

Drug Discovery Workflow Workshop: Using Open PHACTS

May 19-20, 2015

VU University, Amsterdam

Background

The Open PHACTS Project

The Open Pharmacological Concepts Triple Store (Open PHACTS) began as an Innovative Medicines Initiative (IMI) project to address the growing need for access to integrated, interoperable pharmacological data to aid in the drug discovery process. The project's aim was to design and build an open pharmacological information system, bringing together multiple public and pre-competitive data resources into one freely accessible, fully integrated platform.

To guide the development of this platform, Open PHACTS focussed on a series of concrete use cases: questions that real researchers frequently ask when working with data concerning compounds, targets, pathways and diseases. The Open PHACTS Discovery Platform was successfully built to answer many of those questions, and to integrate with real workflows and workflow tools.

A web-based user interface called the Open PHACTS Explorer allows anyone to browse and query the datasets brought together by Open PHACTS. However Open PHACTS also offers free access to an API so that researchers may query the data directly, or incorporate Open PHACTS data into their workflows using tools like KNIME and Pipeline Pilot.

For further background information on the Open PHACTS project, please see the attached publications about the project's outcomes:

- Scientific competency questions as the basis for semantically enriched open pharmacological space development (Azzaoui et al., 2013)
- Drug discovery FAQs: workflows for answering multidomain drug discovery questions (Chichester et al., 2014)

The focus of this workshop will be on using the Open PHACTS [KNIME nodes](#) and [Pipeline Pilot components](#) to interact with the Open PHACTS API, with a particular focus on addressing use cases and research questions similar to the ones described in these publications. Attendees are encouraged to bring along examples of questions that come up in their own research, to discuss and work on at the workshop.

Agenda

Tuesday, 19 May

13:00-13:15 **Welcome**

Antonis Loizou

13:15-14:00 **Overview of the Open PHACTS API: Inputs and Outputs**

Presenter: Christine Chichester

14:00-14:30 **Characteristics of Pipeline Pilot Components**

Presenter: Andrei Caracoti

14:30-15:00 **Examples of Pipeline Pilot Workflows**

Presenter: Jean-Marc Neefs

15:00-15:30 **Characteristics of KNIME Nodes**

Presenter: Daniela Digles

15:30-16:00 **Tea and Coffee Break**

16:00-16:30 **Suggestions for Workflows of Interest**

Chair: Christine Chichester

Facilitator: Kiera McNeice

First Hands-on Session

Facilitators:

- 16:30-18:00
- Christine Chichester (KNIME)
 - Daniela Digles (KNIME)
 - Andrei Caracoti (Pipeline Pilot)
 - Jean-Marc Neefs (Pipeline Pilot)
 - Kiera McNeice
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Dinner for Attendees at De Bosbaan

Hosted by VU University

Agenda

Wednesday, 20 May

Questions from Previous Hands-on Session

09:00-09:30

Chair: Daniela Digles

Facilitator: Kiera McNeice

Second Hands-on Session: Implementing Workflows

Facilitators:

09:30-12:30

- Christine Chichester (KNIME)
 - Daniela Digles (KNIME)
 - Andrei Caracoti (Pipeline Pilot)
 - Jean-Marc Neefs (Pipeline Pilot)
 - Kiera McNeice
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12:30-13:30

Lunch

Wrap-up: Learnings and Feedback

13:30-14:00

Chair: Christine Chichester

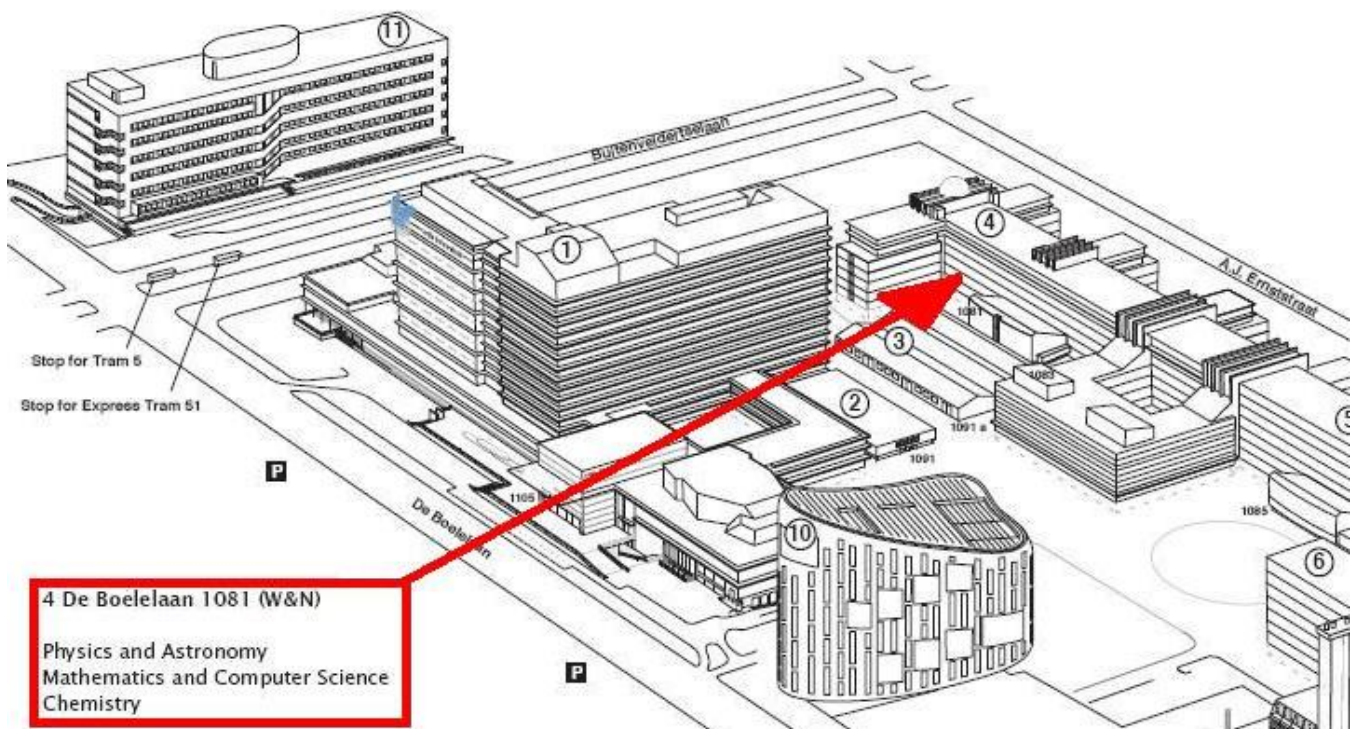
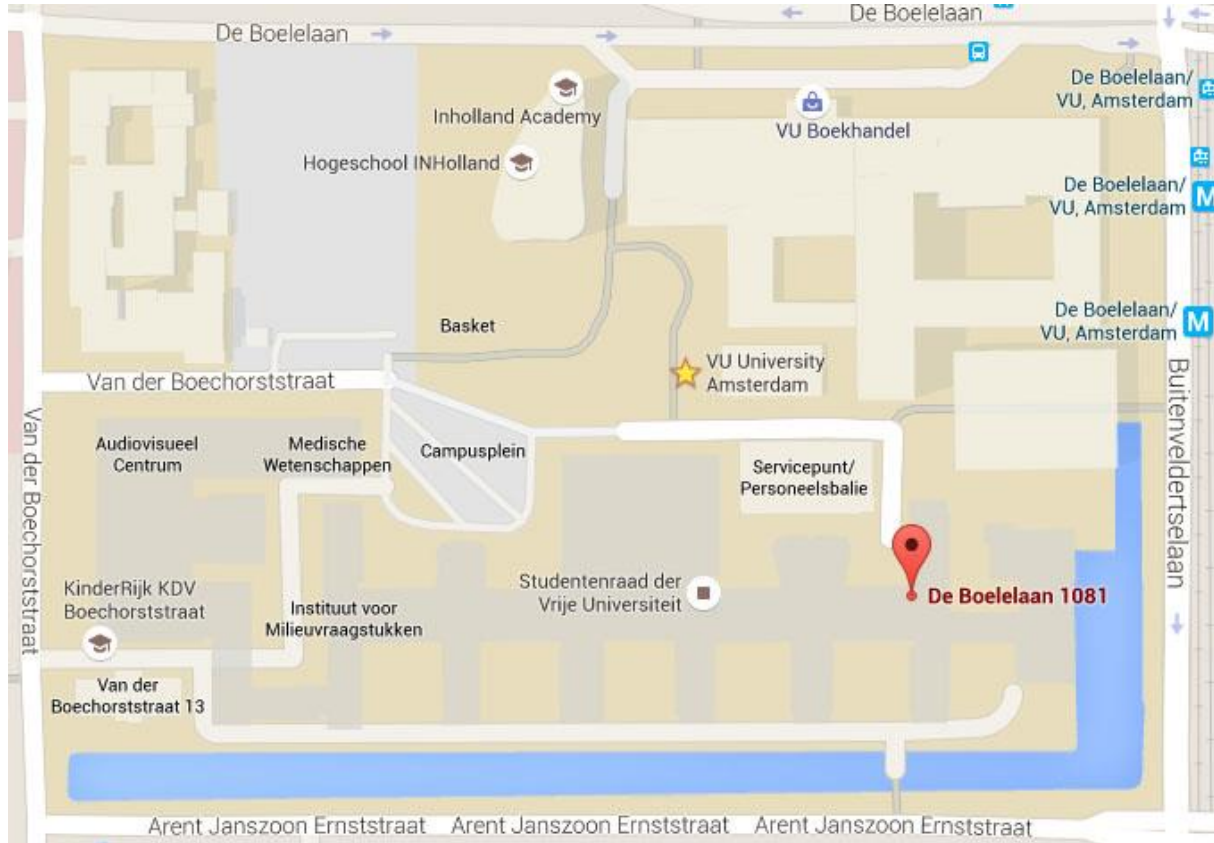
Facilitator: Kiera McNeice

14:00-17:00

Room Open for Networking

Workshop Location

Room WN-C659, [De Boelelaan 1081](#), [VU University, Amsterdam](#)



Restaurant Location

[De Bosbaan, Bosbaan 4, 1182 AG Amstelveen](#)

Workshop facilitators will lead attendees from VU University to De Bosbaan for dinner.

