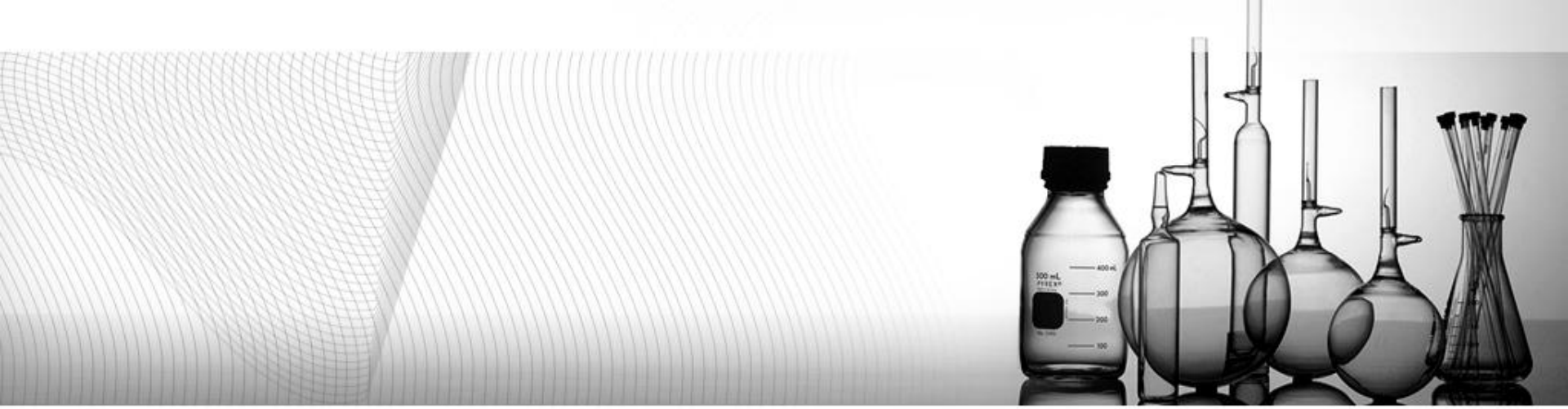

Open PHACTS
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Open PHACTS Foundation

building open semantic data services for life sciences

bryn@openphactsfoundation.org

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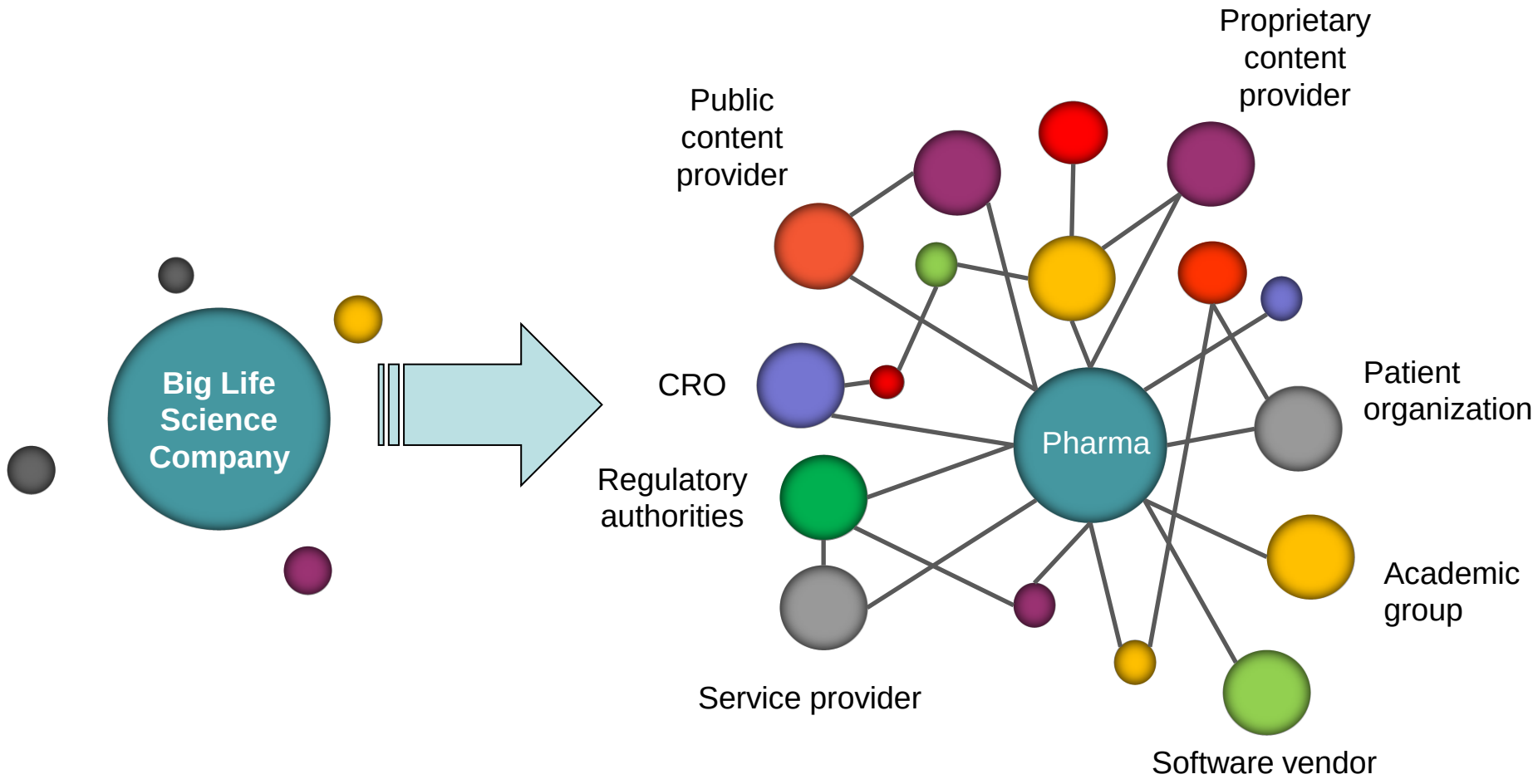
Rapidly Evolving Pharmaceutical Ecosystem



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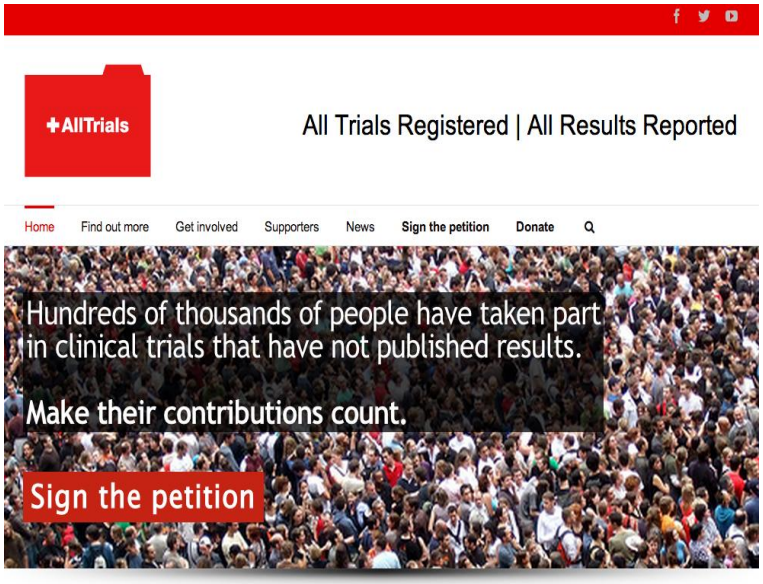
The data world is changing fast



Genomics england

patientslikeme®

open data institute

CHDI FOUNDATION

DATA COMMONS®

Sage BIONETWORKS

imi innovative medicines initiative

Pistoia Alliance

eTRIKS

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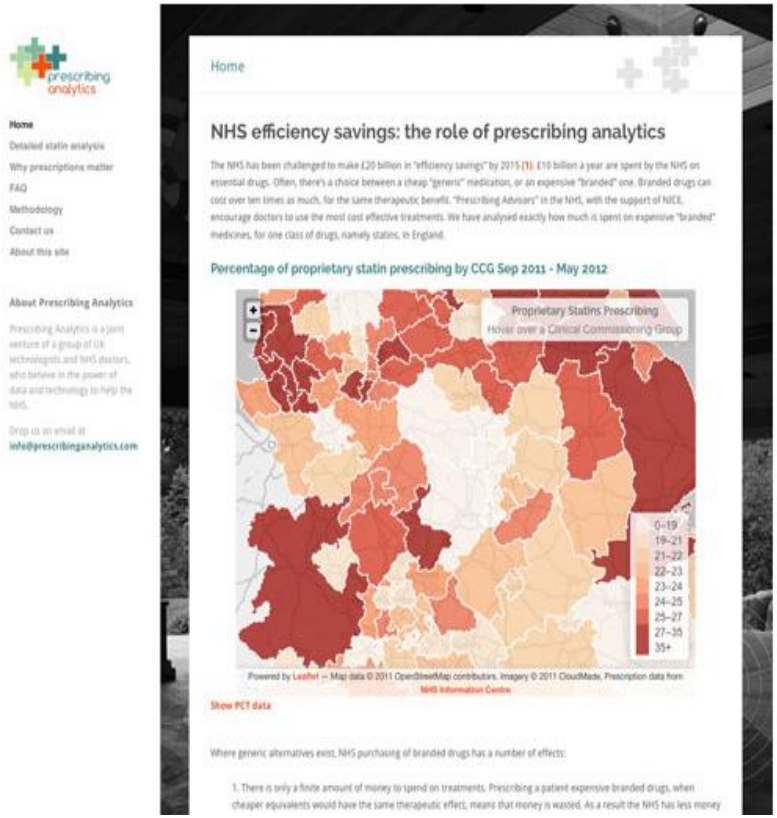
Prescription Savings Worth Millions Identified by ODI incubated company



- Analysis of statin prescribing patterns in UK NHS setting
- Potential saving of £200 million
- Open data transformed into knowledge

- http://theodi.org/news/prescription-savings-worth-millions-identified-odi-incubated-company

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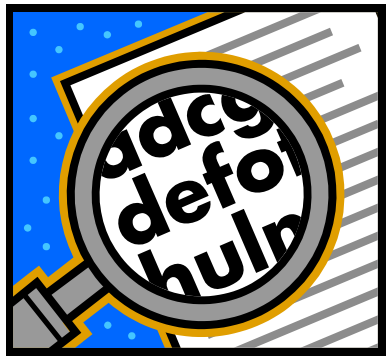
Public Domain Drug Discovery Data

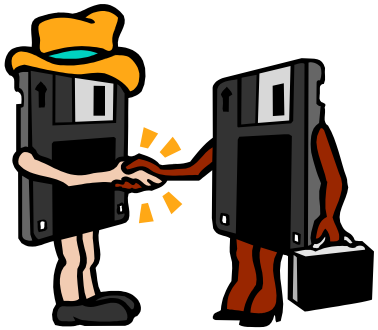


Literature Genbank
Patents PubChem

Databases

Downloads

Firewalled Databases



Data Integration

Data Analysis

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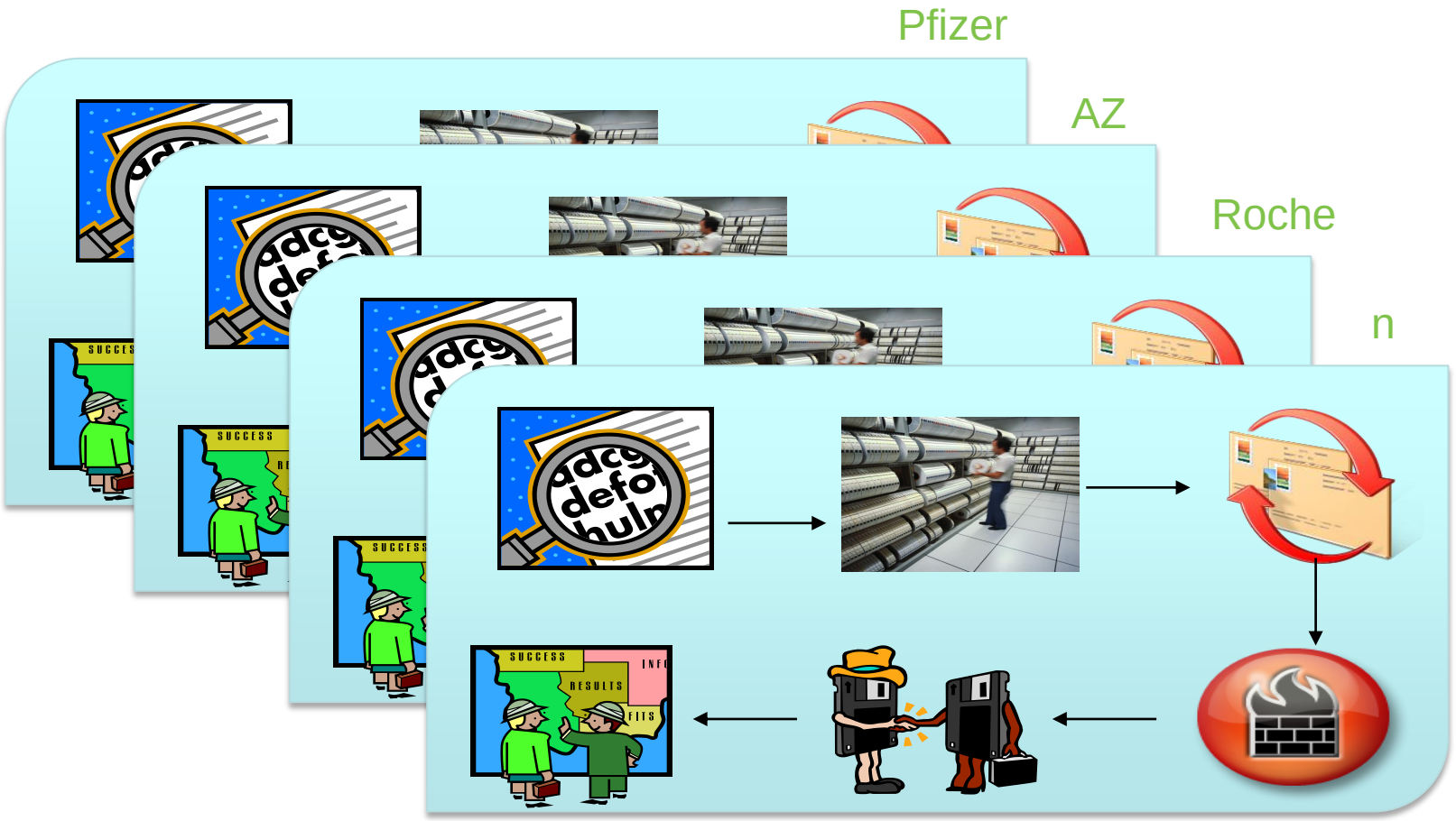
Public Domain Drug Discovery Data

- The Current Situation



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Open PHACTS Mission:

Integrate Multiple Research Biomedical Data Resources Into A Single Open & Free Access Point

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"What is the selectivity profile of known p38 inhibitors?"

"Let me compare MW, logP and PSA for known oxidoreductase inhibitors"

"Find me compounds that inhibit targets in NFkB pathway assayed in only functional assays with a potency <1 µM"

ChEMBL | DrugBank | Gene Ontology | Wikipathways | GeneGo

ChEBI | UniProt | UMLS | neXtProt | GVKBio

ConceptWiki | ChemSpider | DisGeNet | TrialTrove | TR Integrity

ChEMBL Target Class | ENZYME | FDA adverse events | SureChEMBL

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Business Question Driven Approach

Number	sum	Nr of 1	Question
15	12	9	All oxidoreductase inhibitors active <100nM in both human and mouse
18	14	8	Given compound X, what is its predicted secondary pharmacology? What are the on and off,target safety concerns for a compound? What is the evidence and how reliable is that evidence (journal impact factor, KOL) for findings associated with a compound?
24	13	8	Given a target find me all actives against that target. Find/predict polypharmacology of actives. Determine ADMET profile of actives.
32	13	8	For a given
37	13	8	The curren in serine pr
38	13	8	Retrieve al structure (v
41	13	8	A project is compounds the target c level of the
44	13	8	Give me al
46	13	8	Give me th (disease)
59	14	8	Identify all

ELSEVIER

Drug Discovery Today

Volume 18, Issues 17–18, September 2013, Pages 843–852

Review

Scientific competency questions as the basis for semantically enriched open pharmacological space development

Kamal Azzaoui[1], Edgar Jacoby[14], Stefan Senger[2], Emiliano Cuadrado Rodríguez[3], Mabel Loza[3], Barbara Zdrazil[4], Marta Pinto[4], Antony J. Williams[5], Victor de la Torre[6], Jordi Mestres[7], Manuel Pastor[7], Olivier Taboureau[8], Matthias Rarey[9], Christine Chichester[10], Steve Pettifer[11], Niklas Blomberg[12, a], Lee Harland[13], Bryn Williams-Jones[13], Gerhard F. Ecker[4]

Open PHACTS
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Apps

Core Platform

Identity Resolution Service

"Adenosine receptor 2a"

Identifier Management Service

P12374
EC2.43.4
CS4532

Linked Data API (RDF/XML, TTL, JSON)

Semantic Workflow Engine

Data Cache
(Virtuoso Triple Store)

Domain Specific Services

Chemistry Registration Normalisation & Q/C

Indexing

Public Ontologies

VoID
RDF
Db

VoID
Nanopub
RDF
Db

Public Content

VoID
RDF
Db

VoID
Nanopub
RDF
Db

Commercial

VoID
Nanopub
RDF

User Annotations

Open PHACTS
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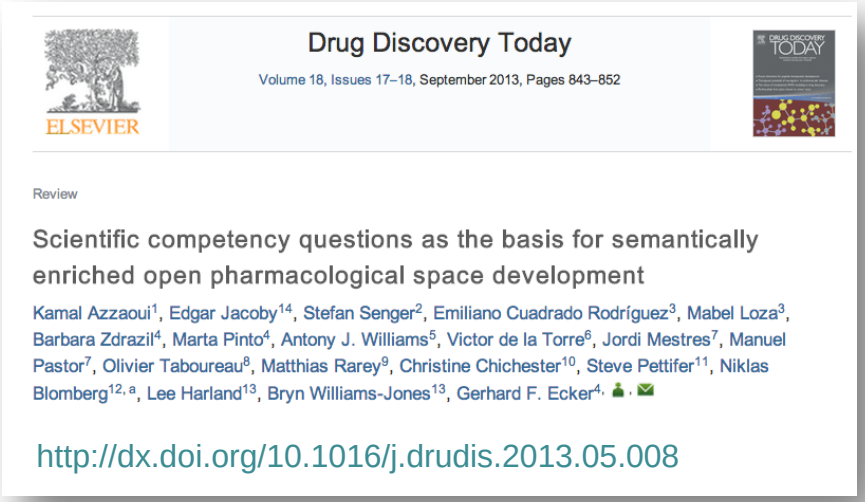
The Open PHACTS Discovery Platform

- **Cloud-Based "Production" Level System. Secure & Private**
- **Guided By Business Questions**
- **Uses Semantic Web Technology <u>But</u> provides a simple REST-ful API for everyone else**



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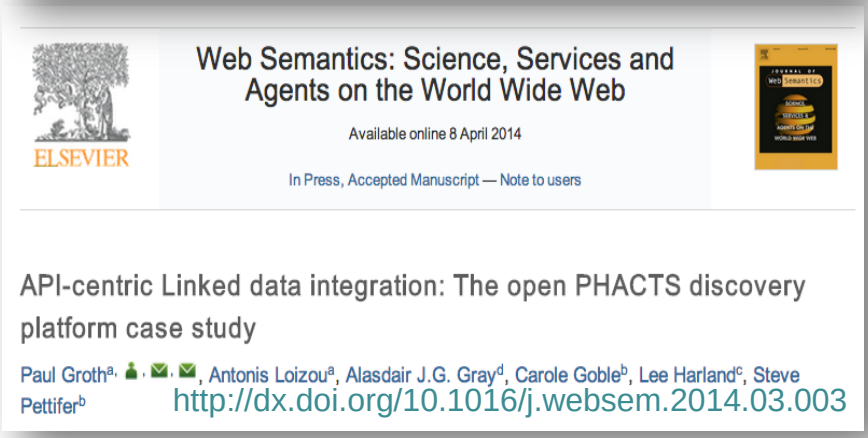
http://dx.doi.org/10.1016/j.drudis.2013.05.008



ELSEVIER

Web Semantics: Science, Services and Agents on the World Wide Web

Available online 8 April 2014

In Press, Accepted Manuscript — Note to users

API-centric Linked data integration: The open PHACTS discovery platform case study

Paul Groth[a], Antonis Loizou[a], Alasdair J.G. Gray[d], Carole Goble[b], Lee Harland[c], Steve Pettifer[b]

http://dx.doi.org/10.1016/j.websem.2014.03.003

Open PHACTS

Open Pharmacological Space

Open PHACTS

Sign in | Sign up

Developer Home | Want help? | Documentation | Get my API keys! | Featured Apps | Workflow

Create!

Build with the Open PHACTS Discovery Platform. The platform provides a convenient API to query across multiple pharmacology datasets.

You'll find complete documentation for the API in our documentation section. You'll need an API key to use the platform. Sign-up is free. For more information on the project, check out www.openphacts.org.

News:

- Let us know if you have a feature request or bug report.
- August 11, 2014 - version 1.4 of the platform is made available.
- June 24, 2014 - Open PHACTS Foundation announces first 3 members.
- January 24, 2014 - version 1.3 of the platform is made available.
- April 22, 2013 - launch of public beta at the 4th Open PHACTS community workshop held at the Royal Society of Chemistry. Great turnout!

Powered By:

ChemSpider Search and share chemistry | OPENLINK SOFTWARE Making Technology Work For You | WikiPathways

ConceptWiki | github SOCIAL CODING | BridgeDb connecting knowledge

ChEMBL | UniProt | DrugBank Open Data Drug & Drug Target Database

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Powered by 3scale

http://dev.openphacts.org

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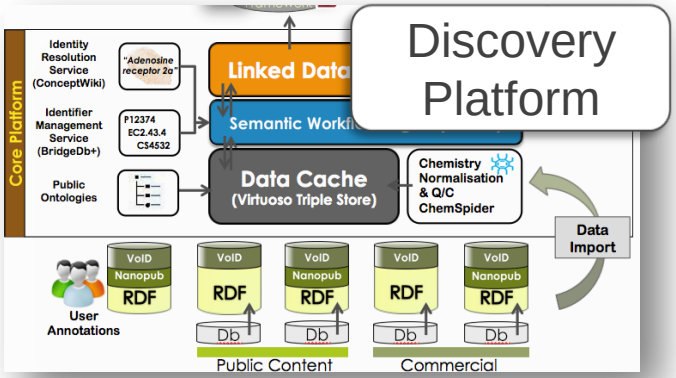
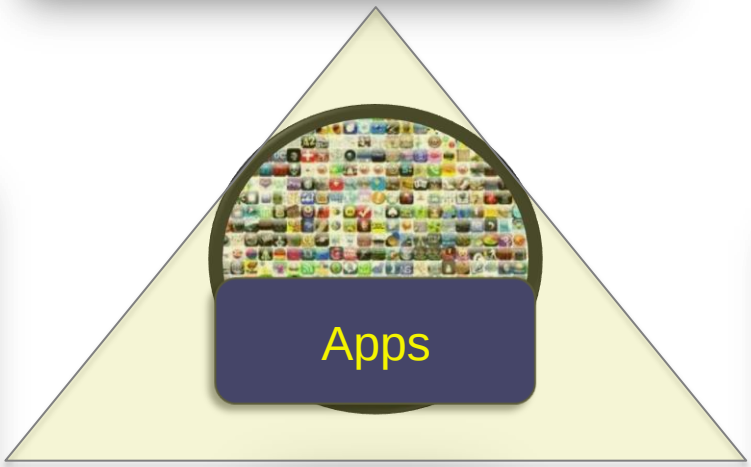
Open PHACTS Elements



API

```
w_uri .
quiv_target .
et_name ;
        void:inDataset <http://www.conceptwiki.
?equiv_target dc:title ?target_name;
        ops:target_organism ?target_organism ;
        ops:targetOfAssay ?equiv_assay ;
        void:inDataset <http://data.kasabi.com/
ops:targetOfAssay owl:inverseOf chembl:hasTarge
?equiv_assay chembl:organism ?assay_organism ;
        chembl:hasDescription ?assay_descriptio
        ops:assayOfActivity ?activity_uri .
ops:assayOfActivity owl:inverseOf chembl:onAssa
?activity_uri chembl:type ?std_type ;
```



Standards

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Names and standards in biomedical science

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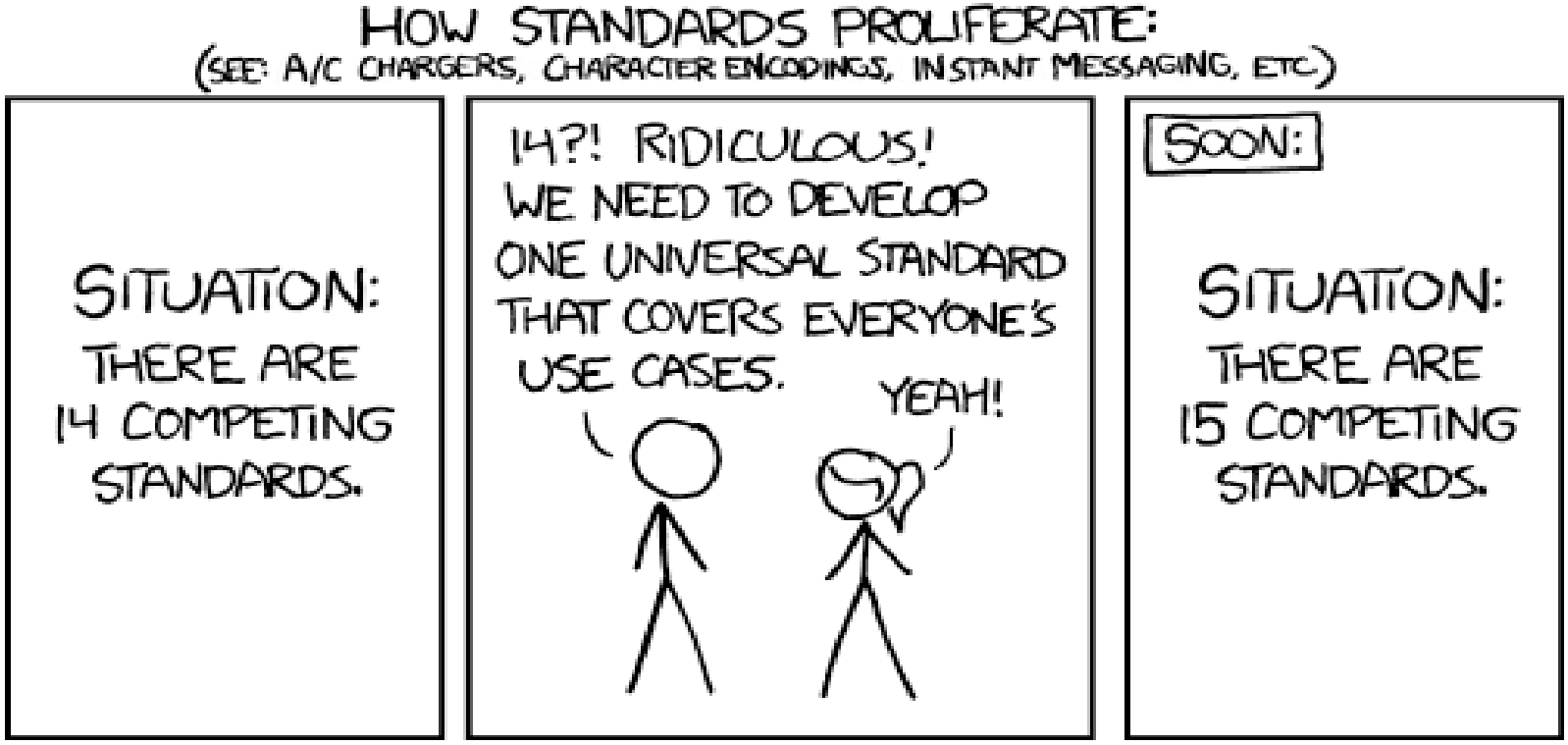

http://imgs.xkcd.com/comics/standards.png

- Basic Semantic web standards
  - SPARQL 1.1, RDF(S), SKOS
- Dataset descriptions
  - Vocabulary of Interlinked Datasets (VoID)
  - VoID linkset descriptions
- QUDT Quantities, Units, Dimensions and Types
- Provenance
  - W3C PROV, PAV, Nanopublications
- BioPortal, ConceptWiki, ChEMBL, identifiers.org, Uniprot, ChemSpider

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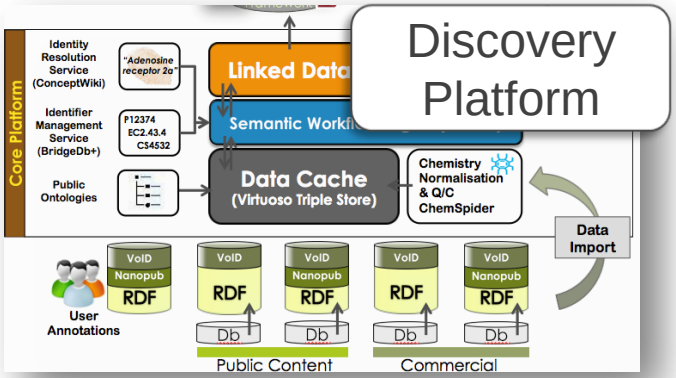
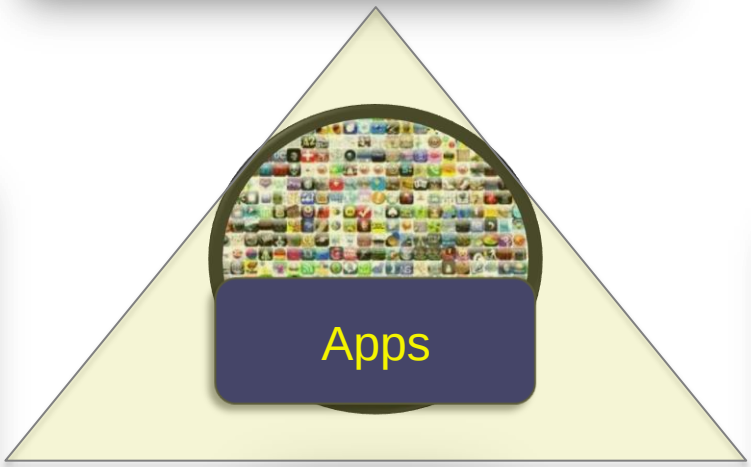
Open PHACTS Elements



API

```
w_uri .
quiv_target .
et_name ;
        void:inDataset <http://www.conceptwiki.
?equiv_target dc:title ?target_name;
        ops:target_organism ?target_organism ;
        ops:targetOfAssay ?equiv_assay ;
        void:inDataset <http://data.kasabi.com/
ops:targetOfAssay owl:inverseOf chembl:hasTarge
?equiv_assay chembl:organism ?assay_organism ;
        chembl:hasDescription ?assay_descriptio
        ops:assayOfActivity ?activity_uri .
ops:assayOfActivity owl:inverseOf chembl:onAssa
?activity_uri chembl:type ?std_type ;
```



Standards

Open PHACTS

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Open PHACTS

Browse and search the data within the Open PHACTS Discovery Platform.

Developed by the University of Manchester and University of Vienna

ChemBioNavigator

Visualise the chemical and biological space of a molecule group in a chemically-aware manner.

Developed by the University of Hamburg and BioSolveIT GmbH

PHARMATREK

Navigate pharmacological space in a flexible and interactive way.

Developed by the Consorci Mar Parc de Salut de Barcelona (PSMAR)

SciBite

Connects the latest news and events in Pharma and Biotech directly to pharmacology data within the Open PHACTS platform.

Developed by SciBite Limited

utopia

Allows the semantic enrichment of scientific articles in PDF format.

Developed by the University of Manchester

GARField

Intuitive predicts target pharmacology based on the Similar Ensemble Approach.

Developed by the Technical University of Denmark

collector

Extracts data to build QSAR predictive models with data from the eTOX project.

Developed by PSMAR as part of the eTOX project

accelrys Pipeline Pilot

A repository of useful Pipeline Pilot components and workflows has been developed.

Open PHACTS - Pipeline Pilot Community

KNIME

A KNIME repository of components and workflows has been developed.

Open PHACTS - KNIME Community

Excel

Queries the Open PHACTS API from Microsoft's Excel spreadsheet software.

Developed by the University of Vienna

AQnowledge Semantics for Science

Identifies significant entities in scientific text, and provides links to Open PHACTS Explorer.

Developed by AQnowledge

he

Helium for Excel Community Edition contains three functions that use the Open PHACTS API.

Developed by Ceiba Solutions

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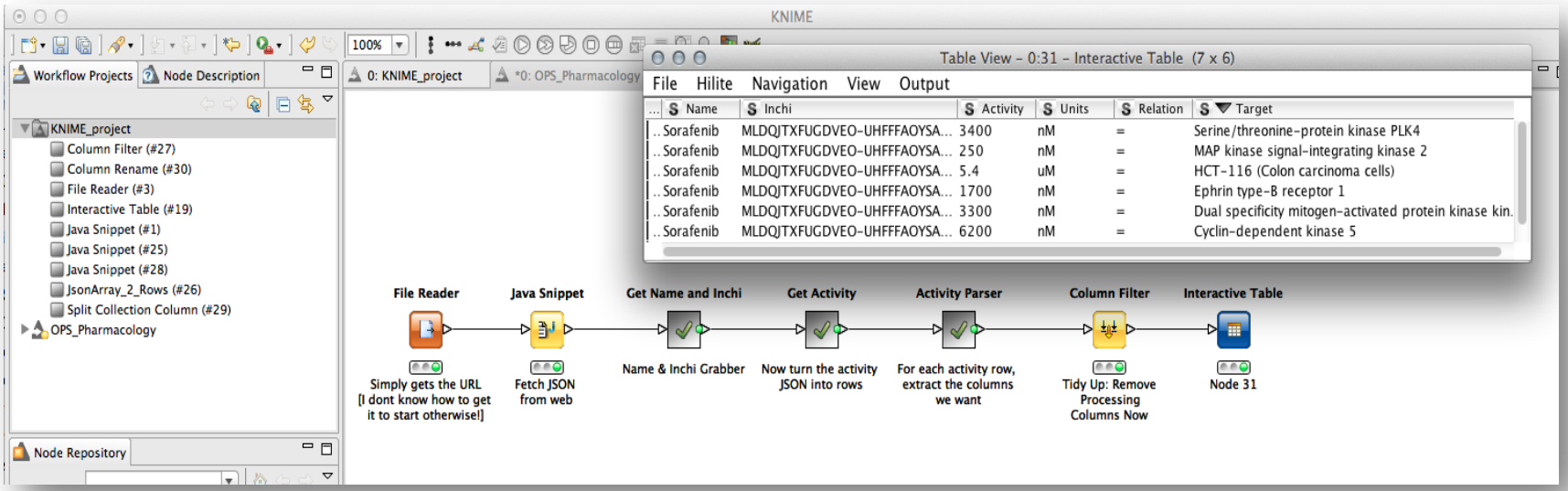

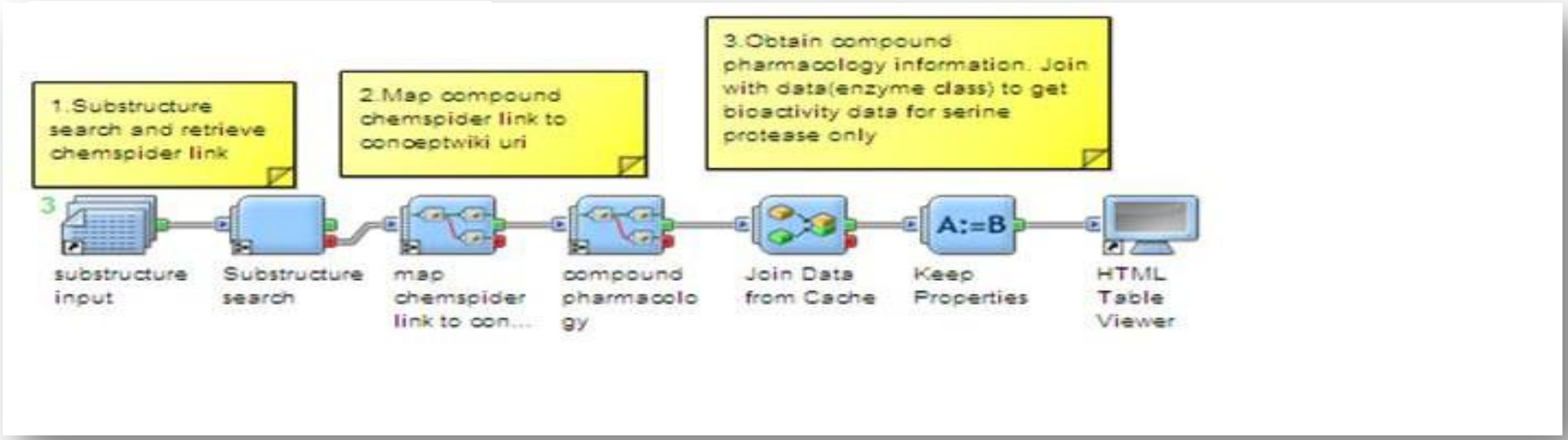

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Open PHACTS Mission:

Integrate Multiple Research Biomedical Data Resources Into A Single Open & Free Access Point

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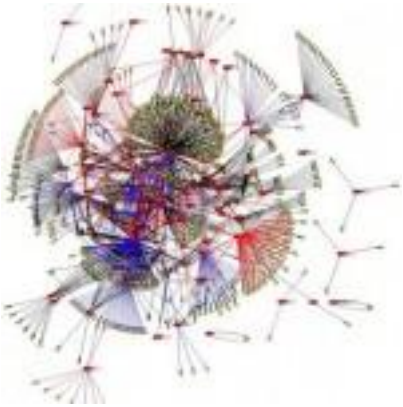
Open Pharmacological Space

Sustaining Impact

- "Software is free like puppies are free - they both need money for maintenance"

- …and more resource for future development

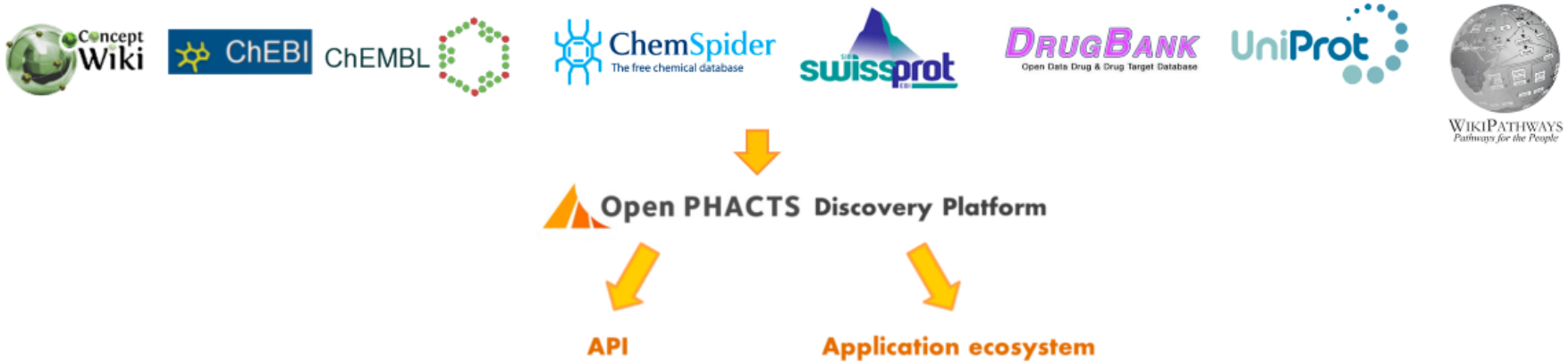


The Open PHACTS Foundation

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.

To reduce the barriers to drug discovery in industry, academia and for small businesses, the Open PHACTS Discovery Platform provides tools and services to interact with multiple integrated and publicly available data sources. To integrate this data, extensive cross-referencing of scientific concepts is needed across all databases.

The Open PHACTS Foundation ensures the sustainability of the Open PHACTS Discovery Platform infrastructure and acts as a hub for relevant scientific research and development.



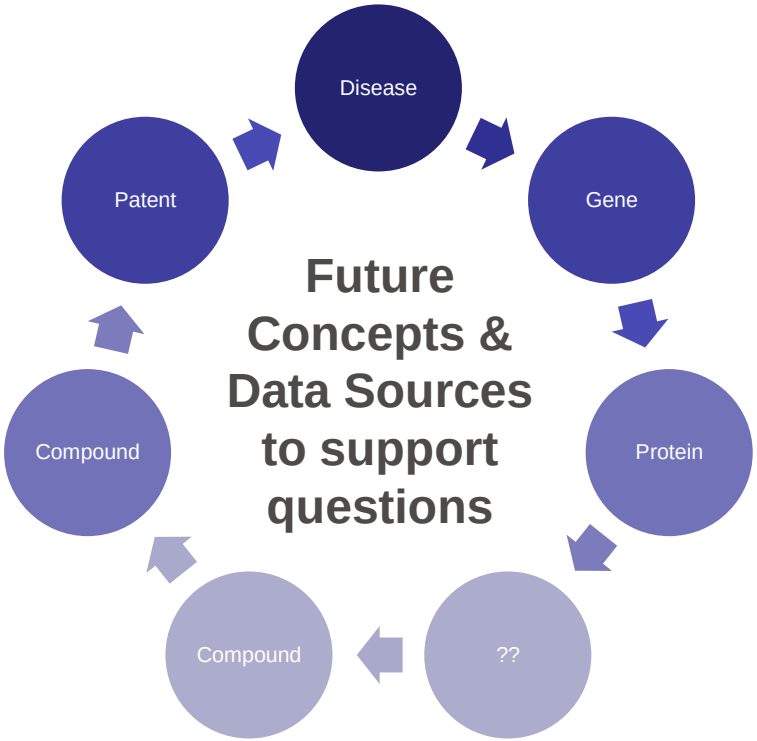
Open PHACTS
Open Pharmacological Space

Powering precompetitive collaborative research

Open PHACTS
Open Pharmacological Space

Open PHACTS has built a unique, flexible and powerful infrastructure for semantic data in life sciences
We have the platform, data, services, experience and capabilities to tackle big data challenges

- Cloud-based ‘production’ level secure and private system
- We are expanding into new data areas
- Comprehensive workflow components for advanced use cases



Open PHACTS
Open Pharmacological Space

- The Open PHACTS Foundation is a UK-based member-owned non-profit company founded to sustain and develop the Open PHACTS infrastructure
- OPF operations are distributed across funded partners to maintain and further develop public:private partnership

- A sought-after partner for Horizon 2020 projects
- Bring industry perspective to new academic partners
- Leverage the heritage of open data services and public:private partnership

BIG DATA EUROPE
Empowering Communities with Data Technologies

OPF is a funded partners in this project, and 5 other pending submissions

Acknowledgements

GlaxoSmithKline – Coordinator
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University of Hamburg, Center for Bioinformatics
BioSolveIT GmBH
Consorci Mar Parc de Salut de Barcelona
Leiden University Medical Centre
Royal Society of Chemistry
Vrije Universiteit Amsterdam
Novartis
Merck Serono
H. Lundbeck A/S
Eli Lilly
Netherlands Bioinformatics Centre
Swiss Institute of Bioinformatics
ConnectedDiscovery
EMBL-European Bioinformatics Institute
Janssen Esteve Almirall
OpenLink Scibite
The Open PHACTS Foundation
Spanish National Cancer Research Centre
University of Manchester
Maastricht University
Aqnowledge
University of Santiago de Compostela
Rheinische Friedrich-Wilhelms-Universität Bonn
AstraZeneca
Pfizer

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