

What is Open PHACTS and why would you care?

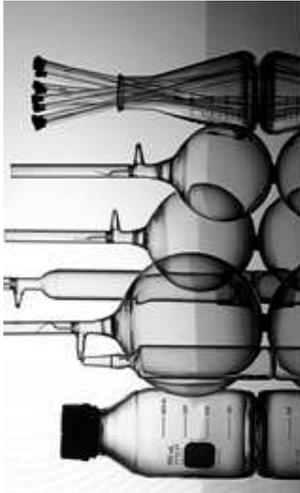
Stefan Senger

Coordinator of the Open PHACTS project

18-Feb-15

Open PHACTS

Open Pharmacological Space



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What is Open PHACTS and why would you care?

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irrdesign English (United Kingdom) 70%



The plan: I take 20 minutes (of your life*), and provide you with answers to 10 questions (on 10 slides)

1. Why (do I think) you should know about Open PHACTS?
2. What is Open PHACTS?
3. Turning data into knowledge: How does the ideal world look like?
4. Why did the world need something like Open PHACTS?
5. What has Open PHACTS set out to do?
6. What has Open PHACTS achieved in just 3 years?
7. What has Open PHACTS done for me/us so far?
8. How does Open PHACTS create impact?
9. What will Open PHACTS do next?
10. Will Open PHACTS have an “afterlife”?



1. Why (do I think) you should know about Open PHACTS?

I think you should know about Open PHACTS because ...

- ... this project is relevant to you. It is trying to make it easier for you to derive knowledge from data.
- ... your input is needed to provide feedback/suggestions and to share your needs so that what the project creates is useful to you.
- ... your help is needed for spotting opportunities and synergies.
- ... it will hopefully (already now) have something to offer that you have a use for.



2. What is Open PHACTS?

Open PHACTS (Pharmacological Concepts Triple Store) is a **Innovative Medicines Initiative** project that started in 2011 and will now run until February 2016, after having been granted a further two year's funding to allow the project to explore new scientific opportunities.

Open PHACTS = 10 EFPIA companies + 15 academic institutions + 6 SMEs

Facts & Figures

Start Date 01/03/2011

Duration 60 months

Contributions €

IMI funding 11 466 433

EFPIA in-kind 6 518 565

Other 2 922 972

Total cost 20 907 970

THE INNOVATIVE MEDICINES INITIATIVE

The Innovative Medicines Initiative (IMI) is Europe's largest public-private initiative aiming to speed up the development of better and safer medicines for patients.

IMI supports collaborative research projects and builds networks of industrial and academic experts in order to boost pharmaceutical innovation in Europe.

IMI is a joint undertaking between the European Union and the pharmaceutical industry association EFPIA.

<http://www.imi.europa.eu>



The European Commission's Seventh Framework Programme contributes €1 billion to the IMI research programme. That amount will be matched by mainly in kind contributions (consisting mostly of research activities) worth at least another €1 billion euro from member companies of the European Federation of Pharmaceutical Industries and Associations (EFPIA).

Partnership

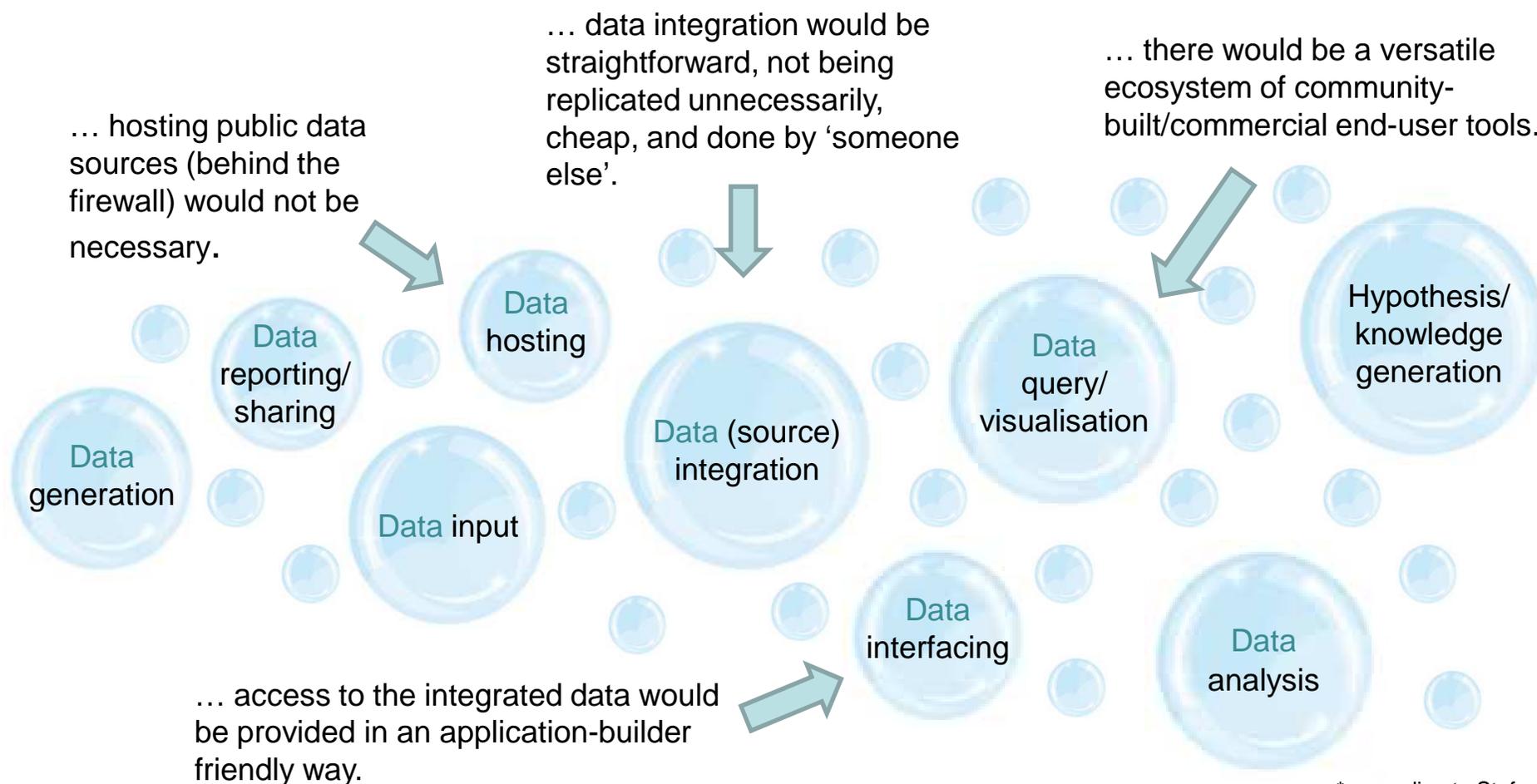


<http://www.imi.europa.eu/content/open-phacts>

<http://www.openphacts.org>



3. Turning data into knowledge: The ideal world*



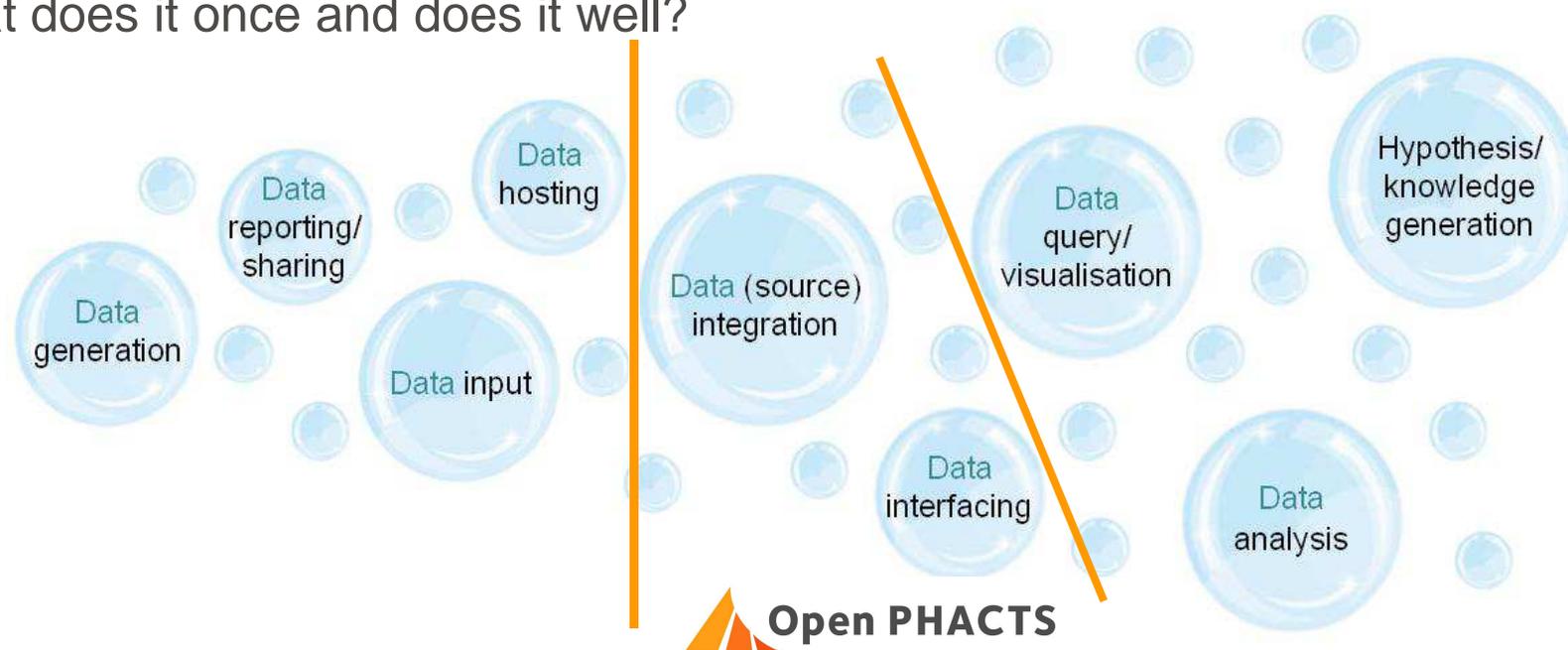
* according to Stefan



4. Why did the world need something like Open PHACTS?

Why continue to **waste** valuable time and resources for integrating public data yourself (possibly over and over again) or '**ignore**' it altogether because it's not easily accessible?

Wouldn't you rather contribute to a **pre-competitive community-driven effort** that does it once and does it well?





5. What has Open PHACTS set out to do?

- **Data integration enabling knowledge generation:** “To reduce the barriers to drug discovery in industry, academia and for small businesses, the Open PHACTS consortium is building the **Open PHACTS Discovery Platform**. This will be **freely available, integrating pharmacological data** from a variety of information resources and providing tools and services to question this integrated data to support pharmacological research.”
- **Open approach:** “The software and data will be available for download and local installation, under an **open source and open access model**.”
- **No project should be an island:** “Throughout the project, a series of recommendations will be developed in conjunction with the community, **building on open standards, to ensure wide applicability of the approaches used for integration of data**.”
“...**semantic technology and principles** are deliberately being adopted to enable the platform to be adapted for application to other subject domains in the future.”



6. What has Open PHACTS achieved in just 3 years? It has...

- ... **identified relevant research questions and prioritised and 'solved' them**
(Drug Discovery Today: <http://dx.doi.org/10.1016/j.drudis.2013.05.008> and <http://dx.doi.org/10.1016/j.drudis.2014.11.006>)
- ... **created the Open PHACTS Discovery Platform**
with **compound-target-pathway-disease data** (e.g. from ChempSpider, ChEMBL, DrugBank, ChEBI, UniProt, Swissprot, neXtProt, WikiPathways, DisGeNet, GeneOntology) accessible via the Open PHACTS **API** (<http://dev.openphacts.org>) or a number of (example) **applications** (e.g. [ChemBioNavigator](#) by BioSolveIT).
- ... worked with the community to develop **open standards**, e.g. for RDF (Resource Description Framework)
- ... worked with data providers in regards to **data licensing** (instead of just 'sucking in' the data), **improving the quality** of the data sources, making them available as RDF (e.g. ChEMBL RDF).
- ... become a well recognised, active member of the community (e.g. look at [this](#))



7. What has Open PHACTS done for us* so far? It has...

- ... allowed us to become part of a **community of companies that all face similar challenges** posed by data-rich R&D, that have realised that it is extremely inefficient to tackle these challenges on their own and that are willing to share their experiences
- ... provided us with a mechanism to '**speak with one voice**' (and hence add more 'weight'). For example, when discussing future developments with data providers (e.g. ChEMBL but also commercial data providers).
- ... **connected us to experts** from various domains who will can call on and also help us to not miss out on relevant opportunities.
- ... provided us with the **opportunity to learn** more about large-scale semantic data integration through a 'real life' Linked Data project that has produced a working platform.



8. How can Open PHACTS create impact?

It can create impact by...

- ... **providing secure access to integrated (public) data (in the cloud) via the Open PHACTS API.** For example, by using the Pipeline Pilot Component Collection or KNIME
- ... **making data integration easier, cheaper, more successful and sustainable.** This includes integration with commercial as well as proprietary data.
- ... allowing us to concentrate on **knowledge generation instead of data integration** (by getting some of the ‘**plumbing**’ done pre-competitively).



9. What will Open PHACTS do next?

Between now and February 2016 Open PHACTS will...

- ... integrate open chemical **patent data** (SureChEMBL)
- ... **enhance pathway data**.
- ... further improve how 'Open PHACTS data' can be accessed via **Pipeline Pilot/KNIME**.
- ... make **tissue expression data** available via the API
- ... start to look at **the integration of proprietary data** and continue to work with commercial data providers
- ... further develop the platform **guided by use cases** (with a focus on target validation and phenotypic screening). **What is it that we want/need?**



10. Will Open PHACTS have an “afterlife”?



The Open PHACTS Foundation

OPF is a not-for-profit membership organisation, supporting the Open PHACTS Discovery Platform:

A sustainable, open, vibrant and interoperable information infrastructure for applied life science research and development.

Press Release



Open PHACTS Foundation announces first three members: GSK, Janssen and Roche

24th June 2014

Cambridge, UK – The not-for-profit Open PHACTS Foundation announced its first three members today – GlaxoSmithKline, Janssen and Roche – who will steer the future of the successor organisation to the Innovative Medicines Initiative (IMI)-funded Open PHACTS project.

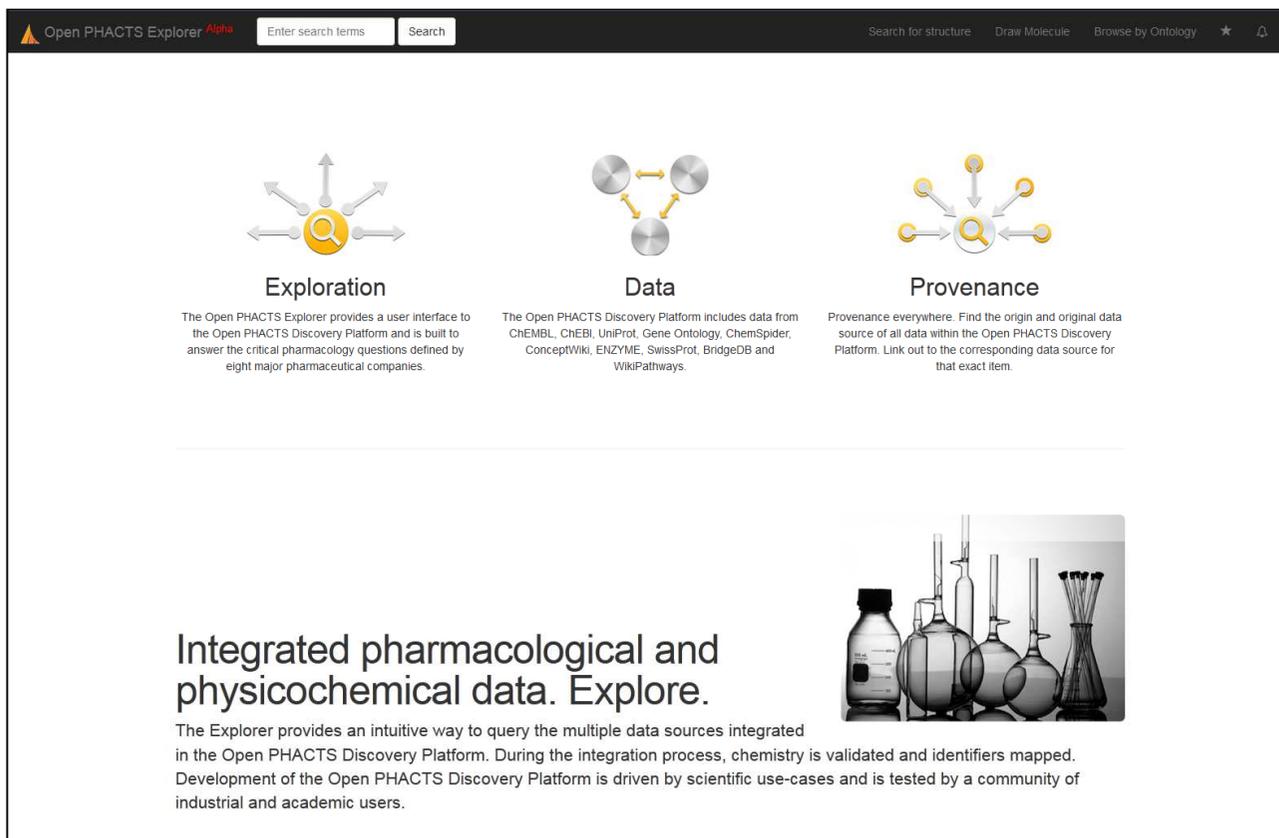
The commitment by these global pharmaceutical industry members signifies a major step in ensuring the sustainability of infrastructure developed during the Open PHACTS project.

Open PHACTS ‘goes global’...

<http://www.openphactsfoundation.org>



No 'rule' without an exception...

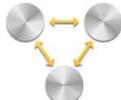


Open PHACTS Explorer ^{Alpha} Search for structure Draw Molecule Browse by Ontology ★ 🔍



Exploration

The Open PHACTS Explorer provides a user interface to the Open PHACTS Discovery Platform and is built to answer the critical pharmacology questions defined by eight major pharmaceutical companies.



Data

The Open PHACTS Discovery Platform includes data from ChEMBL, ChEBI, UniProt, Gene Ontology, ChemSpider, ConceptWiki, ENZYME, SwissProt, BridgeDB and WikiPathways.



Provenance

Provenance everywhere. Find the origin and original data source of all data within the Open PHACTS Discovery Platform. Link out to the corresponding data source for that exact item.

Integrated pharmacological and physicochemical data. Explore.

The Explorer provides an intuitive way to query the multiple data sources integrated in the Open PHACTS Discovery Platform. During the integration process, chemistry is validated and identifiers mapped. Development of the Open PHACTS Discovery Platform is driven by scientific use-cases and is tested by a community of industrial and academic users.



<http://explorer2.openphacts.org>



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Open PHACTS

enabling you to do what you do best.