

Open PHACTS

Deliverable 8.3.4

Run OPS Workshop 4 “Using the Power of Open PHACTS”

Prepared by RSC

Approved by RSC, UNIVIE, CD, Pfizer, LUMC, GSK

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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: 3 years

Nature of the Deliverable	
Report	x
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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

OGI – 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 Introduction

The fourth Open PHACTS Community Workshop was held at Burlington House in London on April 22 and 23, 2013. The Workshop focussed on “Using the Power of Open PHACTS” and featured the public release of the Open PHACTS application programming interface (API) and the first Open PHACTS example apps, ChemBioNavigator and PharmaTrek.

2 Summary of Workshop

The first day featured talks describing the data accessible via the Open PHACTS Discovery Platform and technical aspects of the API. The use of the API by example applications ChemBioNavigator and PharmaTrek was outlined, and the results of the Accelrys Pipeline Pilot Hackathon discussed. The second day involved discussion of Open PHACTS sustainability and plans for the successor organisation, the Open PHACTS Foundation. The afternoon was attended by those keen to further discuss the potential of the Open PHACTS API and the future of Open PHACTS. A publicly available workshop summary is [online](#).

During talks, especially those detailing the Open PHACTS API, a steady stream of signup requests to the API via dev.openphacts.org were received. The hashtag #opslaunch was used to follow reactions to the workshop on Twitter (www.storify.com/Open_PHACTS/open-phacts-api-launch), and showed the response amongst attendees to be overwhelmingly positive.

3 Presentations

Monday 22nd April 2013

Introduction to Open PHACTS ([slides](#))

Lee Harland, Connected Discovery

An introduction to the Open PHACTS Discovery Platform and project.

The Data Available ([slides](#))

Christine Chichester, Swiss Institute of Bioinformatics

Outline of the datasets integrated within Open PHACTS and the platform's concept-based nature.

How does Open PHACTS Work? ([slides](#))

Paul Groth, VU University Amsterdam

Architecture of Open PHACTS and the technical benefits this allows.

Discovery Platform, API Walkthrough ([slides](#))

Paul Groth, VU University Amsterdam

API key walkthrough, outline of a typical application workflow.

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Open PHACTS API Use Example: ChemBioNavigator ([slides](#))

Tim Harder, University of Hamburg and Marcus Gastreich, BioSolveIT

Public release of the example app ChemBioNavigator (www.chembionavigator.org) and outline of its API use.

Open PHACTS API Use Example: PharmaTrek

Jordi Mestres, Consorci Mar Parc de Salut de Barcelona (PSMAR)

Public release of PharmaTrek (www.pharmatrek.org) and discussion of its use of the Open PHACTS API.

Open PHACTS API Use Example: Accelrys Hackathon ([slides](#))

Stefan Senger, GlaxoSmithKline

Illustration of how Pipeline Pilot uses the Open PHACTS API. Presentation of components and workflows created at the Accelrys Hackathon in February.

Tuesday 23rd April 2013

The Open PHACTS Vision: An Open PHACTS Ecosystem ([slides](#))

Lee Harland, Connected Discovery

The aims of Open PHACTS and the unique service it provides.

Open PHACTS Business and Sustainability ([slides](#))

Richard Kidd, Royal Society of Chemistry

Outline of the planned Open PHACTS sustainability model and the successor organisation, the Open PHACTS Foundation.

Open PHACTS: An Academic Researcher's Perspective ([slides](#))

Gerhard Ecker, University of Vienna

Illustration of an academic research group's use of the Open PHACTS API to answer pertinent questions.

Open PHACTS: An Industrial Researcher's Perspective ([slides](#))

Stefan Senger, GlaxoSmithKline

Description of Open PHACTS in an industrial researcher's toolkit.

Breakouts with application builders and developers

4 Attendees

A wide range of organisations were represented at the Community Workshop. Publishers such as Elsevier, Thomson Reuters and Nature Publishing Group were joined by software providers Accelrys, ChemAxon, Dotmatics and IBM. European technology startups Digital Science and Ontoforce were to be found seated alongside attendees from North America from The National Institutes of Health and Carleton University. The variety of organisations

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represented during the two days highlights the far-reaching appeal of the Open PHACTS Discovery Platform.

Affiliation	Name
Digital Science	José Airosa
General Bioinformatics	Nadia Anwar
IBM	Aleksandra Bielen
Innovative Medicines Initiative (IMI)	Colm Caroll
IMAQA	Omer Casher
Numedicus	David Cavalla
GlaxoSmithKline (GSK)	Chris Chau
Swiss Institute of Bioinformatics (SIB)	Christine Chichester
Nature Publishing Group	Laura Croft
European Bioinformatics Institute (EBI)	Samuel Croset
University of Santiago de Compostela (USC)	Emiliano Cuadrado
University College London (UCL)	Bernard de Bono
ChemAxon	Tim Dudgeon
Bio2RDF / Carleton University	Michel Dumontier
University of Vienna	Gerhard Ecker
Maastricht University	Chris Evelo
Syngenta	Mark Forster
BioSolveIT	Marcus Gastreich
Dotmatics	John Gatenby
University of Vienna	Franz Gatterer
Spanish National Cancer Research Center (CNIO)	Francesco Gervasio
Royal Society of Chemistry (RSC)	Jack Gibb
University of Manchester	Alasdair Gray
VU University Amsterdam	Paul Groth
Nature Publishing Group	Tony Hammond
University of Hamburg	Tim Harder
Connected Discovery	Lee Harland
Ian Harrow Consulting Ltd.	Ian Harrow
F. Hoffmann-La Roche	Jérôme Hert
Digital Science	Andrew Hinton
Janssen Pharmaceutica	Edgar Jacoby
Leiden University Medical Center (LUMC)	Mascha Jansen
Royal Society of Chemistry (RSC)	Richard Kidd
Lhasa Limited	Monika Kister
University of Vienna	Katharina Kramler
Optibrium	Chris Leeding
NextMove Software	Daniel Lowe
The Hyve	Pieter Lukasse
Accelrys	Noj Malcolm

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Lhasa Limited	Carol Marchant
MAR Health Park (PSMAR)	Jordi Mestres
Thomson Reuters	Tim Miller
MAR Health Park (PSMAR)	Eva Molero
Metaome Science Informatics	Ramkumar Nandakumar
Janssen Pharmaceutica	Jean-Marc Neefs
Dotmatics	Dan Ormsby
European Bioinformatics Institute (EBI)	George Papadatos
Nature Publishing Group	Michele Pasin
MAR Health Park (PSMAR)	Manuel Pastor
GlaxoSmithKline (GSK)	Stephen Pickett
National Institutes of Health (NIH)	Ajay Pillai
AstraZeneca	Andrew Poirrette
MAR Health Park (PSMAR)	Núria Queralt
AQnowledge	Rishi Ramgolam
University of Santiago de Compostela (USC)	Joseline Ratnam
University of Zürich	Dietrich Rebholz-Schuhmann
IBM	Jeremy Rice
University of Vienna	Lars Richter
University of Vienna	Anika Robl
University of Oxford	Philippe Rocca-Serra
Ontoforce	Stephane Roelandt
F. Hoffmann-La Roche	Lisa Sach-Peltason
NextMove Software	Roger Sayle
Elsevier	Tony Scerri
Hedgehog Research	Eric Schultes
Syngenta	Derek Scuffell
GlaxoSmithKline (GSK)	Stefan Senger
Pistoia Alliance	John Sgouros
Selventa	Ted Slater
Eagle Genomics	William Spooner
KU Leuven	Hilde Stevens
Elsevier	Mike Taylor
Ontoforce	Peter Vandenabeele
AQnowledge	Jan Velterop
Thomson Reuters	Philip Verdemato
Ontoforce	Nicola Vitucci
Maastricht University	Andra Waagmeester
Connected Discovery	Bryn Williams-Jones
GlaxoSmithKline (GSK)	Peter Woollard
University of Bonn	Zhao Xu

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Picture 1. Participants of 4th Open PHACTS Community Workshop.

5 Outcome

The Community Workshop was well attended and the overall response was very positive regarding progress made by the Open PHACTS project. The significant number of signups for API keys during and after the workshop was indicative of the enthusiasm amongst attendees for the Open PHACTS API – helped especially by Paul Groth’s API walkthrough. An attendee from Dotmatics, Dan Ormsby, incorporated use of the Open PHACTS API into an existing app during the API talk, showing the API to be easily accessed and intuitive to use. Breakout discussions in the afternoon of the second day highlighted the eagerness of many community members to start using the API or to become further involved with the Open PHACTS Discovery Platform.