Open PHACTS

Deliverable 5.2.5

CBN major release with refined, full functionality and improved usability, production level testing and documentation

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Definitions

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2 - UNIVIE – Universität Wien – **Managing Entity of IMI JU funding**
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5 - BIT – BioSolveIT GmbH
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24 - SIB – Swiss Institute of Bioinformatics
25 - CD – ConnectedDiscovery
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27 - Janssen – Janssen Pharmaceutica NV
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29 - OPF – The Open PHACTS Foundation
30 - ALM – Laboratorios Almirall S.A.
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1 Introduction

The ChemBioNavigator (CBN) is an exemplar application (eApp) in the context of the Open PHACTS project.

A second prototype of the CBN was released to the consortium members in August 2013 (Deliverable 5.2.4). The major achievements of this release have been structural similarity and substructure pattern search, connection to the Open PHACTS Discovery Platform through the Open PHACTS linked data API, release of a Ruby Gem realizing the Open PHACTS connection, a user interface that is ready for mobile devices, introduction of compound pharmacology data, and direct link out to ChemSpider and the Open PHACTS Explorer.

This deliverable marks the public release of the CBN (www.chembionavigator.org) with refined, full functionality and improved usability, production level testing and documentation.

Since the last deliverable we presented the CBN externally at

- the MedChemRussia Conference, Moscow, Russia (September 2013)
- the European Summerschool at the University of Vienna (September 2013)
- the German Conference on Cheminformatics, Fulda, Germany (November 2013)
- the 247th ACS National Meeting & Exposition, Dallas, Texas, USA (March 2014)
- 6th Open PHACTS Community Workshop in London, GB (June 2014)

2 Functionality and improved usability

While the former development had its focus on the physico-chemical data, for this release biological information about the compounds was incorporated into the CBN.
This includes:

- Import of targets connected by pharmacology data with a selected compound from the Open PHACTS Discovery Platform
- Display of information about targets, which are related to compounds by available activity data
- Retrieving new compounds from the Open PHACTS Discovery Platform, if they are active against the selected target

In analogy to the Compound Panel on the left hand side of the CBN, a Target Panel was introduced on the right hand side. This Target Panel provides data in three tabs Overview, Details and Compounds, to be in perfect symmetry with the Compound Panel on the opposite side. The overview of the available information from the Open PHACTS Discovery Platform about a selected target is shown (if available) together with a picture of the target (the structure as ribbons) as well as linkouts to the databases IntAct and PDB. The Details tab provides, as expected, the provenance of the individual data points. The Compounds tab informs the user about the volume of available activity data and facilitates the download of active compounds for the selected target.

The CBN uses the connection of compounds and targets via pharmacology data in the form of activity values originating from different biological assays. This finally facilitates one of the major goals of the ChemBioNavigator, namely the navigation from compounds to related targets and back to new compound sets.
Together with this new functionality the backend Open PHACTS interface of the CBN was re-factored and amended to work well with the last recent API version. The variety of API calls was extended, such that it now ranges from compound related requests over chemical structure and concept related requests to target related requests. This covers a large part of the Open PHACTS API (Version 1.4) and the CBN shows exemplarily how the different requests can be used in a complementary way.
In addition to the previous compound centric start options, the CBN now also supports sessions starting from a target name search against the Open PHACTS Discovery Platform and the subsequent retrieval of compounds that are active against the given target. This is realized via an integrated concept wiki lookup form that can be used for compound as well as target searches and preserves the simplistic google like look and feel of the ChemBioNavigator starting page.
The current release of the CBN uses the Open PHACTS API version 1.4 via the regularly updated Ruby Gem, which realizes the connection to the Open PHACTS Discovery Platform.
Improvements of the usability are amongst others:

- The distinction between active and inactive assay measurement values for target and compound pharmacology data
- An improved drawing engine for the central drawing area (e.g. animation of dots in the cloud view)
- Highlighting of the selected compound that is currently shown in the compound details panel in the cloud
- Maintenance of tablet compatibility
- Incorporation of a new, more effective browser check

3 Production level testing

Due to the release of the CBN to the consortium in August 2013 and the presentation of it at different meetings and conferences (cf. section 1, above), we were able to gather valuable user feedback.
A sophisticated browser check verifies that the user is accessing the CBN with a modern web browser and a minimum screen resolution to ensure good user experience. If the browser check fails, the user is forwarded to an information page with a listing of compatible web browsers and versions.
The major CBN use cases have been stress tested with a particular focus on the Open PHACTS Discovery Platform connection. This revealed bottlenecks and incorrect response codes that were reported and successfully addressed by the Open PHACTS Discovery Platform tech team.

4 Documentation

For end-users we provide help via tutorial videos as well as an FAQ page, which covers a range of possible workflows. We deliberately abstained from static documentation, as this tends to be ignored by the users, notoriously outdated and/or quite cumbersome to maintain.
The stress-tests of the CBN-platform connection have been documented in the form of a Github issue. Furthermore, we compiled a technical install guide which details the steps that are necessary to set up a CBN server instance.