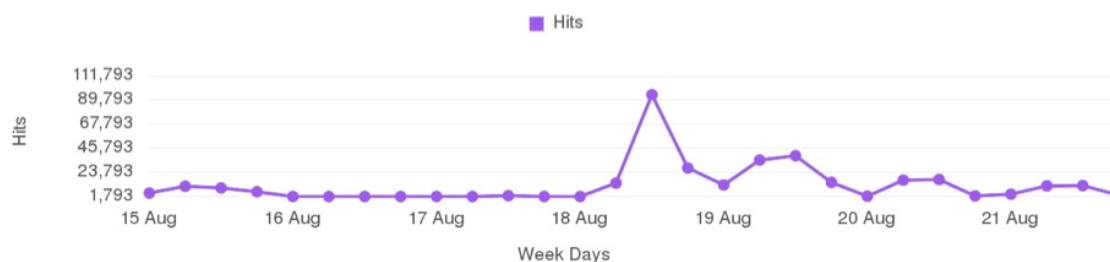
|                    |   |                                |       |
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2014-08-21 - 2014-08-15

## Weekly Report (dev.openphacts.org - API)

Traffic



### Top Users

| Name                 | Hits  |
|----------------------|-------|
| Pfizer               | 90121 |
| Entagen              | 61236 |
| OpenPHACTS Explorer  | 30808 |
| GlaxoSmithKline      | 24212 |
| Newcastle University | 24146 |

### Users

| Plan                  | Users |
|-----------------------|-------|
| Default               | 430   |
| Commercial Data Demo  | 1     |
| OpenPHACTS Developers | 0     |

|                    |   |                                |
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## Appendix 2: Git Hub for Core Developers

The screenshot shows the GitHub interface for the repository 'openphacts / GLOBAL'. The 'Issues' tab is active, displaying a list of 154 open issues and 41 closed issues. The search filter is set to 'is:open is:issue'. The issues list includes:

- #195: Review data stored on open link (IMPORTANT, OpenLink)
- #194: Reduce time chemistry results are stored on server (IMPORTANT, RSC)
- #193: pipe symbol not working for target\_type filter (IMPORTANT, bug, VU)
- #192: Explorer: Target/Compound Class Members (Explorer2, idea)
- #191: Explorer: pharmacology counts on hierarchy browser page (enhancement, Explorer2, idea)
- #190: Explorer: hierarchy browser text hidden (enhancement, Explorer2)
- #189: Explorer: red banner on hierarchy browsing? (enhancement, Explorer2)
- #188: Explorer: target class pharmacology results not loading (CRITICAL, Explorer2)

### Explorer: Structure search handling issue #186

The screenshot shows the details of issue #186, 'Explorer: Structure search handling issue #186', which is currently open. It was opened by danidi 13 days ago and has 3 comments. The issue description states:

The latest changes in the structure search make it quite complicated (or even impossible) to use a SMILES directly for a sub-structure or similarity search. If I add a SMILES in the Compound Structure window, and click on Search with SMILES, I get redirected directly to the compound information page of this compound. The Exact/sub-structure/similarity buttons seem to work only with the SMILES which was initially created by the Draw Structure window. Changing (or copy pasting) a different SMILES (e.g. "CC(CC)CCC1=CC=CC=C1") and clicking on one of the three buttons still searches for the old SMILES. Search for SMILES just tells me there is no compound, but a similarity search with the API gives results.

Comments and actions:

- ianwdunlop was assigned by danidi 13 days ago.
- danidi added Explorer2, bug labels 13 days ago.
- ianwdunlop commented 12 days ago: "There's obviously a bug of sorts here. I think we need a process flow defined of how this structure search page would be used. The page is probably trying to be too clever/do too much for its own good. You are correct that it does not use the smiles a user inputs which is plain wrong."
- ianwdunlop commented 12 days ago.

Labels: bug, Explorer2. Milestone: No milestone. Assignee: ianwdunlop. Notifications: Unsubscribe. 2 participants.