

# Opening up Pharmacological Space: The Open PHACTS API

**@Chris\_Evelo**  
**Dept. Bioinformatics - BiGCaT**  
**Maastricht University**



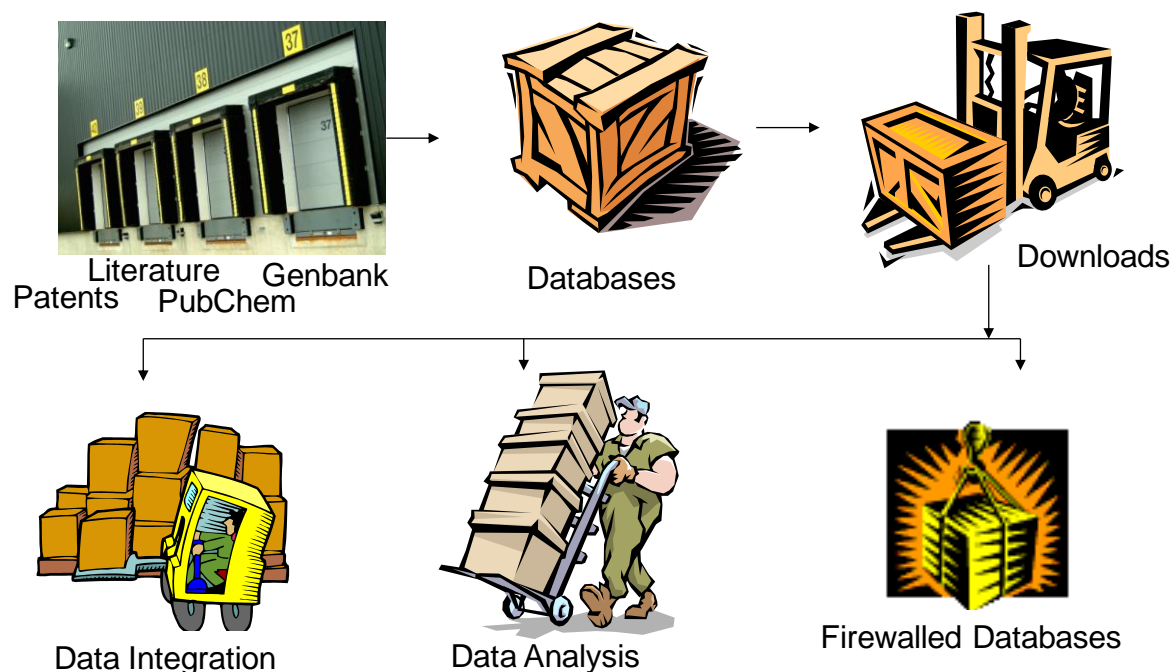
## Fundamental issues:

- ✦ There is a \*lot\* of science outside your walls
- ✦ It's a chaotic space
- ✦ Scientists want to find information quickly and easily
- ✦ Often they just “cant get there”  
(or don't even know where “there” is)
- ✦ And you have to manage it all (or not)



# Pre-competitive Informatics:

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



**Repeat @  
X each  
company**

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



## 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”)...
- Deliver services to support on-going drug discovery programs in pharma and public domain
- *Not just another project*; leading academics in semantics, pharmacology and informatics, driven by solid industry business requirements
- 23 academic partners, 8 pharmaceutical companies, 3 biotech companies
- Work split into clusters:
  - Technical Build (*focus here*)
  - Scientific Drive
  - Community & Sustainability

# The Project

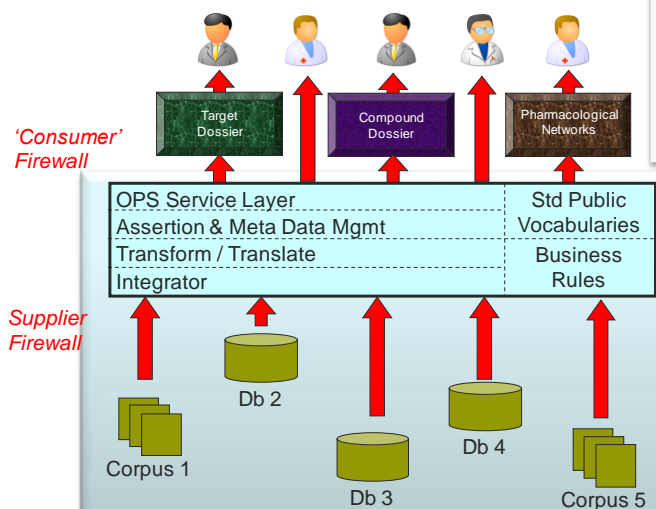


## Major Work Streams

**Build:** OPS service layer and resource integration

**Drive:** Development of exemplar work packages & Applications

**Sustain:** Community engagement and long-term sustainability



### Work Stream 2: Exemplar Drug Discovery Informatics tools

Develop exemplar services to test OPS Service Layer

*Target Dossier (Data Integration)*

*Pharmacological Network Navigator (Data Visualisation)*

*Compound Dossier (Data Analysis)*

### Work Stream 1: Open Pharmacological Space (OPS) Service Layer

Standardised software layer to allow public DD resource integration

- Define standards and construct OPS service layer
- Develop interface (API) for data access, integration and analysis
- Develop secure access models

Existing Drug Discovery (DD) Resource Integration





"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  $\mu$ M"



ChEMBL

DrugBank

Gene  
Ontology

WikiPathways

GeneGo

ChEBI

UniProt

UMLS

GVKBio

ConceptWiki

ChemSpider

TrialTrove

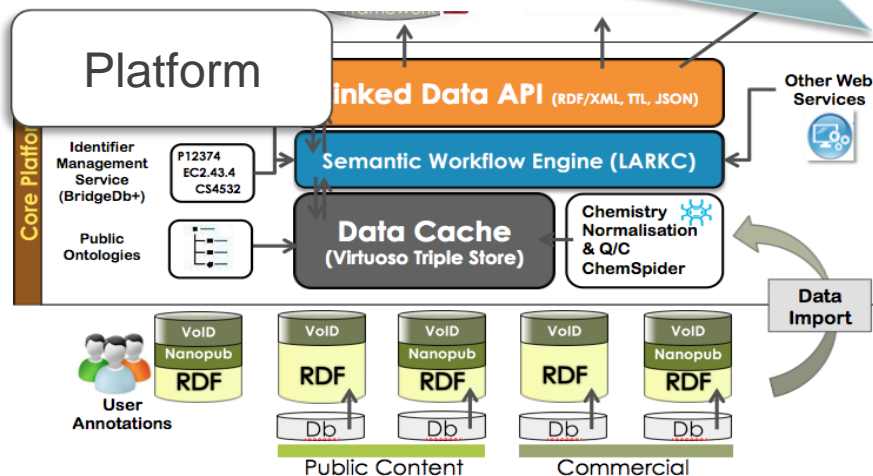
TR Integrity



## 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 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 clinical data for a given list of compounds defined by their chemical structure (with options to match stereochemistry or not).
41	13	8	A project is considering Protein Kinase C Alpha (PRKCA) as a target. What are all the compounds known to modulate the target directly? What are the compounds that may modulate the target directly? i.e. return all cmpds active in assays where the resolution is at least at the level of the target family (i.e. PKC) both from structured assay databases and the literature.
44	13	8	Give me all active compounds on a given target with the relevant assay data
46	13	8	Give me the compound(s) which hit most specifically the multiple targets in a given pathway (disease)
59	14	8	Identify all known protein-protein interaction inhibitors

## “Provenance Everywhere”



### Explorer

**Sildenafil**

Pharmacology Data | View in ChemBioNavigator

Sildenafil (in citrate form), sold under the names Viagra, Revatio and under various other names, is a drug used to treat male erectile dysfunction (impotence) and pulmonary arterial hypertension (PAH), developed by the pharmaceutical company Pfizer. Its primary competitors on the market are tadalafil (Cialis), and vardenafil (Levitra). [Wikipedia]

Hepatic:

ChemSpider ID: **5023**

Molecular Formula:  $C_{22}H_{26}N_4O_6S$

SMILES: O=S(=O)(N1CCN(C)CC1)C4=CC(C)=NC(=O)C3=CC(N2C3CC(C)C(=O)CC4)C(=O)C

Standard InChI: InChI=1S/C22H26N4O6S/c1-5-7-17-19-20(27(4)25-17)22(29)24-21(23-19)16-14-15(8-9-16)32-4-23(30,31)28-12-10-26(31)-13-28/n8-9,14/s-7,10-13H2,1-4H3,(1,23,24,29)

Standard InChIKey: **BNRNUJZRGQAQC-UHFFFAOYSA-N**

Affected Organism: Humans and other mammals

Indication: For the treatment of erectile dysfunction

Melting Point: 189-190 °C

ALogP: 2.2

# H-Bond Receptors: 7

# H-Bond Donors: 1

Mol Weight: 474.576

MW Freebase: 474.576

Polar Surface Area: 117.51

# Rotatable Bonds: 7

### Apps

API

?ops\_item skos:concept

?ops\_item skos:concept

?cw\_uri skos:preference

void:in

?equiv\_target domain

ops:target

ops:target

void:in

ops:targetOfAssay

?equiv\_assay chemical

chembl:chemical

?std\_type ;





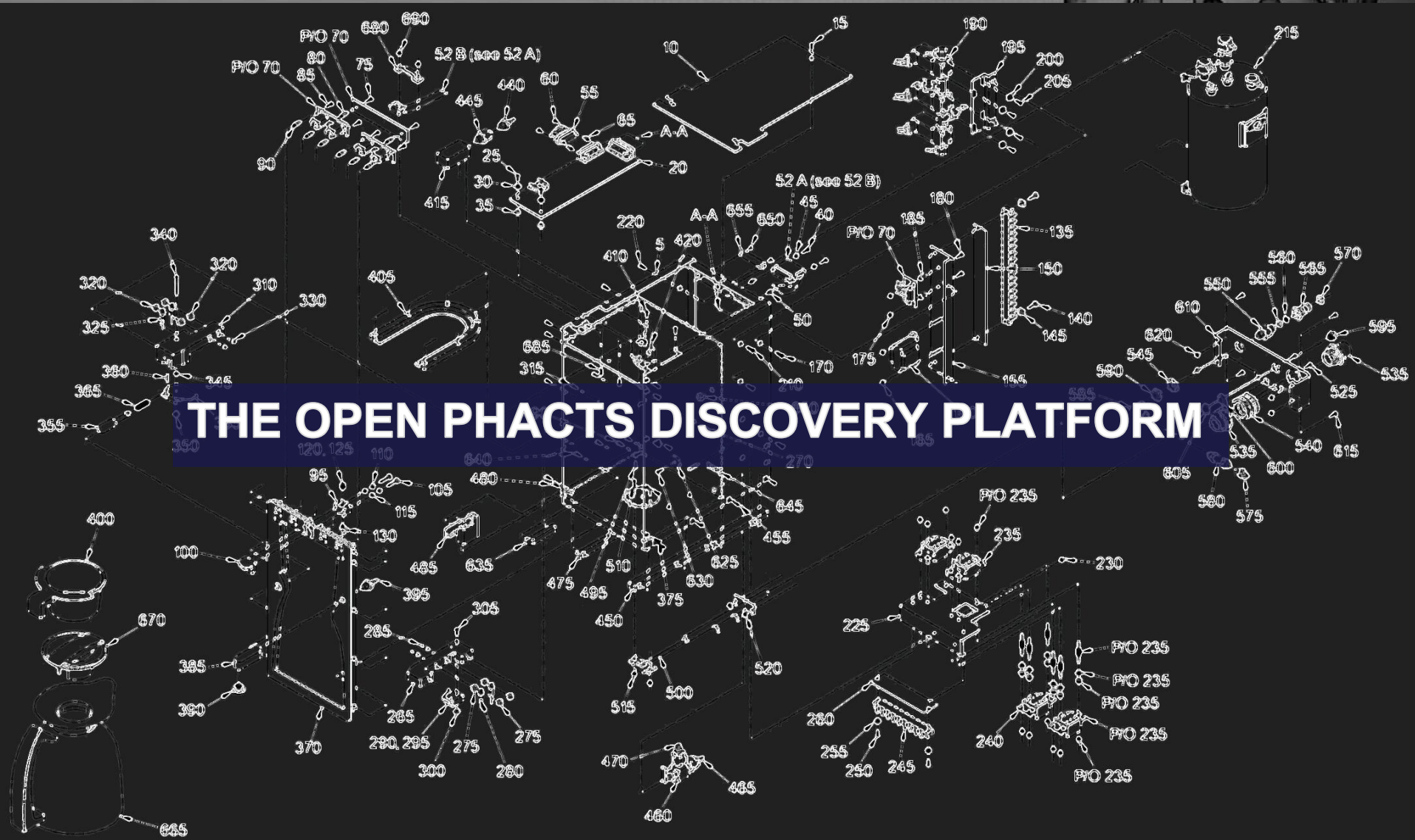


# Open PHACTS

Open Pharmacological Space



## THE OPEN PHACTS DISCOVERY PLATFORM





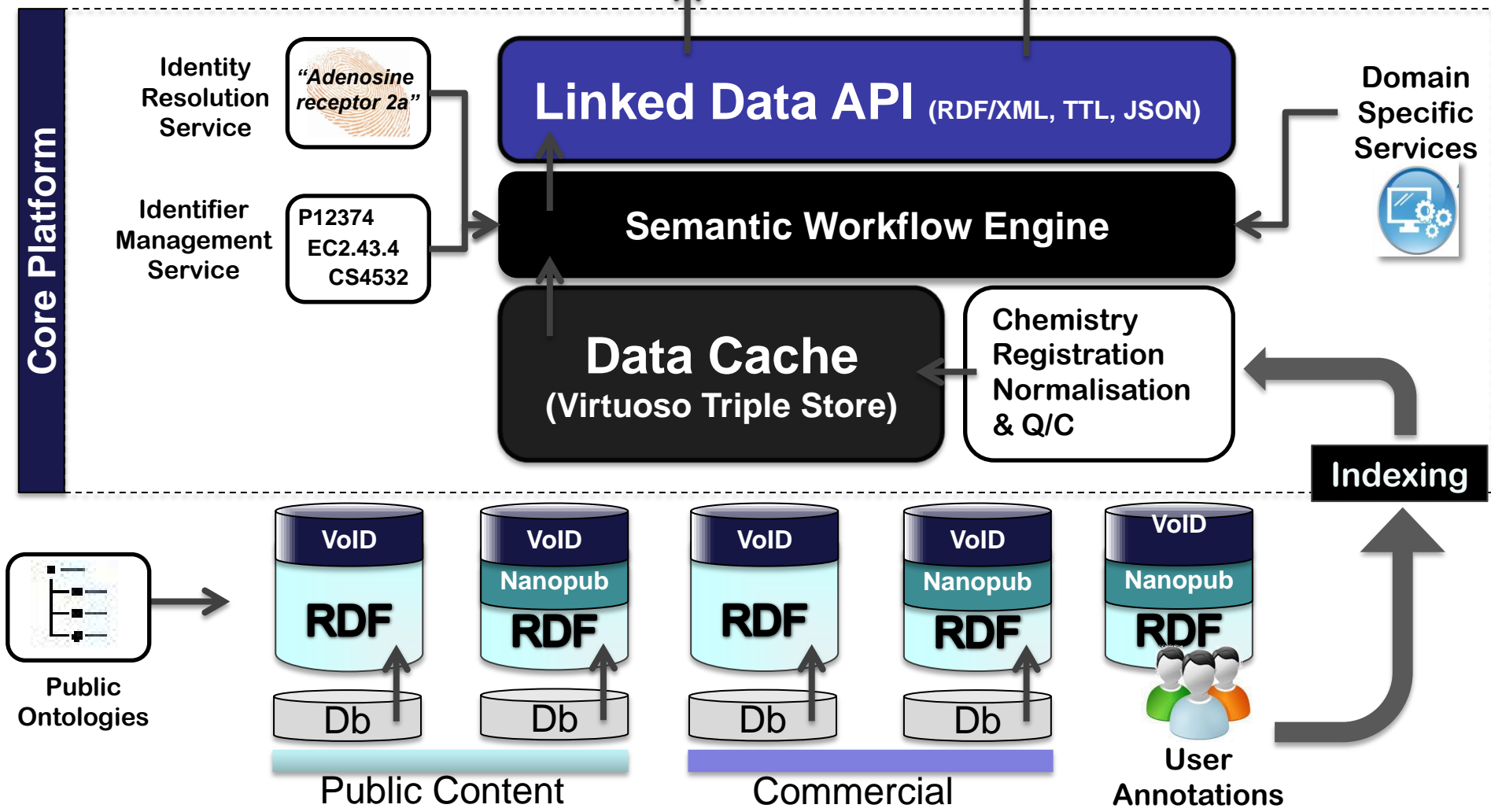
## Contrary to popular belief:

If you produce RDF from two different data sources and put them in a triple store... ***Magic does not happen, and it does not automatically become linked data!***

## You need to link:

- Terms to ontologies
- Ontologies to ontologies
- Identifiers to identifiers
- Text to known concepts
- Chemicals to known structures

# Apps





# Present Content

<u>Source</u>	<u>Initial Records</u>	<u>Triples</u>	<u>Properties</u>
ChEMBL	1,149,792 ~1,091,462 cmpds ~8845 targets	146,079,194	17 cmpds 13 targets
DrugBank	19,628 ~14,000 drugs ~5000 targets	517,584	74
UniProt	536,789	156,569,764	78
ENZYME	6,187	73,838	2
ChEBI	35,584	905,189	2
GO/GOA	38,137	24,574,774	42
ChemSpider/ACD	1,194,437	161,336,857	22 ACD, 4 CS
ConceptWiki	2,828,966	3,739,884	1
WikiPathways	Just added		



## Quantitative Data Challenges

STANDARD_TYPE	UNIT_COUNT
AC50	7
Activity	421
EC50	39
IC50	46
ID50	42
Ki	23
Log IC50	4
Log Ki	7
Potency	11
log IC50	0

STANDARD_TYPE	STANDARD_UNITS	COUNT (*)
IC50	nM	829448
IC50	ug.mL-1	41000
IC50		38521
IC50	ug/ml	2038
IC50	ug ml-1	509
IC50	mg kg-1	295
IC50	molar ratio	178
IC50	ug	117
IC50	%	113
IC50	uM well-1	52

**>5000 types**

Implemented using the Quantities, Dimension, Units, Types  
Ontology (<http://www.qudt.org/>)

**~ 100 units**





**HELLO**  
my name is

~~RS\_2353~~

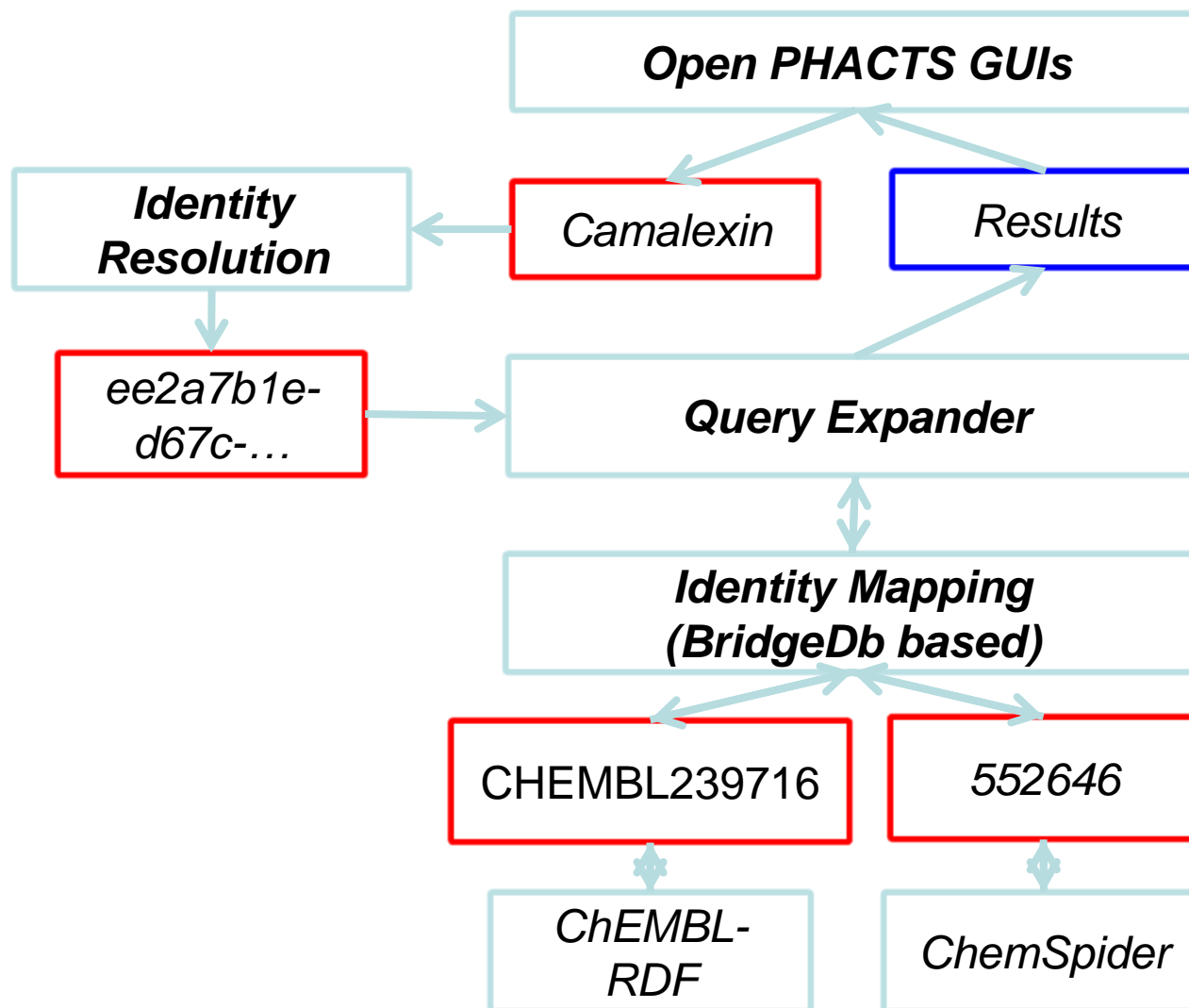
~~GB:29384~~

~~P12047~~

~~X31045~~

~~P12047~~

*Let the IMS take the strain....*





## Chemistry Registration

- Existing chemistry registration system uses standard ChemSpider deposition system: includes low-level structure validation and manual curation service by RSC staff.
- New Registration System in Development
  - Utilizes ChemSpider Validation and Standardization platform including collapsing tautomers
  - Utilizes FDA rule set as basis for standardization (GSK lead)
  - Will generate Open PHACTS identifier (OPS ID)

**Chemistry  
Registration  
Normalisation  
& Q/C**





**Its easy to integrate, difficult to integrate well:**

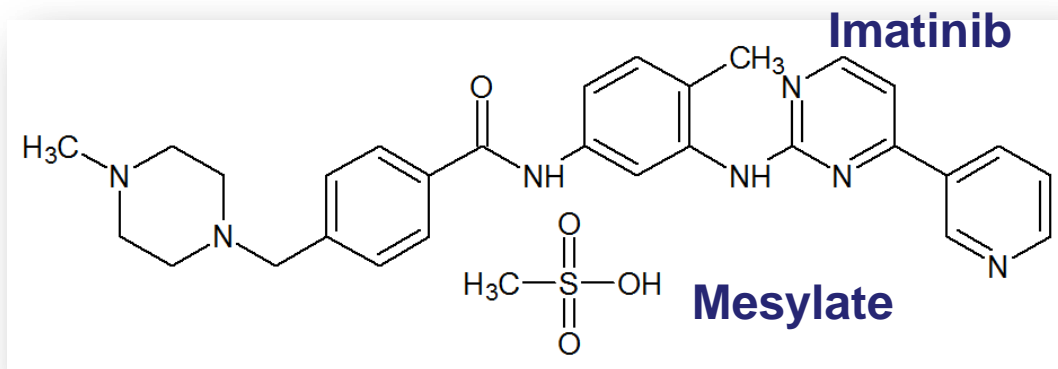
**Type a compound name:**

glee

- Gleevec
- Gleevec



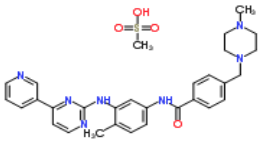
# What Is Gleevec?



**ChemSpider**  
The free chemical database

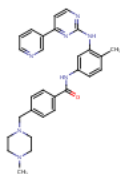
About | More Searches | Web APIs

**Gleevec**



ChemSpider ID: 123596  
Molecular Formula: C<sub>29</sub>H<sub>31</sub>N<sub>7</sub>O<sub>4</sub>S  
Average mass: 589.708400  
Monoisotopic mass: 589.708400  
Systematic name: 4-[[4-methyl-1-piperazinyl]methoxy]phenyl 2-methyl-5-pyridin-2-yl-1H-imidazole-4-carboxylate

**ChemSpider**

Structure	 Download: <a href="#">MOL</a>   <a href="#">SDF</a>   <a href="#">SMILES</a>   <a href="#">InChI</a> Display: <a href="#">2D Structure</a>   <a href="#">3D Structure</a>
Synonyms	<ul style="list-style-type: none"> <li>Imatinib Mesylate</li> <li>Imatinib Methansulfonate</li> <li>STI-571</li> </ul>
Brand names	<ul style="list-style-type: none"> <li>Gleevec</li> <li>Glivec</li> </ul>

**Drugbank**

**Imatinib; 152459-95-5; sti-571 ...**

MW: 493.602740 g/mol MF: C<sub>29</sub>H<sub>31</sub>N<sub>7</sub>O<sub>4</sub>S  
IUPAC name: 4-[[4-methylpiperazin-1-yl]methoxy]phenyl 2-methyl-5-pyridin-2-yl-1H-imidazole-4-carboxylate  
Active in 205 BioAssays Tested in 1376 BioAssays  
CID: 5291  
[Similar Compounds](#) [Same Parent, Connectives](#) (MeSH Keyword)

**Imatinib mesylate; Gleevec; Glivec ...**

MW: 589.708400 g/mol MF: C<sub>30</sub>H<sub>35</sub>N<sub>7</sub>O<sub>4</sub>S  
IUPAC name: methanesulfonic acid; 4-[[4-methylpiperazin-1-yl]methoxy]phenyl 2-methyl-5-pyridin-2-yl-1H-imidazole-4-carboxylate  
Active in 35 BioAssays Tested in 679 BioAssays  
CID: 123596  
[Similar Compounds](#) [Same Parent, Connectives](#) (MeSH Keyword)

**PubChem**





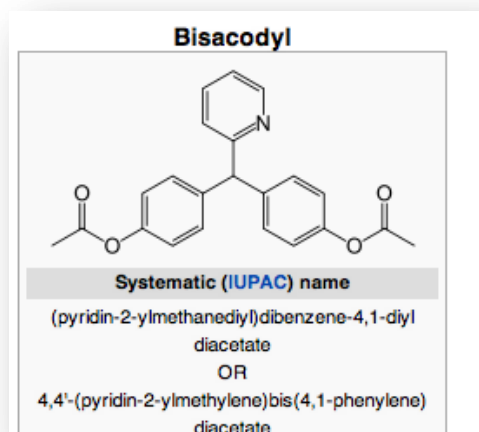
## Dynamic Equality

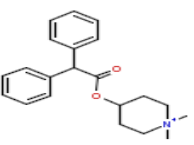
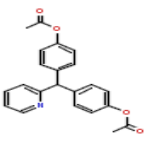


**chemspider:gleevec**

**drugbank:gleevec**

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




<input checked="" type="checkbox"/>	Compound	Synonym
<input checked="" type="checkbox"/>	 <a href="#">CHEMBL168067</a>	Bisacodyl
<input checked="" type="checkbox"/>	 <a href="#">CHEMBL942</a>	Bisacodyl




Home Search

## Terminology

Click on any of the labels to start editing

Term	Authority
Milnacipran	Community, ChemSpider <input type="button" value="trash"/>
<input type="text" value="Enter A Term Here"/>	Community <input type="button" value="trash"/>
(1R,2S)-2-(Aminomethyl)-N,N-diethyl-1-phenylcyclopropanecarboxamide	Community, ChemSpider <input type="button" value="trash"/>
cis-(  )-2-(Aminomethyl)-N,N-diethyl-1-phenylcyclopropanecarboxamide	Community, ChemSpider <input type="button" value="trash"/>
cyclopropanecarboxamide, 2-(aminomethyl)-N,N-diethyl-1-phenyl-, (1R,2S)-	Community, ChemSpider <input type="button" value="trash"/>
92623-85-3	Community, ChemSpider <input type="button" value="trash"/>




**Open PHACTS Explorer**

Navigation

- Compound
- Target
- Pharmacology

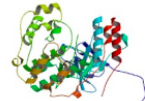
Target by name

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

Target name:

Provenance: ☐ On ☒ Off

Target Data



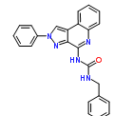
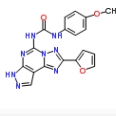
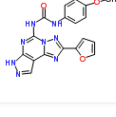
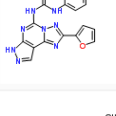

## Mitogen-activated protein kinase 14 (Homo sapiens)

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

Protein name:

☒ Filter
 Provenance: ☐ On ☒ Off

Pharmacology by Target name search results - Total Records: 7887

Structure	Compound Name	Target Name	Target Organism	Assay Organism	Assay Description	Activity Type	Relation	Value	Units	Mol Weight	SMILES	InChI
	urea, N-(phenylmethyl)-N'-(2-phenyl-2H-pyrazolo[3,4-c]quinolin-4-yl)-	Adenosine receptor A3 (Homo sapiens)	Homo sapiens		Displacement of specific [ <sup>125</sup> I]AB-MECA binding at human adenosine A3 receptor expressed in CHO cells	Ki	=	8.3	nM	393.441	O=C(NC(=O)CCCC...	InChI=1S/C
	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 [ <sup>3</sup> H]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
	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
	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
												

explorer.openphacts.org

## Advanced analytics

ChemBioNavigator	Navigating at the interface of chemical and biological data with sorting and plotting options
TargetDossier	Interconnecting Open PHACTS with multiple target centric services. Exploring target similarity using diverse criteria
PharmaTrek	Interactive Polypharmacology space of experimental annotations
UTOPIA	Semantic enrichment of scientific PDFs

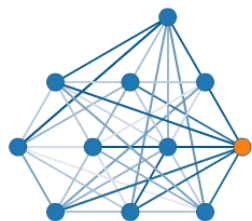
## Predictions

GARFIELD	Prediction of target pharmacology based on the Similar Ensemble Approach
eTOX connector	Automatic extraction of data for building predictive toxicology models in eTOX project

# Target dossier (CNIO)

## Front-end framework to visualize biological data

### P53\_HUMAN PROTEIN INTERACTION NETWORK



**NAME:** CDKN1A\_HUMAN, Cyclin-dependent kinase inhibitor 1

**GENES:** cdkn1a, cap20, cdkn1, cip1, mda6, pic1, sdi1, waf1

**TAXONOMY:** Homo sapiens, Human

**TISSUE:** Eye, Lung, Epithelium

**FUNCTION:** May be the important intermediate by which p53 mediates its role as an inhibitor of cellular proliferation in

#### Protein Annotations

**NAME:** P53\_HUMAN, Cellular tumor antigen p53

**GENES:** tp53, p53

**TAXONOMY:** Homo sapiens, Human

**TISSUE:** Kidney, Lung carcinoma, Blood, Ovarian adenocarcinoma, Glial cell, Glial tumor

**SUBCELLULAR LOCATION:** Interaction with BANP promotes nuclear localization.

**FUNCTION:** Acts as a tumor suppressor in many tumor types; induces growth arrest or apoptosis depending on the physiological circumstances and cell type. Involved in cell cycle regulation as a trans-activator that acts to negatively regulate cell division by controlling a set of genes required for this process. One of the activated genes is an inhibitor of cyclin-dependent kinases. Apoptosis induction seems to be mediated either by stimulation of BAX and FAS antigen expression, or by repression of Bcl-2 expression. Implicated in Notch signaling cross-over.

Dna

Proteins

Pathways

Literature

Synthetic Parts

SEARCH

Nucleotides

Proteins

Literature

Synthetic parts

HISTORY

P04637

p53

UniProtID	Gene	Protein Name	Protein Full Name	Ta
P04637,Q15086,Q150	TP53,P53	P53_HUMAN	Cellular tumor antigen p53	Ho
P02340,Q9QUP3	Tp53,P53,Trp53	P53_MOUSE	Cellular tumor antigen p53	Mi
P10361,O09168,Q4K1	Tp53,P53	P53_RAT	Cellular tumor antigen p53	Ra
Q29537,Q9TV78	TP53,P53	P53_CANFA	Cellular tumor antigen p53	Ca
Q42578	PER53,P53,A15g0672	PER53_ARATH	Peroxidase 53	Ar
Q13625,Q12892,Q867	TP53BP2,ASPP2,BBF	ASPP2_HUMAN	Apoptosis-stimulating of p53 protein 2	Ho
P56424	TP53,P53	P53_MACMU	Cellular tumor antigen p53	Ma
Q12888,Q2M1Z7,Q4L	TP53BP1	TP53B_HUMAN	Tumor suppressor p53-binding protein 1	Ho
Q9TUB2	TP53,P53	P53_PIG	Cellular tumor antigen p53	St
Q09185,P97258,P977	TP53,P53	P53_CRIGR	Cellular tumor antigen p53	Cr

Protein Annotations

**NAME:** P53\_HUMAN, Cellular tumor antigen p53

**GENES:** tp53, p53

**TAXONOMY:** Homo sapiens, Human

**TISSUE:** Kidney, Lung carcinoma, Blood, Ovarian adenocarcinoma, Glial cell, Glial tumor, Colon adenocarcinoma, Embryonic kidney, Embryonic kidney, Embryonic kidney

**SUBCELLULAR LOCATION:** Interaction with BANP promotes nuclear localization.

**FUNCTION:** Acts as a tumor suppressor in many tumor types; induces growth arrest or apoptosis depending on the physiological circumstances and cell type. Involved in cell cycle regulation as a trans-activator that acts to negatively regulate cell division by controlling a set of genes required for this process. One of the activated genes is an inhibitor of mutation of BAX and FAS antigen over.

	Cancers	Literature Score
NOTCH1	Brain [C], lymphomagenesis [NCI], 189 more ...	0
BRAF	Adrenocortical [C], well-differentiated thyroid carcinoma [NCI], 282 more ...	0.457
CDH1	BiliaryTract [C], skin tumor [NCI], 156 more ...	0
BCL2	Brain [C], waldenstroms macroglobulinemia [NCI], 1233 more ...	0
NRAS	Adrenocortical [C], childhood acute lymphocytic leukemia [NCI], 406 more ...	0.249
PTEN	AutonomicGanglia [C], lipomatosis [NCI], 568 more ...	0
SOCS1	Brain [C], barrett's adenocarcinoma [NCI], 163 more ...	0
MMP2	Colorectal [C], urothelial cancers [NCI], 637 more ...	0
GNAQ	Melanoma [C]	0

15



Page 1

of 13

Displaying 1 to 15 of 181 items





### TARGETS

p38 alpha homo

**Mitogen-activated protein kinase 14 (Homo sapiens)**  
Amino Acid, Peptide, or Protein

**alpha thalassemia/mental retardation syndrome X-linked homolog (human) protein, mouse**  
Amino Acid, Peptide, or Protein

You have 1 targets selected

**Mitogen-activated protein kinase 14 (Homo sapiens)**  
Amino Acid, Peptide, or Protein

☐ connect

### LIGANDS

**2(1H)-quinazolinone, 5-(2-chloro-4-fluorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-7-(4-piperidinyl)-**

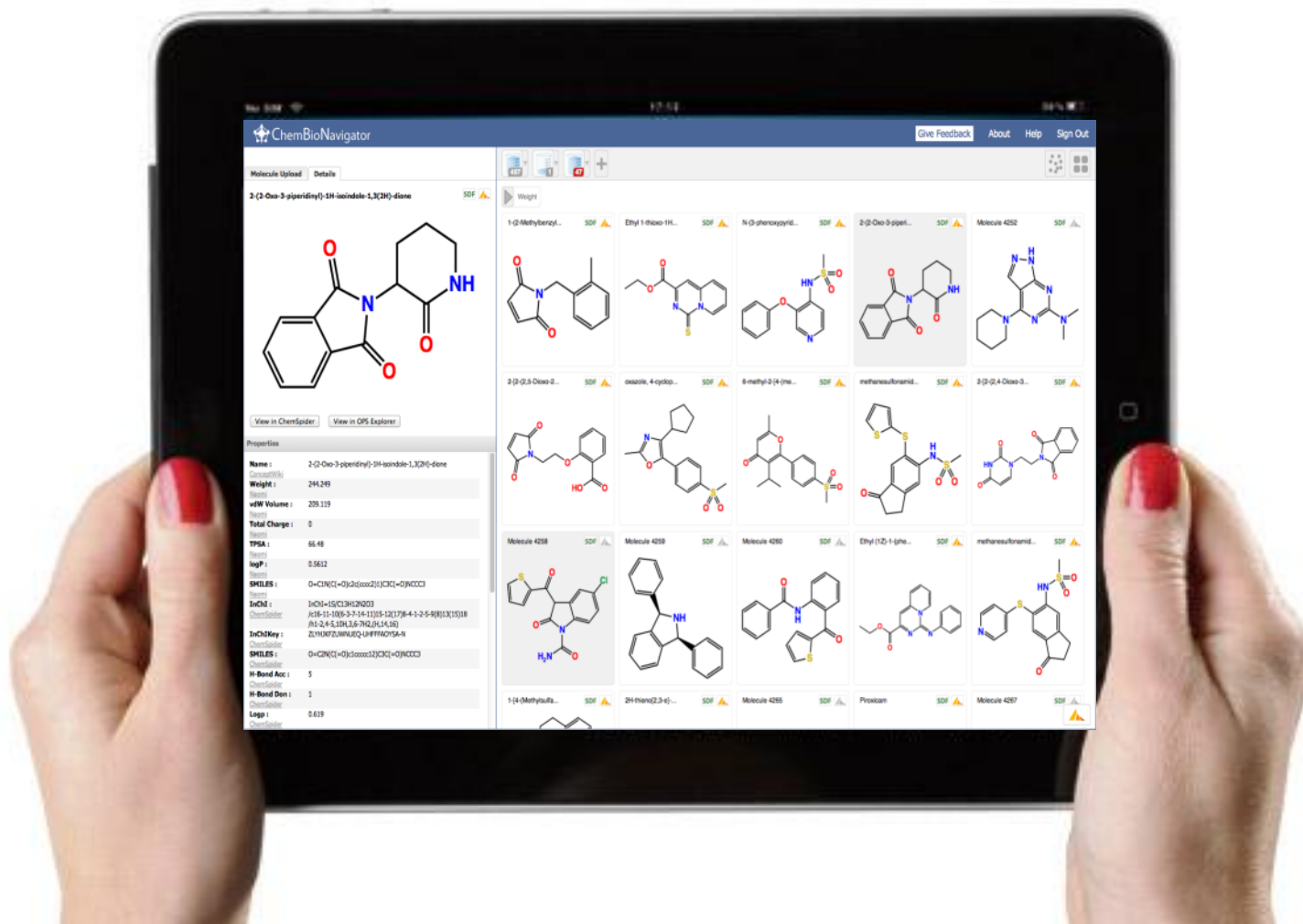
**2(1H)-quinazolinone, 5-(2-chloro-4-fluorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-7-(4-piperidinyl)-**

**2(1H)-quinazolinone, 5-(2-chlorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-7-(1-piperazinylmethyl)-**

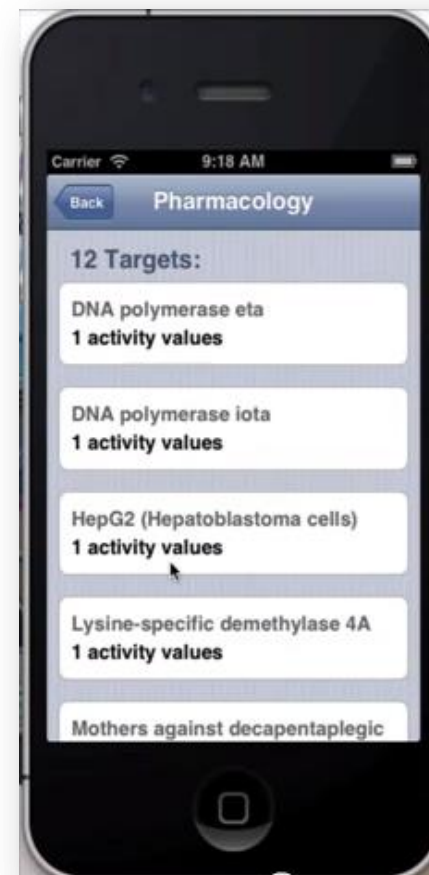
### Interaction Map

35 TARGETS  
546 MOLECULES  
Min annotation [8.00]  
Max annotation [10.41]

☒ Expand target space



9 of 16 pages







KNIME

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

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

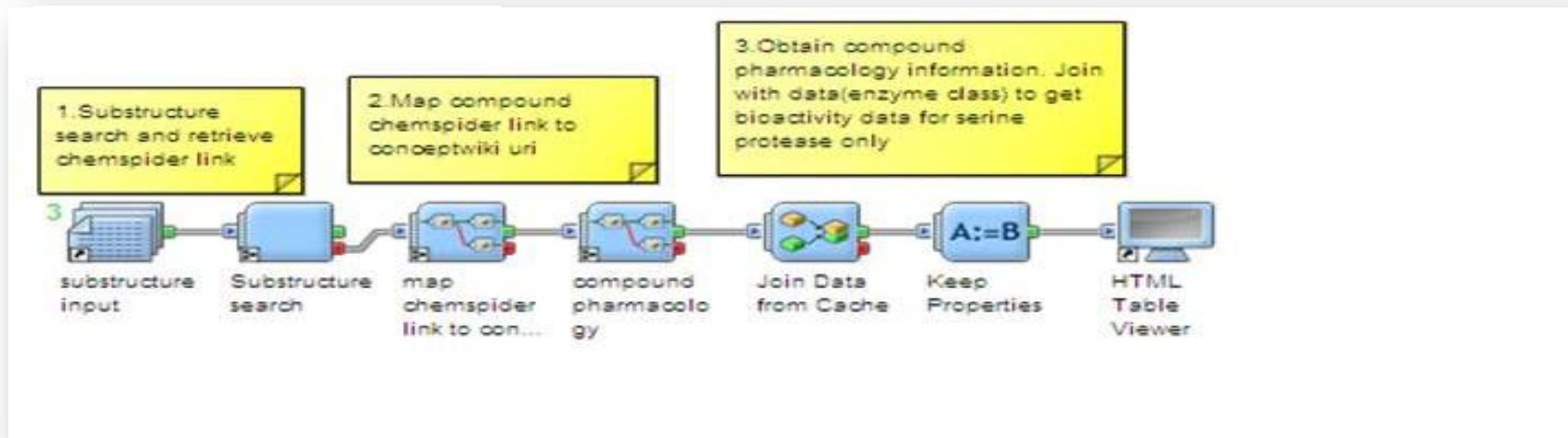
Workflow Diagram:

```

graph LR
    FileReader[File Reader] --> JavaSnippet[Java Snippet]
    JavaSnippet --> GetNameInchi[Get Name and Inchi]
    GetNameInchi --> GetActivity[Get Activity]
    GetActivity --> ActivityParser[Activity Parser]
    ActivityParser --> ColumnFilter[Column Filter]
    ColumnFilter --> InteractiveTable[Interactive Table]
  
```

Node Descriptions:

- 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







Chrome File Edit View History Bookmarks Window Help

Open PHACTS - YouTube

www.youtube.com/user/OpenPHACTS/videos

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Open PHACTS Explorer - Search Compounds by Name

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Open PHACTS Explorer - View Pharmacology by Compound

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Open PHACTS Explorer - Search for Target Information by Name

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The Open PHACTS Explorer

610 views 4 months ago

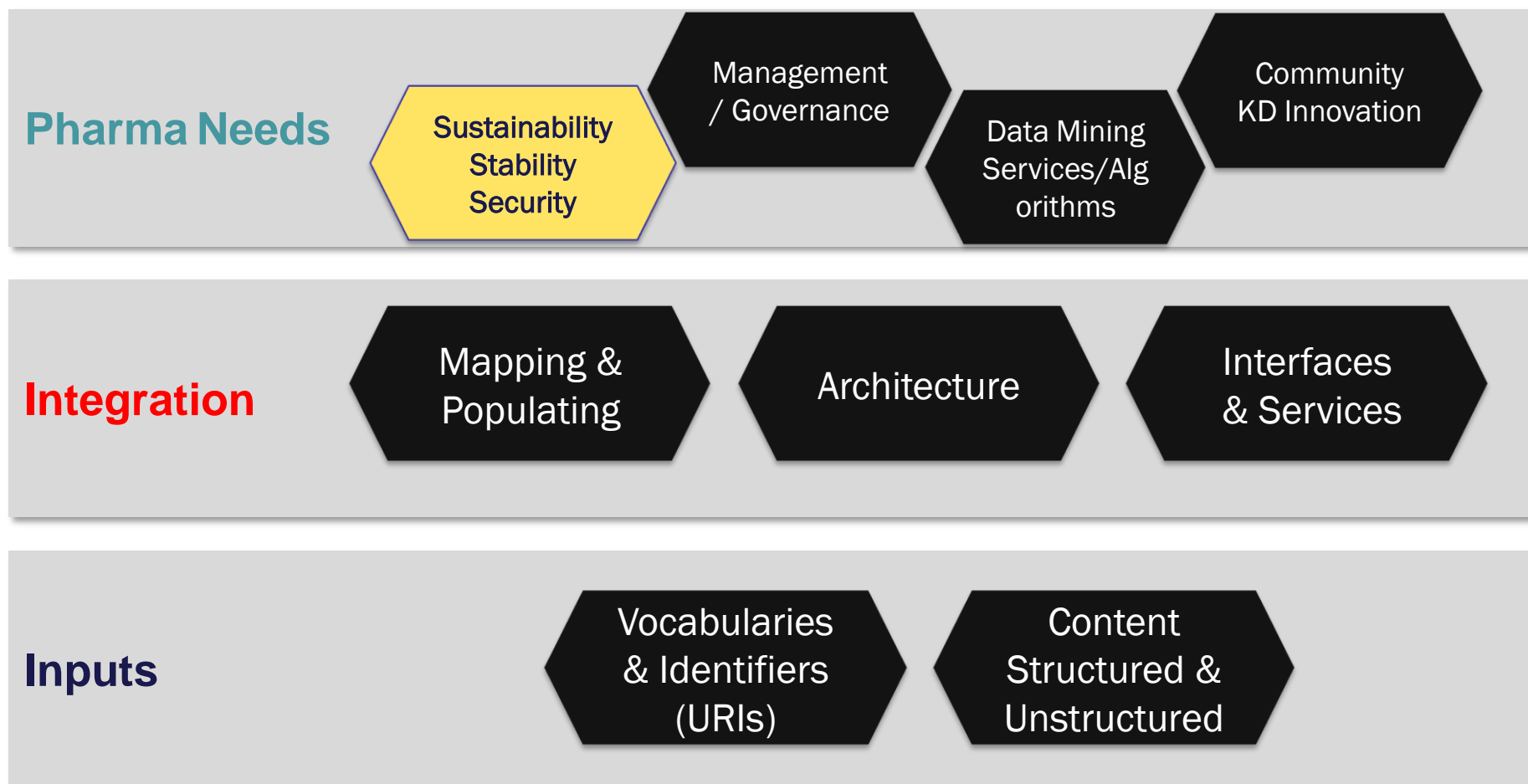
Open PHACTS 6 Month Lashup Demo

1,173 views 1 year ago

www.youtube.com/user/OpenPHACTS



# A Precompetitive Knowledge Framework



## Associated partners

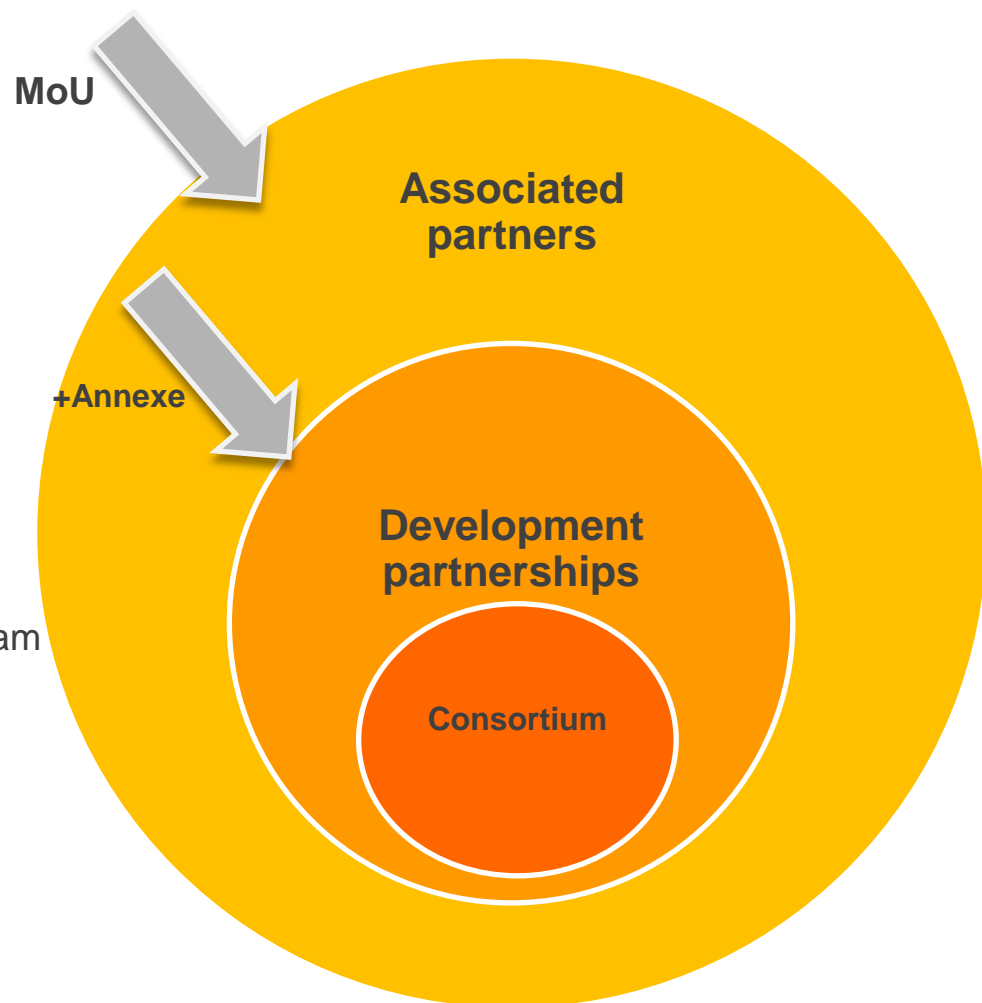
Organisations, most will join here  
Support, information  
Exchange of ideas, data, technology  
Opportunities to demo at community webinars  
Need MoU

## Development partnerships

Influence on API developments  
Opportunities to demo ideas & use cases to core team  
Need MoU and annexe

## Consortium

28 current members

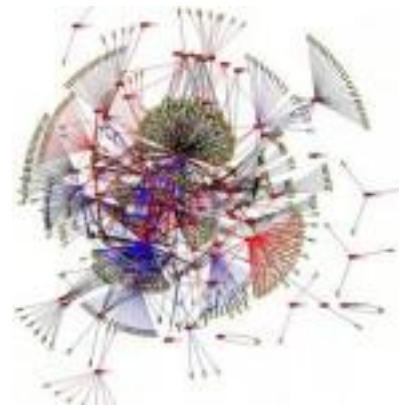


# Sustaining Impact

✦ “Software is free like puppies are free - they both need money for maintenance”



✦ ...and more resource for future development





## The Open PHACTS community ecosystem







A UK-based not-for-profit  
member owned company

Publish

Maintain and develop the  
Open PHACTS Platform

‘Research based’ organisation

Many different types of member

Develop and build the Open  
PHACTS community

Develop and contribute to  
data standards

Innovate

Become partner in  
other consortia

Provide stable API services

Precompetitive

Develop and build new value-  
added analytical methods

Promote and build interoperable  
data beyond Open PHACTS



## Becoming part of the Open PHACTS Foundation

### Members

A UK-based not-for-profit  
member owned company

- ❖ membership offers early access to platform updates and releases
  - ❖ the opportunity to steer research and development directions
  - ❖ receive technical support
  - ❖ work with the ecosystem of developers and semantic data integrators around Open PHACTS
- 
- ❖ tiered membership
  - ❖ familiar business and governance model

# Open PHACTS Project Partners



**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

University of Santiago de Compostela

Rheinische Friedrich-Wilhelms-Universität Bonn

AstraZeneca

GlaxoSmithKline

Esteve

Novartis

Merck Serono

H. Lundbeck A/S

Eli Lilly

Netherlands Bioinformatics Centre

Swiss Institute of Bioinformatics

ConnectedDiscovery

EMBL-European Bioinformatics Institute

Janssen

OpenLink



[pmu@openphacts.org](mailto:pmu@openphacts.org)



- ❖ **Access to a wide range of interconnected data** – easily jump between pharmacology, chemistry, disease, pathways and other databases without having to perform complex mapping operations
- ❖ **Query by data type, not by data source** (“Protein Information” not “Uniprot Information”)
- ❖ **API queries that seamlessly connect data** (for instance the Pharmacology query draws data from ChEMBL, ChemSpider, ConceptWiki and Drugbank)
- ❖ **Strong chemistry representation** – all chemicals reprocessed via Open PHACTS chemical registry to ensure consistency across databases
- ❖ **Built using open community standards**, not an ad-hoc solution. Developed in conjunction with 8 major pharma (so your app will speak their language!)
- ❖ **Simple, flexible data-joining** (join compound data ignoring salt forms, join protein data ignoring species)
- ❖ **Provenance everywhere** – every single data point tagged with source, version, author, etc
- ❖ **Nanopublication-enabled**. Access to a rich dataset of established and emerging biomedical “assertions”
- ❖ **Professionally Hosted** (Continually Monitored)
- ❖ **Developer-friendly JSON/XML methods. Consistent API** for multiple services
- ❖ **Seamless data upgrades**. We manage updates so you don’t have to
- ❖ **Community-curation** tools to enhance and correct content
- ❖ Access to a **rich application network** (many different App builders)
- ❖ **Toolkits** to support many different languages, workflow engines and user applications
- ❖ **Private and secure**, suitable for confidential analyses
- ❖ **Active & still growing** through a unique public-private partnership