Open PHACTS

Deliverables

D 6.19 Organisation of prototype user group meeting

D 8.3.6 Run Open PHACTS Workshop 6 "Open PHACTS for Academia"

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

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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: 42 months

Nature of the Deliverable	
Report	x
Prototype	
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:

  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
  Lilly – Eli Lilly
  NBIC – Stichting Netherlands Bioinformatics Centre
  SIB – Swiss Institute of Bioinformatics
  ConnDisc – Connected Discovery
  EBI – European Bioinformatics Institute
  Janssen – Janssen Pharmaceutica
  OGL – 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.

1   Introduction

The sixth Open PHACTS Community Workshop was held at Burlington House, Piccadilly, London on 26th June 2014. The Workshop focussed on introducing members of the academic community to the Open PHACTS Discovery Platform, and encouraging use of it within their research and teaching workflows.

2   Summary of Workshop

The morning session featured an introduction to the Open PHACTS Discovery Platform and app ecosystem, and presentations on applications that query the Open PHACTS API (ChemBioNavigator and PharmaTrek) followed by academic use cases from the Universities of Vienna and Maastricht.

The afternoon session involved interactive discussions and workshops on technical aspects of using workflow tools and code to query the Open PHACTS API. These hands-on sessions were thoroughly enjoyed by participants, many of whom suggested them to be the most engaging way to learn how to use the Open PHACTS API.

3   Presentations

Session I

The Open PHACTS Discovery Platform
Bryn Williams-Jones, Connected Discovery
An introduction to the Open PHACTS Discovery Platform and project.

The Open PHACTS Application Ecosystem
Lee Harland, Connected Discovery
Outline of the applications that make up the Open PHACTS app ecosystem.

Apps: ChemBioNavigator
Katrin Stierand, University of Hamburg
Overview of the ChemBioNavigator: an app which queries the Open PHACTS API and allows visualisation of the chemical and biological space of a molecule group in a chemically-aware manner.

Apps: PharmaTrek
Jordi Mestres, IMIM
Overview of PharmaTrek: an app which queries the Open PHACTS API and allows the navigation of pharmacological space in a flexible and interactive way.

Academic use case: ErbB signaling
Daniela Digles, University of Vienna
Using Open PHACTS KNIME workflows to investigate the epidermal growth factor receptor (ErbB) signaling pathway, which is associated with cancer and neurodegenerative diseases.

Academic use case: Programming in the Life Sciences
Egon Willighagen, Maastricht University
Highlighting the use of the Open PHACTS API for teaching at Maastricht University.

<u>**Session II**</u>

How to use the Open PHACTS API
Christine Chichester, SIB
An introduction to the Open PHACTS API.

Connecting to the Open PHACTS API via Python / Pipeline Pilot
Robert Campbell, GSK
Querying the Open PHACTS API using Python / Pipeline Pilot.

Developing your own app
Ian Dunlop, University of Manchester
Integrating an application with the Open PHACTS API.

Using the Open PHACTS API with KNIME
Daniela Digles, University of Vienna
Using KNIME, an open source analytics platform, to build workflows without the need of programming knowledge.

Open PHACTS and MOE, Google Spreadsheet
Lars Richter, University of Vienna
Implementation of the Open PHACTS API within MOE (Molecular Operating Environment).

4   Attendees

First Name	Last Name	Affiliation
Sune	Askjær	LEO Pharma
Michael	Barnes	Queen Mary University of London
Ian	Bruno	CCDC
Robert	Campbell	GSK
Christine	Chichester	SIB
Sandesh	Chopade	Indian Institute of Technology Kanpur
William	Collier	University of Warwick
Bernard	de Bono	University College London
Ulrik	de Lichtenberg	LEO Pharma
Hans	De Winter	University of Antwerp
Daniela	Digles	University of Vienna
Ian	Dunlop	University of Manchester
Gerhard	Ecker	University of Vienna
Jack	Gibb	Royal Society of Chemistry
Phillip	Gould	University of Warwick
Lee	Harland	Connected Discovery
Douglas	Kell	University of Manchester

Richard	Kidd	Royal Society of Chemistry
Richard	Lewis	University of Cambridge
Caroline	Low	Imperial College London
Andrew	Marsh	University of Warwick
Jordi	Mestres	IMIM
Danielle	Newby	Universities of Kent/Greenwich
Sally	Oxenford	University College London
John	Pinney	Imperial College London
Lars	Richter	University of Vienna
Lars	Sandberg	University of Dundee
Matthew	Seddon	University of Sheffield
Stefan	Senger	GSK
Maxim	Sharifi	University of Kent
Katrin	Stierand	University of Hamburg
Chris	Swain	Cambridge MedChem Consulting
Andreas	Tielmann	Merck
Ben	Wahab	University of Sussex
Bryn	Williams-Jones	Connected Discovery
Egon	Willighagen	Maastricht University
Matthew	Wright	LHASA

5   Feedback

"*It was an excellent and most useful day!*"

"*The afternoon session with Daniela was particularly useful as were the case study sessions (I especially liked the teaching one – maybe this is something we can use here at some point).*"

"*Definitely feel that this is the way forward for semantic and systems pharmacology*"

6   Outcome

The 6th Community Workshop was well attended and the overall response was highly positive. Interactive sessions in the afternoon highlighted the eagerness of many academic community members to query the API and learning how to integrate it into their teaching or research workflows.