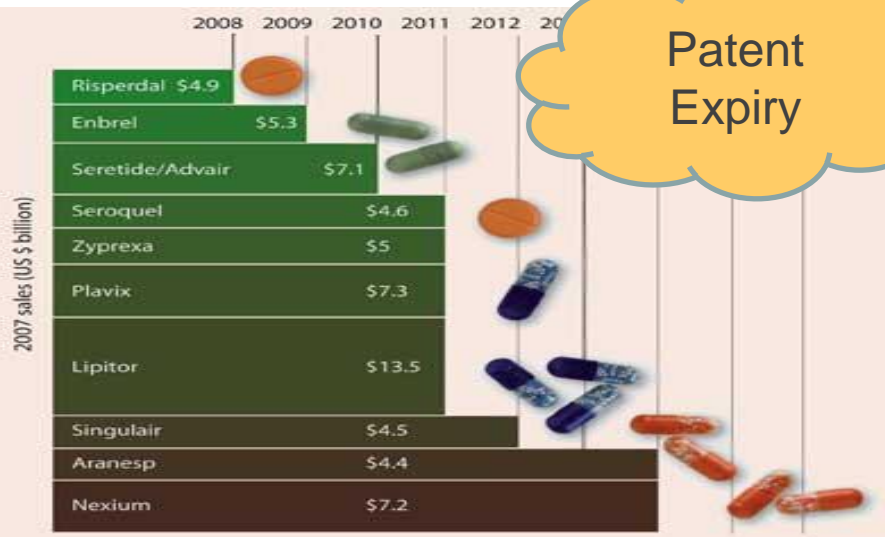


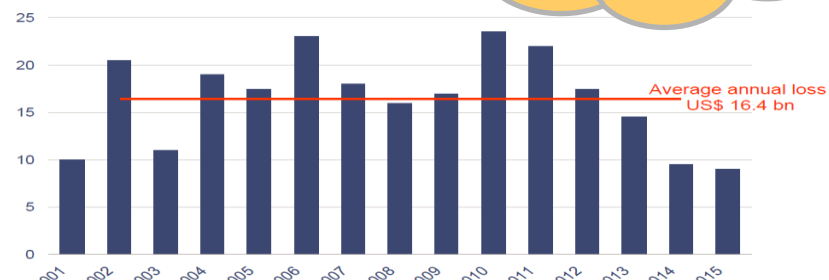
The Open PHACTS Discovery Platform

Semantic Data Integration for Life Sciences



Resulting in a sales revenue

Value of patent expiries 2001-2015 (constant US\$)



\$157 billion sales exposed to generic competition by 2015

PricewaterhouseCoopers LLP

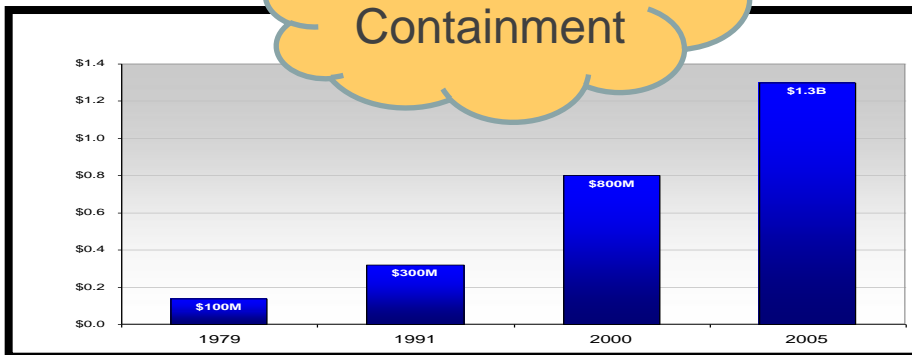
Source: IMS Health Midas

7

PwC - Pharma 2020 - Value of Patent Expiries

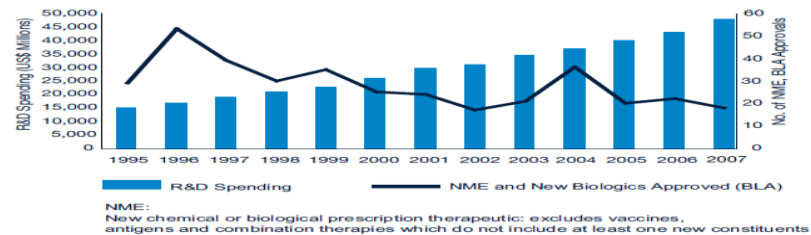
<http://www.rsc.org/chemistryworld/Issues/2009/January/PharmaRefocusesOnThePatentCliff.asp>

Cost Containment



Improve R&D Productivity

Figure 1: The decline in R&D productivity



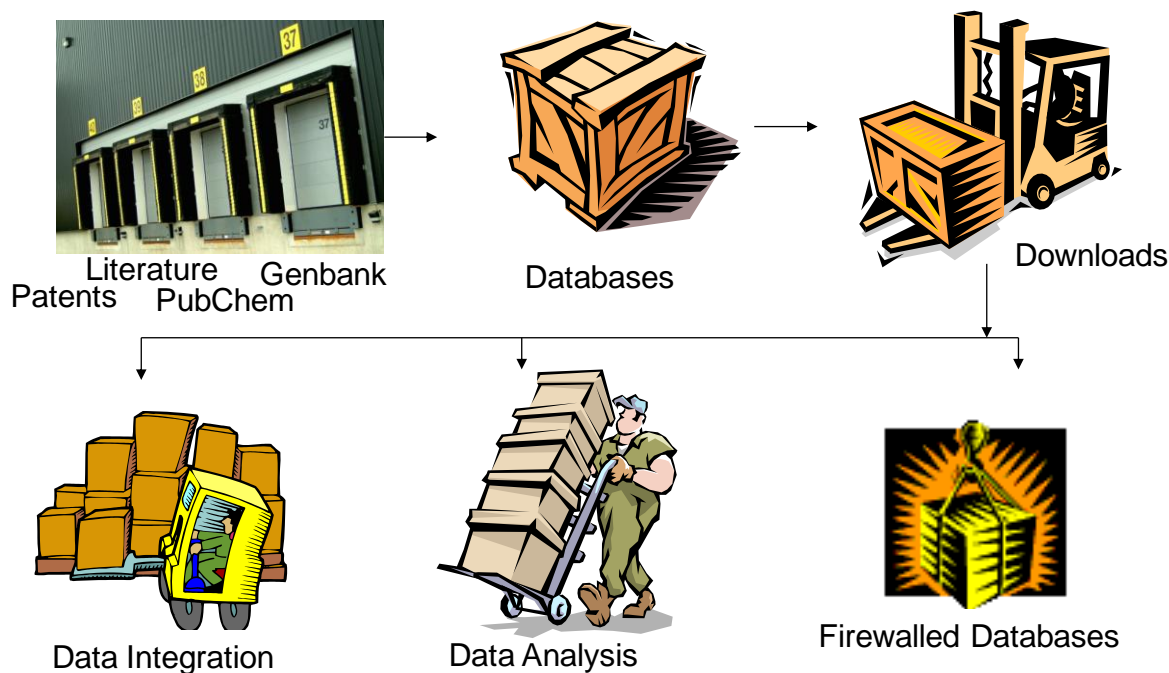
Source: FDA CDER, PhRMA and PricewaterhouseCoopers analysis

Note: Data on R&D spending for non-PhRMA companies are not included here.



Pre-competitive Informatics:

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



**Repeat @
X each
company**

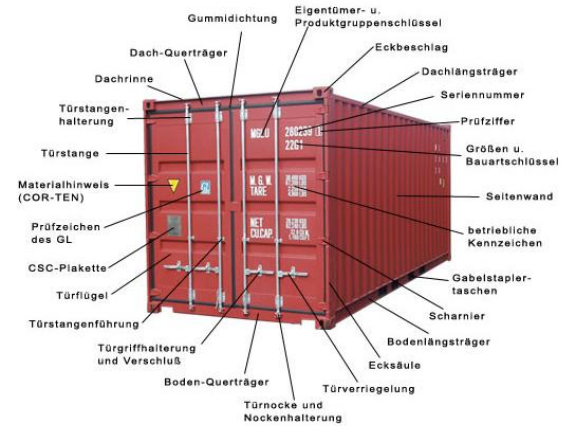


Over the last decade

- 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





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



Open PHACTS Mission:
Integrate Multiple Research
Biomedical Data Resources
Into A Single **Open & Free**
Access Point



"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 <math>< 1 \mu\text{M}</math>"



ChEMBL

DrugBank

Gene
Ontology

Wikipathways

GeneGo

ChEBI

UniProt

UMLS

GVKBio

ConceptWiki

ChemSpider

TrialTrove

TR Integrity



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 current in serine pr
38	13	8	Retrieve all structure (v
41	13	8	A project is compounds the target o level of the
44	13	8	Give me all
46	13	8	Give me th (disease)
59	14	8	Identify all



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 Azzaoui¹, Edgar Jacoby¹⁴, Stefan Senger², Emiliano Cuadrado Rodríguez³, Mabel Loza³, Barbara Zdrzil⁴, Marta Pinto⁴, Antony J. Williams⁵, Victor de la Torre⁶, Jordi Mestres⁷, Manuel Pastor⁷, Olivier Taboureau⁸, Matthias Rarey⁹, Christine Chichester¹⁰, Steve Pettifer¹¹, Niklas Blomberg¹², a, Lee Harland¹³, Bryn Williams-Jones¹³, Gerhard F. Ecker⁴.  



The Open PHACTS Discovery Platform

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




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

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



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>



HOW STANDARDS PROLIFERATE:
(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC.)



<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



HELLO
my name is

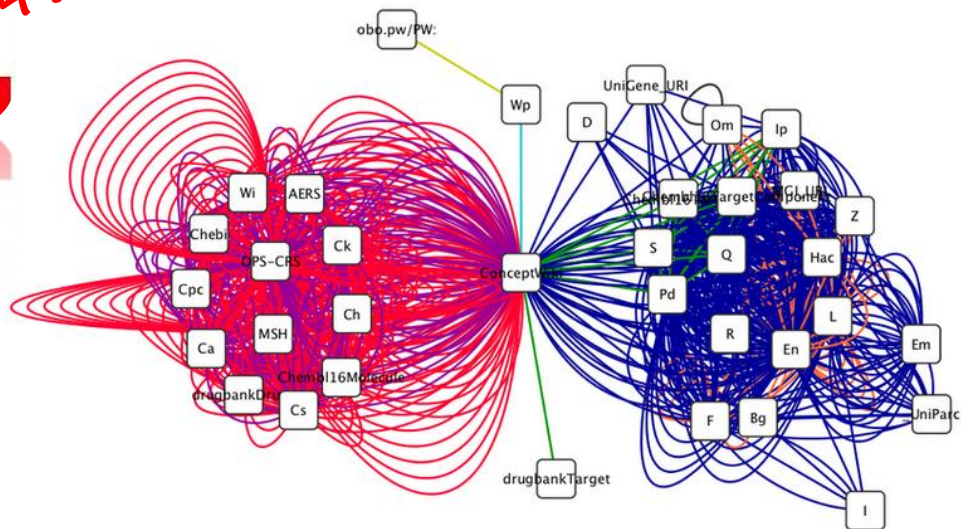
~~RS_2353~~

~~GB:29384~~

~~P12047~~

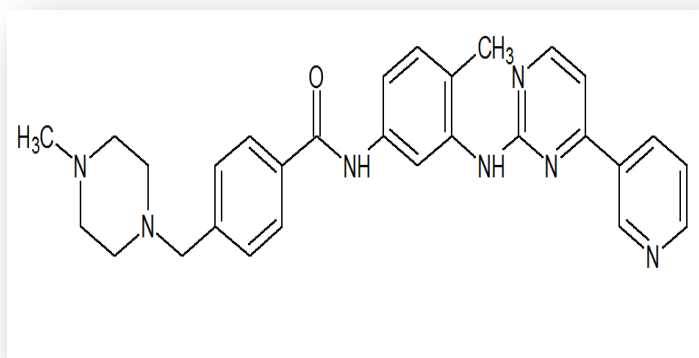
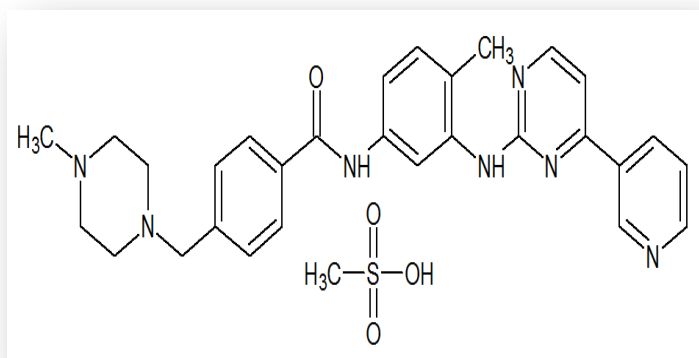
~~X31045~~

P12047





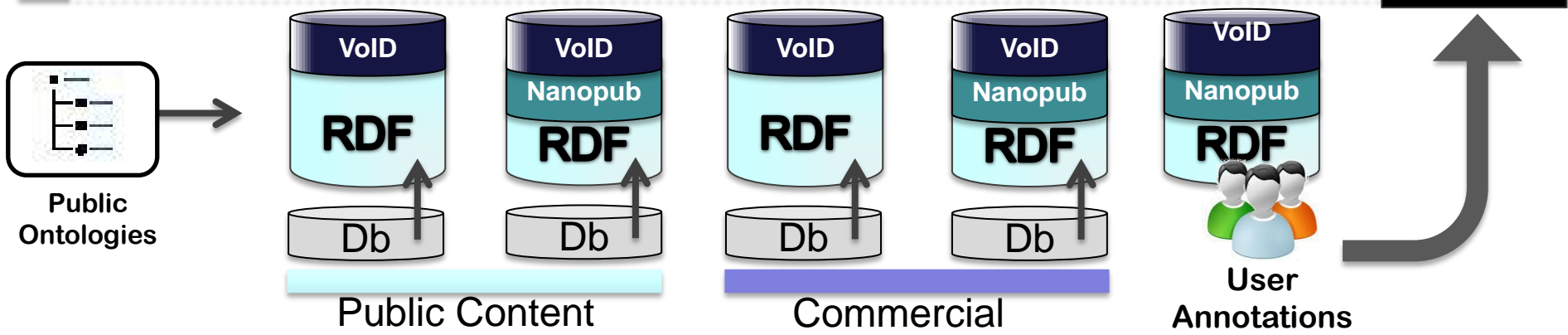
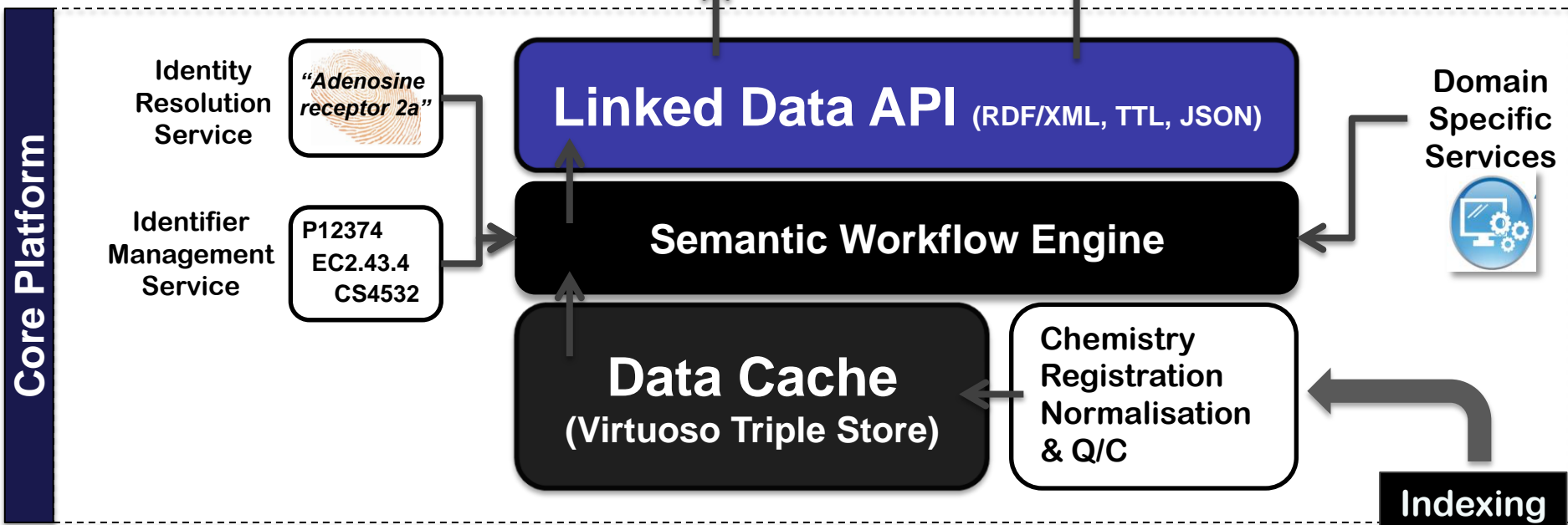
Are These Two Molecules The Same(*)



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



Apps



[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®



ConceptWiki



github
SOCIAL CODING



BridgeDb
connecting knowledge



ChEMBL



UniProt



DRUGBANK
Open Data Drug & Drug Target Database



Open PHACTS Support Portal

Welcome
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[Home](#)

[Solutions](#)

[Forums](#)

How can we help you today?

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

Posted by **Lee Madland**, a year ago



The Application Ecosystem

Browsers



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

[Open PHACTS Explorer »](#)



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

[SciBite »](#)

Predictions



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

[GARfield »](#)



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



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

[ChemBioNavigator »](#)



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

[PharmaTrek »](#)



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

[Target Dossier »](#)



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

[Utopia »](#)

Workflow Integration



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

[Pipeline Pilot Components »](#)



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

[KNIME Repository »](#)



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

[Helium for Excel »](#)



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 »](#)



ChemBioNavigator

Molecule Upload Details

2-(2-Oxo-3-piperidinyl)-1H-isindole-1,3(2H)-dione

View in ChemSpider View in OPS Explorer

Properties

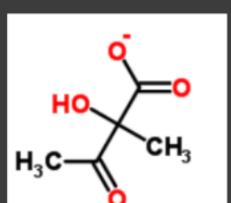
Name: 2-(2-Oxo-3-piperidinyl)-1H-isindole-1,3(2H)-dione
 Molecular Weight: 244.249
 vdw Volume: 205.119
 Total Charge: 0
 TPSA: 66.48
 logP: 0.562
 SMILES: O=C1NC(=O)C2=CC=CC=C2C1=CN3CCCC3=O
 InChI: InChI=1S/C13H12N2O3/c16-11-10(-2)-7-14-11(15)-12(17)-4-1-2-5-6(13)/15118/h1-2,4-5,10h,13,6-7h2,11,14,16/z11/t12/w1/b2-4/q11/p15-18
 InChIKey: ZJHNFZQWALBQ-UPFFH915A-H
 SMILES: O=C1NC(=O)C2=CC=CC=C2C1=CN3CCCC3=O
 H-Bond Acc: 5
 H-Bond Don: 1
 LogP: 0.619

Grid of molecules:

- 1-(2-Methylbenzyl)-2-oxo-1,2,3,4-tetrahydroisoindol-3-one
- Ethyl 1-thioxo-1H-imidazo[4,5-b]pyridine-2-carboxylate
- N-(2-phenoxypyridin-5-yl)acetamide
- 2-(2-Oxo-3-piperidinyl)-1H-isindole-1,3(2H)-dione
- Molecule 4262
- 2-(2-Oxo-3-piperidinyl)-1H-isindole-1,3(2H)-dione
- oxazole, 4-cyano-2-thio-
- 6-methyl-2-(4-methylphenyl)-1,2,4-triazole
- methanesulfonamide
- 2-(2-(2,4-Dioxo-3,4-dihydro-1,2,4-triazin-5-yl)ethyl)-1H-imidazo[4,5-b]pyridine-2-carboxylate
- Molecule 4258
- Molecule 4259
- Molecule 4260
- Ethyl (1Z)-1-phenyl-1H-imidazo[4,5-b]pyridine-2-carboxylate
- methanesulfonamide
- 1-(4-Methylsulfonylphenyl)-2-oxo-1,2,3,4-tetrahydroisoindol-3-one
- 2H-Pheno(2,3-e)-[1,2,4]triazole
- Molecule 4265
- Procainamide
- Molecule 4267



Utopia Documents - pcbi.1000976 1..16
Back to overview



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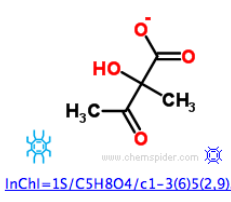
Table 4: The 13 most highly connected drugs in the network.

Drug	Intended Targets	Total Number of Connections	Connected <i>Mtb</i> proteins with Solved Structures
Albendazole	Retinoic acid receptor RXR- α , β & γ , retinoic acid receptor α , β & γ -1A2, cellular retinoic acid binding protein 1&2	98	<i>arcG</i> , <i>hspD</i> , <i>hspC</i> , <i>opp123</i> , <i>embR</i> , <i>glnA</i> , <i>hnhA</i> , <i>lpxX</i> , <i>NDX</i> , <i>RD7E</i> , <i>pcA</i> / <i>pcB</i> , <i>purN</i> , <i>Rv1264</i> , <i>Rv3776</i>
Levofloxacin	Topoisomerase, thyroid hormone receptor α & β -1, thyroxine-binding globulin, myocystatin homolog, serum albumin	63	<i>argK</i> , <i>hspD</i> , <i>hspA</i> , <i>hspB</i> , <i>glnA</i> , <i>glnB</i> , <i>hspK</i> , <i>hspL</i> , <i>hspM</i> , <i>hspN</i> , <i>Rv1234</i> , <i>Rv1636</i> , <i>secA1</i> , <i>zmpC</i>
Methotrexate	Dihydrofolate reductase, serum albumin	48	<i>argK</i> , <i>anfF</i> , <i>cmaA2</i> , <i>opp121</i> , <i>opp151</i> , <i>lpx</i> , <i>mmaA4</i> , <i>panC</i> , <i>Rv1636</i> , <i>TE31.7</i>
Estradiol	Estrogen receptor	38	<i>argK</i> , <i>hspD</i> , <i>opp121</i> , <i>opp151</i> , <i>hnhA</i> , <i>mecA</i> , <i>plefB</i> , <i>Rv1264</i> , <i>Rv1636</i> , <i>hspC</i>
Rifampin	DNA-directed RNA polymerase beta chain, ophiactin nuclear receptor PXR, multidrug resistance protein 1	34	<i>hnhA</i> , <i>lpxC</i> , <i>lpxK</i> , <i>lpxM</i> , <i>mecA</i> , <i>ppqB</i> , <i>Rv1636</i>
Ahydroxytamoxifen	Estrogen receptor, estrogen receptor β , epoxide hydrolase 2, multidrug resistance protein 1, tyrosine phosphatase	33	<i>argK</i> , <i>opp151</i> , <i>hnhA</i> , <i>hspD</i> , <i>hspK</i> , <i>plefB</i> , <i>plefE</i> , <i>Rv1264</i> , <i>Rv1636</i> , <i>hspC</i>
Amantadine	Dopamine receptor D1A2, matrix protein 2	32	(homology models only)
Ribavirin	Estrogen receptor, estrogen receptor β	28	<i>hspD</i> , <i>hnhA</i> , <i>mecA</i> , <i>plefB</i> , <i>plefE</i> , <i>pcA</i> / <i>pcB</i> , <i>Rv1264</i> , <i>Rv1636</i> , <i>hspC</i> , <i>hspE</i>
Ropivacaine	Serum albumin, gamma-aminobutyric acid receptor subunit α 1-1, fatty acid amide hydrolase	24	<i>opp151</i> , <i>glnA</i> , <i>hnhA</i>
Didanosine	HIV-1 protease, Gag-Pol polyprotein	23	<i>hnhA</i> , <i>lpxC</i>
Ribavirin	HIV-1 protease	22	<i>acdD3</i> , <i>anfF</i> , <i>fadE</i> , <i>lpxC</i> , <i>panC</i> , <i>serA1</i> , <i>TE31.7</i>
Zidovudine	HIV-1 protease, Gag-Pol polyprotein	22	<i>opp123</i> , <i>secE</i> , <i>hnhA</i> , <i>lpxC</i> , <i>panC</i>
Lopinavir	HIV-1 protease, Gag-Pol polyprotein, protease	22	<i>lpxC</i> , <i>mecA</i> , <i>hspD</i> , <i>hspK</i>
Penciclovir	Capsase-1, γ -lappa chain V-B region GOL	20	<i>glnE</i> , <i>hnhA</i> , <i>mecA</i> , <i>Rv1264</i> , <i>Rv1636</i>
Nelfinavir	HIV-1 protease	20	<i>fadE</i> , <i>plefB</i> , <i>serA1</i>

The intended targets of the drugs are given as well as the solved *Mtb* proteins to which they are connected in the network. Those genes that were present in the GSMN-TB metabolic reconstruction are underlined and, of these, those whose knockout resulted in a maximal theoretical growth rate of zero or close to zero have been highlighted in bold. Note that only cross-fold connections are considered here. doi:10.1371/journal.pcbi.1000976.t004

synthase III), *panC* (panama—beta-alanine ligase) and *serA1* (D-Typhosphoglycerate dehydrogenase). Amantadine has connections to homology models only and so was excluded from this study. Although lopinavir may not inhibit any essential metabolic proteins, some of the proteins that *panC* and *serA1* are connected to be interesting anti-tubercular targets. eukaryotic-type protein kinase, has survival of mycobacteria in host cell. In addition, the GSMN-TB multiple gene knockouts and three drugs, while the protein kinases and poly(ADP-ribose) polymerase synthase bind human protein kinase inhibitors and farnesyl-diphosphate synthase inhibitors, respectively. Although this result is not surprising, the fact that similar drugs and similar

acetolactate



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InChI=1S/CSH8O4/c1-3(6)5(2,9)...

acetolactate

2-acetylacrylate

In enzymology, a 2-acetylacrylate mutase is an enzyme that catalyzes the chemical reaction 2-acetylacrylate + H₂O \rightleftharpoons 3-hydroxy-2-methyl-2-oxobutanoate + H⁺. This enzyme has one substrate, 2-acetylacrylate, and one product, 3-hydroxy-2-methyl-2-oxobutanoate. This enzyme belongs to the family of isomerases, specifically those intramolecular transferases transferring other groups. The systematic name of this enzyme class is 2-acetylacrylate methylmutase.

[View Wikipedia web page...](#)

Acetolactate decarboxylase

In enzymology, an acetolactate decarboxylase is an enzyme that catalyzes the chemical reaction (S)-2-hydroxy-2-methyl-3-oxobutanoate + H₂O \rightleftharpoons (R)-2-acetoin + CO₂. Hence, this enzyme has one substrate, (S)-2-hydroxy-2-methyl-3-oxobutanoate, and two products, (R)-2-acetoin and CO₂. This enzyme belongs to the family of lyases, specifically the carboxy-lyases, which cleave carbon-carbon bonds.

[View Wikipedia web page...](#)

ACETOLACTATYNI-CPLX

Bifunctional acetoxybutanoate synthase / acetolactate synthase (IlvN) carries out both the first step in valine biosynthesis and the second step in isoleucine biosynthesis. The IlvN protein complex catalyzes the conversion of pyruvate and oxobutanoate into 2-aceto-2-hydroxy-butyrate and the conversion of pyruvate into 2-acetylacrylate. Both reactions generate carbon dioxide as a product [CITS: [4608700][370104][7009323][6181375][3011751][1632601]]. This enzyme has a wide substrate range *in vitro* [CITS: [15558598]]. This bifunctional enzyme is a tetramer comprising two IlvB subunits and two IlvN subunits. Its apparent molecular weight rises above the expected weight for this configuration when pyruvate is added *in vitro* [CITS: [6360995]]. The IlvB large subunit can catalyze the reaction in isolation and is not inhibited by valine in the manner of the holoenzyme. However the Vmax for the reaction as catalyzed by only IlvB is

[Look up](#)

9 of 16 pages



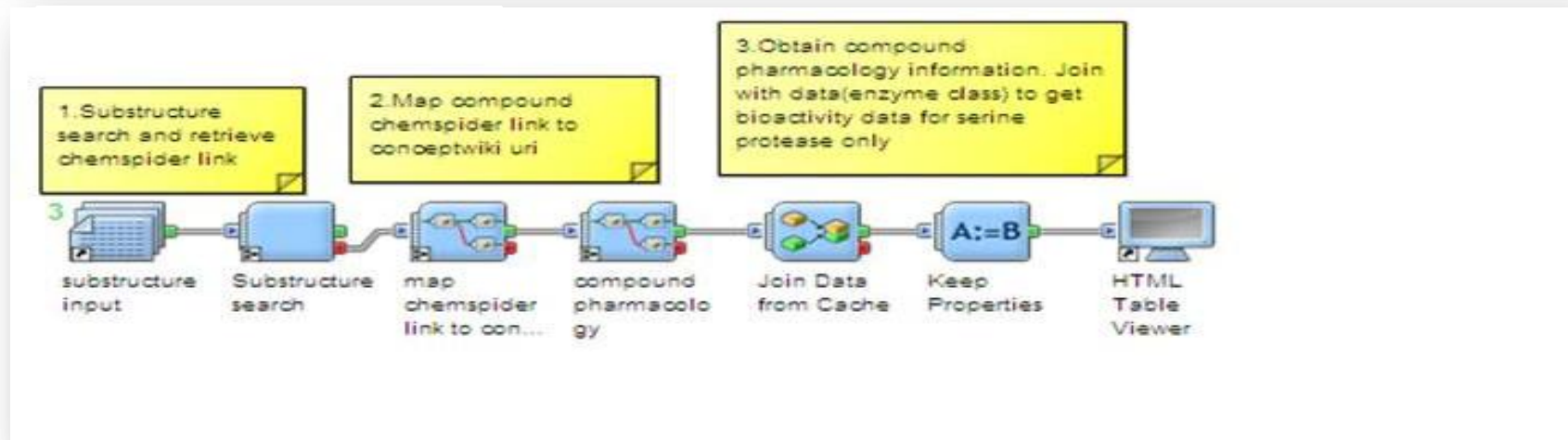
KNIME

Table View - 0:31 - Interactive Table (7 x 6)

Name	Inchi	Activity	Units	Relation	Target
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	3400	nM	=	Serine/threonine-protein kinase PLK4
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	250	nM	=	MAP kinase signal-integrating kinase 2
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	5.4	uM	=	HCT-116 (Colon carcinoma cells)
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	1700	nM	=	Ephrin type-B receptor 1
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	3300	nM	=	Dual specificity mitogen-activated protein kinase kin.
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	6200	nM	=	Cyclin-dependent kinase 5

Workflow Nodes:

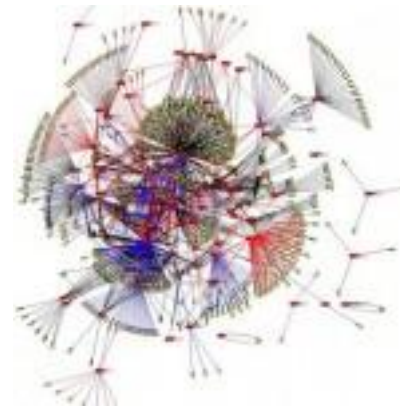
- File Reader**: Simply gets the URL [I dont know how to get it to start otherwise!]
- Java Snippet**: Fetch JSON from web
- Get Name and Inchi**: Name & Inchi Grabber
- Get Activity**: Now turn the activity JSON into rows
- Activity Parser**: For each activity row, extract the columns we want
- Column Filter**: Tidy Up: Remove Processing Columns Now
- Interactive Table**: Node 31





Sustaining Impact

- ✦ “Software is free like puppies are free - they both need money for maintenance”
- ✦ ...and more resource for future development





Open PHACTS Mission:
Integrate Multiple Research
Biomedical Data Resources
Into A Single **Open & Free**
Access Point



Open PHACTS Associate Partner Community

The image displays a diverse array of logos representing the Open PHACTS Associate Partner Community. The logos are arranged in a grid-like fashion around a central dark grey rounded rectangle containing the text "Open PHACTS Associate Partner Community".

Visible logos include:

- Academic and Research Institutions:** Universität Wien, DTU, Universität Hamburg, VU Amsterdam, Leids Universitair Medisch Centrum, Maastricht University, The University of Manchester, USC, universität bonn, ESTEVE, NOVARTIS, MERCK, Lindbeck, AstraZeneca, SIB (Swiss Institute of Bioinformatics), EMBL-EBI, janssen, OPENLINK SOFTWARE, syngenta, THOMSON REUTERS, VIVO.
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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.



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Membership Benefits



Integrated data:	
Pharmacological	
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Pathways	

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.

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
-

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

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

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Nominate and vote for the Board of Trustees

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Get involved in projects and collaborate

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Acknowledgements



GlaxoSmithKline – Coordinator

Universität Wien – Managing entity

Technical University of Denmark
University of Hamburg, Center for
Bioinformatics

BioSolveIT GmbH

Consorti Mar Parc de Salut de Barcelona

Leiden University Medical Centre

Royal Society of Chemistry

Vrije Universiteit Amsterdam

Novartis

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Janssen Esteve Almirall

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