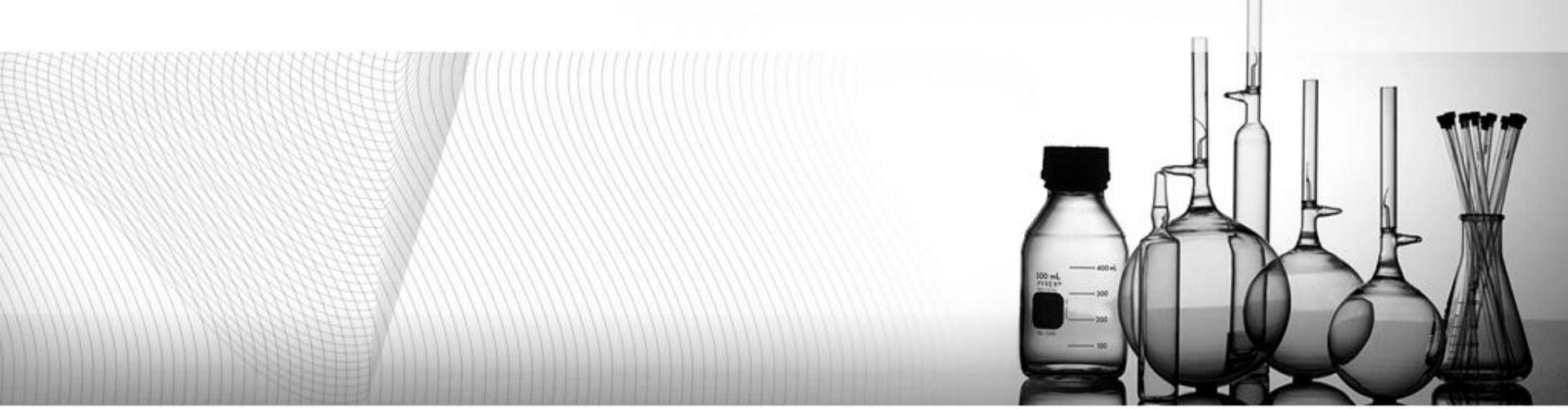

Open PHACTS
Open Pharmacological Space

Open PHACTS – The use of open data for *in silico* models

Gerhard F. Ecker
Dept. of Pharmaceutical Chemistry, Univ Vienna
Gerhard.f.ecker@univie.ac.at; www.openphacts.org

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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

Approaching complex research questions needs integration of data sources

Open PHACTS
Open Pharmacological Space

The Need

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

Azzaoui et al., *Drug Discov Today* 2013, 843-52

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The User

The Explorer is a user-friendly, full featured interface that allows scientists to explore and interrogate integrated biological and chemical data

The API allows searches along the concepts of

compound – target – pathway - disease

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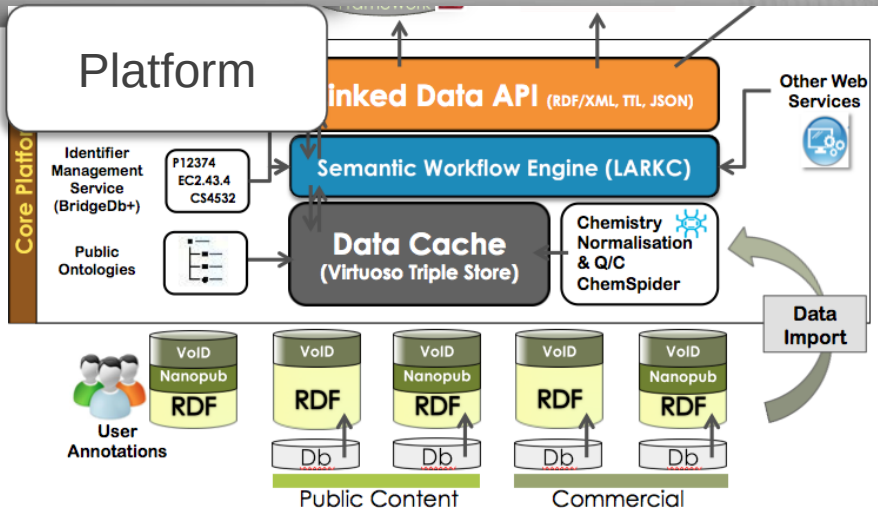
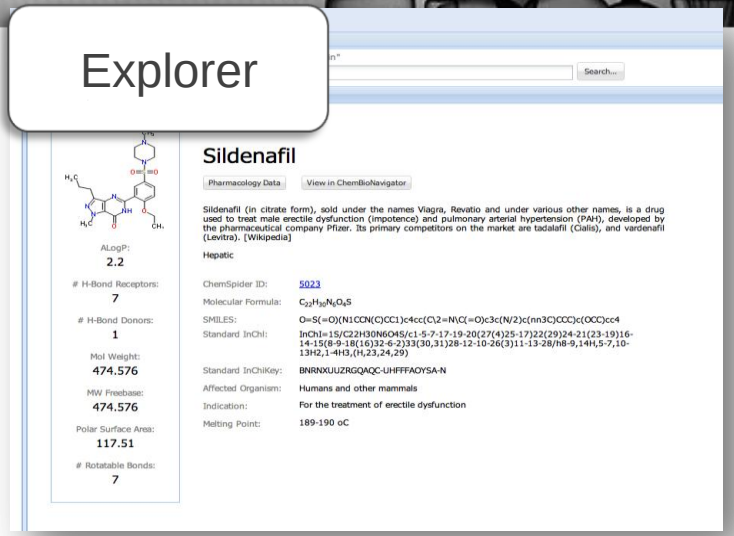
Platform



Explorer



Apps

API

Standards

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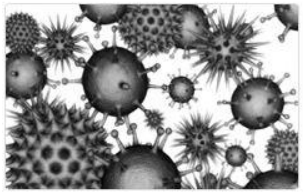
STANDARD_TYPE	UNIT_COUNT
AC50	7
Activity	421
EC50	39
IC50	46
ID50	42
Ki	23
Log IC50	4
Log Ki	7
Potency	11
log IC50	0

>5000 types

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
IC50	p.p.m.	51
IC50	ppm	36
IC50	uM-1	25
IC50	nM kg-1	25
IC50	milliequivalent	22
IC50	kJ m-2	20

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

~ 100 units



Menu Explorer

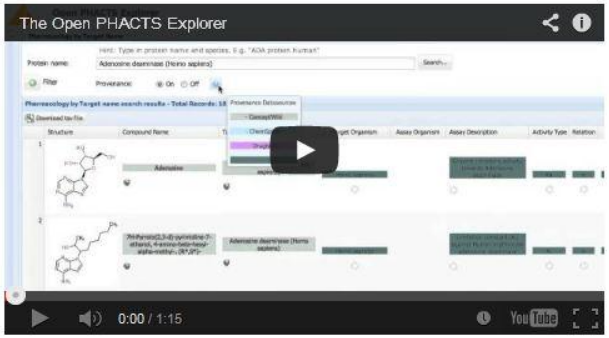
- Welcome
- The Project
- Explorer Release Notes
- Tutorials
- The Data
- Terms and Conditions
  - Terms of Use
  - Privacy Statement
  - Licensing
  - Take-down policy

Welcome to the Open PHACTS Explorer

We are pleased to present the first public release of the beta Open PHACTS Explorer.

The Open PHACTS Explorer allows multiple sources of publicly-available pharmacological and physicochemical data to be intuitively queried, and makes data provenance accessible at every step. The Open PHACTS Explorer was built to answer critical pharmacological questions as defined by academic and pharmaceutical industry scientists.

To get started watch our tutorial introduction, visit the tutorials page or click on the registration link :



This is the first public release of the Open PHACTS Explorer, and we look forward to and value your feedback and comments .

Explorer

Registration and access to the Open PHACTS Explorer

Known issues with beta Open PHACTS Explorer

Feedback

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Explorer

www.openphacts.org

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Open Pharmacological Space

Open PHACTS Explorer

Navigation

- Compound
  - Compound by name
  - Compound by structure
- Target
  - Target by name
- Pharmacology
  - Pharmacology by Enzyme family
  - Pharmacology by Compound
  - Pharmacology by Target

Help and Feedback

API Status

TSV Downloads

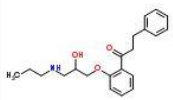
Compound by name

Hint: Type in compound name. E.g. "Aspirin"

Compound name: Propafenone Search

Provenance: On Off

Compound by Name search results



ALogP: 3.4

H-Bond Acceptors: 4

H-Bond Donors: 2

Mol Weight: 341.444

MW Freebase: 341.444

Polar Surface Area (Å2): 58.6

Rotatable Bonds: 11

Propafenone

Pharmacology Data | Structure Search | ChemSpider Info

An antiarrhythmia agent that is particularly effective in ventricular arrhythmias. It also has weak beta-blocking activity. The drug is generally well tolerated. [PubChem]

Metabolized primarily in the liver where it is rapidly and extensively metabolized to two active metabolites, 5-hydroxypropafenone and N-depropylpropafenone. These metabolites have antiarrhythmic activity comparable to propafenone but are present in concentrations less than 25% of propafenone concentrations.

ChemSpider ID:	4763
Molecular Formula:	$C_{21}H_{27}NO_3$
SMILES:	O=C(c1ccccc1OCC(O)CNCCC)CCc2ccccc2
Standard InChI:	InChI=1S/C21H27NO3 /c1-2-14-22-15-18(23)16-25-21-11-7-6-10-19(21)20(24)13-12-17-8-4-3-5-9-17 /h3-11,18,22-23H,2,12-16H2,1H3
Standard InChiKey:	JWHAUXFOSRPERK-UHFFFAOYSA-N
Protein Binding:	97%
Toxicity:	Symptoms of propafenone overdose (usually most severe within the first 3 hours) may include convulsions (rarely), heartbeat irregularities, low blood pressure, and sleepiness.

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Navigation

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- Target
  - Target by name
- Pharmacology
  - Pharmacology by Enzyme family
  - Pharmacology by Compound
  - Pharmacology by Target

Help and Feedback

API Status

TSV Downloads

Compound by name | Pharmacology by Compound name

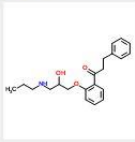
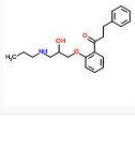
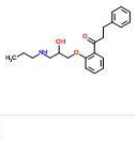
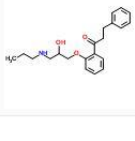
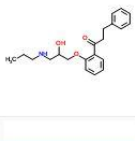
Hint: Type in compound name. E.g. "Aspirin" and select a result

Compound name: Propafenone Search...

Filter Provenance: On Off

Pharmacology by Compound name search results - Total Records: 122

Prepare tsv file

	Structure	Compound Name	Target Names	Target Organisms	Assay Organism	Assay Description	Activity Type	Relation	Value	Units	SMILES	InChi	InChi Key	Pubmed ID
1		Propafenone	P-glycoprotein 1	Homo sapiens		Compound was tested for inhibition of daunomycin efflux in the resistant human T-lymphoblast cell line CEM vcr1000.	EC50	=	320	nM	O=C(c1ccccc1O...	InChI=1S/C21H...	JWHAUXFOSRP...	9767638
2		Propafenone	L5178Y (Lymphoma cells)	Mus musculus	Mus musculus	Compound was tested for inhibition of rhodamine 123 efflux in mdr 1 transfectant L5178Y VMDRI C.06 mouse lymphoma cells; nd=Not determined					O=C(c1ccccc1O...	InChI=1S/C21H...	JWHAUXFOSRP...	9767638
3		Propafenone				Calculated membrane partition coefficient (Kmemb)	Log Kmemb	=	0.7		O=C(c1ccccc1O...	InChI=1S/C21H...	JWHAUXFOSRP...	15027870
4		Propafenone				Volume of distribution in man (IV dose)	Vdss	=	3.6	L.kg-1	O=C(c1ccccc1O...	InChI=1S/C21H...	JWHAUXFOSRP...	12061889
5		Propafenone				Unbound fraction (plasma)	Fraction fr...	=	0.05		O=C(c1ccccc1O...	InChI=1S/C21H...	JWHAUXFOSRP...	12061889
6														

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Open PHACTS Explorer

Navigation

- Compound
  - Compound by name
  - Compound by structure
- Target
  - Target by name
- Pharmacology
  - Pharmacology by Enzyme family
  - Pharmacology by Compound
  - Pharmacology by Target

Help and Feedback

API Status

TSV Downloads

Compound by name | Pharmacology by Compound name | Compound Structure Search | Target by name

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

Target name: Multidrug resistance protein 1A (Mus musculus) Search

Provenance: On Off

Target Data

Multidrug resistance protein 3 (Mus musculus)

Pharmacology Data

Description:	Multidrug resistance protein 3
Synonyms:	ATP-binding cassette sub-family B member 1A, CHEMBL2573, MDR1A, Multidrug resistance protein 3, P-glycoprotein 3
Specific Function:	Energy-dependent efflux pump responsible for decreased drug accumulation in multidrug-resistant cells.
Keywords:	Hydrolase, Phosphoprotein, 3D-structure, ATP-binding, Cell membrane, Complete proteome, Direct protein sequencing, Glycoprotein, Membrane, Nucleotide-binding, Reference proteome, Repeat, Transmembrane, Transmembrane helix, Transport
PDB Entry:	3G61 3G5U 3G60

Open PHACTS Explorer

Navigation

- Compound
  - Compound by name
  - Compound by structure
- Target
  - Target by name
- Pharmacology
  - Pharmacology by Enzyme family
  - Pharmacology by Compound
  - Pharmacology by Target

Help and Feedback

API Status

TSV Downloads

Compound by name | Pharmacology by Compound name | Compound Structure Search | Target by name | Compounds active against enzyme family | Pharmacology by Target Name

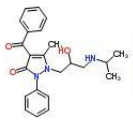
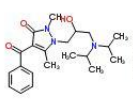
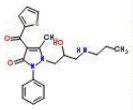
Hint: Type in protein name and species. E.g. "ADA protein human" and select a result

Protein name: Multidrug resistance protein 1 (Homo sapiens) Search...

Filter Provenance: On Off

Pharmacology by Target name search results - Total Records: 2563

Prepare tsv file

	Structure	Compound Name	Target Name	Target Organism	Assay Organism	Assay Description	Activity Type	Relation	Value	Units	Mol Weight	SMILES	InChi	InChi Key
1		4-benzoyl-1-[2-hydroxy-3-(propan-2-ylamino)propyl]-5-methyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one	Multidrug resistance protein 1 (Homo sapiens)	Homo sapiens		Compound was tested for inhibition of daunomycin efflux in the resistant human T-lymphoblast cell line CEM vcr 1000.	EC50	=	83180	nM	393.479	O=C2\C(=C(/N(...	InChI=1S/C23H...	VZPAOCHCLZMT...
2		1,3-dimethyl-4-[(E)-phenyl(propylimino)methyl...pyrazol-5-ol	Multidrug resistance protein 1 (Homo sapiens)	Homo sapiens		Compound was tested for inhibition of daunomycin efflux in the resistant human T-lymphoblast cell line CEM vcr 1000.	EC50	=	272500	nM	257.331	CCC/N=C(\c1cc...	InChI=1S/C15H...	GJPFQWWTOPA...
3		4-benzoyl-1-[3-(dipropan-2-ylamino)-2-hydroxypropyl]-2,5-dimethyl-1,2-dihydro-3H-pyrazol-3-one	Multidrug resistance protein 1 (Homo sapiens)	Homo sapiens		Compound was tested for inhibition of daunomycin efflux in the resistant human T-lymphoblast cell line CEM vcr 1000.	EC50	=	24120	nM	373.489	O=C1\C(=C(/N(...	InChI=1S/C21H...	UYZSJNDVHQW...
4		1-[2-Hydroxy-3-(propylamino)propyl]-5-methyl-2-phenyl-4-(2-thienylcarbonyl)-1,2-dihydro-3H-pyrazol-3-one	Multidrug resistance protein 1 (Homo sapiens)	Homo sapiens		Compound was tested for inhibition of daunomycin efflux in the resistant human T-lymphoblast cell line CEM vcr 1000.	EC50	=	72440	nM	399.507	O=C(C=2C(=O)...	InChI=1S/C21H...	JCKJIYACBBEC...
5		1-[2-hydroxy-3-(propan-2-ylamino)propyl]-5-methyl-2-phenyl-4-(3-phenylpropanoyl)-1,2-dihydro-3H-pyrazol-3-one	Multidrug resistance protein 1 (Homo sapiens)	Homo sapiens		Compound was tested for inhibition of daunomycin efflux in the resistant human T-lymphoblast cell line CEM vcr 1000.	EC50	=	11750	nM	421.532	O=C2\C(=C(/N(...	InChI=1S/C25H...	DNSZEGKDVYSK...
6														

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Provenance

Open PHACTS Explorer

Navigation

- Compound
- Target
- Pharmacology
  - Pharmacology by Enzyme family
  - Pharmacology by Compound
  - Pharmacology by Target

TSV Downloads

Home | Pharmacology by Target Name

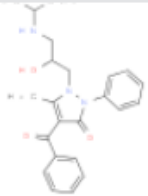
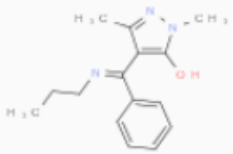
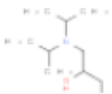
Hint: Type in protein name and species. E.g. "Adenosine rece

Protein name: Multidrug resistance protein 1 (Homo sapiens)

Filter Provenance: On Off

Pharmacology by Target name search results - Total Records: 5204

Prepare tsv file

	Structure	Compound Name	Target Name
		4-benzoyl-1-[2-hydroxy-3-(propan-2-ylamino)propyl]-5-methyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one	P-glycoprotein 1
2		1,3-dimethyl-4-[(E)-phenyl(propylimino)methyl]-pyrazol-5-ol	P-glycoprotein 1
3		4-benzoyl-1-[3-(dipropan-2-ylamino)-2-hydroxypropyl]-2,5-dimethyl-1,2-dihydro	P-glycoprotein 1

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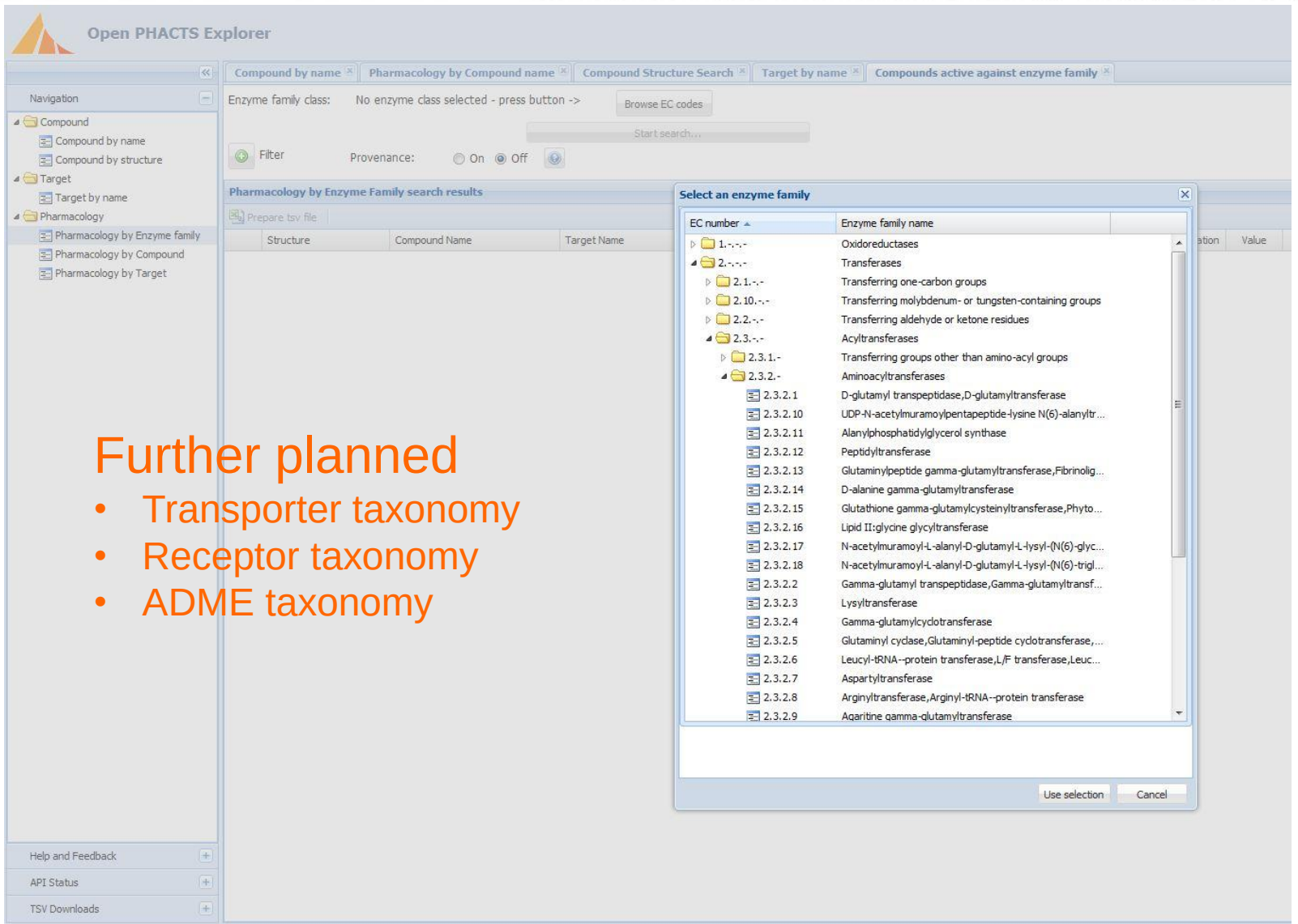
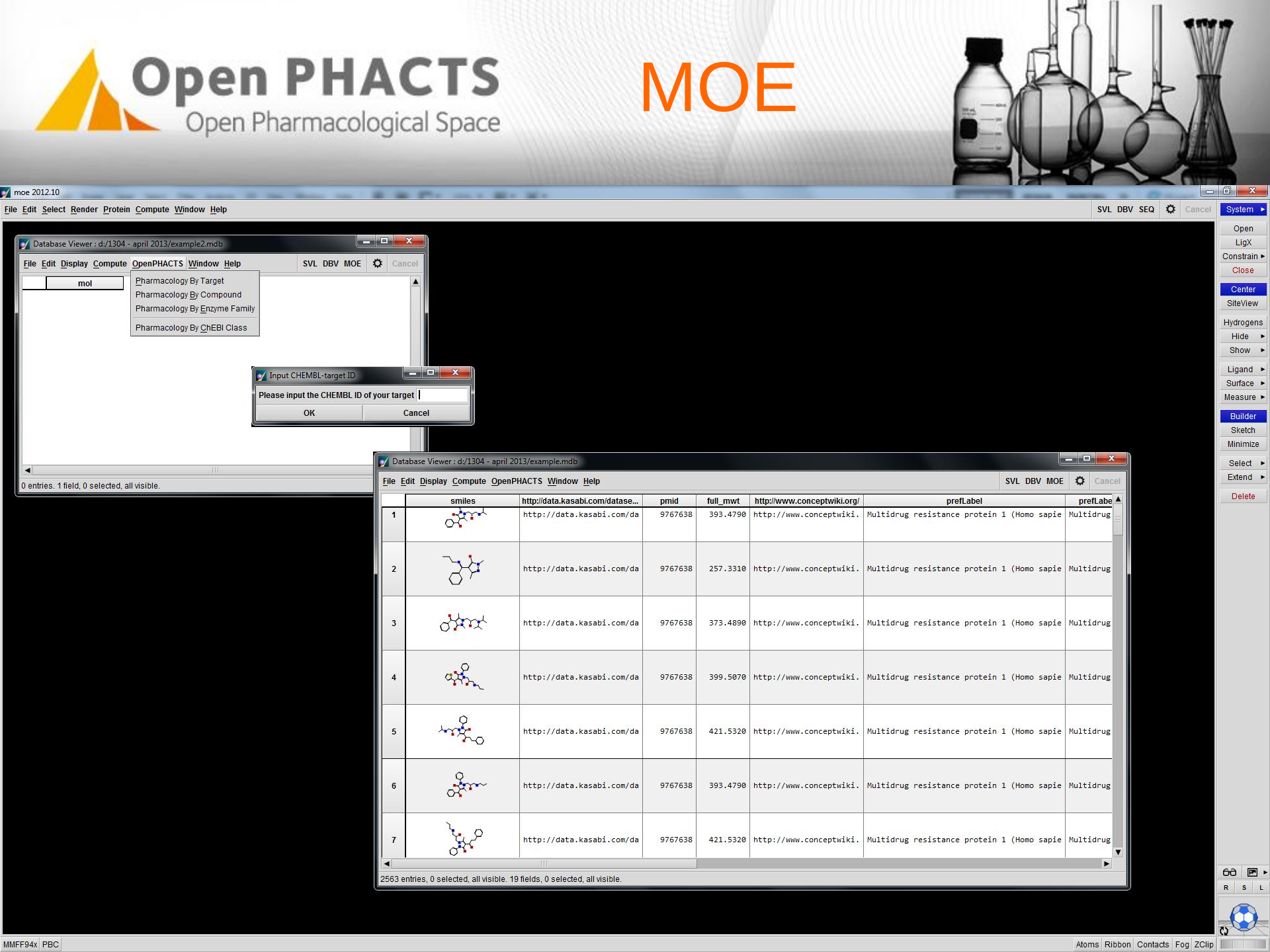
Target Taxonomy



Further planned

- Transporter taxonomy
- Receptor taxonomy
- ADME taxonomy


Open PHACTS
Open Pharmacological Space
MOE
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
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
0 entries. 1 field, 0 selected, all visible.
Input CHEMBL-target ID
Please input the CHEMBL ID of your target
OK
Cancel
Database Viewer : d:/1304 - april 2013/example.mdb
File Edit Display Compute OpenPHACTS Window Help
SVL DBV MOE
Cancel
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.
MMFF94x PBC
Atoms Ribbon Contacts Fog ZClip

Open PHACTS
Open Pharmacological Space

Example applications

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

Open PHACTS
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PharmaTrek

PHARMATREK

TARGETS

p38 alpha homo

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

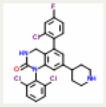
alpha thalassemia/mental retardation syndrome X-linked homolog (human) protein, mouse
Amino Acid, Peptide, or Protein

You have 1 targets selected

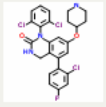
Mitogen-activated protein kinase 14 (Homo sapiens)
Amino Acid, Peptide, or Protein

connect

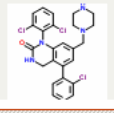
LIGANDS



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

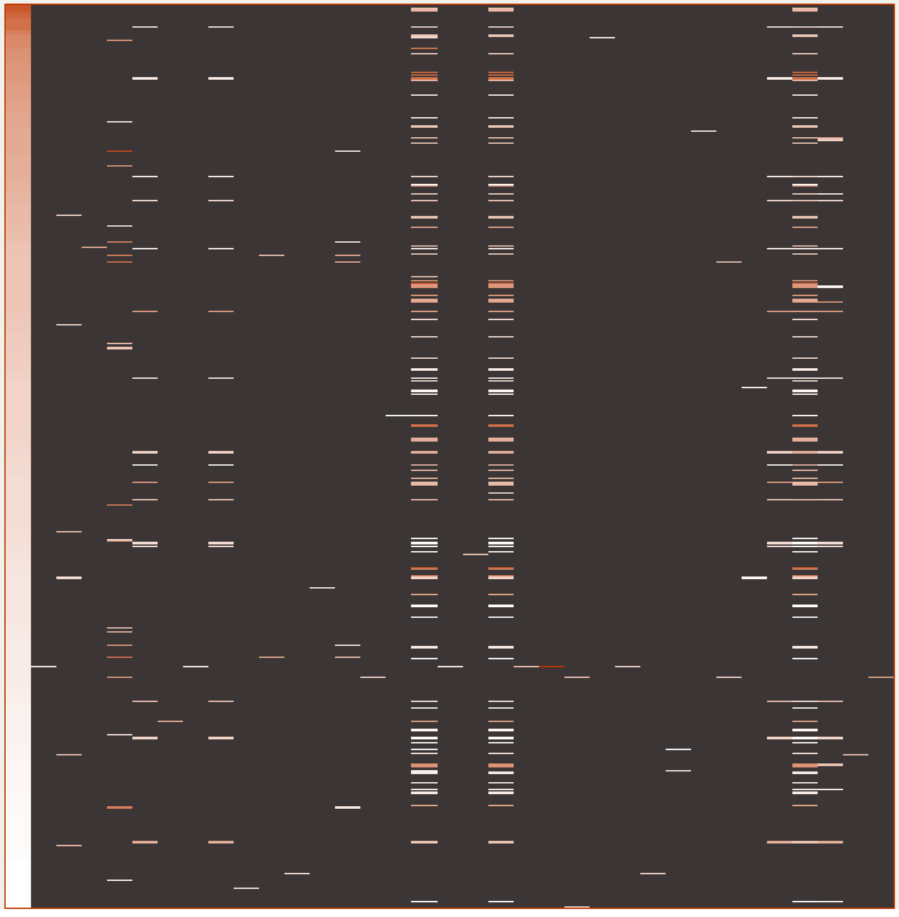


2(1H)-quinazolinone, 5-(2-chloro-4-fluorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-7-(4-piperidinyloxy)-



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

Open PHACTS
Open Pharmacological Space

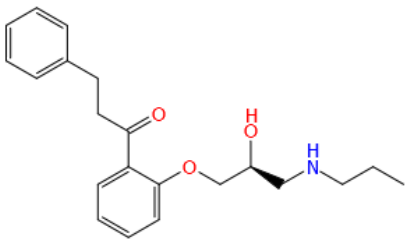
ChemBioNavigator

www.chembionavigator.com

ChemBioNavigator | Save session | Give Feedback | About | Help | Start Over

Selected Compound:
1-(2-{[(2S)-2-Hydroxy-3-(propylamino)propyl]oxy}phen...

Overview | Details | Pharmacology | Publications | Pathways

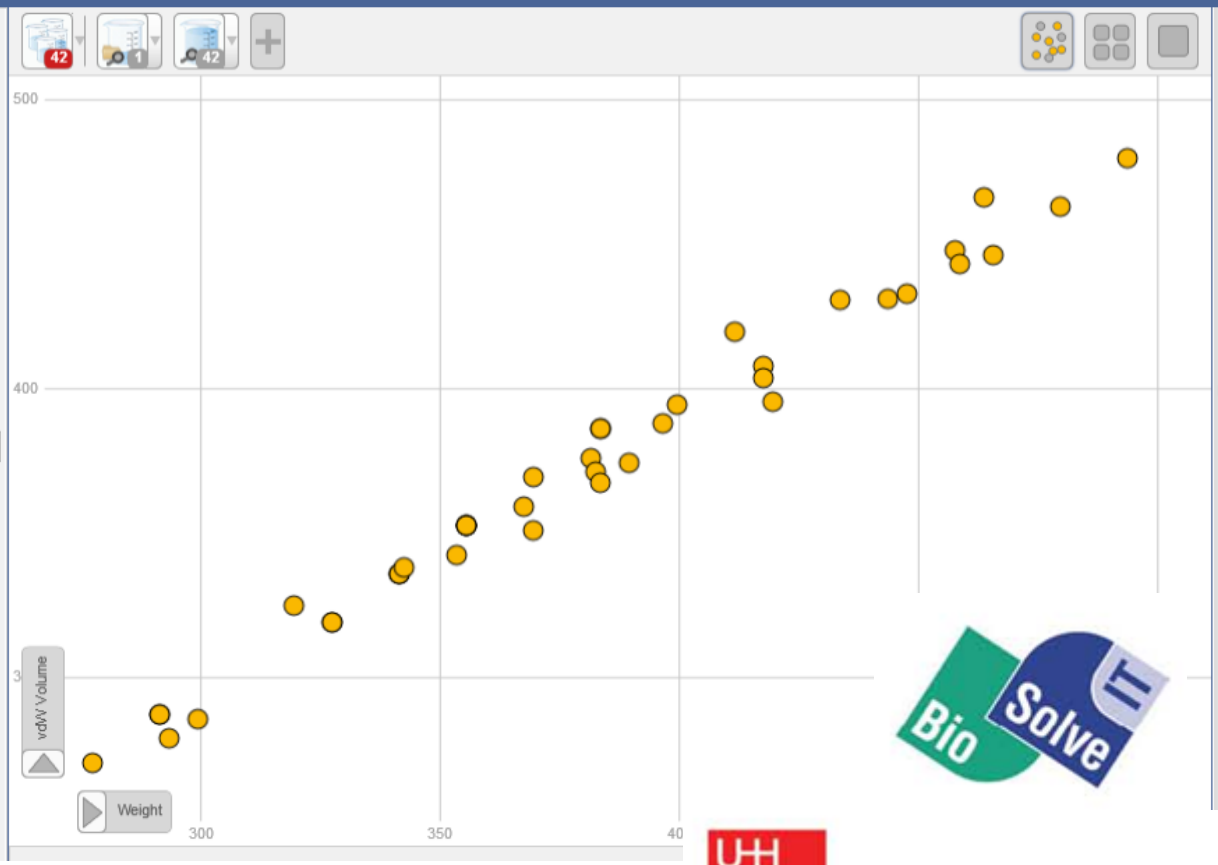


View in ChemSpider | View in Open PHACTS

SMILES	O=C(c1c(OC[C@@H](O)CNCCC)cccc1)CCc2ccccc2
InChI	InChI=1S/C21H27NO3.ClH /c1-2-14-22-15-18(23)16-25-21-11-7-6-10-19(21)20(24)13-12-17-8-4-3-5-9-17;/h3-11,18,22-23H,2,12-16H2,1H3;1H/t18-;/m0./s1
InChI Key	XWIHRGFIPXWGEF-FERBBOLQSA-N
Weight	341.448
logP	3.2414

Find more molecules by :

advanced options ▼ | Similarity Search



Developed by the University of Hamburg and BioSolveIT

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

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Open Pharmacological Space

COLLECTOR, AN APPLICATION FOR GATHERING BIOACTIVITY DATA FROM THE OPS PLATFORM

Manuel Pastor

collector

eTOX

UNIVERSITAT POMPEU FABRA

prbb Parc Recerca Biomèdica Barcelona

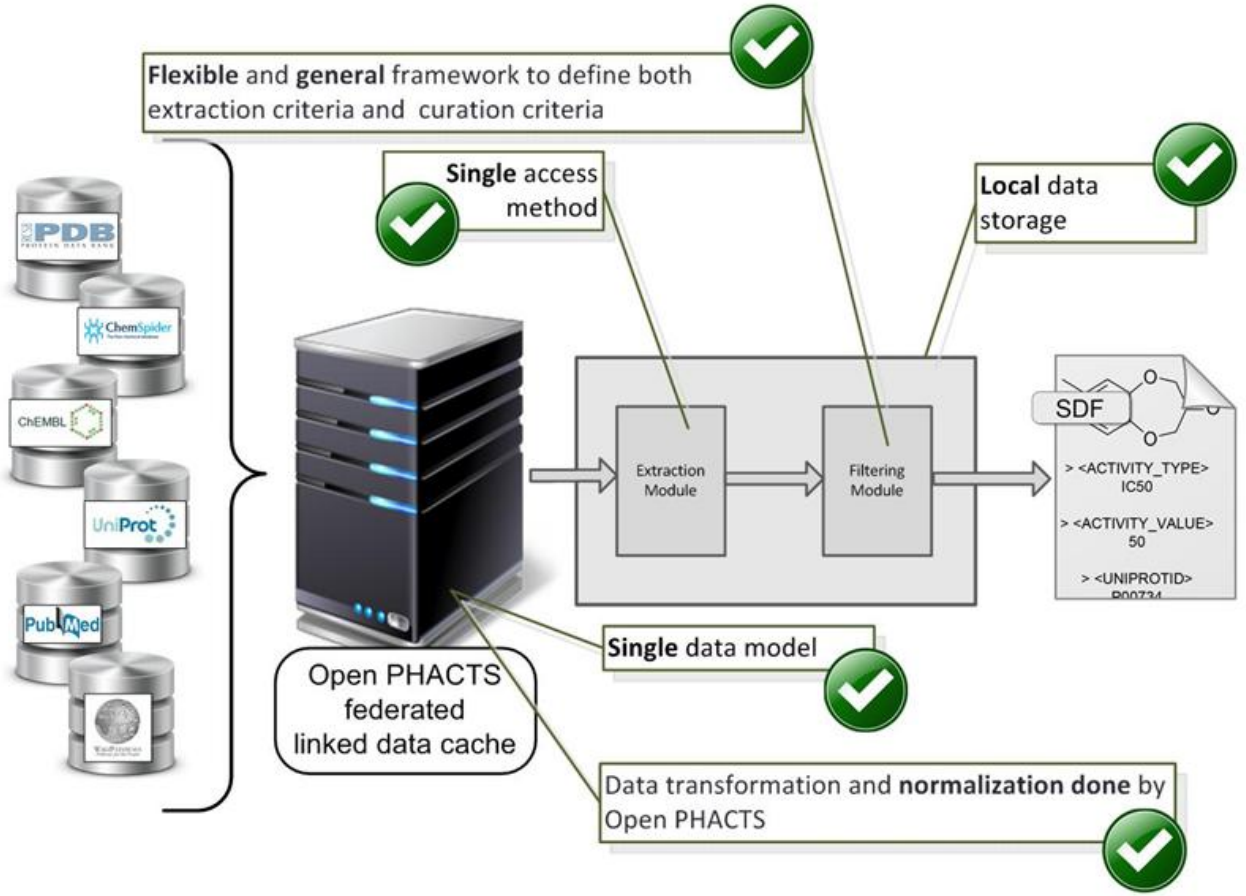
IMIM Institut de Recerca Hospital del Mar

Parc de Salut MAR Barcelona

GRIB

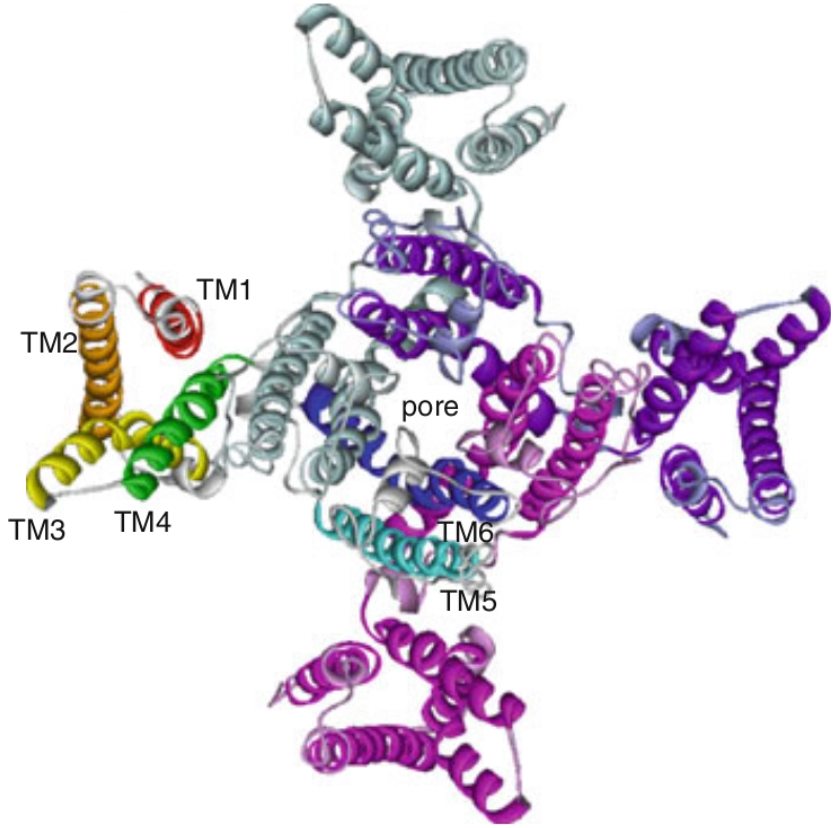
RESEARCH PROGRAMME ON BIOMEDICAL INFORMATICS

Collector: architecture overview



TRPV1

- Transmembrane receptor
- Tetramer
- Non-selective cation channel
- Peripheral nervous system
- Activation → influx of cations → depolarization of membrane → pain perception
- Prolonged activation – desensitization



Lee et al., J Comput Aided Mol Des (2011) 25: 317-37

TRPV1

Firefox | Louis Armstrong New Orleans Interna... | Google Kalender | Register for Open PHACTS Explorer | Open PHACTS

explorer.openphacts.org/#!p=PharmByTargetNameForm&u=http://www.conceptwiki.org/concept/f1c37c53-63c3-4107-a688-12d4dc082ef3

molecular informatics journal

Open PHACTS Explorer

Navigation

- Compound
- Target
- Pharmacology
  - Pharmacology by Enzyme family
  - Pharmacology by Compound
  - Pharmacology by Target

Help and Feedback

API Status

TSV Downloads

Pharmacology by Target Name

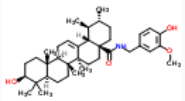
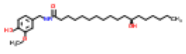
Hint: Type in protein name and species. E.g. "ADA protein human" and select a result

Protein name: Transient receptor potential cation channel subfamily V member 1 (Homo sapiens) Search...

Filter Provenance: On Off

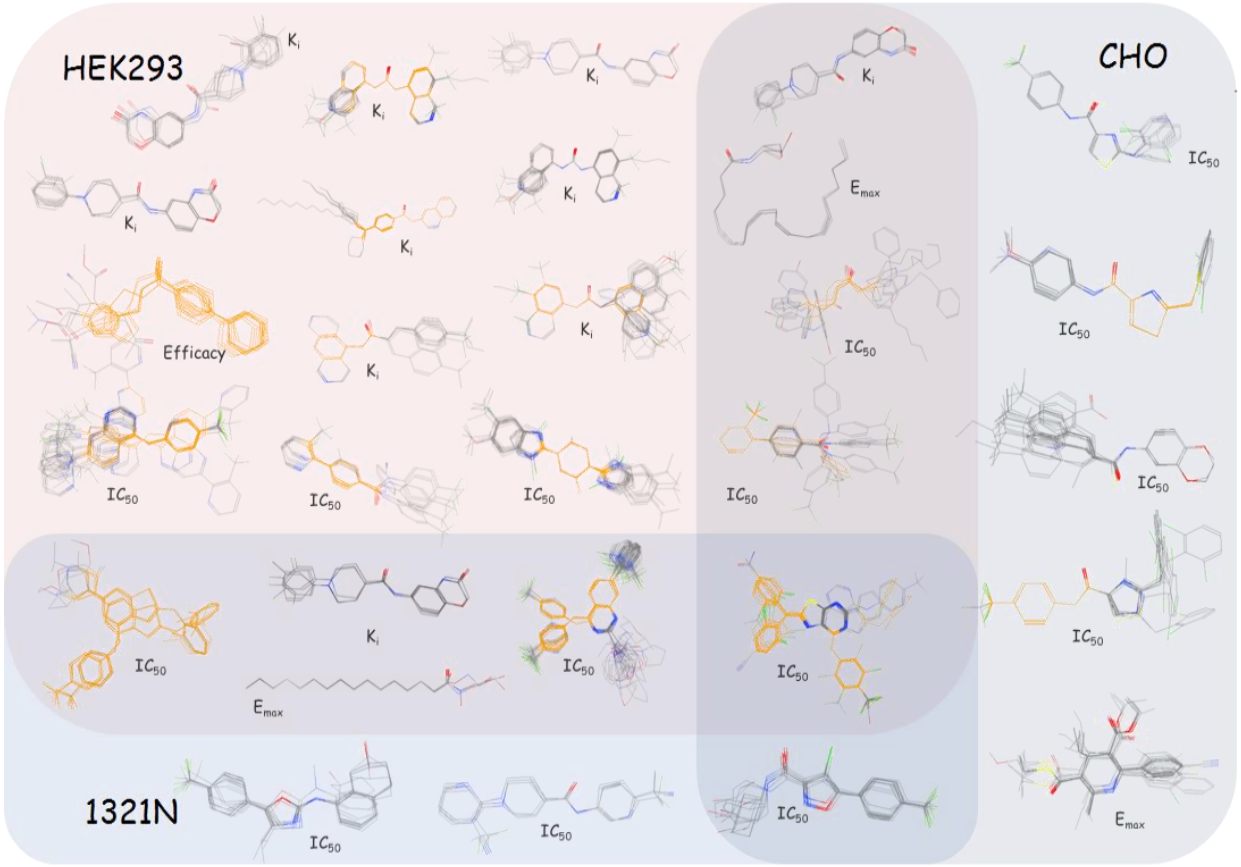
Pharmacology by Target name search results - Total Records: 2328

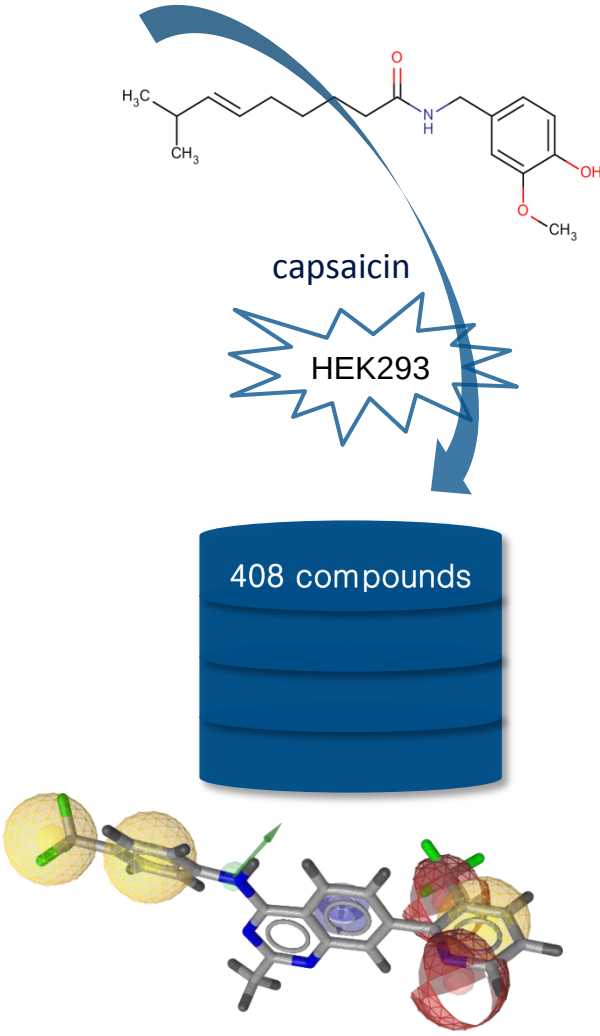
Prepare tsv file

	Structure	Compound Name	Target Name	Target Organism	Assay Organism	Assay Description	Activity Type	Relation	Value	U
1		(3beta)-3-hydroxy-N-(4-hydroxy-3-methoxybenzyl)urs-12-en-28-amide	Transient receptor potential cation channel subfamily V member 1 (Homo sapiens)	Homo sapiens		Percent absolute effect obtained with ionomycin, measured by the entry of [Ca2+] into human embryonic kidney HEK293 cells overexpressing hVR1	Response	=	14.3	
2		(3beta)-3-hydroxy-N-(4-hydroxy-3-methoxybenzyl)urs-12-en-28-amide	Transient receptor potential cation channel subfamily V member 1 (Homo sapiens)	Homo sapiens	Homo sapiens	[Ca2+] influx into human embryonic kidney HEK293 cells overexpressing human VR1 (NM = non-measurable)				
3		(12R)-12-hydroxy-N-(4-hydroxy-3-methoxybenzyl)octadecanamide	Transient receptor potential cation channel subfamily V member 1 (Homo sapiens)	Homo sapiens		Percent absolute effect obtained with ionomycin, measured by the entry of [Ca2+] into human embryonic kidney HEK293 cells overexpressing hVR1	Response	=	69.7	

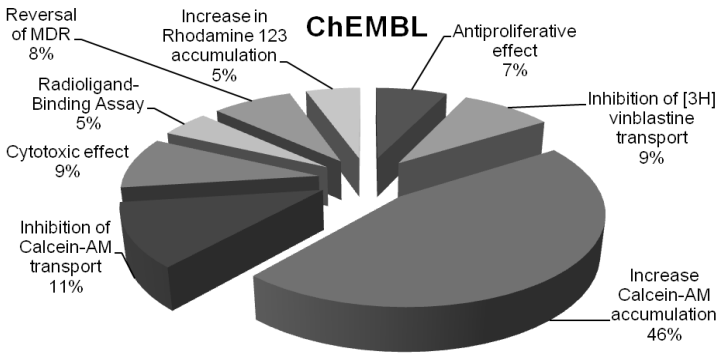
TRPV1

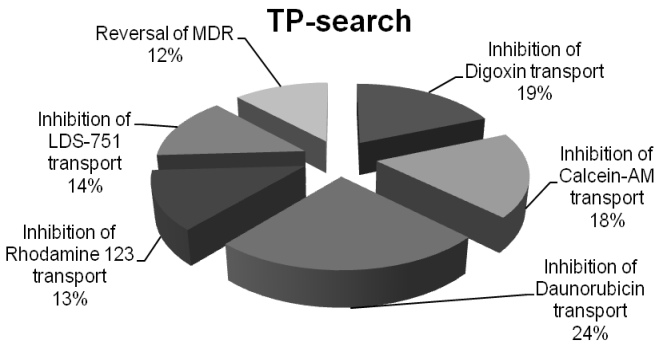
hTRPV1 → 2328 ligands from Open PHACTS

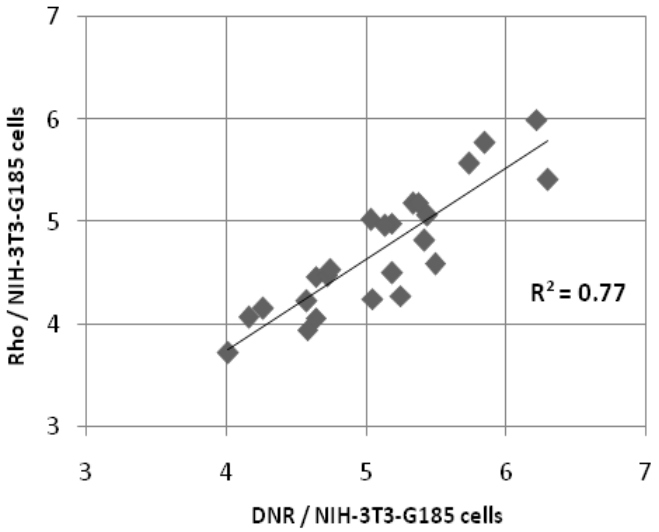




Goldmann D, Mol Inform 2013.







molecular informatics

SPECIAL ISSUE

DOI: 10.1002/minf.201200059

Annotating Human P-Glycoprotein Bioassay Data

Barbara Zdrazil,[a] Marta Pinto,[a] Poongavanam Vasanthanathan,[a] Antony J. Williams,[b] Linda Zander Balderud,[c] Ola Engkvist,[c] Christine Chichester,[d] Anne Hersey,[e] John P. Overington,[e] and Gerhard F. Ecker*[a]

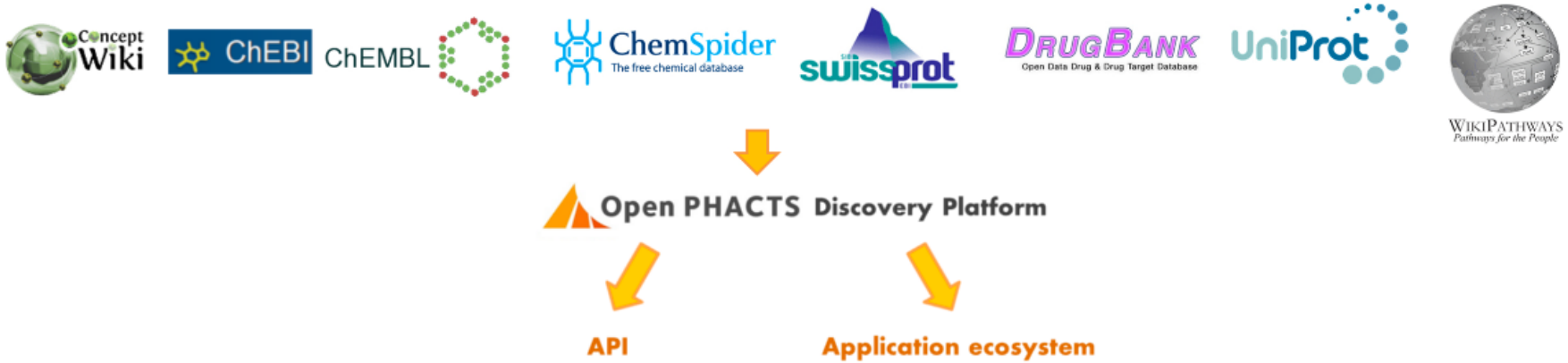
Develop assay ontology
Create tools for semiautomatic combination
Propose reference compounds

The Open PHACTS Foundation

OPF is a not-for-profit membership organisation, supporting the Open PHACTS Discovery Platform:
A sustainable, open, vibrant and interoperable information infrastructure for applied life science research and development.

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

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



Open PHACTS
Open Pharmacological Space

Open PHACTS Project Partners

www.openphacts.org

Project Contacts:

GSK – Coordinator
(Stefan Senger)

Universität Wien – Managing entity
(Gerhard Ecker)