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

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

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 - OGL – OpenLink Group Ltd
29 - OPF – The Open PHACTS Foundation
30 - ALM – Laboratorios Almirall S.A.
31 - SciBite – SciBite Limited

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)
- Use of 3 scale as an API provider, providing extensive management and tracking capabilities
- 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 and the Open PHACTS API at dev.openphacts.org. Feedback from users is gathered via the support portal available at support.openphacts.org (tickets and forum) or alternatively via email to support@openphacts.org.

Related publications:

Paul Groth, Antonis Loizou, Alasdair J.G. Gray, Carole Goble, Lee Harland, Steve Pettifer, API-centric Linked Data integration: The Open PHACTS Discovery Platform case study, Web Semantics: Science, Services and Agents on the World Wide Web, Available online 8 April 2014, ISSN 1570-8268
http://dx.doi.org/10.1016/j.websem.2014.03.003.

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.

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). As outlined in D 3.2.6 (A full technical sustainability plan delivered and signed off by TTF and EC to continue Open PHACTS beyond the duration of the Open PHACTS project and consortium), the Open PHACTS Foundation has successfully signed a contract with UNIMAN to provide technical resource for maintaining the platform. This represents a major step forward in the long term stability of the system.

4 Secure access implemented

The Open PHACTS API is accessible via dev.openphacts.org, which is secured with an SSL certificate. The system is now fully secured and private in accordance with a detailed specification worked out between the Open PHACTS team, Open Link and EFPIA. The full document is available at http://www.openphactsfoundation.org/security.

Appendix 1: Selection of usage reports

2014-08-31 - 2014-08-25

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

Top Users: University (202978 hits), University (152650), Explorer (39333), SME (34390), Pharma (24268)

2014-05-14 - 2014-05-08

Weekly Report (dev.openphacts.org)
Traffic

Top Users: University (81284 hits), Explorer (54638), Pharma (40786), Pharma (24256), Pharma (16456)

2014-08-21 - 2014-08-15

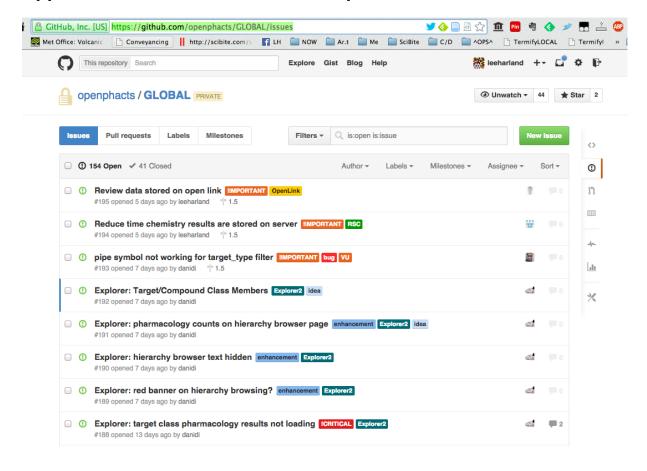**Weekly Report** (dev.openphacts.org - API)
Traffic

Top Users: Pharma (90121 hits), Commercial Organisation (61236), Explorer (30808), Pharma (24212), University (24146)

Appendix 2: Git Hub for Core Developers

Explorer: Structure search handling issue #186

Edit   New issue

ⓘ Open   **danidi** opened this issue 13 days ago · 3 comments

danidi commented 13 days ago

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.

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
You're receiving notifications because you're subscribed to this repository.

2 participants

🔒 Lock issue