Open PHACTS

Deliverable 5.2.4

Second prototype of CBN including substructure and pattern search, API to OPS data layer and access to most OPS data sources, release to public

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Nature of the Deliverable	
Report	
Prototype	x
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
  E.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 ChemBioNavigator (CBN) is an exemplar application (eApp) in the context of the Open PHACTS project. A first prototype of the CBN was released to the consortium members in early 2012 and very valuable feedback was collected in the following weeks.

This deliverable marks the release of the second CBN prototype to the consortium members (see 3 Availability for login details). Major advancements include:

- Structural similarity and substructure pattern search
- Connects to the OPS-platform through the new OPS linked data API
- Ruby Gem (software package) realizing the OPS connection released
- User interface matured and is ready for mobile devices
- Introduction of pharmacology data
- Direct link out to other eApps and the OPS Explorer

Since the release of the first prototype, significant progress was made: The user interface matured further and now allows intuitive browsing of compounds on mobile devices. The CBN was connected to the new OPS linked data API, allowing to retrieve additional meta information such as the provenance information alongside the actual data. This connection was realized by developing a Ruby Gem which has since been released as open source software under the MIT license. The Gem represents a data abstraction layer allowing to quickly implement new API methods. Using this free package, developers new to the OPS platform can quickly set up a connection to the OPS data API. Additionally, we introduced the possibility to perform structural similarity as well as substructure searches for small molecules against the OPS compound database.

Further progress was made on the inter eApp collaboration where a common format for deep links in between applications was implemented allowing one-click transfers of datasets from one eApp to another. Please note that those links may be disabled in the application until all eApps are publicly released. In addition, the close collaboration with the OPS explorer developers resulted in sharing of code such as small widgets that could be reused with only small modifications necessary.

We presented the CBN in the form of a scientific publication (Stierand et.al., Mol. Inf. 2012, 31, 543-546). Further, we presented the CBN at both the EuroQSAR Meeting in Vienna (August 2012) as well as the EFMC Meeting in Berlin (September 2012).

2   Delayed Release

The release of the CBN had originally been planned for September 2012 but was postponed until the OPS platform was publicly released. Delays in finding a proper hosting provider for the OPS platform service had delayed its release until recently. Thus, during their meeting in

Vienna, August 2012, the project steering committee decided to push back the release of the eApps accordingly.

This deliverable marks an internal release to the consortium members. The public release of the CBN is planned for the Open PHACTS Community Workshop (London, April 22nd – 23rd). This staged release plan was agreed on with the project release manager.

3   Availability

The current release is available for internal dissemination and evaluation under the URL mentioned below. Since this is a project-internal release, the website is password protected.

Link: http://cbn.zbh.uni-hamburg.de
Username: cbn
Password: cbn4ops

4   Feedback and Testing

Feedback can be given directly from the CBN website using the *Give Feedback* button in the top navigation bar or by emailing to cbn@zbn.uni-hamburg.de. After the presentation of the first prototype to the consortium members in early 2012, we received around 100 comments that way.

One of the main goals of this internal release is to gather feedback from the consortium members. This will help both preparing the CBN for the public release in April as well as guiding the future development for the remainder of the project. Additionally, a series of more systematic tests is in planning with the OPS Test Group at the University of Vienna.