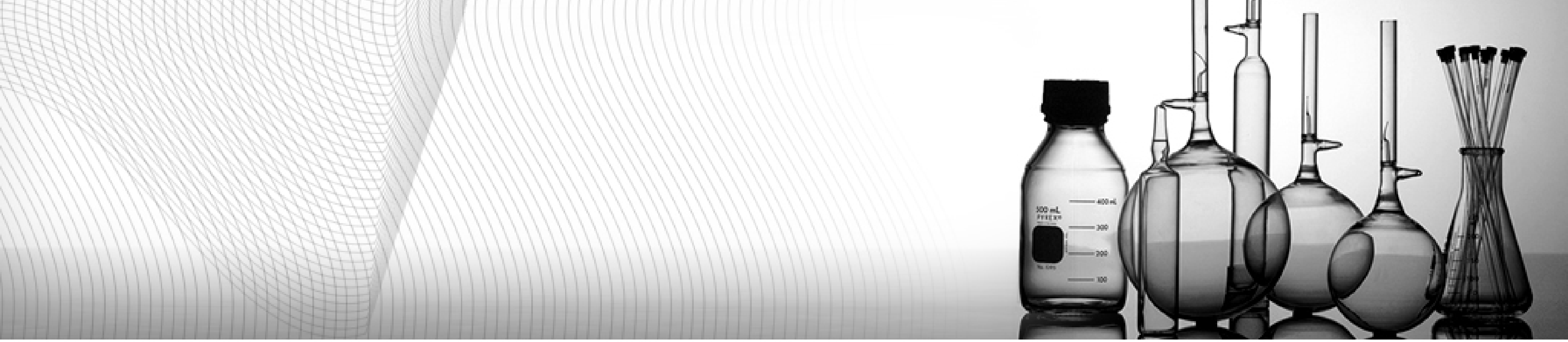


Open PHACTS
Open Pharmacological Space

A Data Platform for Drug Discovery

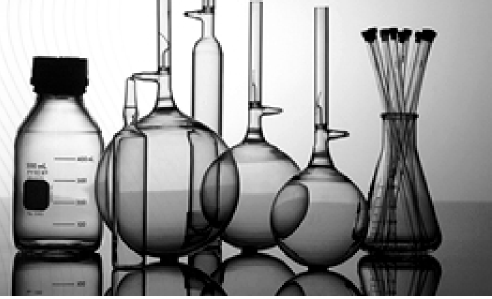
Paul Groth (@pgroth)
http://www.few.vu.nl/~pgroth

VU VRIJE UNIVERSITEIT AMSTERDAM

1. WHY
2. THE PLATFORM
3. APPS
4. THE FUTURE

Open PHACTS

Open Pharmacological Space



Pfizer

universität wien

RSC | Advancing the Chemical Sciences

130 jaar VU VRIJE UNIVERSITEIT AMSTERDAM

AstraZeneca

gsk GlaxoSmithKline

DTU

UHH Universität Hamburg

cnio

MANCHESTER 1824

ESTEVE closer to you

NOVARTIS

35th anniversary Maastricht University Leading in Learning!

AQnowledge™ Semantics for Science

MERCK

Lundbeck

Bio Solve IT

Parc de Salut Barcelona MAR

USC UNIVERSIDADE DE SANTIAGO DE COMPOSTELA

universitätbonn

Lilly

LUMC

janssen

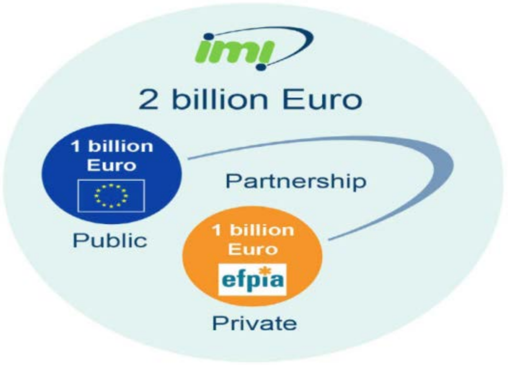
EMBL-EBI

connecteddiscovery

nbic

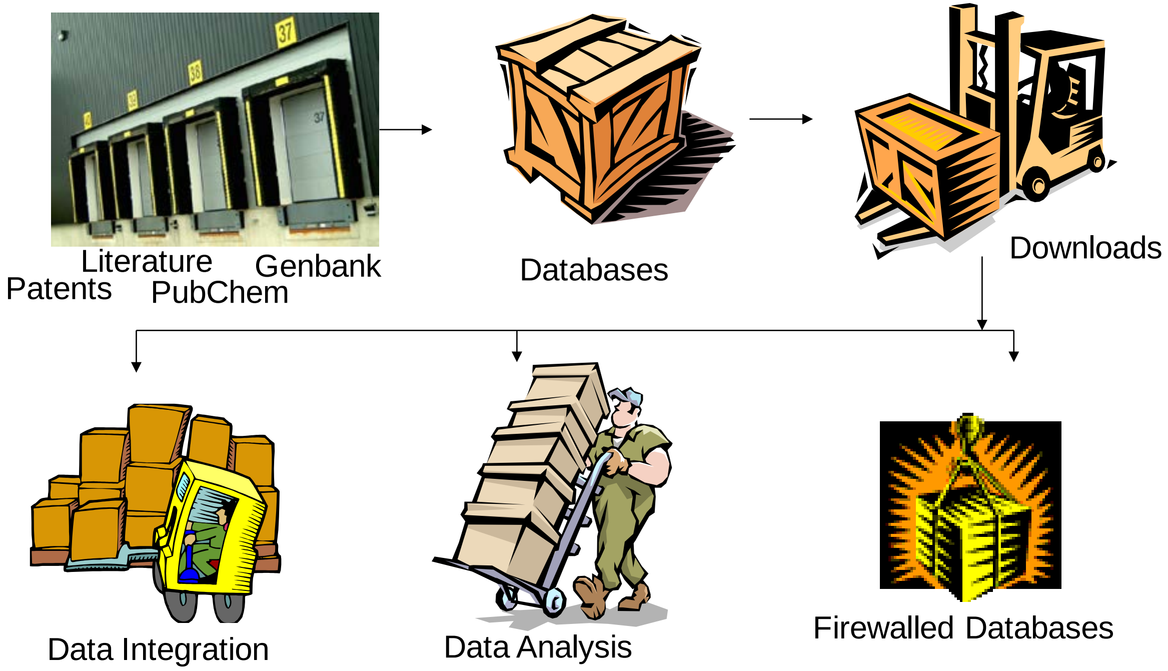
OPENLINK SOFTWARE Making Technology Work For You®

SIB Swiss Institute of Bioinformatics



Pre-competitive Informatics:

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



Literature Genbank
Patents PubChem

Databases

Downloads

Data Integration

Data Analysis

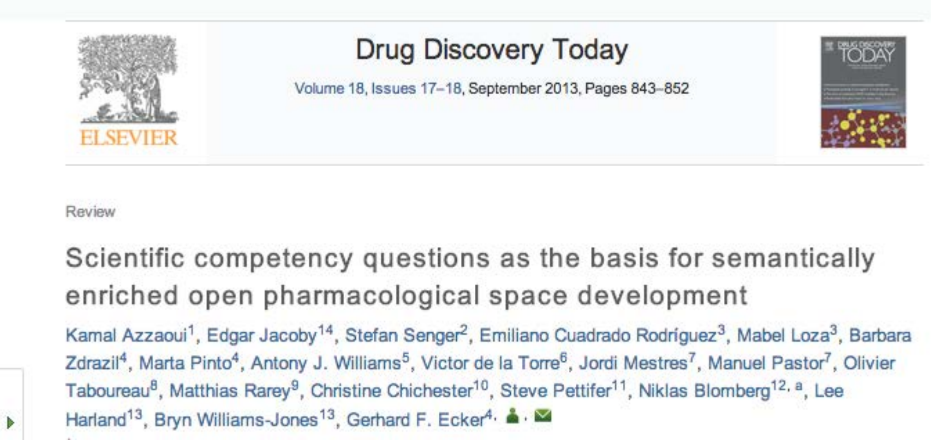
Firewalled Databases

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

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 interaction profile, give me compounds similar to it.
37	13	8	The current Factor Xa lead series is characterised by substructure X. Retrieve all bioactivity data in serine protease assays for molecules that contain substructure X.
38	13	8	Retrieve all experimental and cli structure (with options to match
41	13	8	A project is considering Protein compounds known to modulate the target directly? i.e. return all level of the target family (i.e. PK
44	13	8	Give me all active compounds o
46	13	8	Give me the compound(s) which (disease)
59	14	8	Identify all known protein-protei



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,] ✉

http://www.sciencedirect.com/science/article/pii/S1359644613001542

"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

Open PHACTS

Open Pharmacological Space

▶ 1st Hackathon

▶ Hackathon 2

▶ GUI Hackathon

▶ Focused User Feedback

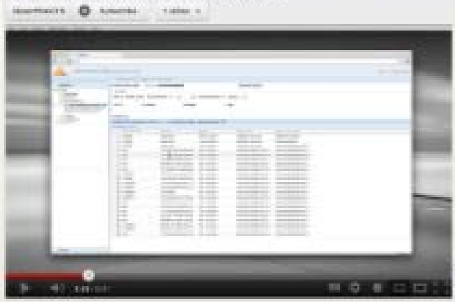
▶ Hackathon 3

▶ Alpha for public release

▶ Platform On Hosting Provider

▶ Revised Platform Implementation

Open PHACTS 6 Month Lashup Demo



▶ Hosting Selected

OPENLINK SOFTWARE Making Technology Work For You!®

▶ Hosting Partner On-board

▶ Drive Team In-Place

▶ Project Start

▶ Tech Team Kickoff

▶ Prototype

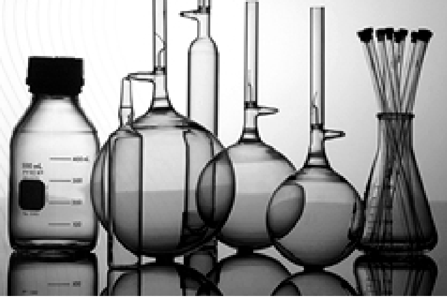
▶ Linked Data API

▶ Usathon

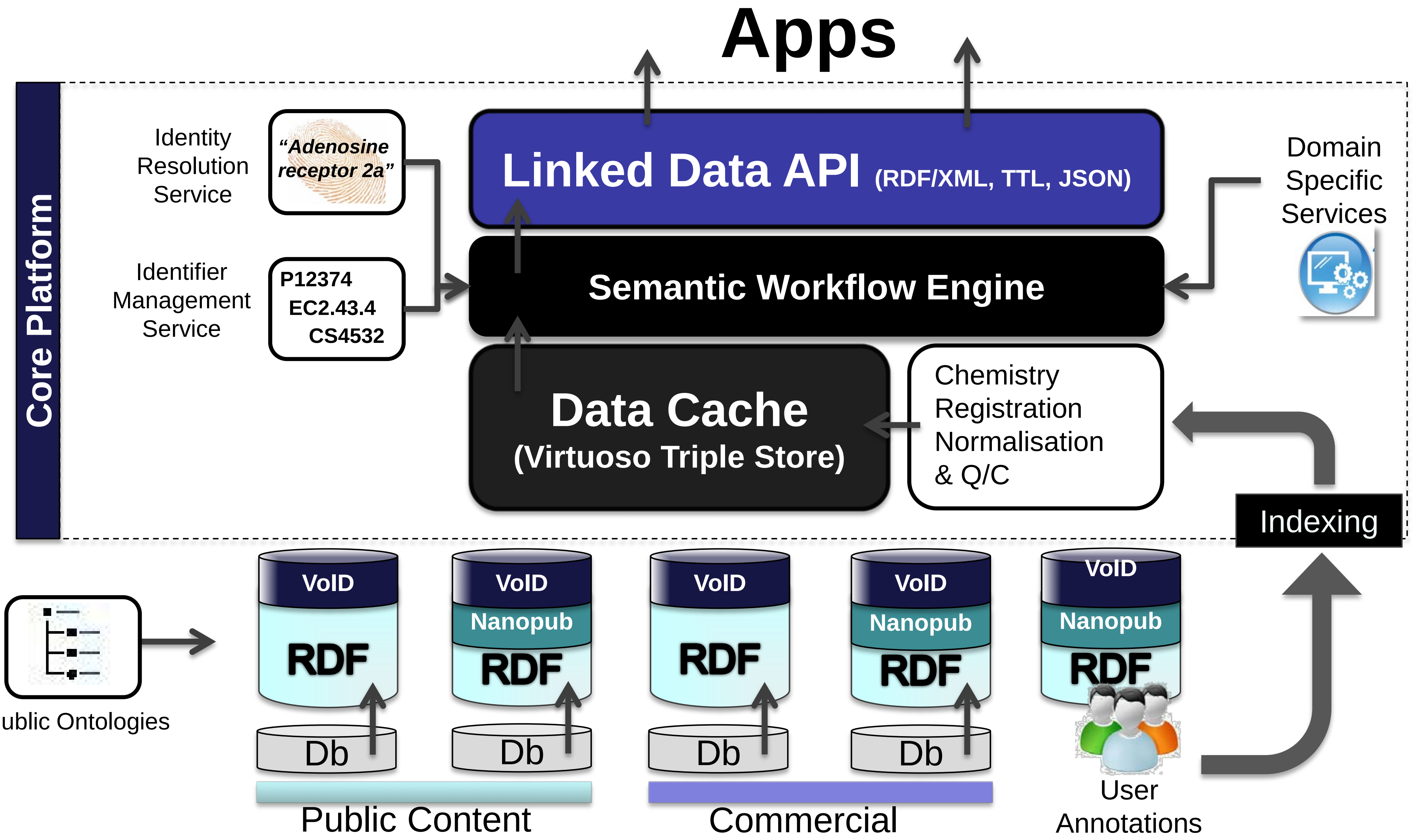
▶ Public Release

Open Phacts

										2012												2013				
b	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May



THE OPEN PHACTS DISCOVERY PLATFORM



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

Domain Specific Services

Data Cache
(Virtuoso Triple Store)

Chemistry Registration Normalisation & Q/C

Indexing

Public Ontologies

VoID
RDF
Db

VoID
Nanopub
RDF
Db

VoID
RDF
Db

VoID
Nanopub
RDF
Db

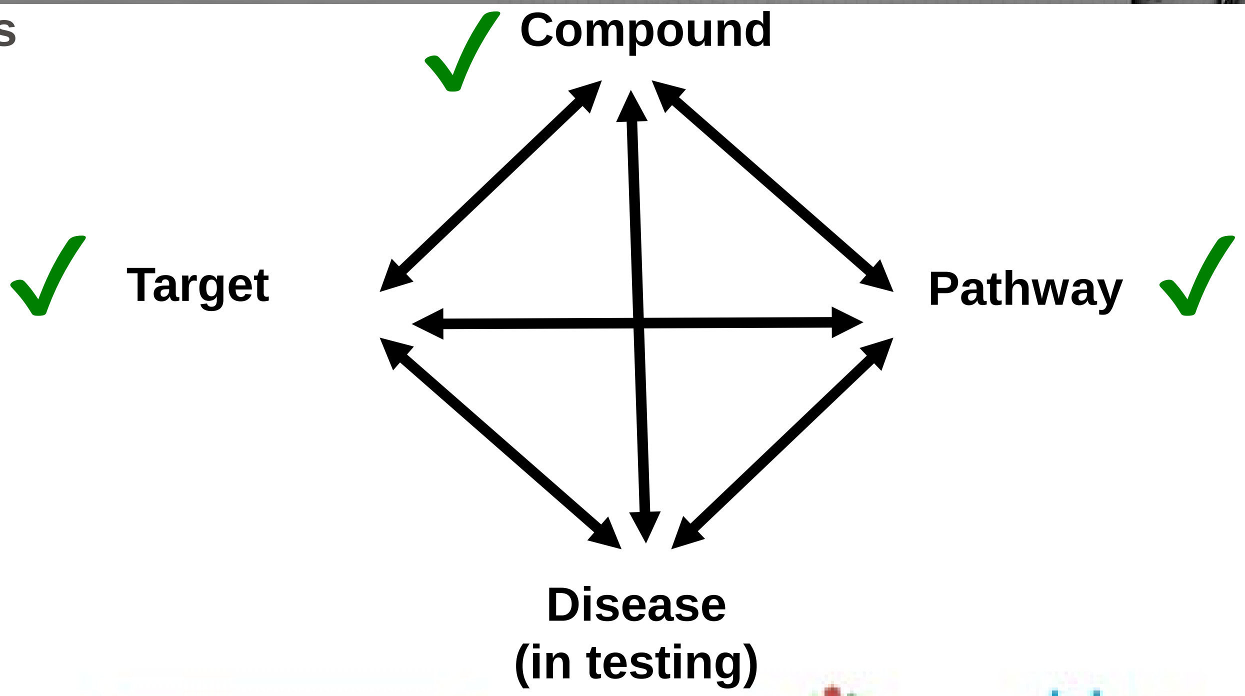
VoID
Nanopub
RDF

User Annotations

Public Content

Commercial

Data Sources


✓ Compound

✓ Target

Pathway ✓

Disease
(in testing)

Concept Wiki

ChEBI

ChEMBL

ChemSpider
The free chemical database

swissprot

DrugBank
Open Data Drug & Drug Target Database

UniProt

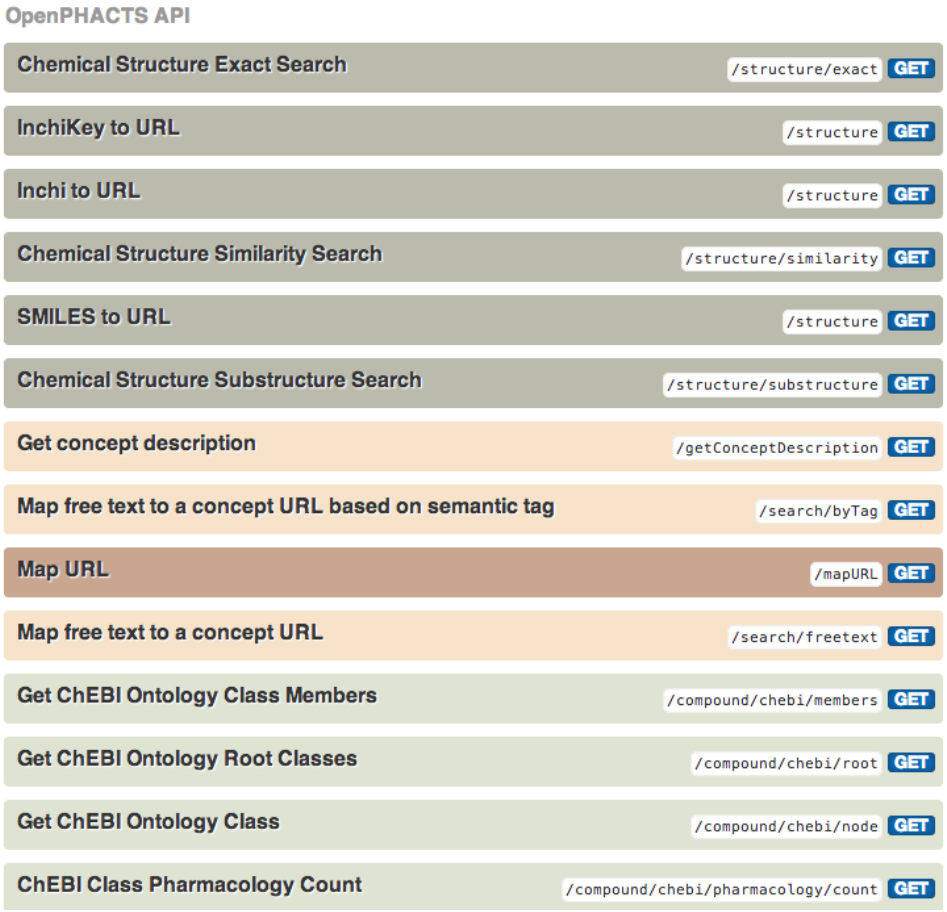
WikiPathways
Pathways for the People

GeneOntology
Unifying Biology

Open PHACTS

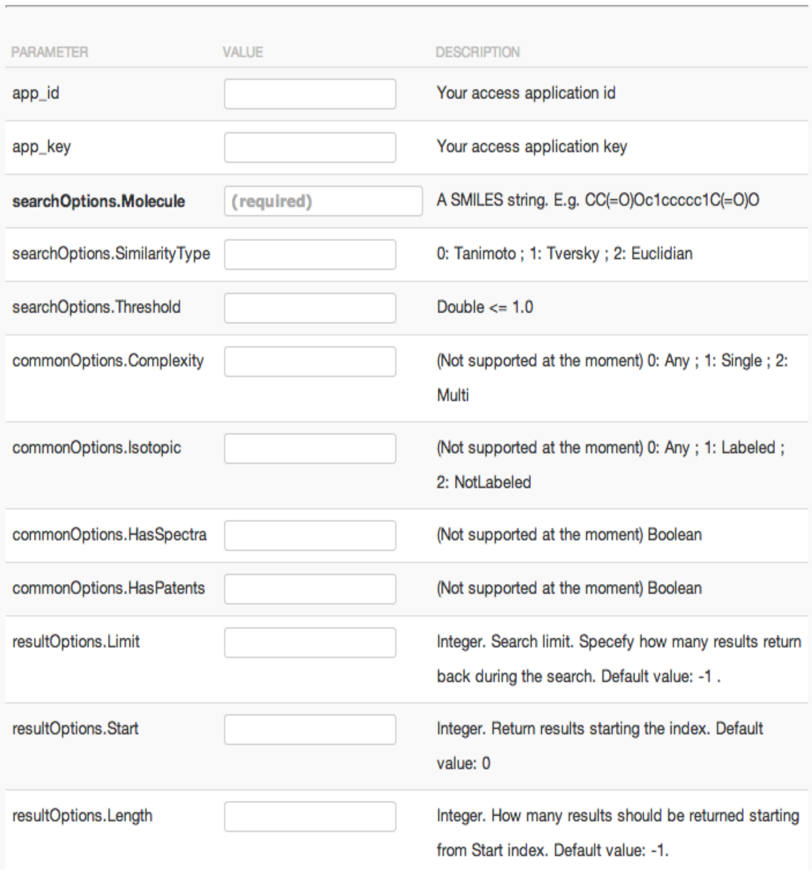
Open Pharmacological Space

Play! *https://dev.openphacts.org/*



OpenPHACTS API

Chemical Structure Exact Search	/structure/exact	GET
InchiKey to URL	/structure	GET
Inchi to URL	/structure	GET
Chemical Structure Similarity Search	/structure/similarity	GET
SMILES to URL	/structure	GET
Chemical Structure Substructure Search	/structure/substructure	GET
Get concept description	/getConceptDescription	GET
Map free text to a concept URL based on semantic tag	/search/byTag	GET
Map URL	/mapURL	GET
Map free text to a concept URL	/search/freetext	GET
Get ChEBI Ontology Class Members	/compound/chebi/members	GET
Get ChEBI Ontology Root Classes	/compound/chebi/root	GET
Get ChEBI Ontology Class	/compound/chebi/node	GET
ChEBI Class Pharmacology Count	/compound/chebi/pharmacology/count	GET



PARAMETER	VALUE	DESCRIPTION
app_id		Your access application id
app_key		Your access application key
searchOptions.Molecule	(required)	A SMILES string. E.g. CC(=O)Oc1ccccc1C(=O)O
searchOptions.SimilarityType		0: Tanimoto ; 1: Tversky ; 2: Euclidian
searchOptions.Threshold		Double <= 1.0
commonOptions.Complexity		(Not supported at the moment) 0: Any ; 1: Single ; 2: Multi
commonOptions.Isotopic		(Not supported at the moment) 0: Any ; 1: Labeled ; 2: NotLabeled
commonOptions.HasSpectra		(Not supported at the moment) Boolean
commonOptions.HasPatents		(Not supported at the moment) Boolean
resultOptions.Limit		Integer. Search limit. Specefy how many results return back during the search. Default value: -1 .
resultOptions.Start		Integer. Return results starting the index. Default value: 0
resultOptions.Length		Integer. How many results should be returned starting from Start index. Default value: -1.

Secure Cloud Hosted + Virtualized

Triple Store

- Virtuoso 7 column store
- Scale to > 100 billion triples

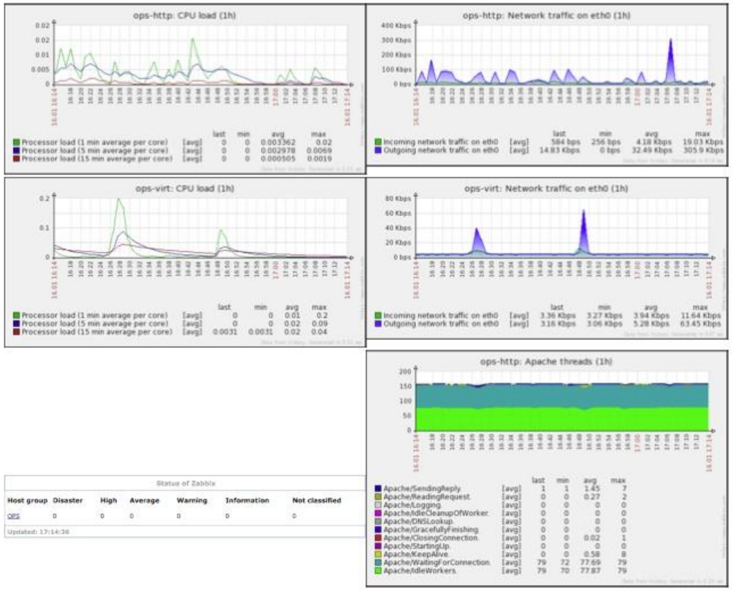
Network

- AMX-IS
- Extensive memcache
- Monitored

Hardware (development)

- 2 x Intel Xeon E5-2640 - 384 GB DDR3 1333MHz RAM - 1.5 TB SSD - 3TB 7200rpm

OPENLINK
SOFTWARE
Making Technology Work For You®



		last	min	avg	max
🟩 Processor load (1 min average per core)	[avg]	0	0	0.003362	0.02
🟦 Processor load (5 min average per core)	[avg]	0	0	0.002978	0.0069
🟥 Processor load (15 min average per core)	[avg]	0	0	0.000505	0.0019

		last	min	avg	max
🟩 Incoming network traffic on eth0	[avg]	584 bps	256 bps	4.18 Kbps	19.03 Kbps
🟦 Outgoing network traffic on eth0	[avg]	14.83 Kbps	0 bps	32.49 Kbps	305.9 Kbps

		last	min	avg	max
🟩 Processor load (1 min average per core)	[avg]	0	0	0.01	0.2
🟦 Processor load (5 min average per core)	[avg]	0	0	0.02	0.09
🟥 Processor load (15 min average per core)	[avg]	0.0031	0.0031	0.02	0.04

		last	min	avg	max
🟩 Incoming network traffic on eth0	[avg]	3.36 Kbps	3.27 Kbps	3.94 Kbps	11.64 Kbps
🟦 Outgoing network traffic on eth0	[avg]	3.16 Kbps	3.06 Kbps	5.28 Kbps	63.45 Kbps

		last	min	avg	max
Apache/SendingReply	[avg]	1	1	1.45	7
Apache/ReadingRequest	[avg]	0	0	0.27	2
Apache/Logging	[avg]	0	0	0	0
Apache/IdleCleanupOfWorker	[avg]	0	0	0	0
Apache/DNSLookup	[avg]	0	0	0	0
Apache/GracefullyFinishing	[avg]	0	0	0	0
Apache/ClosingConnection	[avg]	0	0	0.02	1
Apache/StartingUp	[avg]	0	0	0	0
Apache/KeepAlive	[avg]	0	0	0.58	8
Apache/WaitingForConnection	[avg]	79	72	77.69	79
Apache/IdleWorkers	[avg]	79	70	77.87	79

Status of Zabbix

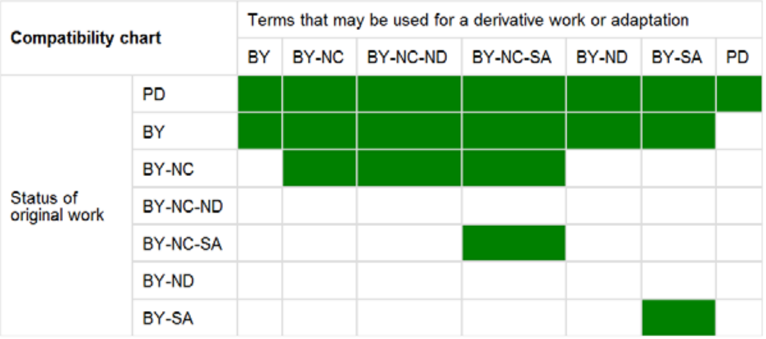
Host group	Disaster	High	Average	Warning	Information	Not classified
OPS	0	0	0	0	0	0

Updated: 17:14:36

Dealing With The *Really* Tough Parts

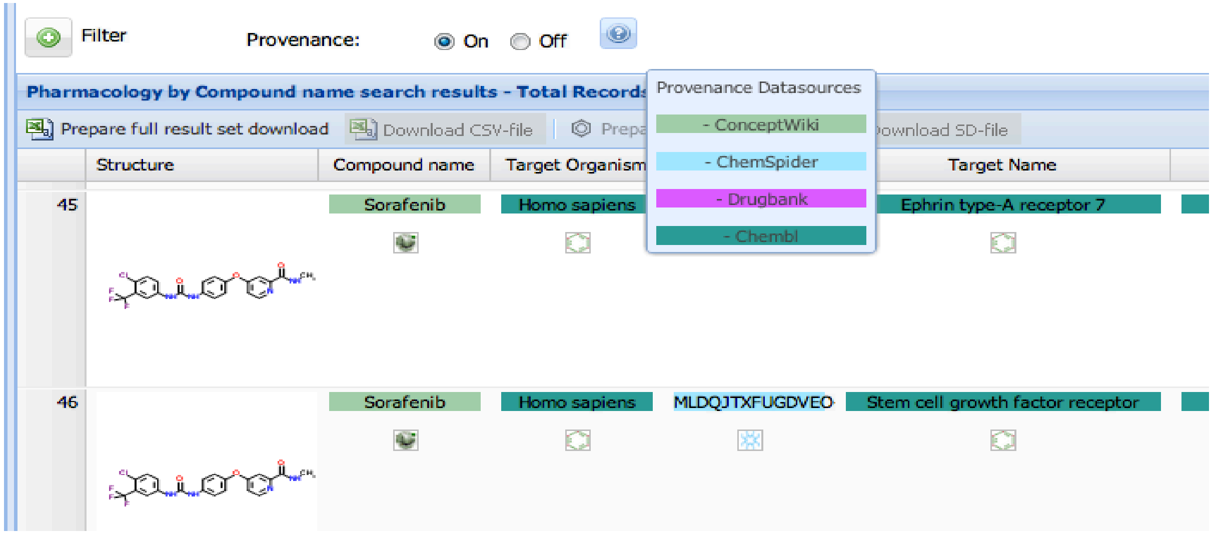
Data Licensing

John
Wilbanks
http://del-fi.org/



Compatibility chart		Terms that may be used for a derivative work or adaptation						
		BY	BY-NC	BY-NC-ND	BY-NC-SA	BY-ND	BY-SA	PD
Status of original work	PD	🟩	🟩	🟩	🟩	🟩	🟩	🟩
	BY	🟩	🟩	🟩	🟩	🟩	🟩	
	BY-NC		🟩	🟩	🟩			
	BY-NC-ND							
	BY-NC-SA				🟩			
	BY-ND							
	BY-SA						🟩	

Open PHACTS
Open Pharmacological Space



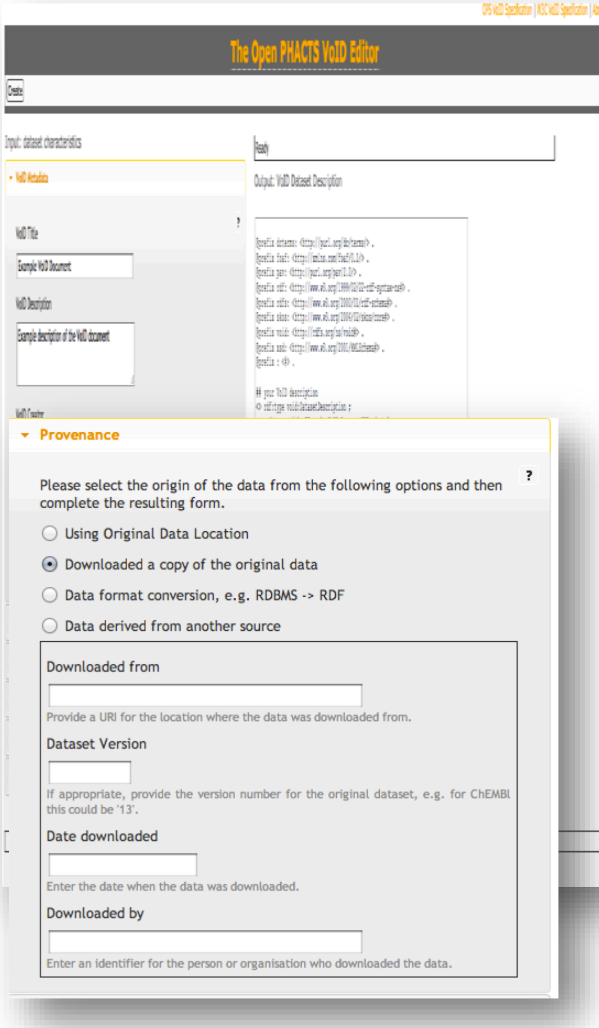
Filter | Provenance: ● On ○ Off

Provenance Datasources
- ConceptWiki
- ChemSpider
- Drugbank
- Chembl

Pharmacology by Compound name search results - Total Records

Prepare full result set download | Download CSV-file | Prepa… | …ownload SD-file

	Structure	Compound name	Target Organism		Target Name
45		Sorafenib	Homo sapiens		Ephrin type-A receptor 7
46		Sorafenib	Homo sapiens	MLDQJTXFUGDVEO	Stem cell growth factor receptor



The Open PHACTS VoID Editor

Input: dataset characteristics

Output: VoID Dataset Description

VoID Title: Example VoID Document

VoID Description: Example description of the VoID document

▾ Provenance

Please select the origin of the data from the following options and then complete the resulting form.

○ Using Original Data Location
● Downloaded a copy of the original data
○ Data format conversion, e.g. RDBMS -> RDF
○ Data derived from another source

Downloaded from

Provide a URI for the location where the data was downloaded from.

Dataset Version

If appropriate, provide the version number for the original dataset, e.g. for ChEMBL this could be '13'.

Date downloaded

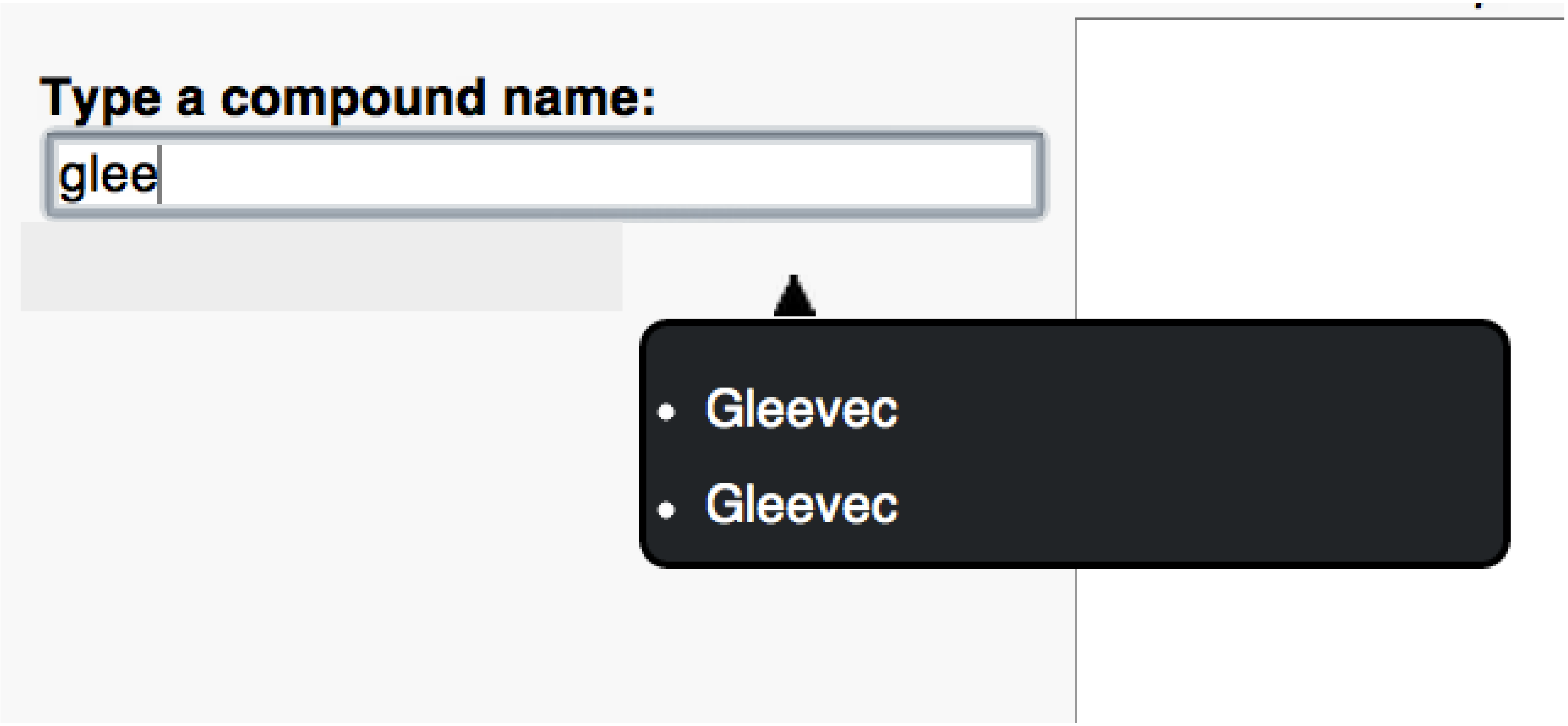
Enter the date when the data was downloaded.

Downloaded by

Enter an identifier for the person or organisation who downloaded the data.

Provenance everywhere

Its easy to integrate, difficult to integrate well:

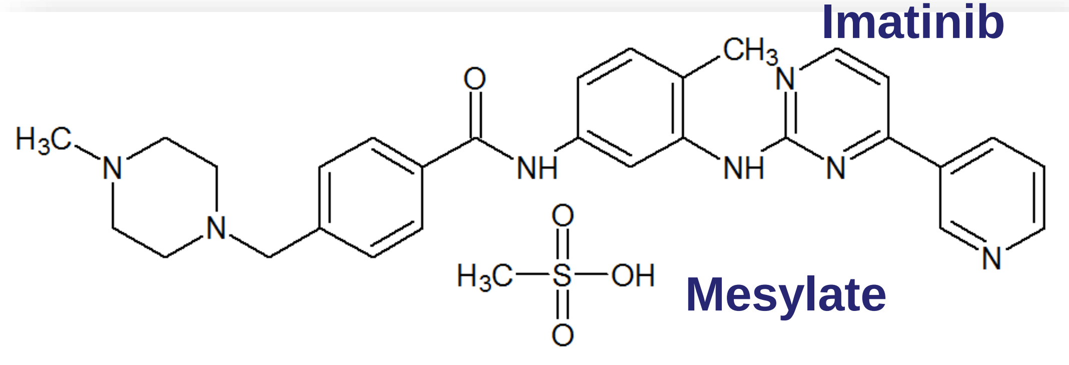


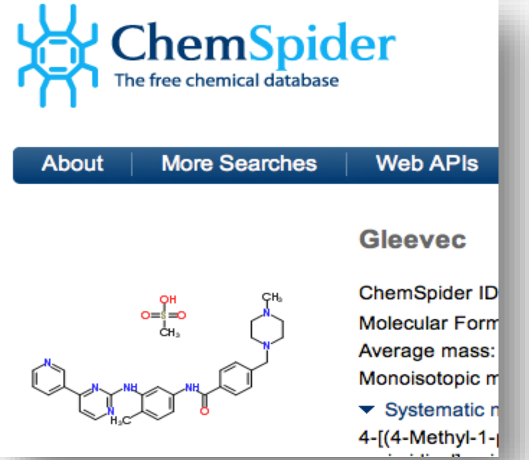
Type a compound name:

glee

- Gleevec
- Gleevec

What Is Gleevec?





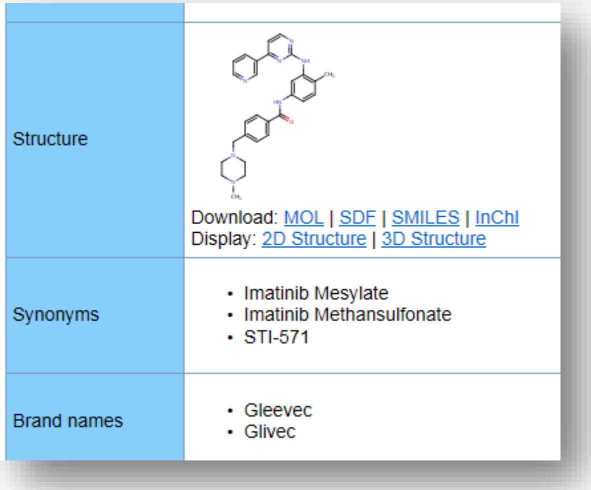
ChemSpider
The free chemical database

About | More Searches | Web APIs

Gleevec

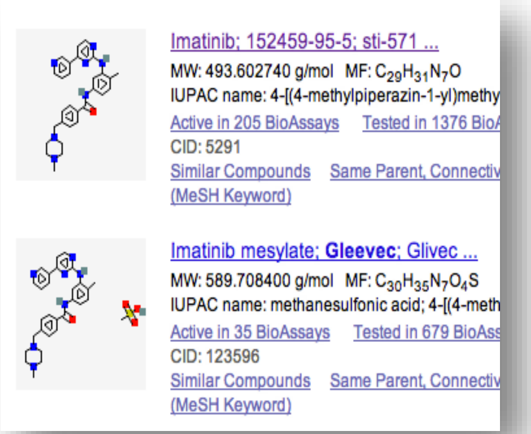
ChemSpider ID
Molecular Form
Average mass:
Monoisotopic m
Systematic n
4-[(4-Methyl-1-(

ChemSpider



Structure	Download: MOL | SDF | SMILES | InChI Display: 2D Structure | 3D Structure
Synonyms	• Imatinib Mesylate • Imatinib Methansulfonate • STI-571
Brand names	• Gleevec • Glivec

Drugbank

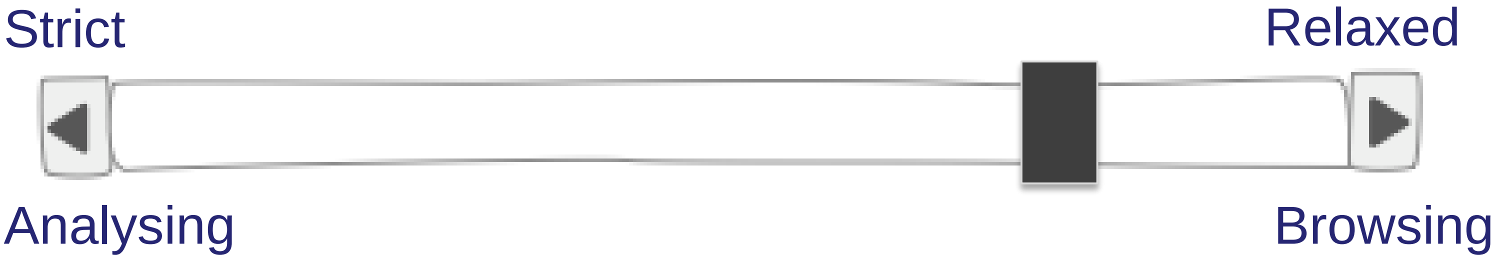


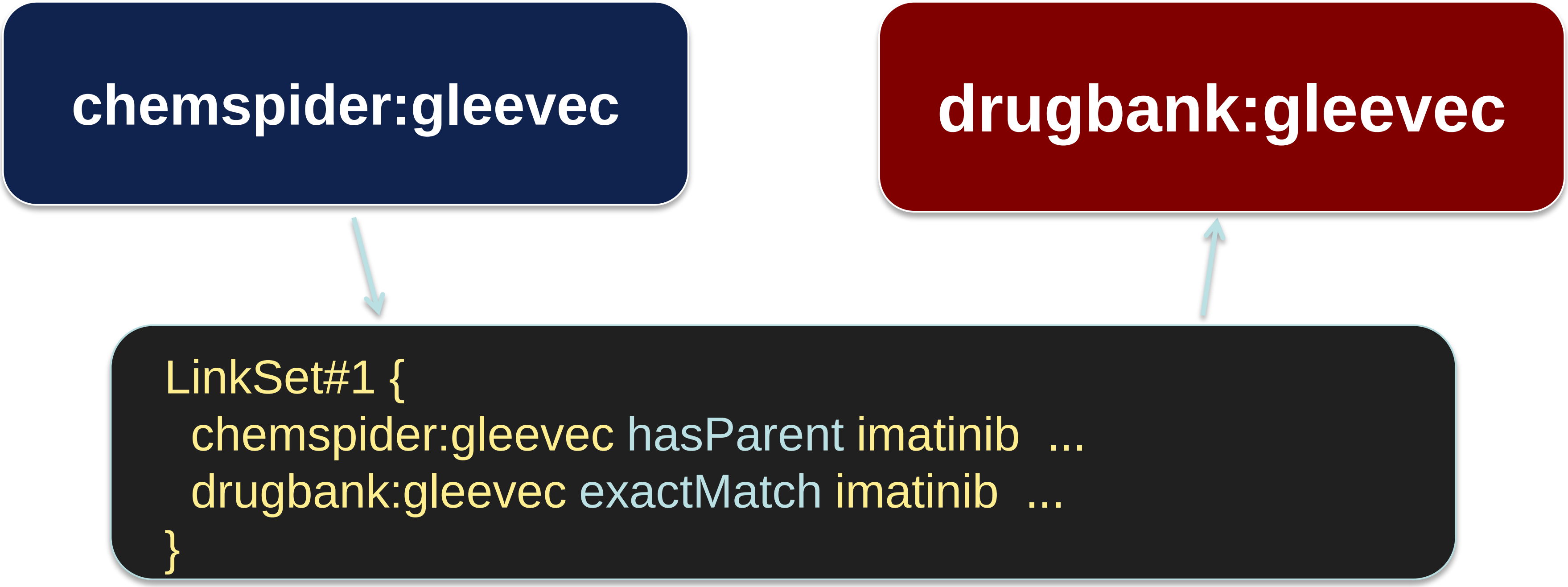
Imatinib; 152459-95-5; sti-571 ...
MW: 493.602740 g/mol MF: $C_{29}H_{31}N_7O$
IUPAC name: 4-[(4-methylpiperazin-1-yl)methy
Active in 205 BioAssays Tested in 1376 BioA
CID: 5291
Similar Compounds Same Parent, Connectiv
(MeSH Keyword)

Imatinib mesylate; Gleevec; Glivec ...
MW: 589.708400 g/mol MF: $C_{30}H_{35}N_7O_4S$
IUPAC name: methanesulfonic acid; 4-[(4-meth
Active in 35 BioAssays Tested in 679 BioAss
CID: 123596
Similar Compounds Same Parent, Connectiv
(MeSH Keyword)

PubChem

Dynamic Equality

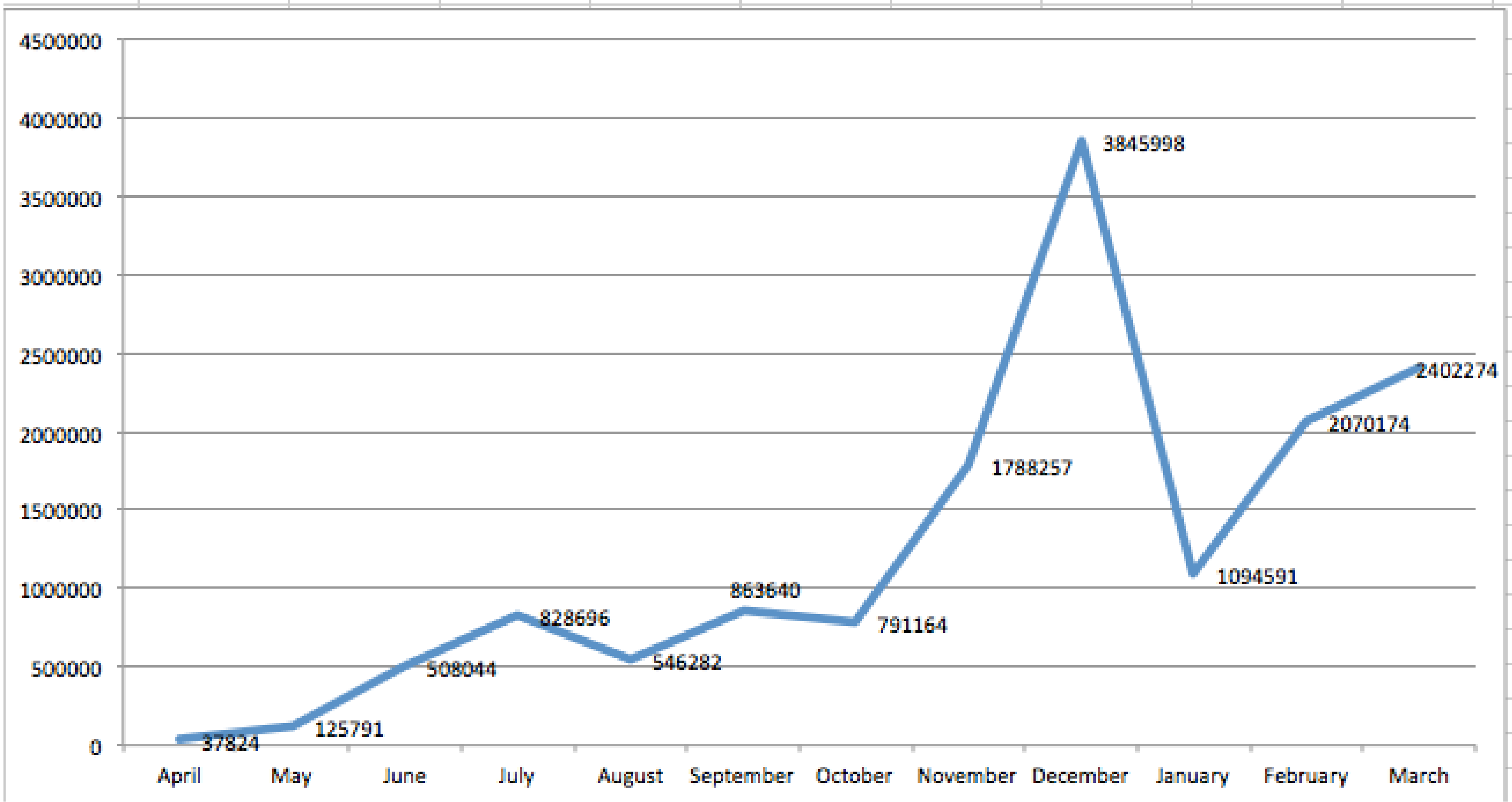


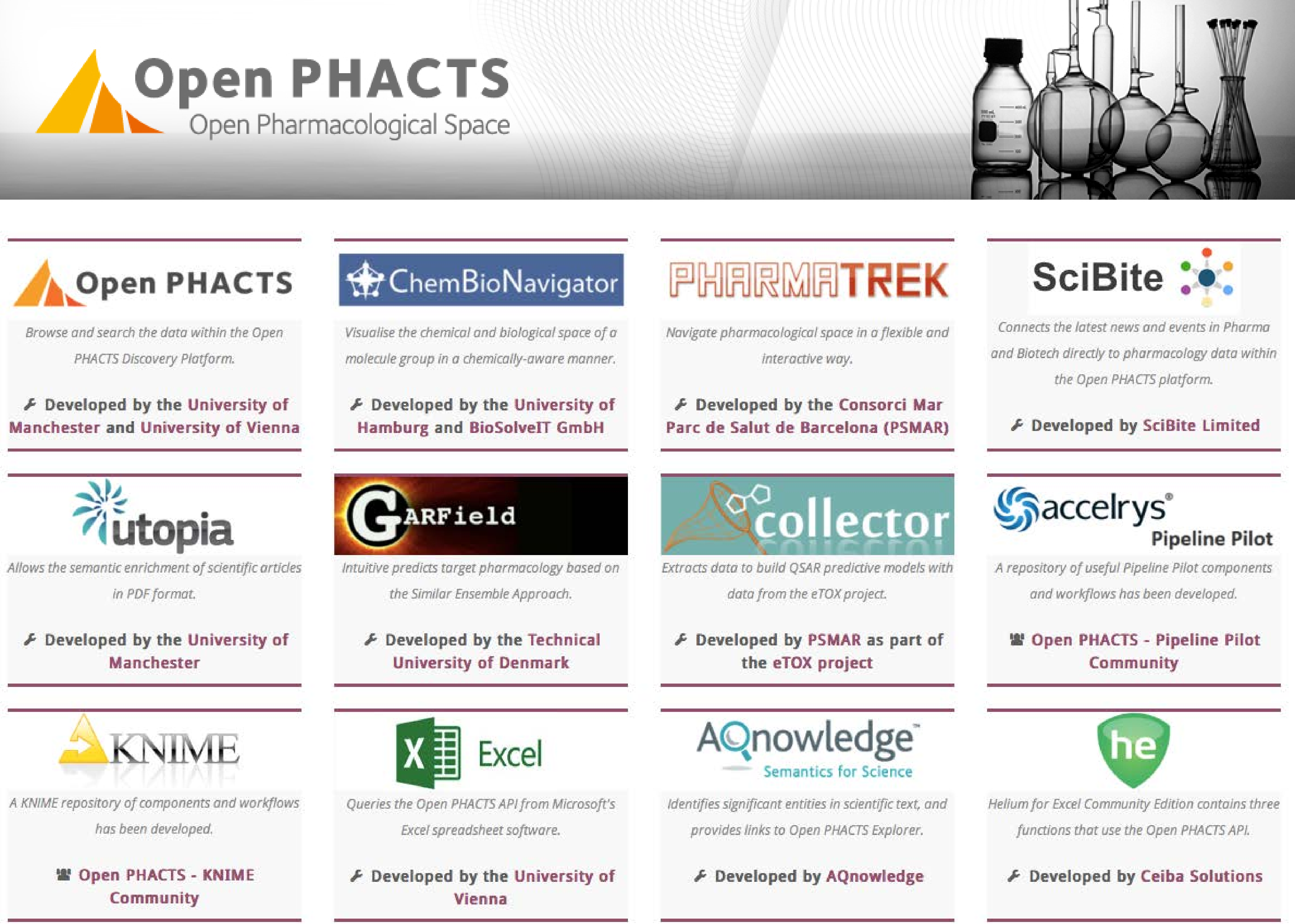


```
LinkSet#1 {
  chemspider:gleevec hasParent imatinib  ...
  drugbank:gleevec exactMatch imatinib  ...
}
```

APPS

API Hits (April 2013 – March 2014)





Open PHACTS

Open Pharmacological Space

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

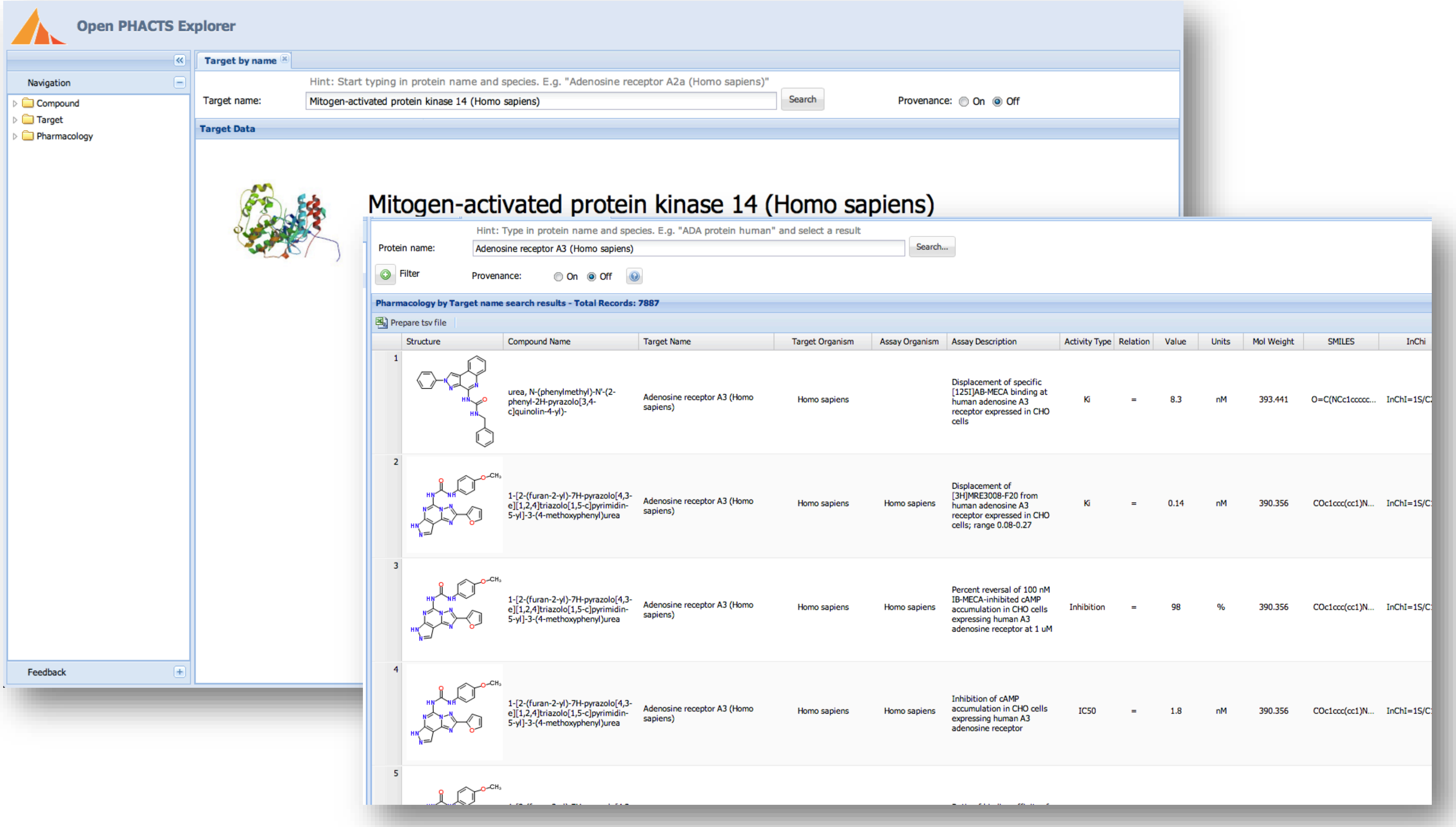
he

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

Developed by Ceiba Solutions

Open PHACTS

Open Pharmacological Space



Open PHACTS Explorer

Navigation

- Compound
- Target
- Pharmacology

Feedback

Target by name

Hint: Start typing in protein name and species. E.g. "Adenosine receptor A2a (Homo sapiens)"

Target name: Mitogen-activated protein kinase 14 (Homo sapiens) Search

Provenance: ○ On ● Off

Target Data

Mitogen-activated protein kinase 14 (Homo sapiens)

Hint: Type in protein name and species. E.g. "ADA protein human" and select a result

Protein name: Adenosine receptor A3 (Homo sapiens) Search...

Filter

Provenance: ○ On ● Off

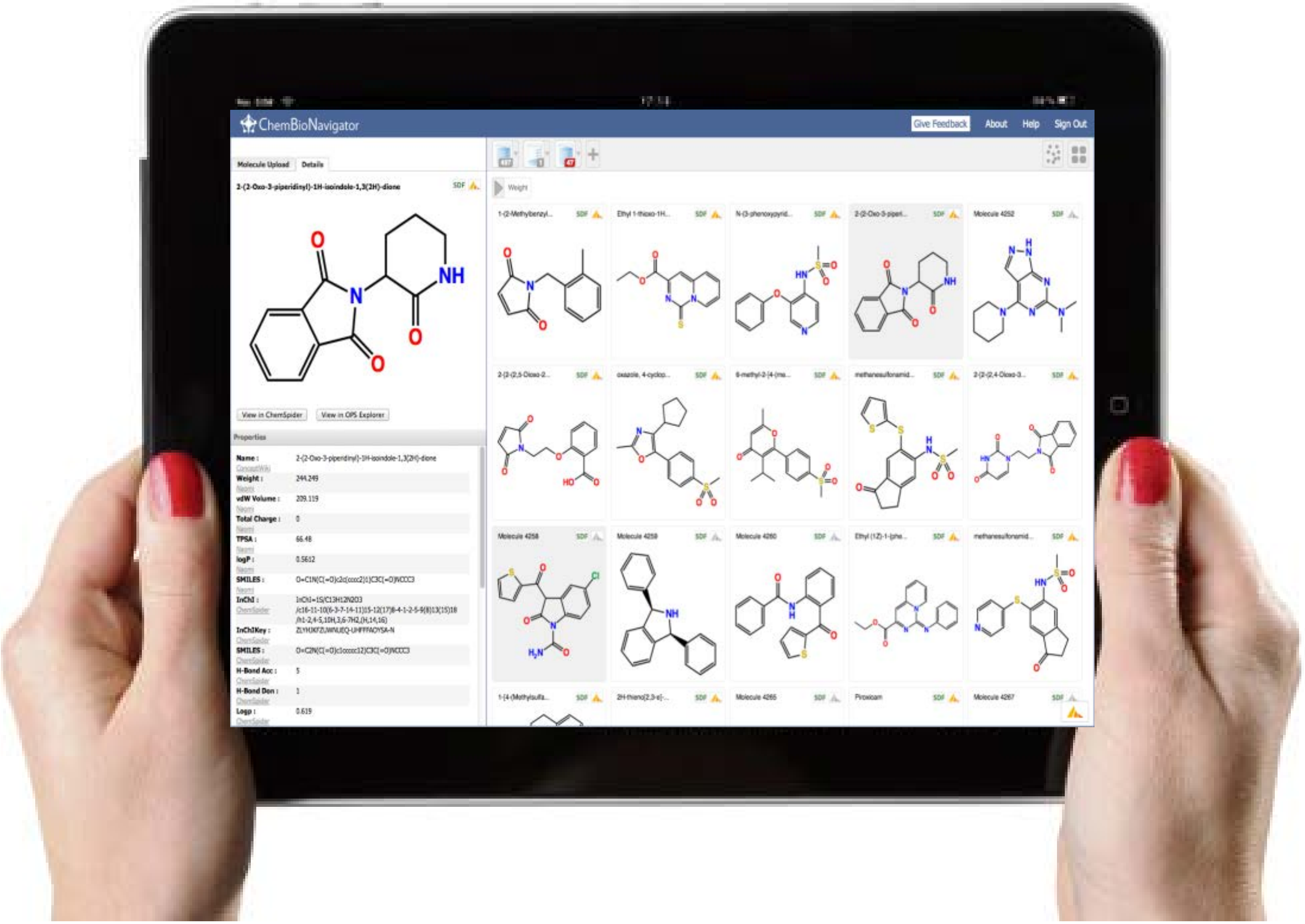
Pharmacology by Target name search results - Total Records: 7887

Prepare tsv file

	Structure	Compound Name	Target Name	Target Organism	Assay Organism	Assay Description	Activity Type	Relation	Value	Units	Mol Weight	SMILES	InChi
1		urea, N-(phenylmethyl)-N'-(2-phenyl-2H-pyrazolo[3,4-c]quinolin-4-yl)-	Adenosine receptor A3 (Homo sapiens)	Homo sapiens		Displacement of specific [125I]AB-MECA binding at human adenosine A3 receptor expressed in CHO cells	Ki	=	8.3	nM	393.441	O=C(NCc1ccccc...	InChI=1S/C
2		1-[2-(furan-2-yl)-7H-pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidin-5-yl]-3-(4-methoxyphenyl)urea	Adenosine receptor A3 (Homo sapiens)	Homo sapiens	Homo sapiens	Displacement of [3H]MRE3008-F20 from human adenosine A3 receptor expressed in CHO cells; range 0.08-0.27	Ki	=	0.14	nM	390.356	COc1ccc(cc1)N...	InChI=1S/C
3		1-[2-(furan-2-yl)-7H-pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidin-5-yl]-3-(4-methoxyphenyl)urea	Adenosine receptor A3 (Homo sapiens)	Homo sapiens	Homo sapiens	Percent reversal of 100 nM IB-MECA-inhibited cAMP accumulation in CHO cells expressing human A3 adenosine receptor at 1 uM	Inhibition	=	98	%	390.356	COc1ccc(cc1)N...	InChI=1S/C
4		1-[2-(furan-2-yl)-7H-pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidin-5-yl]-3-(4-methoxyphenyl)urea	Adenosine receptor A3 (Homo sapiens)	Homo sapiens	Homo sapiens	Inhibition of cAMP accumulation in CHO cells expressing human A3 adenosine receptor	IC50	=	1.8	nM	390.356	COc1ccc(cc1)N...	InChI=1S/C
5													

http://explorer.openphacts.org

ChemBioNavigtor

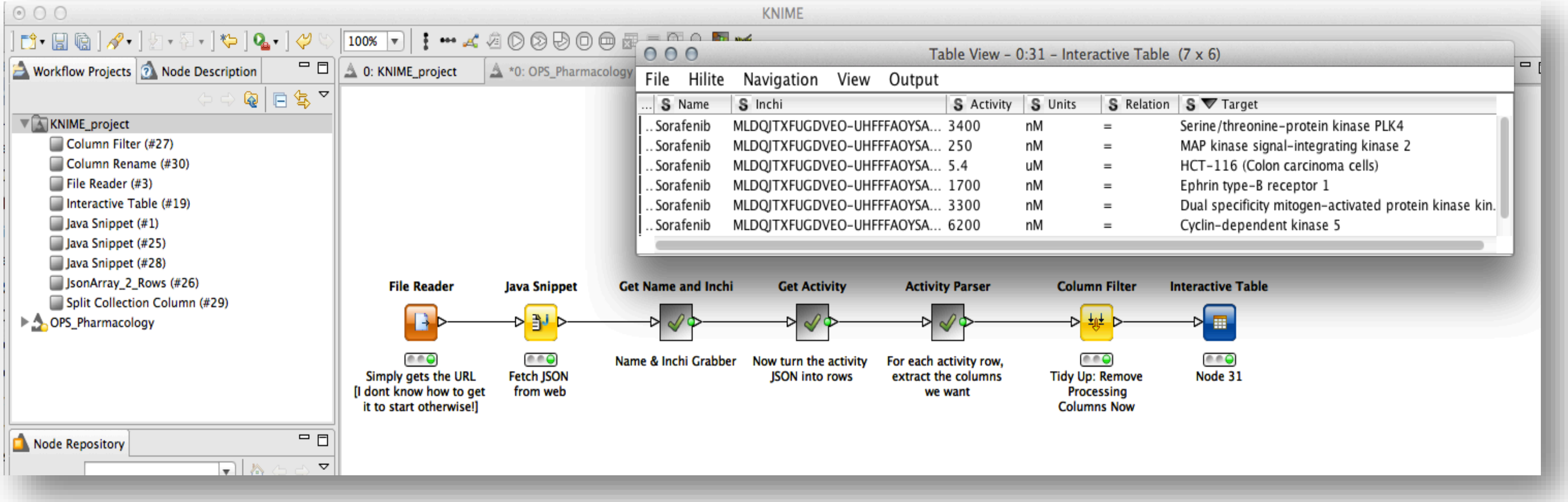


2-(2-Oxo-3-piperidinyl)-1H-isoindole-1,3(2H)-dione

Properties

Name : ConceptWiki	2-(2-Oxo-3-piperidinyl)-1H-isoindole-1,3(2H)-dione
Weight : [illegible]	244.249
vdW Volume : [illegible]	209.119
Total Charge : [illegible]	0
TPSA : [illegible]	66.48
logP : [illegible]	0.5612
SMILES : [illegible]	O=C1N(C(=O)c2c(cccc2)1)C3C(=O)NCCC3
InChI : ChemSpider	InChI=1S/C13H12N2O3 /c16-11-10(6-3-7-14-11)15-12(17)8-4-1-2-5-9(8)13(15)18 /h1-2,4-5,10H,3,6-7H2,(H,14,16)
InChIKey : ChemSpider	ZLYHIKFZUWNUEQ-UHFFFAOYSA-N
SMILES : ChemSpider	O=C2N(C(=O)c1ccccc12)C3C(=O)NCCC3
H-Bond Acc : ChemSpider	5
H-Bond Don : ChemSpider	1
Logp : ChemSpider	0.619

Open PHACTS
Open Pharmacological Space



- KNIME_project
  - Column Filter (#27)
  - Column Rename (#30)
  - File Reader (#3)
  - Interactive Table (#19)
  - Java Snippet (#1)
  - Java Snippet (#25)
  - Java Snippet (#28)
  - JsonArray_2_Rows (#26)
  - Split Collection Column (#29)
- OPS_Pharmacology

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

...	S Name	S Inchi	S Activity	S Units	S Relation	S 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

Simply gets the URL [I dont know how to get it to start otherwise!]

Fetch JSON from web

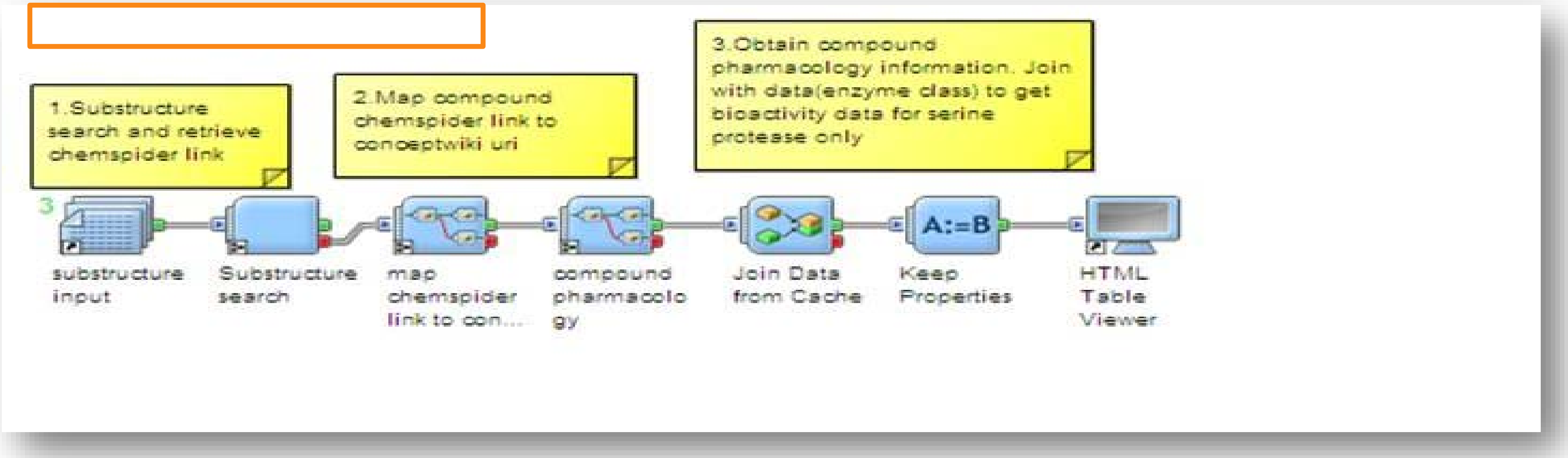
Name & Inchi Grabber

Now turn the activity JSON into rows

For each activity row, extract the columns we want

Tidy Up: Remove Processing Columns Now

Node 31



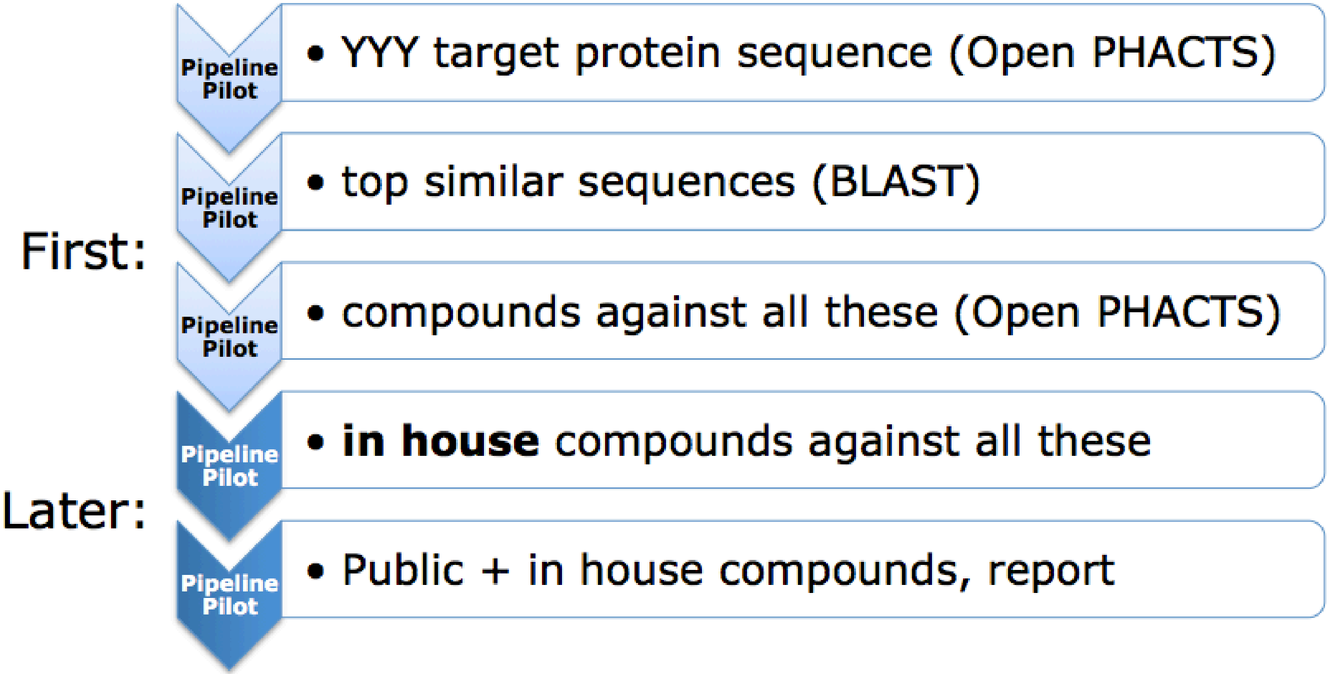
1.Substructure search and retrieve chemspider link

2.Map compound chemspider link to conceptwiki uri

3.Obtain compound pharmacology information. Join with data(enzyme class) to get bioactivity data for serine protease only

Open PHACTS Use Case: Neuroscience / Oncology

- Which compounds are associated with YYY and related targets to design a focused set?



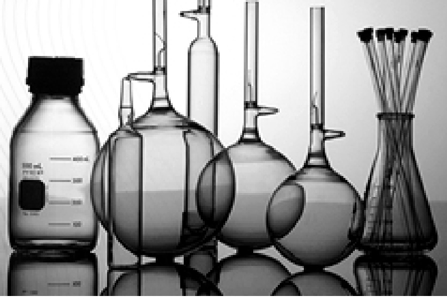
First:

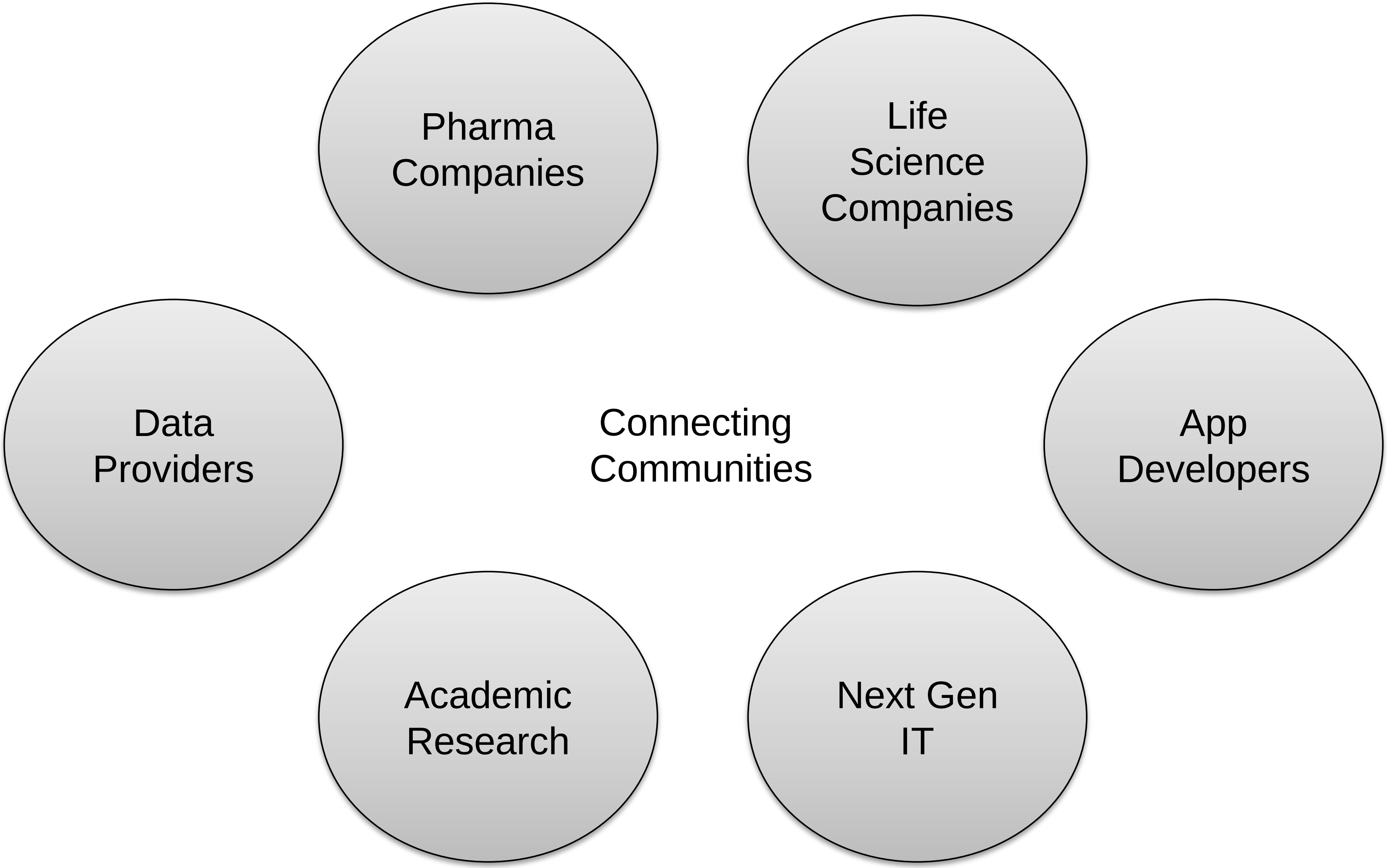
- Pipeline Pilot • YYY target protein sequence (Open PHACTS)
- Pipeline Pilot • top similar sequences (BLAST)
- Pipeline Pilot • compounds against all these (Open PHACTS)

Later:

- Pipeline Pilot • **in house** compounds against all these
- Pipeline Pilot • Public + in house compounds, report

THE FUTURE





Pharma Companies

Life Science Companies

Data Providers

Connecting Communities

App Developers

Academic Research

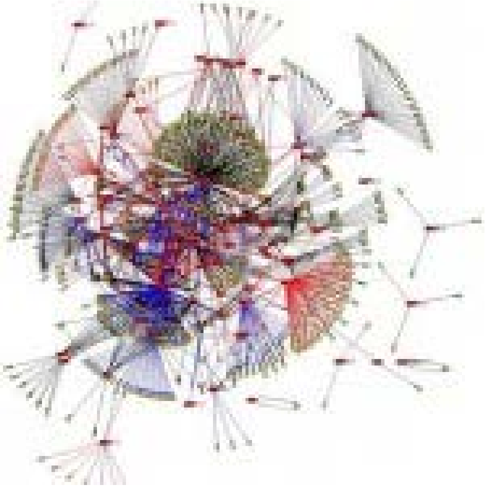
Next Gen IT

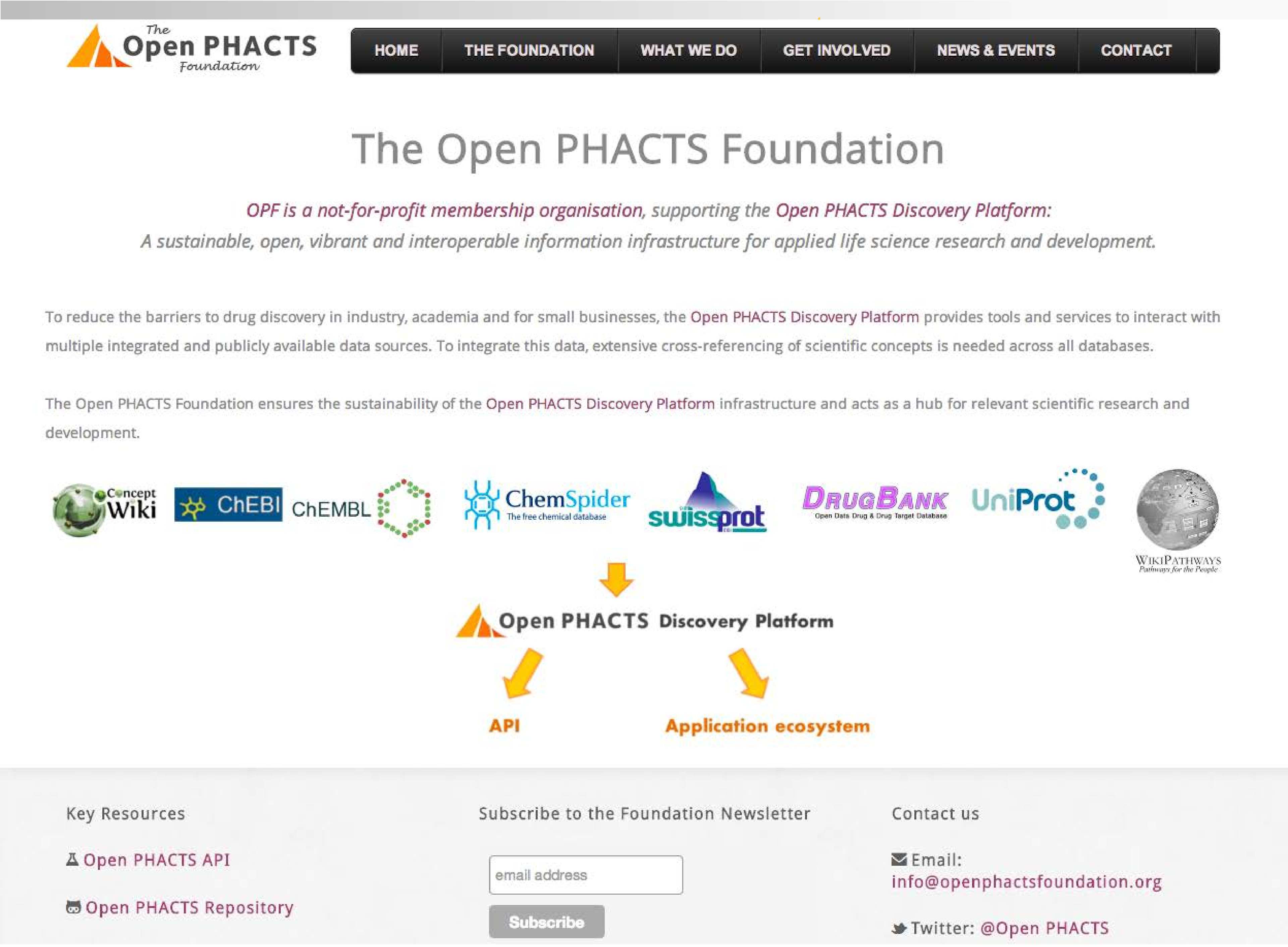
Sustaining Impact

Open PHACTS
Open Pharmacological Space

- “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.

Key Resources

Open PHACTS API

Open PHACTS Repository

Subscribe to the Foundation Newsletter

Contact us

✉ Email:
info@openphactsfoundation.org

Twitter: @Open PHACTS

Pfizer Limited – Coordinator

Universität Wien – Managing entity

Technical University of Denmark

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

Spanish National Cancer Research Centre

University of Manchester

Maastricht University

Aqnowledge

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Rheinische Friedrich-Wilhelms-Universität Bonn

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Eli Lilly

Netherlands Bioinformatics Centre

Swiss Institute of Bioinformatics

ConnectedDiscovery

EMBL-European Bioinformatics Institute

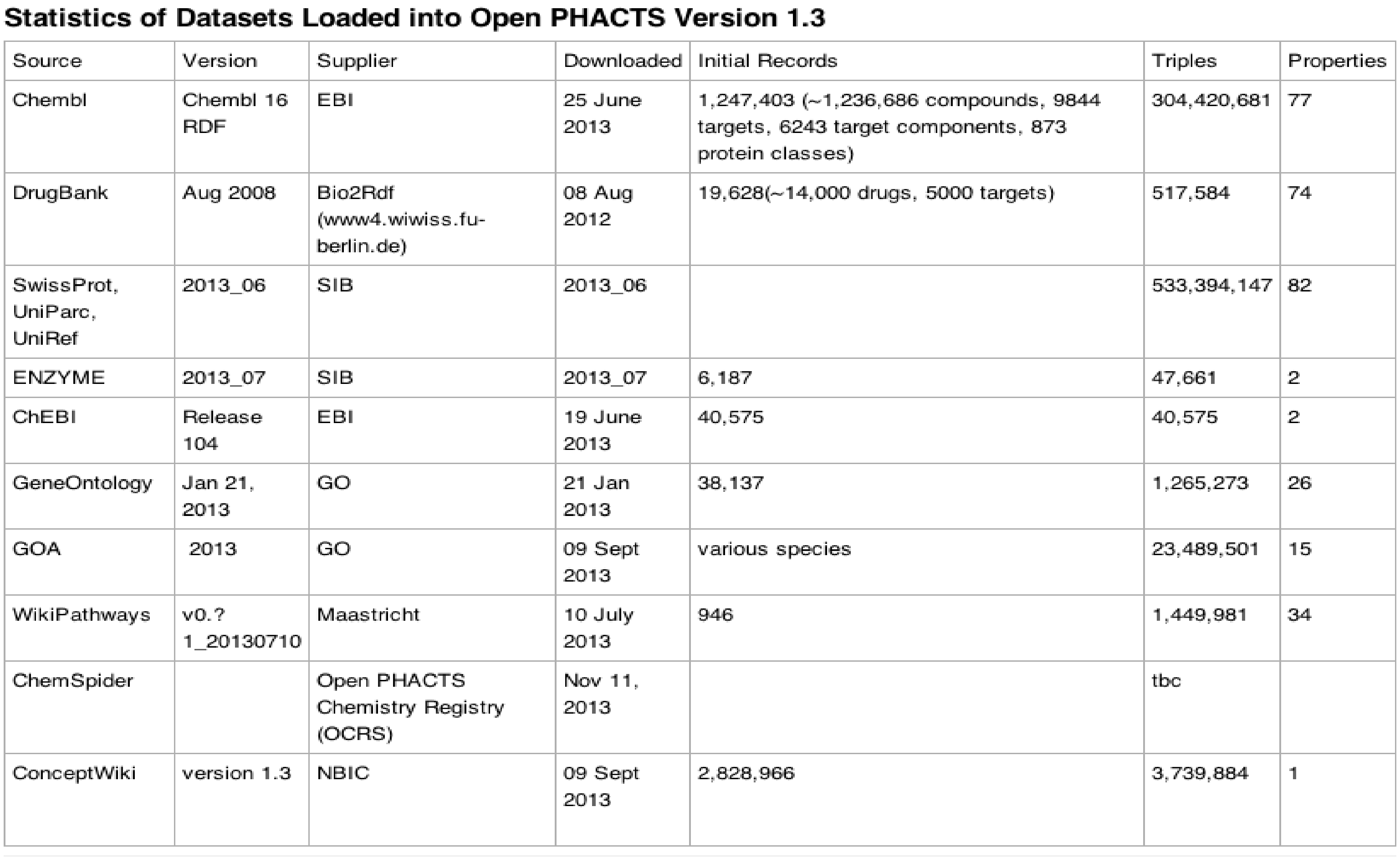
Janssen

OpenLink

pmu@openphacts.org @Open_PHACTS Open PHACTS

Backup

Present Content

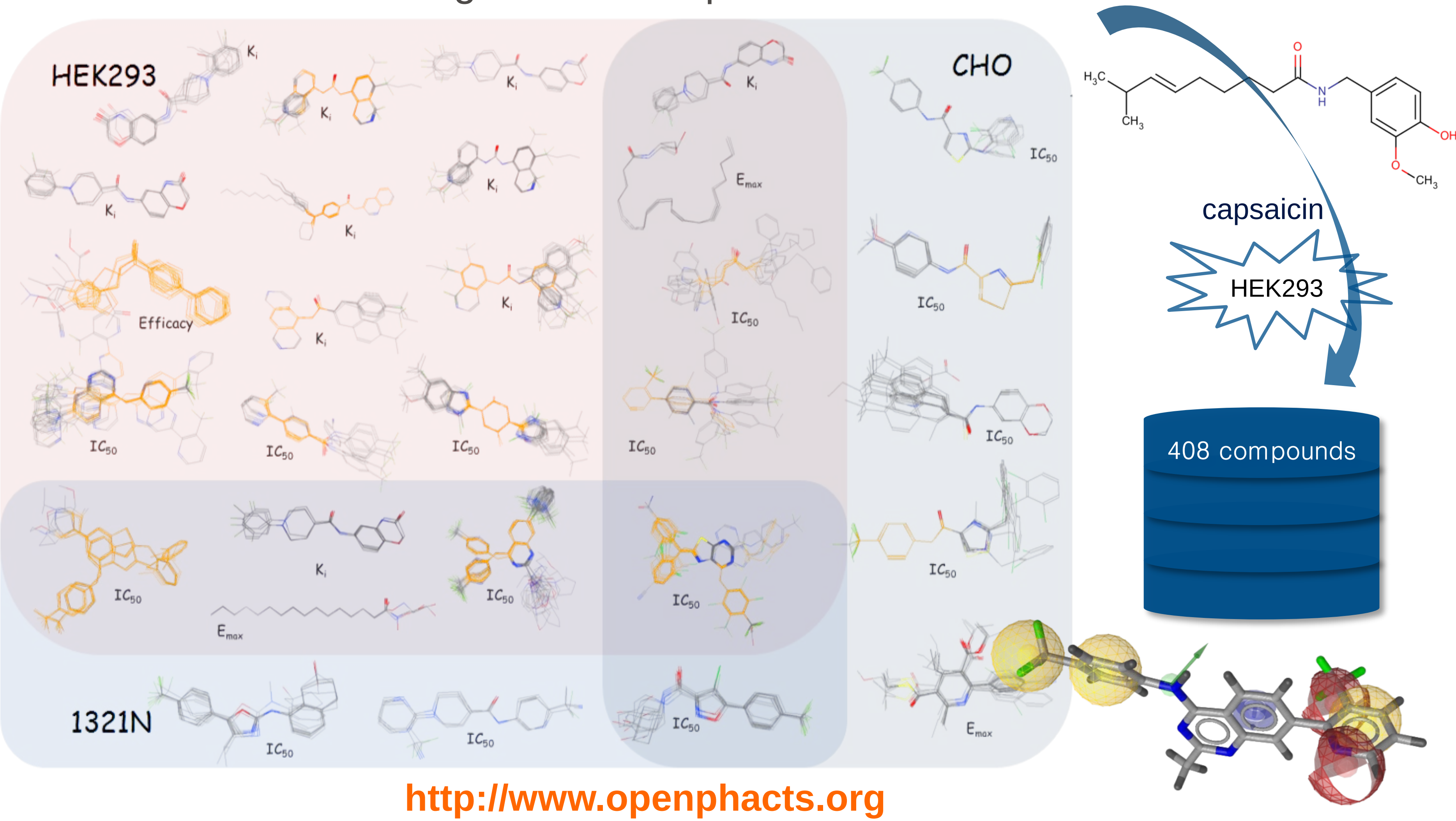


Statistics of Datasets Loaded into Open PHACTS Version 1.3

Source	Version	Supplier	Downloaded	Initial Records	Triples	Properties
Chembl	Chembl 16 RDF	EBI	25 June 2013	1,247,403 (~1,236,686 compounds, 9844 targets, 6243 target components, 873 protein classes)	304,420,681	77
DrugBank	Aug 2008	Bio2Rdf (www4.wiwiss.fu-berlin.de)	08 Aug 2012	19,628(~14,000 drugs, 5000 targets)	517,584	74
SwissProt, UniParc, UniRef	2013_06	SIB	2013_06		533,394,147	82
ENZYME	2013_07	SIB	2013_07	6,187	47,661	2
ChEBI	Release 104	EBI	19 June 2013	40,575	40,575	2
GeneOntology	Jan 21, 2013	GO	21 Jan 2013	38,137	1,265,273	26
GOA	2013	GO	09 Sept 2013	various species	23,489,501	15
WikiPathways	v0.?1_20130710	Maastricht	10 July 2013	946	1,449,981	34
ChemSpider		Open PHACTS Chemistry Registry (OCRS)	Nov 11, 2013		tbc	
ConceptWiki	version 1.3	NBIC	09 Sept 2013	2,828,966	3,739,884	1

TRPV1

hTRPV1 → 2328 ligands from Open PHACTS

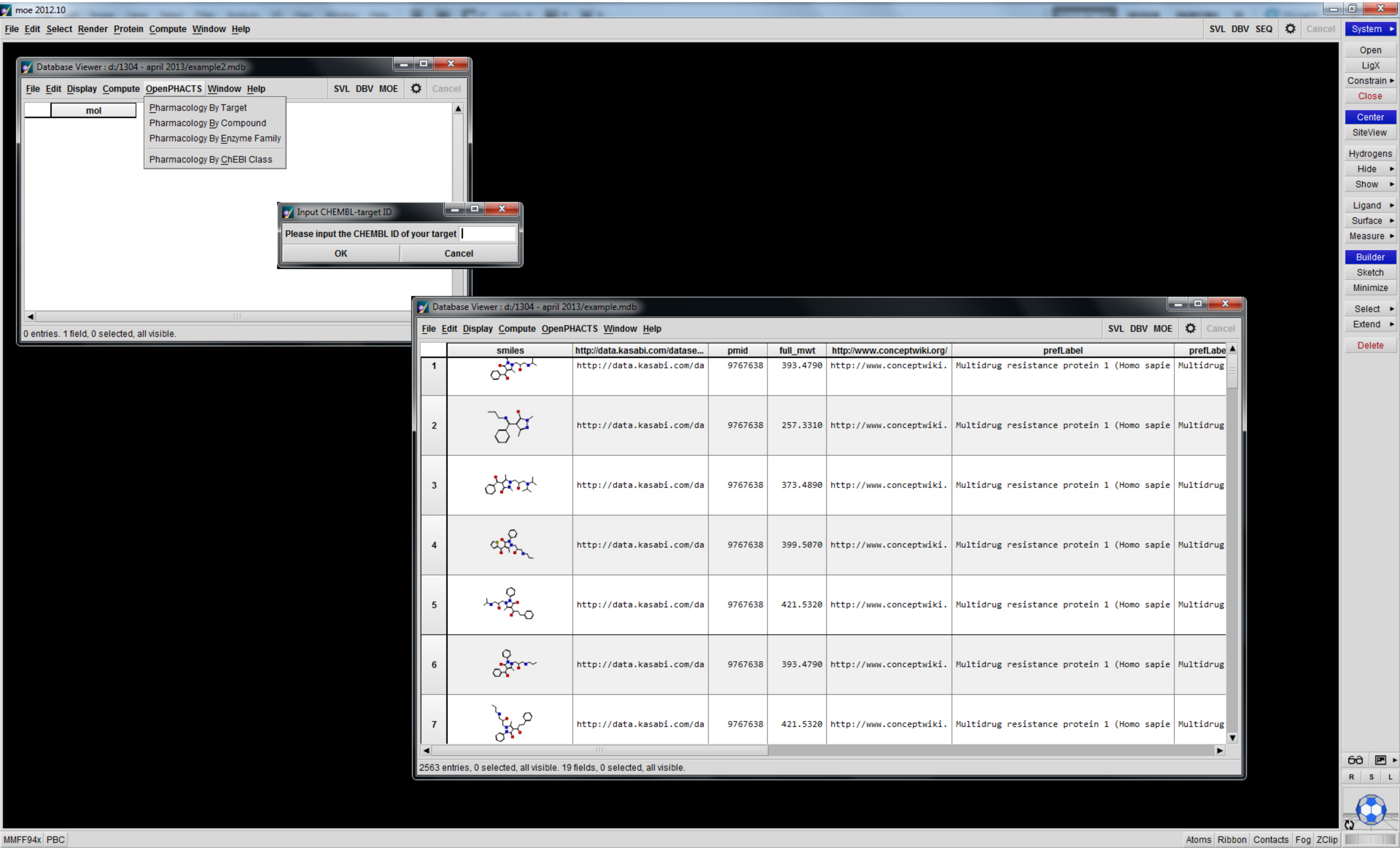


capsaicin

HEK293

408 compounds

http://www.openphacts.org


moe 2012.10
File Edit Select Render Protein Compute Window Help
SVL DBV SEQ Cancel
System
Open
LigX
Constrain
Close
Center
SiteView
Hydrogens
Hide
Show
Ligand
Surface
Measure
Builder
Sketch
Minimize
Select
Extend
Delete
R S L
MMFF94x PBC
Atoms Ribbon Contacts Fog ZClip
Database Viewer : d:/1304 - april 2013/example2.mdb
File Edit Display Compute OpenPHACTS Window Help
SVL DBV MOE Cancel
mol
Pharmacology By Target
Pharmacology By Compound
Pharmacology By Enzyme Family
Pharmacology By ChEBI Class
Input CHEMBL-target ID
OK
Cancel
Database Viewer : d:/1304 - april 2013/example.mdb
File Edit Display Compute OpenPHACTS Window Help
SVL DBV MOE Cancel

0 entries. 1 field, 0 selected, all visible.

Please input the CHEMBL ID of your target

	smiles	http://data.kasabi.com/datase...	pmid	full_mwt	http://www.conceptwiki.org/	prefLabel	prefLabe
1		http://data.kasabi.com/da	9767638	393.4790	http://www.conceptwiki.	Multidrug resistance protein 1 (Homo sapie	Multidrug
2		http://data.kasabi.com/da	9767638	257.3310	http://www.conceptwiki.	Multidrug resistance protein 1 (Homo sapie	Multidrug
3		http://data.kasabi.com/da	9767638	373.4890	http://www.conceptwiki.	Multidrug resistance protein 1 (Homo sapie	Multidrug
4		http://data.kasabi.com/da	9767638	399.5070	http://www.conceptwiki.	Multidrug resistance protein 1 (Homo sapie	Multidrug
5		http://data.kasabi.com/da	9767638	421.5320	http://www.conceptwiki.	Multidrug resistance protein 1 (Homo sapie	Multidrug
6		http://data.kasabi.com/da	9767638	393.4790	http://www.conceptwiki.	Multidrug resistance protein 1 (Homo sapie	Multidrug
7		http://data.kasabi.com/da	9767638	421.5320	http://www.conceptwiki.	Multidrug resistance protein 1 (Homo sapie	Multidrug

2563 entries, 0 selected, all visible. 19 fields, 0 selected, all visible.