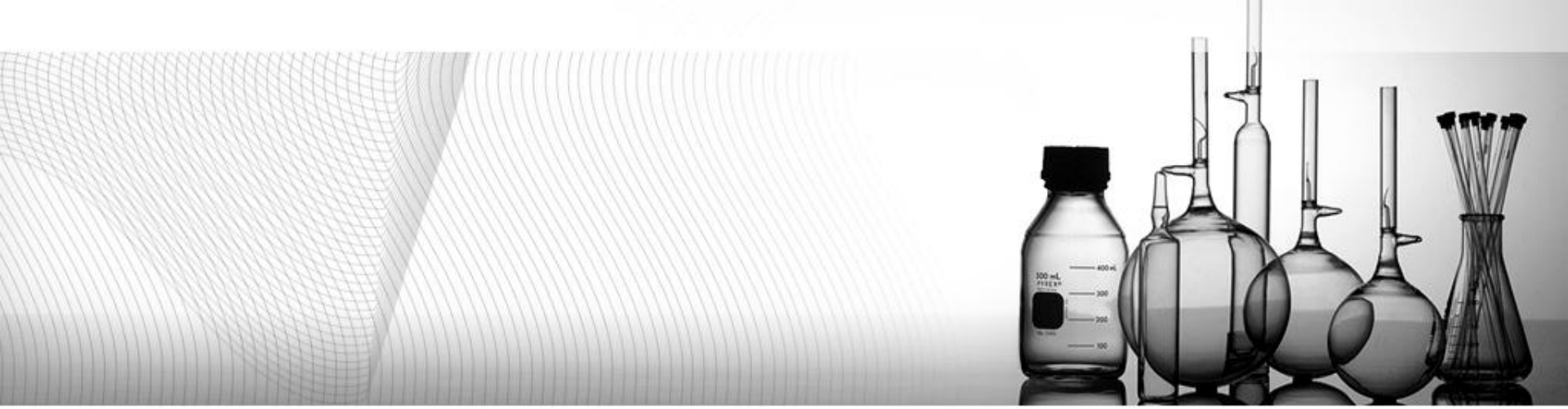


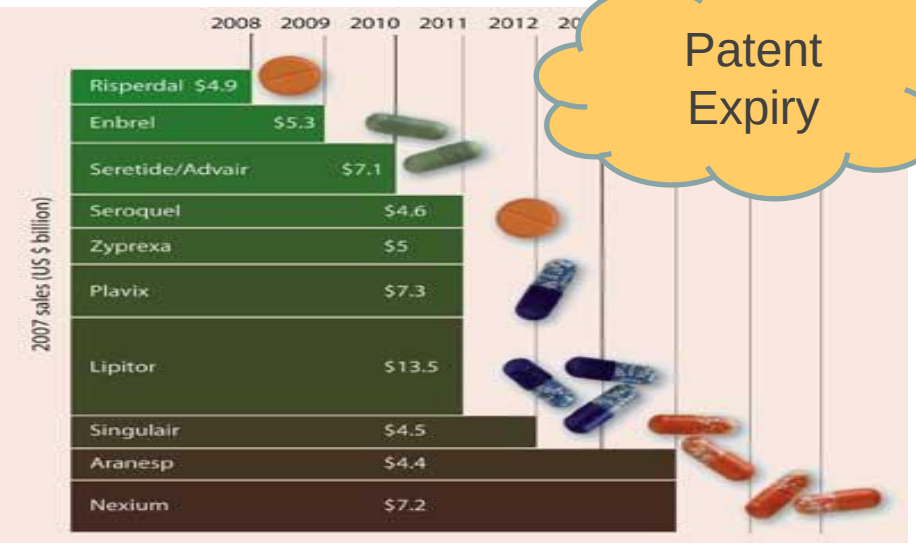
Open PHACTS
Open Pharmacological Space

The Open PHACTS Discovery Platform

Semantic Data Integration for Life Sciences

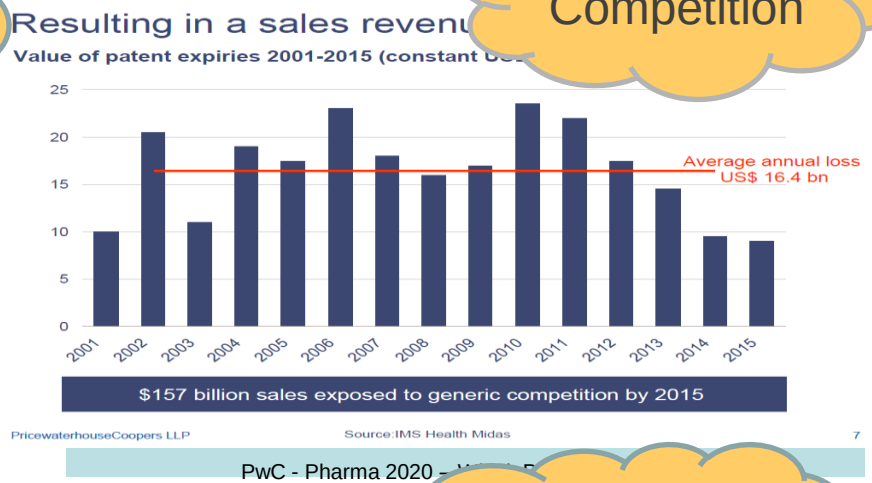
Open PHACTS

Open Pharmacological Space



Patent Expiry

Generic Competition

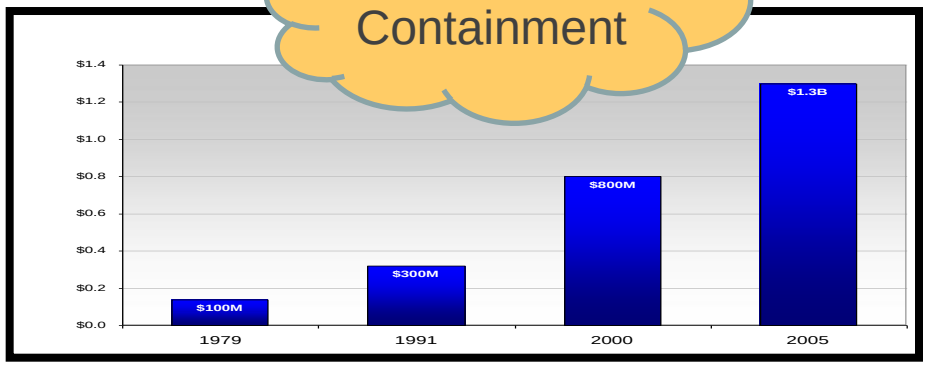


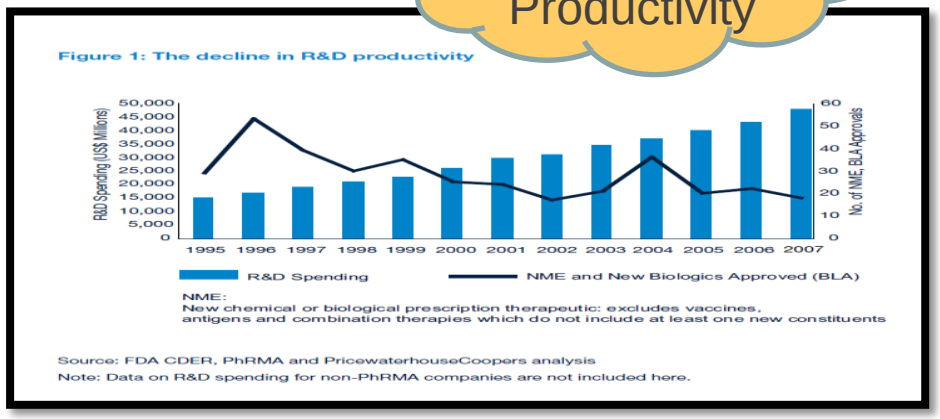
PwC - Pharma 2020 –

http://www.rsc.org/chemistryworld/Issues/2009/January/PharmaRefocusesOnThePatentCliff.asp

Improve R&D Productivity

Cost Containment





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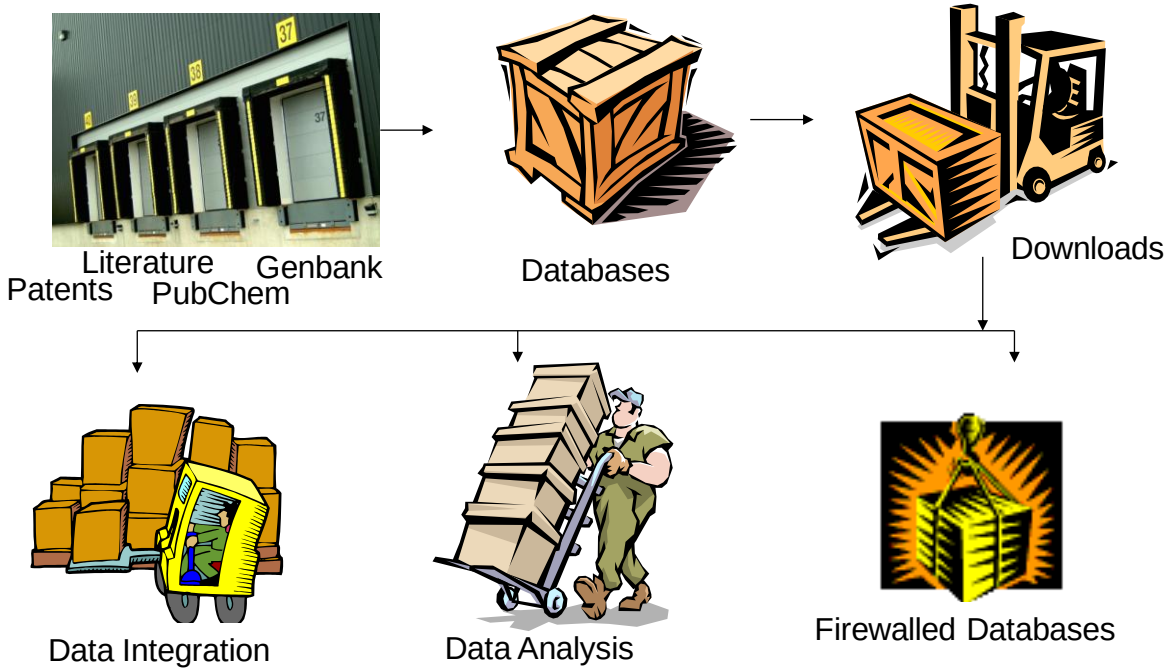
Open Pharmacological Space

Pre-competitive Informatics:

Pharma are all accessing, processing, storing & re-processing external research data



X Repeat @ each company

Lowering industry firewalls: pre-competitive informatics in drug discovery
Nature Reviews Drug Discovery (2009) 8, 701-708 doi:10.1038/nrd2944

Open PHACTS
Open Pharmacological Space

Over the last decade

- Data has become more open
- Data has become better represented (Standards)
- Major providers are becoming more organised (NCBI, EBI, FDA)

BUT

Integration across sources, and across providers is still a gap

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Open Pharmacological Space

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The Innovative Medicines Initiative

- EC funded public-private partnership for pharmaceutical research
- Focus on key problems
  - Efficacy, Safety, Education & Training, **Knowledge Management**

The Open PHACTS Project

- Create a *semantic integration hub ("Open Pharmacological Space")…*
- *Runs 2011-2014, ENSO till 2016*
- Deliver services to support on-going drug discovery programs in pharma and public domain
- Leading academics in semantics, pharmacology and informatics, driven by solid industry business requirements
- 31 academic partners, 9 pharmaceutical companies, 3 software SMEs
- Work split into clusters:
  - Technical Build
  - Scientific Drive
  - Community & Sustainability

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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 | GVKBio

ConceptWiki | ChemSpider | TrialTrove | TR Integrity

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Open Pharmacological Space

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

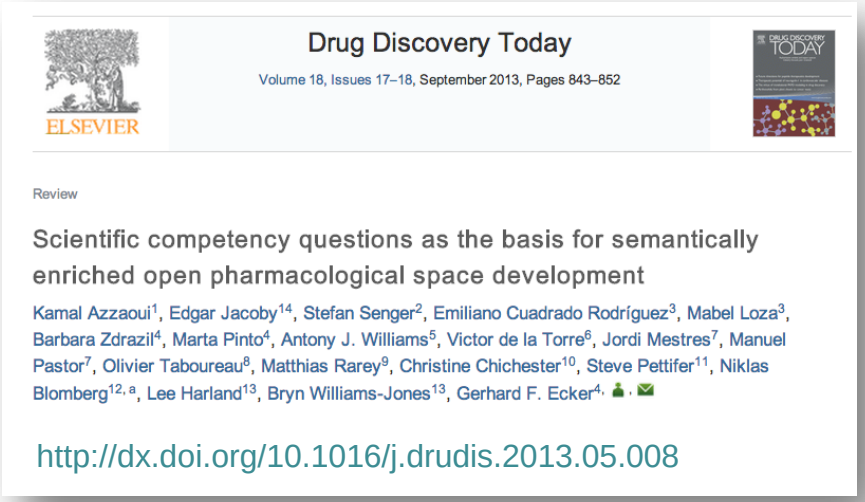
Scientific competency questions as the basis for semantically enriched open pharmacological space development

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
Open Pharmacological Space

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**



ELSEVIER

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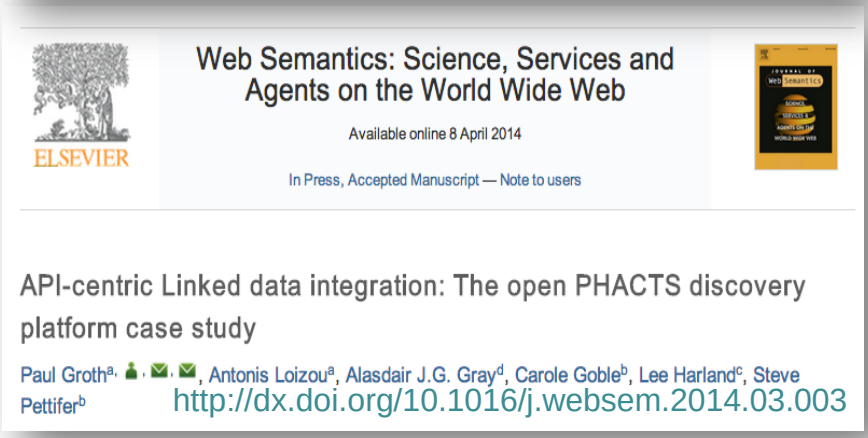
http://dx.doi.org/10.1016/j.drudis.2013.05.008



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

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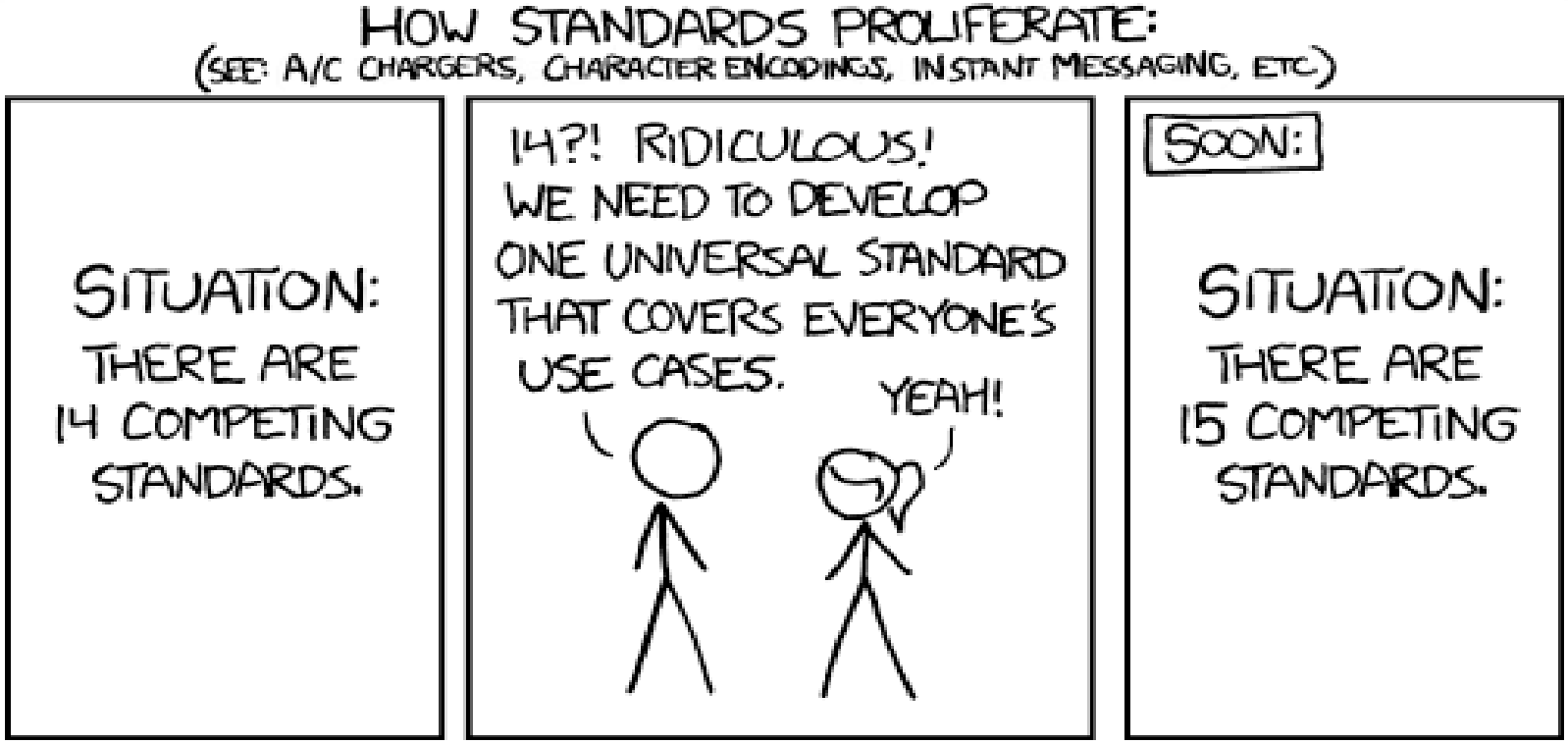
Open Pharmacological Space



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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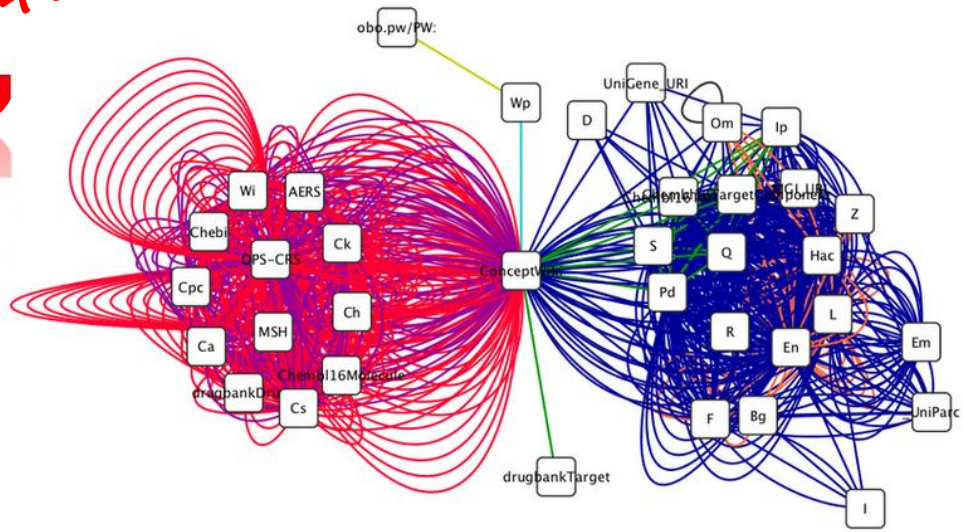
HELLO
my name is

~~RS_2353~~

~~GB:29384~~

~~P12047~~

~~X31045~~ P12047



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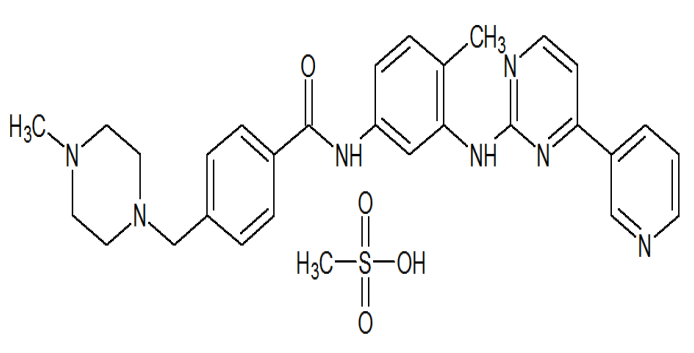
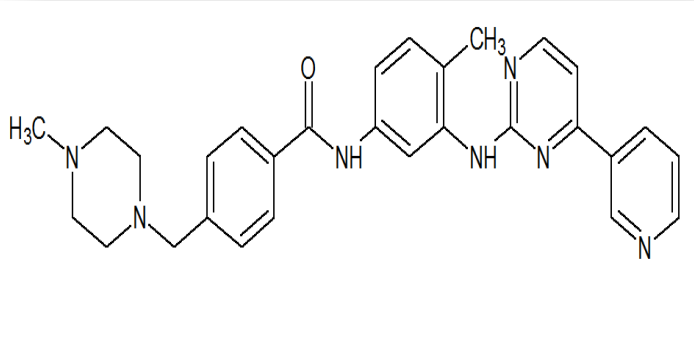
Are These Two Molecules The Same(*)





*Really: Is it sensible to combine data associated with these two molecules?

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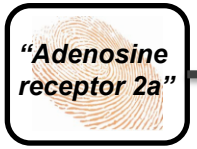
Apps

Core Platform

Identity Resolution Service



Identifier Management Service

P12374
EC2.43.4
CS4532

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

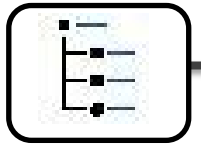
Semantic Workflow Engine

Data Cache
(Virtuoso Triple Store)

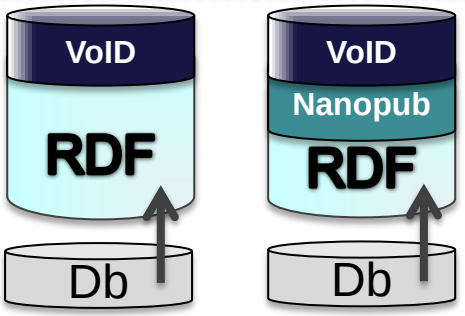
Domain Specific Services

Chemistry
Registration
Normalisation
& Q/C

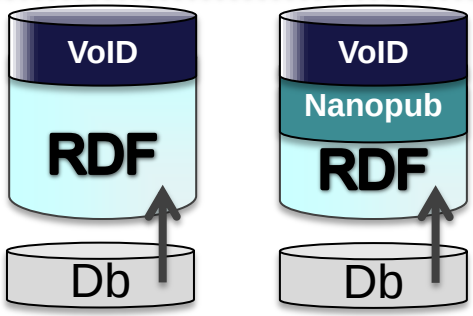
Indexing



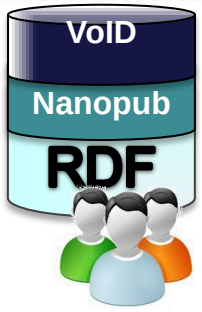
Public Ontologies



Public Content



Commercial



User Annotations

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

Powered by 3scale

http://dev.openphacts.org

Open PHACTS Support Portal

Welcome
Login **Sign up**

Home | Solutions | Forums

How can we help you today?

Enter your search term here... SEARCH

Login or Signup to submit a new ticket

Check ticket status

Knowledge base

General Overview

Platform FAQ (11)

- Current System Status
- Are there rate limits to the API?
- What is the current production version of t...
- How can I download your entire dataset?
- Do you provide a SPARQL End Point?

» See all 11 articles

Release Notes (2)

- 1.3 API
- 1.4 API

Getting started (2)

- How do I get access to the API?
- Reviewing API query results: Copy query U...

Support portal FAQ (2)

- How do I add a solution to the portal?
- One of your solutions should be changed, ...

Community forums

Showing recent updates

Start a new topic

Open PHACTS Forums

Announcements (4)

- System Issues
  Posted by **Open PHACTS**, a year ago ,
  Last Reply by Open PHACTS a year ago
- Developers Mailing List
  Posted by **Open PHACTS**, a year ago
- Staying Up To Date
  Posted by **Open PHACTS**, a year ago

» See all 4 topics

General Discussion (4)

- New Datasets

support.openphacts.org

Open PHACTS

Open Pharmacological Space

The Open PHACTS Foundation

Home | The Foundation | What We Do | Get Involved | News & Events | Contact Us

The Application Ecosystem

Browsers

Open PHACTS

Browse and search the data within the Open PHACTS Discovery Platform. Developed by the University of Manchester and University of Vienna

Open PHACTS Explorer »

SciBite

Connects the latest news and events in Pharma and Biotech directly to Open PHACTS pharmacology data. Developed by SciBite Limited

SciBite »

Predictions

GARField

Intuitive predicts target pharmacology based on the Similar Ensemble Approach. Developed by the Technical University of Denmark

GARField »

collector

Extracts data to build QSAR predictive models with data from the eTOX project. Developed by PSMAR as part of the eTOX project

Collector »

Advanced Analytics

ChemBioNavigator

Visualise the chemical and biological space of a molecule group. Developed by the University of Hamburg and BioSolveIT GmbH

ChemBioNavigator »

PHARMATREK

Navigate pharmacological space in a flexible and interactive way. Developed by the Consorci Mar Parc de Salut de Barcelona (PSMAR)

PharmaTrek »

Target Dossier

Interconnecting Open PHACTS data with multiple target centric services. Developed by the Spanish National Cancer Research Centre (CNIO)

Target Dossier »

utopia

Allows the semantic enrichment of scientific articles in PDF format. Developed by the University of Manchester

Utopia »

Workflow Integration

accelrys Pipeline Pilot

A repository of useful Pipeline Pilot components and workflows has been developed. Developed by the Open PHACTS Scientific Community

Pipeline Pilot Components »

KNIME

A KNIME repository of components and workflows has been developed. Developed by the Open PHACTS Scientific Community

KNIME Repository »

he

Helium for Excel Community Edition contains three functions that use the Open PHACTS API. Developed by Ceiba Solutions

Helium for Excel »

AQnowledge Semantics for Science

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

AQnowledge »

How do I build my own application?

The Open PHACTS API allows external applications to query the data within the Open PHACTS Discovery Platform. The data can be combined with other datasets, analysed and visualised in any number of ways.

Open PHACTS Services »

Would you like your application mentioned on this page?

If you have an application or application idea that could use the Open PHACTS API, please contact us and we can tell our growing community of developers, app users and scientists.

Contact us »

http://www.openphactsfoundation.org/apps.html

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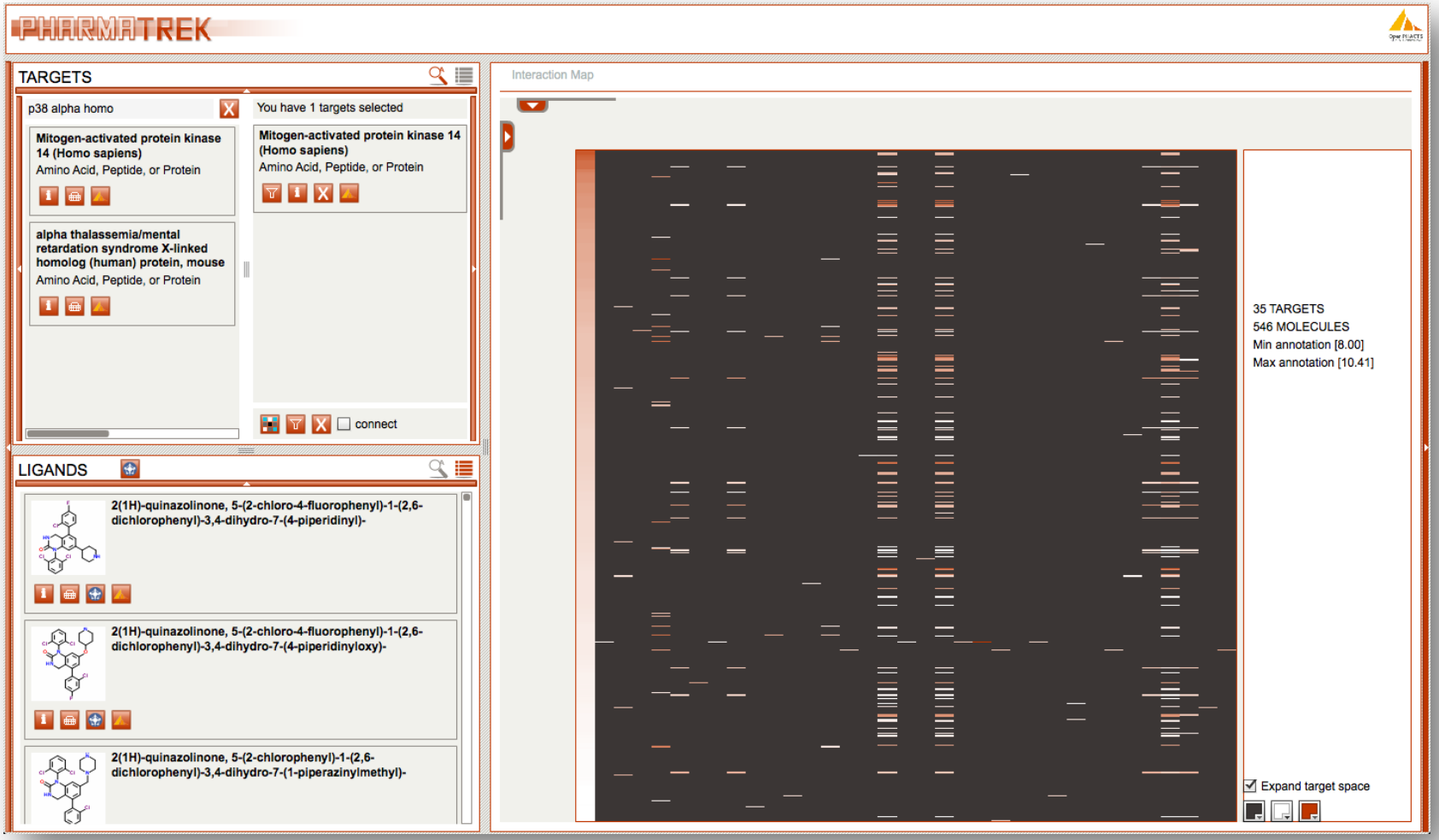

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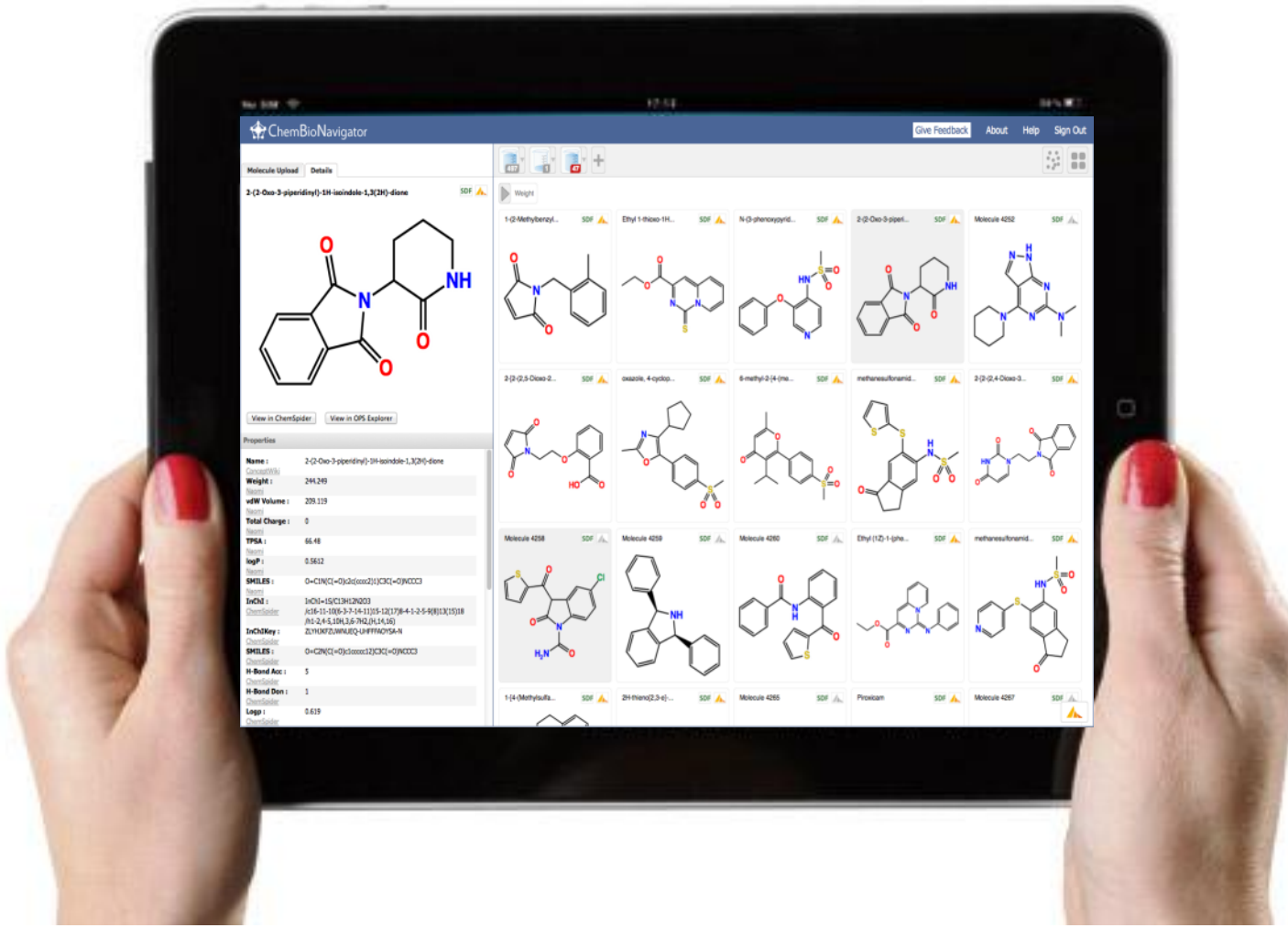
Open Pharmacological Space



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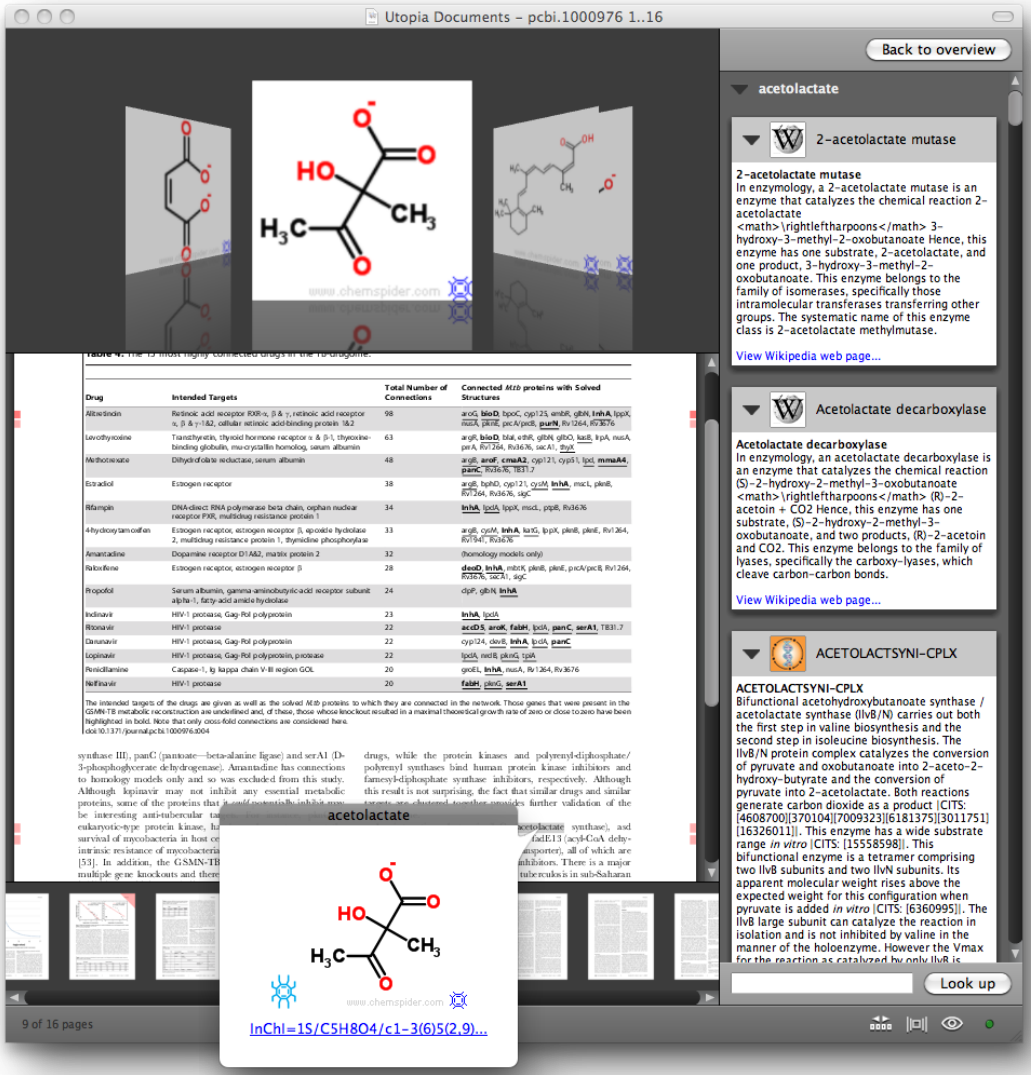

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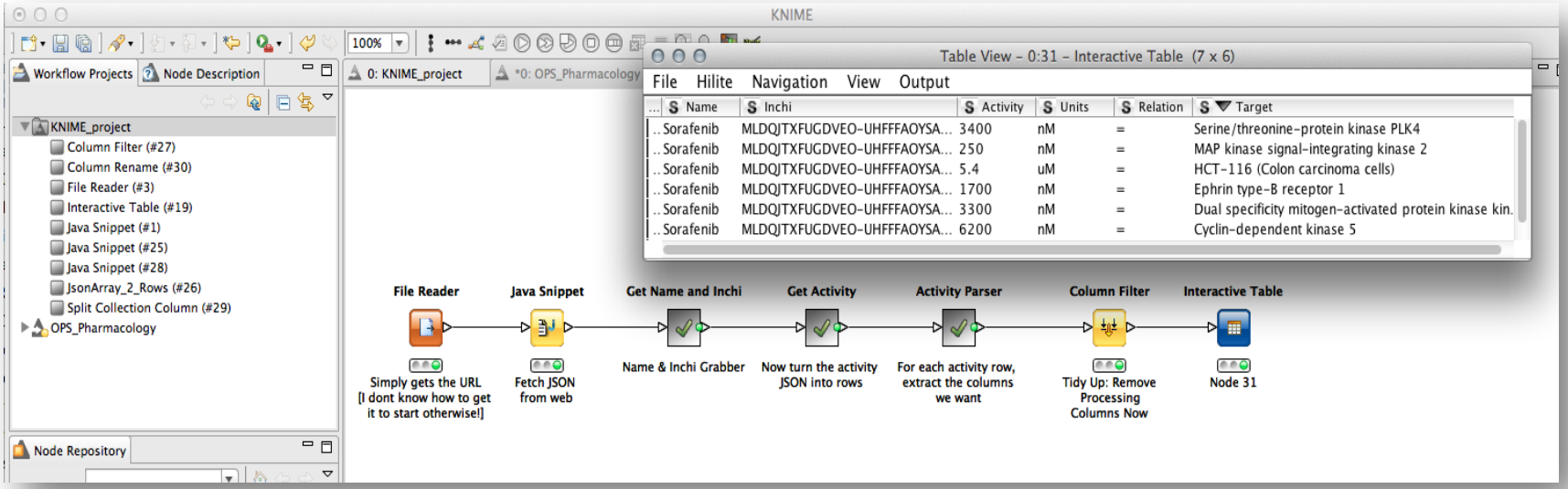

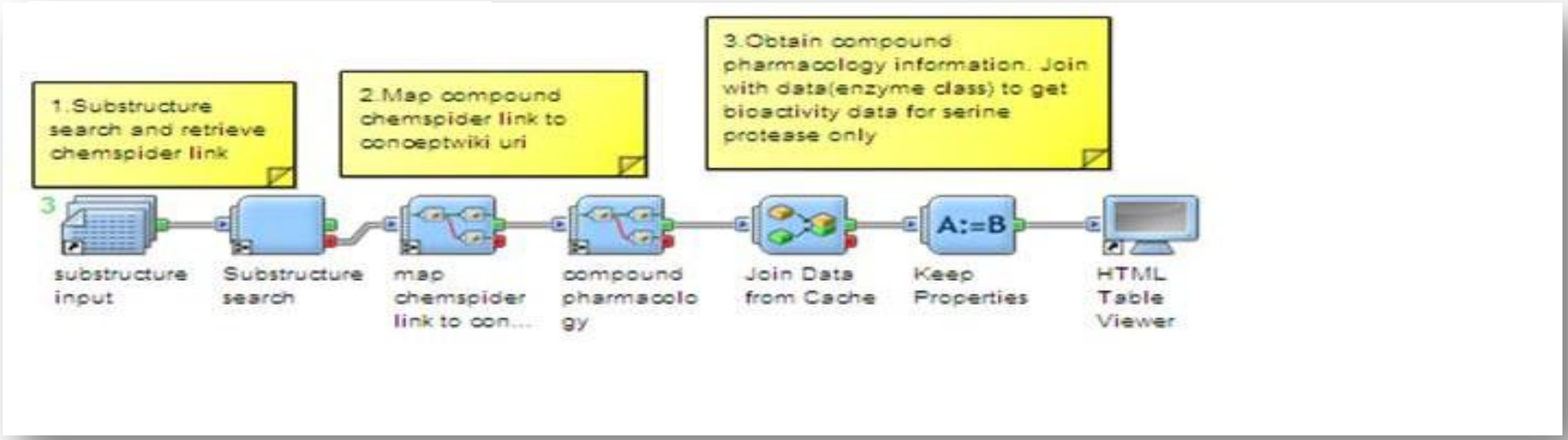

Open PHACTS
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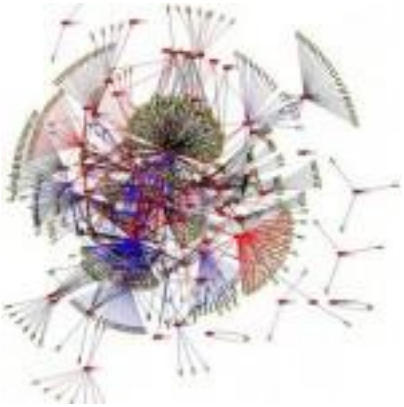
Sustaining Impact

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

- …and more resource for future development



Open PHACTS
Open Pharmacological Space

Open PHACTS Mission:

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

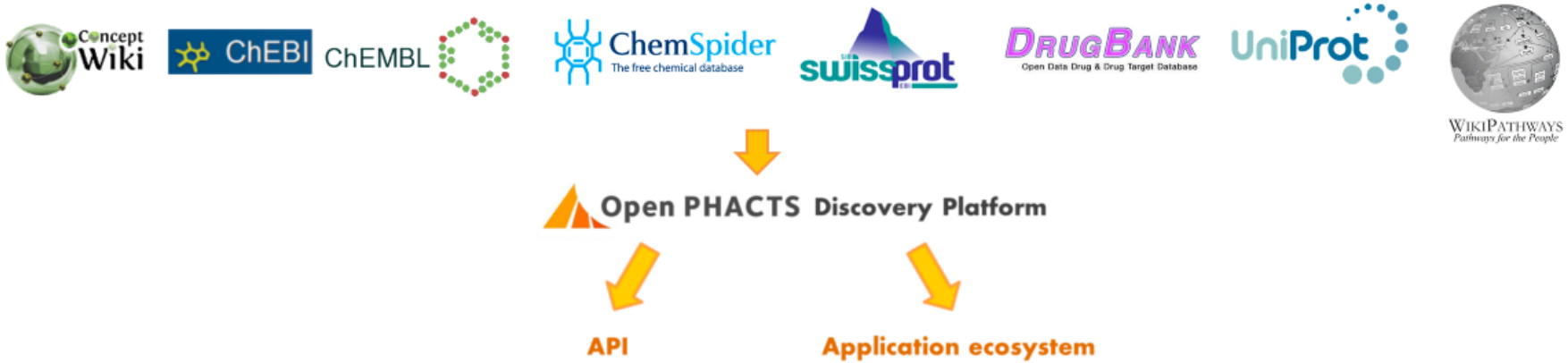

Open PHACTS
Open Pharmacological Space
Open PHACTS Associate Partner Community

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.



Membership Benefits

The Open PHACTS Foundation

The not-for-profit Foundation maintains the Open PHACTS Discovery Platform, a versatile infrastructure of integrated biomedical data, and actively engages an ecosystem of industry and academic semantic web experts.

Integrated data:

- Pharmacological
- Physicochemical
- Disease
- Gene
- Pathways

Steer the direction

- Prioritise new projects
- Get involved with Foundation governance
- Identify development opportunities
- Propose new data sources to include
- Develop new use-cases and workflows
- [illegible]

Training opportunities

Enjoy training opportunities by experts.

Early access to releases

Members have early access to infrastructure and platform updates and new releases, including a locally installable system

Engage a community of experts and peers

The Foundation serves a unique and vibrant scientific community, facilitating collaboration between the pharma industry, academia & SMEs.

Influence the security policy

Membership Levels

[illegible] turnover. Pay in cash or by donating people-hours to the Foundation.

Full — Nominate and vote for the Board of Trustees

Contributing — Vote for the Board of Trustees

Individual **Non-voting** — Get involved in projects and collaborate

www.openphactsfoundation.org

info@openphactsfoundation.org

Open PHACTS Foundation
c/o Royal Society of Chemistry,
Thomas Graham House,
Science Park, Cambridge, CB4 0WF

[illegible]

bryn@openphactsfoundation.org

Acknowledgements

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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
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The Open PHACTS Foundation
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Maastricht University
Aqnowledge
University of Santiago de Compostela
Rheinische Friedrich-Wilhelms-Universität Bonn
AstraZeneca
Pfizer

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