



Open PHACTS | News

Welcome to the 3rd Open PHACTS Newsletter.

This newsletter contains information about the new [Workflow Integration Portal](#), our open access Drug Discovery Today [paper](#) and other recent project information.

Open PHACTS project extended for 6 months

We are pleased to announce that the Open PHACTS project will be extended for 6 months until the end of August 2014. The newly established Open PHACTS Foundation will now 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.

Open PHACTS workflow integration portal now available

[Pipeline Pilot components/workflows](#) and [KNIME nodes/workflows](#) have been developed to integrate with the Open PHACTS API. The portal to these workflow integration collections can be found at dev.openphacts.org/workflow. Many thanks to Accelrys for supporting the development of the Pipeline Pilot components.

Invitation to Open PHACTS training event

We invite you to the 1st Open PHACTS training event, 19-20 September 2013 in Vienna. This event is in collaboration with the [Vienna Summer School for Drug Design](#). The Open PHACTS training event is free of charge, but you will need to bring your own laptop.

If you are interested in participating please register with [Katharina Kramler](#).

Using the Open PHACTS API - Webinar video

Interested in learning about the [Open PHACTS API](#)? Watch Paul Groth's webinar to get to know about the data and technical setup, and to learn what can be done using the API. Watch the webinar [here](#).

Helium for Excel Community Edition uses Open PHACTS API

The June release of the [Helium for Excel Community Edition](#) from [Ceiba Solutions](#) contains three functions that use the Open PHACTS API. This short [video](#) shows what these functions do.

AQnowledge Bookmarklet links to Open PHACTS Explorer

The browser-based [Bookmarklet](#) developed by [AQnowledge](#) identifies significant entities in scientific text, and provides links to further information such as the corresponding entry in the Open PHACTS Explorer.

Open PHACTS Explorer updates

Updates to the [Open PHACTS Explorer](#) have been implemented. See the [release notes](#) and let us know what you think.

Recent Publications

- "[Scientific competency questions as the basis for semantically enriched open pharmacological space development](#)" published in Drug Discovery Today (open access)
- "[On the Formulation of Performant SPARQL Queries](#)" by Antonis Loizou and Paul Groth (open access).

Recent Presentations

- Christian Brenninkmeijer and Chris Evelo presented on Scientific Lenses and the [Open PHACTS API](#) at the ISMB/ECCB 2013 Conference in Berlin, July 21-23.
- Andra Waagmeester presented a poster "Visualizing Linked Open Data in Biological Pathways and Networks" at the ISMB/ECCB 2013 SIGs & Tutorials Meeting in Berlin, July 19-20.
- Gerhard Ecker presented [The Open Pharmacological Concepts Triple Store](#) at the Translational Knowledge Management in Pharmaceutical R&D Meeting in Brussels, July 11-12.
- Marcus Gastreich represented Open PHACTS at RICT 2013 - Drug Discovery and Selection in Nice, France, July 3-5.
- Lee Harland presented "[Mashing Up Drug Discovery: There's an API for that](#)" at the RSC CICAG New Developments in Chemical Information: Best Practice meeting in London, July 3.
- Gerhard Ecker gave a talk entitled "Integrated approaches - from docking poses to prediction of side effects" at the 18th Joint Meeting on Medicinal Chemistry 2013 in Lublin, Poland, July 1-2.
- Ronald Siebes from VU Amsterdam gave a talk entitled "[Easy Access to Pharmacology Data: The Open PHACTS KNIME Nodes](#)" at the KNIME User Day UK in London, 25 June.
- Open PHACTS exhibited at FMC 2013 - Frontiers in Medicinal Chemistry in San Francisco, June 23-26.
- Bryn Williams-Jones presented "[Open PHACTS: a precompetitive infrastructure for pharmacological research](#)" at the Infotech conference "Using R&D IT to extract maximum value from increasing data volumes to accelerate scientific decision making" in London, June 19-20.
- Andrew Leach gave a talk entitled "[Open PHACTS - Data integration for all](#)" at the 14th Annual Drug Discovery Summit in Geneva, Switzerland, June 10-11.
- Paul Groth presented the Open PHACTS project in 10th ESWC 2013 in Montpellier, France, May 26-30.
- Christian Herhaus presented "[Addressing Research Questions by Integration of Open PHACTS with Pipeline Pilot](#)" at Accelrys Solutions for Enhancing Research Innovations: An Interactive Seminar in Mainz, Germany, May 14.

Recent Mentions of Open PHACTS

- The ChEMBL-og featured a [blogpost](#) on the Open PHACTS workflow integration portal
- "[Metabolomics and systems pharmacology: why and how to model the human metabolic network for drug discovery](#)" published in Drug Discovery Today
- "[Semantic Medical Prescriptions – Towards Intelligent and Interoperable Medical Prescriptions](#)" at the Seventh IEEE International Conference on Semantic Computing ICSC 2013 (open access)
- "[Message-Passing Interface for Java Applications: Practical Aspects of Leveraging High Performance Computing to Speed and Scale Up the Semantic Web](#)" published in International Journal on Advances in Software (open access)
- "[Improving data and knowledge management to better integrate health care and research](#)" published in Journal of Internal Medicine (open access)
- "[Querying over Federated SPARQL Endpoints - A State of the Art Survey](#)" Digital Enterprise Research Institute (DERI) Technical Report 2013-06-07 (open access)
- "[Ovopub: Modular data publication with minimal provenance](#)" (open access)
- "[Chemical information matters: an e-Research perspective on information and data sharing in the chemical sciences](#)" published in Chemical Society Reviews
- "[Micropublications: a Semantic Model for Claims, Evidence, Arguments and Annotations in Biomedical Communications](#)" submitted to Journal of Biomedical Semantics (open access)
- "[The ChEMBL database as linked open data](#)" published in Journal of Cheminformatics (open access)
- "[PAV ontology: Provenance, Authoring and Versioning](#)" submitted to Journal of Biomedical Semantics (open access)
- "[Applicability of the Nano-publication Concept for Fostering Open Access in Developing and Transition Countries](#)" Proceedings of the 5th Belgrade International Open Access Conference 2012 (open access)
- "[Towards the Collaborative Curation of the Registry underlying identifiers.org](#)" published in Database (open access)
- "[New Approaches in Data Integration for Systems Chemical Biology](#)" published in Current Topics in Medicinal Chemistry
- "[Drug and Disease Model Resources: A Consortium to Create Standards and Tools to Enhance Model-Based Drug Development](#)" published in CPT: Pharmacometrics & Systems Pharmacology (open access)
- "[Cheminformatics and the Semantic Web: adding value with linked data and enhanced provenance](#)" published in Computational Molecular Science
- "[Shifting from the single to the multitarget paradigm in drug discovery](#)" published in Drug Discovery Today (open access)

Recent Associate Partners

We are pleased to welcome Ceiba Solutions, CRS4, DIQA, eTox, the Integrative Bioinformatics Group from Newcastle University, LEO Pharma and Metaome Science Informatics as [Open PHACTS Associated Partners](#).



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