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

June 2014
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

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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
  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
<table>
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<tr>
<th>Open PHACTS</th>
<th>Deliverables: Organisation of prototype user group meeting + Run Open PHACTS Workshop 6</th>
<th>Deliverable: 6.19 + 8.3.6</th>
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<tr>
<td>IMI - 115191</td>
<td>Author: Jack Gibb (RSC)</td>
<td>Version: 1.0</td>
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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.

**Session II**
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

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<tr>
<th>First Name</th>
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<tbody>
<tr>
<td>Sune</td>
<td>Askjær</td>
<td>LEO Pharma</td>
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<tr>
<td>Michael</td>
<td>Barnes</td>
<td>Queen Mary University of London</td>
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<tr>
<td>Ian</td>
<td>Bruno</td>
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<td>Robert</td>
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<td>Sandesh</td>
<td>Chopade</td>
<td>Indian Institute of Technology Kanpur</td>
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<tr>
<td>William</td>
<td>Collier</td>
<td>University of Warwick</td>
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<tr>
<td>Bernard</td>
<td>de Bono</td>
<td>University College London</td>
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<tr>
<td>Ulrik</td>
<td>de Lichtenberg</td>
<td>LEO Pharma</td>
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<tr>
<td>Hans</td>
<td>De Winter</td>
<td>University of Antwerp</td>
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<tr>
<td>Daniela</td>
<td>Digles</td>
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<td>Ian</td>
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<tr>
<td>Gerhard</td>
<td>Ecker</td>
<td>University of Vienna</td>
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<tr>
<td>Jack</td>
<td>Gibb</td>
<td>Royal Society of Chemistry</td>
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<td>Phillip</td>
<td>Gould</td>
<td>University of Warwick</td>
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<tr>
<td>Lee</td>
<td>Harland</td>
<td>Connected Discovery</td>
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<tr>
<td>Douglas</td>
<td>Kell</td>
<td>University of Manchester</td>
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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.