

Dear Colleague

Welcome to the Open PHACTS Newsletter. The 4th Open PHACTS Community Workshop was held in London last week, and featured the public release of the Open PHACTS API.

This newsletter contains information about the Community Workshop and other recent project information.

Using the Power of Open PHACTS: Community Workshop, 22-23 April 2013, London

The 4th Open PHACTS Community Workshop focussed on the possibilities of Open PHACTS and the Open PHACTS API, emphasising Open PHACTS as a data service provider that can be integrated with and aid the development of third party applications. Many thanks to all workshop attendees!

For those of you who did not attend, the workshop summary and presentations can be found here.

Public Release of the API

The <u>Open PHACTS API</u> was publicly released at the Community Workshop in London. The Open PHACTS API allows third party applications to use the data present within the Open PHACTS Discovery Platform, and for organisations to integrate internal and external data.

Open PHACTS Explorer

The <u>Open PHACTS Explorer is now online</u>, providing an intuitive interface to query the data present within the Open PHACTS Discovery Platform. Tutorials for using the Open PHACTS Explorer are <u>available</u>. All feedback is valued and will help us build a better product!

Public Release of ChemBioNavigator and PharmaTrek

The first Open PHACTS example apps, <u>ChemBioNavigator</u> and <u>PharmaTrek</u>, were publicly released at the 4th Community Workshop. <u>ChemBioNavigator</u> allows the user to visualise the chemical and biological space of a molecule group in a chemically-aware manner.

<u>PharmaTrek</u> navigates pharmacological space in a flexible and interactive way, by accessing the content of ChEMBL via the Open PHACTS Discovery Platform.

Recent Presentations and Publications

- "On the Formulation of Performant SPARQL Queries" by Antonis Loizou and Paul Groth.
- Gerhard Ecker gave a talk at the Joint ASTOX-ÖPhG-ASAC-ÖGGM-CCC Scientific Symposium in Vienna entitled "Integrated systems for predicting toxicity and drugdrug interactions".
- CSHALS 2013 Conference on Semantics in Healthcare and Life Science in Boston: Alasdair Gray held a tech talk on Open PHACTS.
- Claus Stie Kallesøe gave a talk at Open Source Days 2013, Copenhagen "Open Source in the Pharma and Biotech Industries".
- "Partnerships and Open Innovation in Drug Discovery" by Gerhard Ecker at Informa LifeScience's Annual Drug Discovery Innovations 2013
- 2nd QNano Integrating Conference 2013 in Prague, Egon Willighagen presented a poster.
- SMI conference: Advances and Progress in Drug Design in London, Andrew Leach gave a talk entitled "Open PHACTS: data integration for all".
- Open PHACTS was well represented at the ACS National Meeting & Exposition in New Orleans with various posters and presentations. "Open PHACTS: Meaningful linking of preclinical drug discovery knowledge"; "Architecture for an open science molecular compound database" (Egon Willighagen); "About the impact of open access bioassay data on cheminformatic approaches" and "RSC chemical validation and standardization platform: A potential path to quality-conscious databases" (Ken Karapetyan).

Open PHACTS code now on GitHub

The Open PHACTS code repository is now available as an open source community project on GitHub. The central GUI API, GUI components code, API configuration files, Open PHACTS Explorer code and more can be found on the <u>GitHub Open PHACTS page</u>.

Accelrys Hackathon & Community Website

The Open PHACTS – Accelrys Hackathon was held in Cambridge on February 20th. Pipeline Pilot components and workflows were developed to query the Open PHACTS API, answering various key scientific competency questions proposed by Open PHACTS EFPIA members. The Hackathon results and on-going Open PHACTS API discussions can be found on the <u>Accelrys Community Open PHACTS group website</u>.

Recent Associated Partners

This year we are pleased to welcome Accelrys, Bio2RDF, DIQA, Inte:ligand, Linked Data Benchmark Council, The OpenBEL Project, Oxford e-Research Centre, Phortos Consultants, Prestwick, The Scripps Research Institute, Syngenta and TW2Informatics as Open PHACTS Associated Partners.







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