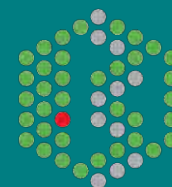


ChEMBL Database: Meeting Chemical and Biological Information needs of Scientists of the Future

Anne Hersey

EMBL-EBI



Outline

- Background
- ChEMBL
 - What is it
 - Applications
 - Data Integration
- Challenges for the future

Getting Drugs to Market is difficult and costly

- Cost of bringing a new drug to market is \$1.8billion



- Clinical development (Phase 1-3) accounts for 63% of cost
- Only 8% of new molecules make it from candidate selection to a marketed drug
- Takes 13.5 years to discover and develop a drug
- Need ~10 molecules a year entering clinical development to achieve 1 launched drug per year



Changing Landscape

- Patent Cliff
- Pharma Site Closures

- More academic, SME research
- Precompetitive initiatives

GlaxoSmithKline to shed 380 research jobs in Harlow

A pharmaceutical giant is to close one of its research units in Essex with the loss of about 380 jobs.

One third of the workforce is to be made redundant after projects for pain relief, anxiety and depression drugs



BBC Essex
Sport, travel, weather, more to do, features and more

SEE ALSO

AstraZeneca announces plans to close Loughborough site

One of Leicestershire's major employers is to shut its operation with the loss of almost 1,200 jobs.

Managers at AstraZeneca's research facility on the outskirts of Loughborough are to be made

The firm



WHERE I LIVE



BBC Leicester
Sport, travel, weather, things to do, features and much more

amid profit rise

Pistoia Alliance | Lowering Barriers to R&D Innovation

Search...

Newsletter Sign-Up | Contact Us | Join | Member Login

ABOUT | WORKING GROUPS | INDUSTRY CHALLENGES | NEWS & EVENTS | OUTPUTS | BLOG

Precompetitive Collaboration.

Infosys, AstraZeneca, the Royal Society of Chemistry, and EMBL-EBI are doing it.

Are you ready to collaborate?

1 February 2011 Last updated at 18:02

3.3K Share

Pfizer to close UK research site

Drug maker Pfizer is to close its research and development (R&D) facility in Kent, which employs 2,400 people.

The move has raised concerns that the UK is losing highly-skilled jobs and about the private sector's ability to absorb cuts in the public sector.

The Unite union said the roles were "exactly the sort of jobs we need to keep in this country".



Pfizer described the facilities in Sandwich as "excellent"

Business Secretary Vince Cable said the firm's

GSK and Online Communities Create Unique Alliance to Stimulate Open Source Drug Discovery for Malaria

f Like | t Tweet | in Share | +1

-- GSK becomes first company to freely share chemical structures on 13,500 molecules from its compound library

-- Alliances formed with leading scientific research communities from private industry and public-domain data providers

ChEMBL Database

Press Release

EMBL-EBI



Open access to large-scale drug discovery data

Data on drugs and small molecules is placed in the public domain, helping the discovery and development of new medicines

Hinxton, 23 July 2008 – The Wellcome Trust has awarded £4.7 million (£5.8 million) to EMBL's European Bioinformatics Institute (EMBL-EBI) to support the transfer of a large collection of information on the properties and activities of drugs and a large set of drug-like small molecules from publicly listed company Galapagos NV to the public domain. It will be incorporated into the EMBL-EBI's collection of open-access data resources for biomedical research and will be maintained by a newly established team of scientists at the EMBL-EBI. These data lie at the heart of translating information from the human genome into successful new drugs in the clinic.

The human genome sequence provided a molecular 'parts list' for a human being, comprising all the genes and proteins that are encoded by our genetic blueprint. But to develop new medicines, it is important to catalogue how each of these 'parts' interacts with drugs and drug-like molecules. This interface of the genome with chemistry is a core part of the new scientific area of chemogenomics. For the past eight years, researchers at BioFocus DPI, the service division of Galapagos, have been integrating the existing collections of information in these two areas to develop a set of well-structured chemogenomic databases that can be used to help determine whether a particular molecule has the right properties to make an effective drug. BioFocus DPI licensed this information to pharmaceutical and biotech companies worldwide. As part of the Wellcome Trust grant announced today, the EBI will obtain the rights to the databases from BioFocus DPI. The award will make it possible to provide free access to this information for all researchers. "The scientific community worldwide will greatly benefit from unrestricted access to these data. It will aid their efforts in predictive drug discovery," says Galapagos CEO Onno

van de Stolpe. "Galapagos has successfully accelerated its research programs with these, and BioFocus DPI used the data to deliver on its contracts with customers. After this transfer, which we hope will contribute to the advancement of drug discovery research by improving access to the data that we have collected, we will continue to use these resources."

The transfer will empower academia to participate in the first stages of drug discovery for all therapeutic areas, including major diseases of the developing world. In future it could also result in improved prediction of drug side-effects. "We are excited to be able to provide information that defines the effects of a large number of small molecules on the body, and link this to the proteins that these molecules interact with, as part of our mission to provide wide access to bioinformatics tools to promote scientific progress and disseminate cutting-edge technologies to industry," says EMBL-EBI Director Janet Thornton. "With this transfer, we aim to facilitate faster and better drug discovery. It speaks to the importance of this information for translational research that the Wellcome Trust has chosen to support this particular transfer with sufficient long-term funding."

This unprecedented transfer of pharmaceutical data resources from the private sector to the public domain will have the greatest impact on researchers in academia and in small companies on limited budgets. "The Wellcome Trust has a strong commitment to making vital research tools freely available to the academic research community," says Dr Alan Schafer, Head of Molecular and Physiological Sciences at the Wellcome Trust. "Enabling these previously proprietary data to enter the public domain will allow researchers worldwide to make free use of knowledge essential for drug discovery." ●

- Open access bioactivity database (since 2009)
- Manually extracted data from Med Chem literature
- Gives users access to curated SAR data
- Open repository for deposited datasets
- Integration of subset of PubChem data

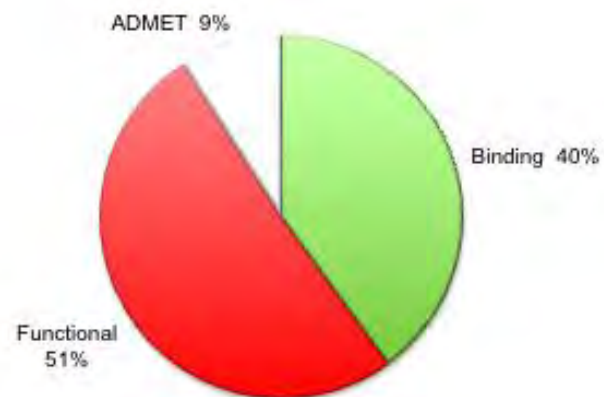


ChEMBL Database

- Freely available (searchable and downloadable) resource for drug discovery
- Updated regularly with new data
- Secure searching <https://www.ebi.ac.uk/chembl/db>

Assays are classified as:

- Binding measurements
- Functional assays
- ADME/toxicity data



ChEMBL11

Targets: 8,603

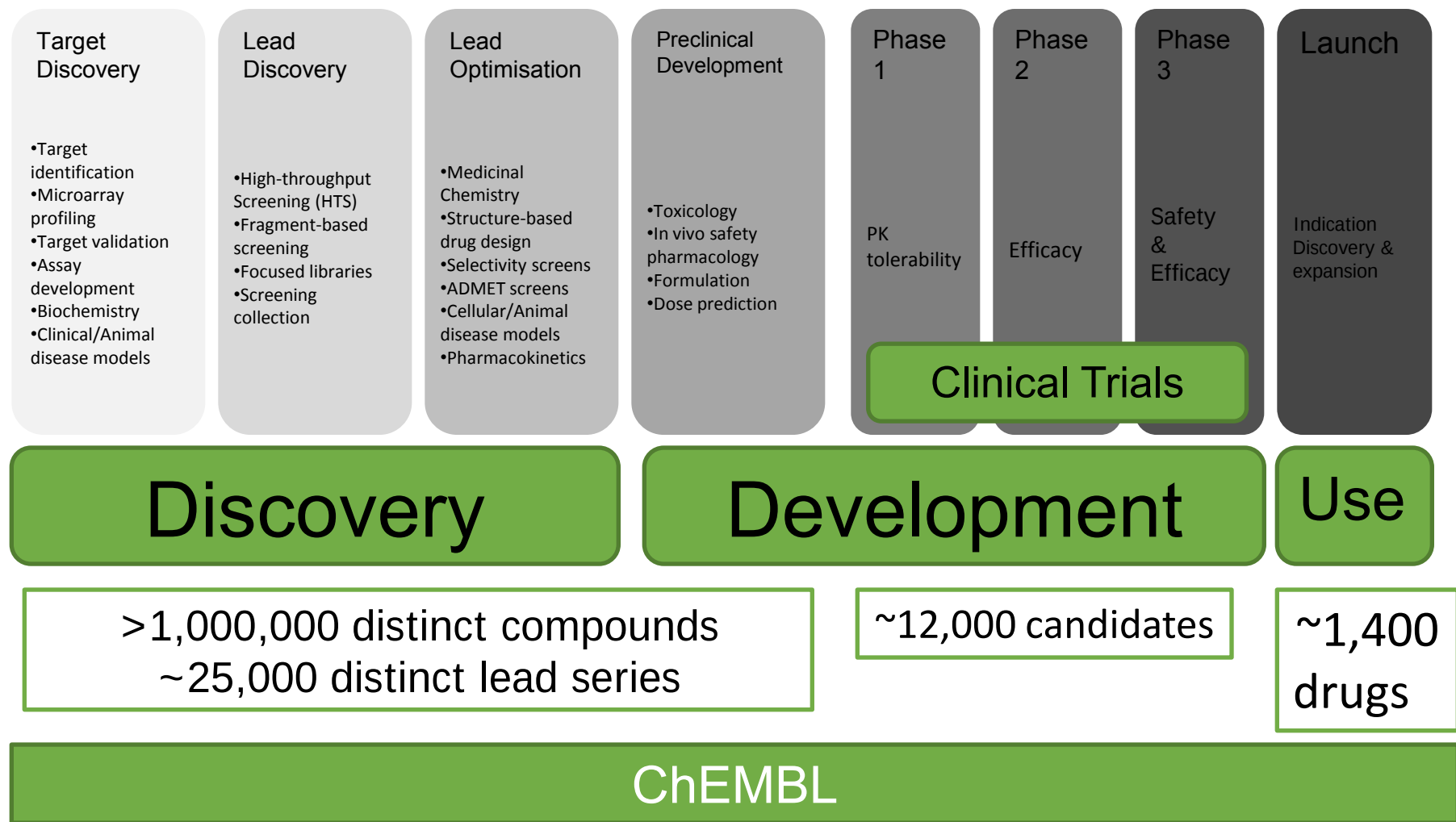
Compounds: 1,060,258
(~350K from PubChem)

Activities: 5,479,146

Publications: 42,516

5420 proteins
1481 organisms
1431 cell lines

Drug Discovery Data in ChEMBL



Accessing ChEMBL Data

The screenshot displays the ChEMBL website interface. A green arrow points from the 'Web Services' link in the left sidebar to the 'ChEMBL Web Services' section. Another green arrow points from the 'Getting Started' section to the 'Getting Started with Java' subsection. A third green arrow points from the 'Getting Started with Java' subsection to the 'Getting Started' section.

Index of ftp://ftp.ebi.ac.uk/pub/databases/chembl/

Name	Size	Last Modified
BioTorrents		22/02/2011 11:32:00
ChEMBLNTD		19/05/2010 00:00:00
ChEMBLdb		
GPCRSARfari		
KinaseSARfari		
VEHICLE		

ChEMBL Web Services

ChEMBL REST API Methods

Using the ChEMBL web service API users can retrieve data from the ChEMBL database in a programmatic fashion. The following list defines the methods:

1. [Get compound by ChEMBLID](#)
2. [Get compound by Standard InChIKey](#)
3. [Get individual compound bioactivities](#)
4. [Get target by ChEMBLID](#)
5. [Get target by UniProt Accession Identifier](#)
6. [Get target by RefSeq Accession Identifier](#)
7. [Get individual target bioactivities](#)
8. [Get all targets](#)
9. [Get assay by ChEMBLID](#)
10. [Get individual assay bioactivities](#)

How to use the ChEMBL REST API

We have provided a [Java](#) client and also [Perl](#) and [Python](#) scripts to help get you started with using the ChEMBL RESTful Web Service API.

Getting Started with Java

The chemblRestClient java client contains all of the dependencies necessary for interacting with the ChEMBL REST Web Service API. Below are the following steps:

1. Download the [chemblRestClient](#) jar file
2. Copy the 'Example' class code below to 'Example.java'
3. Compile [Example.java](#)

```
javac -cp ./chemblRestClient.jar Example.java
```

4. Run the executable

```
java -cp ./chemblRestClient.jar Example
```

```
import java.util.List;
import org.springframework.context.ApplicationContext;
import org.springframework.context.support.ClassPathXmlApplicationContext;
import uk.ac.ebi.chemblservice.restclient.ChemblRestClient;
import uk.ac.ebi.chemblservice.model.Assay;
import uk.ac.ebi.chemblservice.model.Compound;
import uk.ac.ebi.chemblservice.model.Target;
import uk.ac.ebi.chemblservice.model.Bioactivity;

public class Example
{
    public static void main( String[] args )
    {
        ApplicationContext applicationContext = new ClassPathXmlApplicationContext( "applicationContext.xml" );
        ChemblRestClient chemblClient = applicationContext.getBean( "chemblRestClient", ChemblRestClient.class );

        /***** Uncomment sections as required *****/
    }
}
```

ChEMBLdb Statistics

- DB: ChEMBL_09
- Targets: 8,091
- Compound records: 758,082
- Distinct compounds: 658,075
- Activities: 3,030,317

<https://www.ebi.ac.uk/chembl>

Use Case 1 - Searching by Target

- What is known about chemical structures that bind to a specific protein (ZAP70)?
- What is known about their potency/selectivity/ADMET Properties
- Is there any protein structure data?

Use Case 1 Searching by target in ChEMBL

EMBL-EBI [Help](#) [Feedback](#)

[Databases](#) [Tools](#) [Research](#) [Training](#) [Industry](#) [About Us](#) [Help](#) [Site Index](#)

ChEMBL

[ChEMBLdb](#)
[ChEMBL-NTD](#)
[Kinase SARfari](#)
[GPCR SARfari](#)
[DrugEBility](#)
[ChEMBL Group](#)
[Downloads](#)
[Web Services](#)
[FAQ](#)

ChEMBLdb Statistics

- DB: ChEMBL_11
- Targets: 8,603
- Compound records: 1,195,368
- Distinct compounds: 1,060,258
- Activities: 5,479,146
- Publications: 42,516

ChEMBL Blog

- [Lipinski Seminar - Cancelled](#)
- [Opinion: The Inventive and Creative Industries - Patents and Copyright](#)

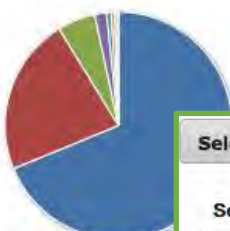
EBI > Databases > Small Molecules > ChEMBL Database > Target Search > Target Classification Hierarchy

[Activity Source Filter](#)

Browse ☒ Protein Target Tree ☐ Taxonomy Tree

Click arrows to navigate tree

- Enzyme (3219)
 - Kinase (595)
 - Protein Kinase (593)
 - Ser Thr (408)
 - Tyr (133)
 - Ser Thr Tyr (32)
 - His (10)
 - Guanylate cyclase (4)
 - Ser (3)
 - Endoribonuclease (2)
 - Ser Thr (1)
 - Protease (402)
 - Phosphatase (70)
 - Phosphodiesterase (57)
 - Cytochrome P450 (55)
 - Aminoacyltransferase (1)
 - Reductase (1)
 - Membrane receptor (555)
 - Ion channel (338)
 - Transporter (136)
 - Transcription Factor (102)
 - Cytosolic other (102)
 - Secreted (57)
 - Structural (29)
 - Surface antigen (26)
 - Membrane other (16)
 - Adhesion (14)
 - Nuclear other (13)



Selected Bioactivity Sources

Selected	Source	Counts
☒	Scientific Literature	3079587 (65.97%)
☒	PubChem BioAssays	1473189 (31.56%)
☒	GSK Malaria Screening	81198 (1.74%)
☒	Novartis Malaria Screening	22788 (0.49%)
☒	Sanger Institute Genomics of Drug Sensitivity in Cancer	5984 (0.13%)
☒	St Jude Malaria Screening	5456 (0.12%)

Choose Sources to include in search

Retrieving Bioactivity Data

Target Report Card

Target Details

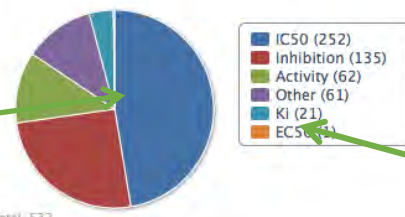
Target ID	CHEMBL2803
Target Type	PROTEIN
Preferred Name	Tyrosine-protein kinase ZAP-70
Synonyms	Tyrosine-protein kinase ZAP-70; 70 kDa zeta-associated protein; Syk-related tyrosine kinase
Organism	Homo sapiens
Description	Tyrosine-protein kinase ZAP-70
Protein Target Classification	enzyme kinase protein kinase tyr tk syk

Database Links

UniProt	P43403
PDB	1M61 1U59 2OQ1 2OZO

Bioactivity Summary

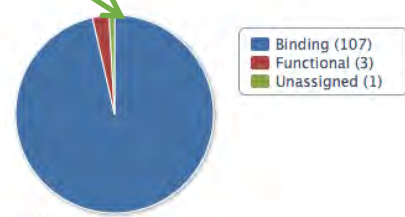
ChEMBL Activity Types for Target CHEMBL2803



Total: 532

Assay Summary

ChEMBL Assays for Target CHEMBL2803



Total: 111

Sequence data

3D Structures

Display all
bioactivity data for
target

Click pie chart to
retrieve particular
end-points

Summary of
bioactivity/assay/com
pound data available
for target

Select the activities and conditions you desire:

Activity (#Endpoints)	Condition	Value
Ki (nM) (2.1)	<	10000

Add

Activity	Condition	Value
IC50	lessthan	10000
Ki	lessthan	10000

Delete Delete

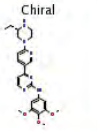
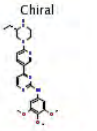
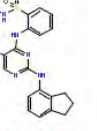
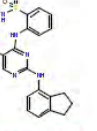
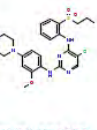
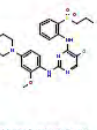
Step 2: Filter

Filter on IC50 <10uM

168 ZAP70 IC50 or Ki values <10uM

ChEMBL Bioactivity Search Results: 168

1 2 3 4 5 6 [Next] [End] Please select....

Parent	Ingredient	Bioactivity	Activity Comment	Operator	Value	Units	Assay ChEMBL ID	Assay Source	Assay Type	Description	ChEMBL Target ID	Target Name	Organism	Target Mapping	Curated By	Reference	Name in Reference
 ChEMBL112346	 ChEMBL112346	IC50		=	8	nM	ChEMBL824029	Scientific Literature	B	Inhibition of Zeta-chain (TCR) associated protein kinase 70 kDa phosphorylation of polyGly-Tyr.	ChEMBL2803	Tyrosine-protein kinase ZAP-70	Homo sapiens	Homologous protein	Expert	Bioorg. Med. Chem. Lett. (1999) 9:23:3351	20
 ChEMBL575048	 ChEMBL575048	IC50		=	10	nM	ChEMBL1037893	Scientific Literature	B	Inhibition of human GST-fused ZAP-70 expressed in Sf9 cells	ChEMBL2803	Tyrosine-protein kinase ZAP-70	Homo sapiens	Protein	Intermediate	Eur. J. Med. Chem. (2009) 44:12:4793	26
 ChEMBL573483	 ChEMBL573483	IC50		=	10	nM	ChEMBL1037893	Scientific Literature	B	Inhibition of human GST-fused ZAP-70 expressed in Sf9 cells	ChEMBL2803	Tyrosine-protein kinase ZAP-70	Homo sapiens	Protein	Intermediate	Eur. J. Med. Chem. (2009) 44:12:4793	1

Compound structures

Activity values

Assay details

Target details

References

Use Case 2 – Searching by Structure

- What compounds contain a particular substructure?
- What is known about their bioactivities?
- What other data exists
 - Clinical Trials, 3D structures, drug data etc

Use Case 2 - Structure Searching

The screenshot shows the ChEMBL Compound Search page. A green box labeled "name" points to the search input field. A green box labeled "Lists of Identifiers" points to the "List Search" section, which includes radio buttons for "SMILES Search", "ChEMBL ID Search", and "Keyword Search", and a text area for entering identifiers. A green box labeled "Types of synonyms:" points to a list of synonyms: Research codes, Trade names, and INN, USAN. A green box labeled "Different sketchers" points to the "Compound Sketcher" dropdown menu, which lists "Please select...", "JME", "Marvin", and "JDraw".

name

Lists of Identifiers

Types of synonyms:

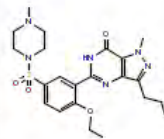
- Research codes
- Trade names
- INN, USAN

Different sketchers

Compound Report Card

Summary

Compound ID	CHEMBL192
Compound Name	sildenafil
Synonyms	UK-92480, Sildenafil, UK-92480-10, Sildenafil Citrate, Sildenafil citrate
Approved Drug	Yes
Trade Names	Viagra, Revatio



CHEMBL192

names

Approved Drug Features



Clinical Trials

Clinical Trials

Number of clinical trials registered at clinicaltrials.gov	324
---	-----

Parent Properties

Mol. Weight	ALogP	Num Ro5 Violations	Num Rotatable Bonds	Passes Rule-Of-Three	Med Chem Friendly
474.6	2.25	0	7	No	Yes

Parent ACD Properties

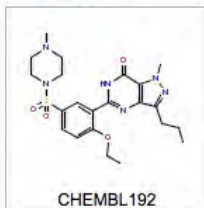
Acidic pKa	Basic pKa	LogP	LogD	Species
10.052	6.027	2.468	2.449	NEUTRAL

Representations

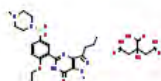
Molfile	Download Molfile
Molecular Formula	C22H30N6O4S
Canonical SMILES	<chem>CCCC1nn(C)c2C(=O)NC(=Nc12)c3cc(ccc3OCC)S(=O)(=O)N4CCN(C)CC4</chem> Download SMILES
Standard InChI	InChI=1S/C22H30N6O4S/c1-5-7-17-19-20(27(4)25-17)22(29)24-21(... Download InChI
Standard InChI Key	BNRNXUZRGAQC-UHFFFAOYSA-N Download InChI Key

Properties

Molecule Forms



CHEMBL192



CHEMBL1737

Structure

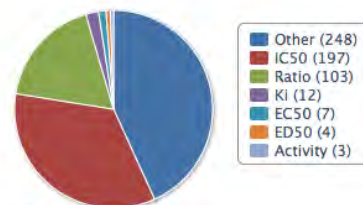
Database Links

ChEBI	ChEBI:9139
ChemSpider	ChemSpider:BNRNXUZRGAQC-UHFFFAOYSA-N
DrugBank	DB00203
PDBe	VIA - VIA (PDBe Entries)
PubChem	SID: 26748898 SID: 50085897
Wikipedia	Sildenafil

Links

Bioactivity Summary

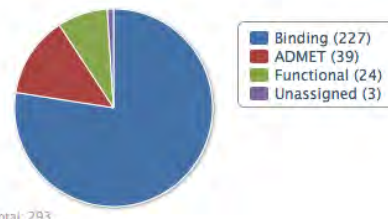
ChEMBL Activity Types for Compound CHEMBL192



Bioactivities

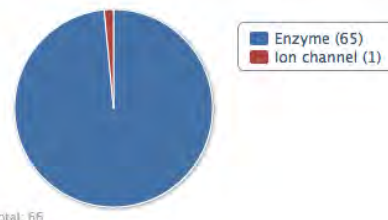
Assay Summary

ChEMBL Assays for Compound CHEMBL192



Protein Target Summary

ChEMBL Protein Target Classes for Compound CHEMBL192



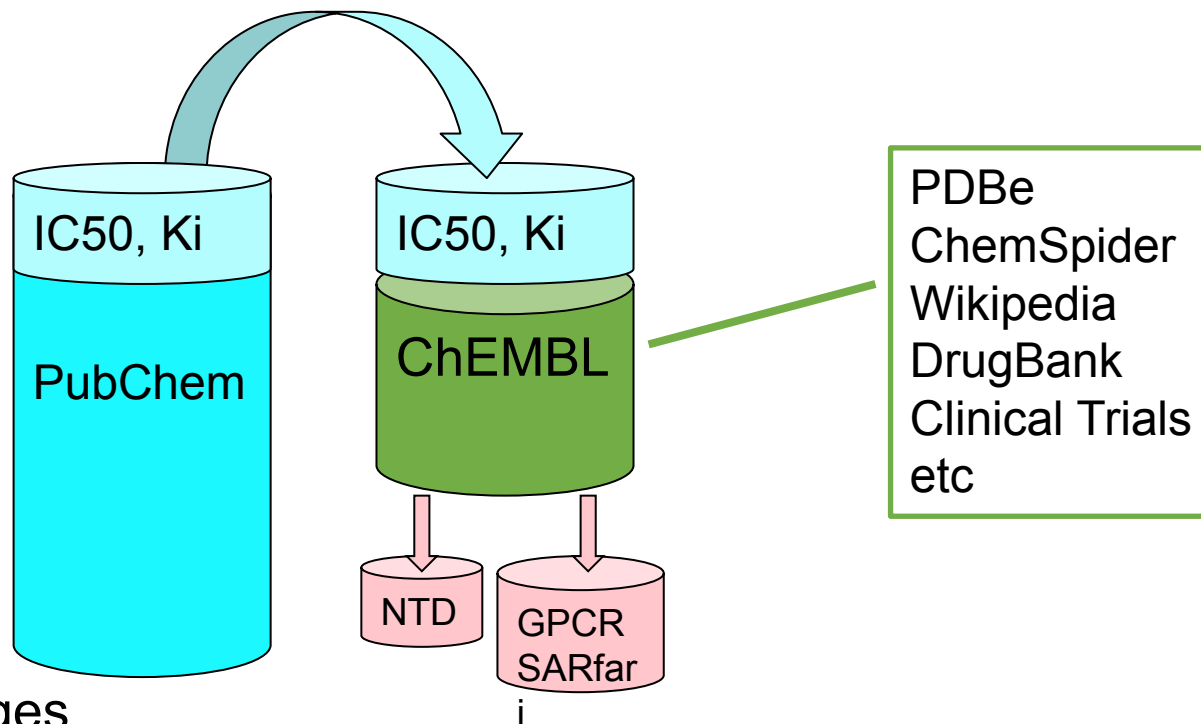
Chemistry Challenges

- Standardise representations of chemical structures
- Needs to be largely automated (1 chemistry curator)
- Will be mistakes - some from abstraction but some in papers
- Software packages interpret structures differently particularly when converting between structure formats

Standardisation Protocol

- Based on FDA Substance Registration System User's Guide
 - <http://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/default.htm>
- Standard InChI is used to identify unique structures
- Parent compounds and salts are registered with different ChEMBL_IDs and the relationship is recorded in database
- Stereochemistry is retained and recorded where known
- Tautomers of the same compound are registered with a single ChEMBL ID (merged on standard InChI)

Integration with other Resources



Challenges

- Data from different sources have different business rules
- Maintaining and updating database with new data
- Links to other resources vs integration
- More data sources becoming available
- Scalability

UniChem

FRIDAY, 25 NOVEMBER 2011

UniChem - An EBI compound structure cross-referencing resource

un1Chem

We have faced for some time some issues with compound integration with ChEMBL - specifically the loading of compound sets into ChEMBL for cross referencing, between for example, ChEBI, PDBe compounds, *etc.* The ChEMBL update cycle is relatively slow with respect to some other resources, and there is inevitable thrash with compounds not being present, especially for exciting new data. Without doing something different for compound integration, we were starting to face a scenario where we had a compound table with many millions of compounds without any bioactivity data, and following this the inevitable slowdown in searching, *etc.*

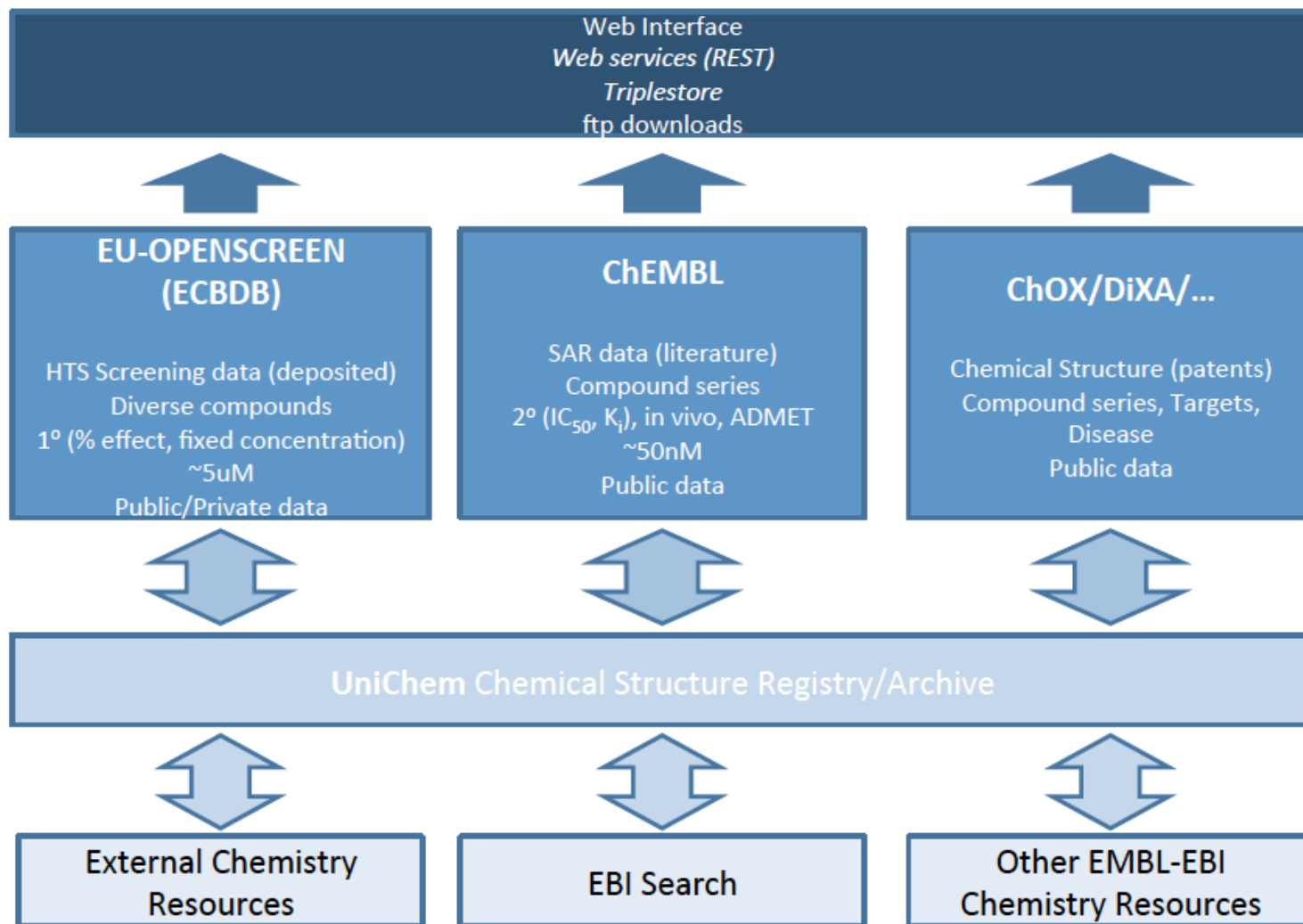
We also had some issues facing us about curation of other people's primary data, changing compound structures, or their rendering, *etc.*

So, we decided to set up an external system to resolve cross-references between various databases. This is a very simple Standard InChI lookup, containing compounds from resources such as ChEMBL, ChEBI, PDBe, DrugBank, KEGG, BindingDB, PubChem, and so forth. UniChem can also handle versioning of the contained resources. We will be migrating various components of the current ChEMBL interface across to use web services on UniChem, this way, the cross links will always be fresh and correct, and we can focus on curation and optimisation of ChEMBL content. There are some other resources, like ZINC, STITCH, and ChemSpider, for example, that would be great to integrate, if we can get hold of the required data.

What is UniChem ?

- A 'Unified Chemical Identifier' system
- A system for cross-referencing chemical structures and their identifiers between databases
- Enables tracking of 'id-to-structure' assignments over time
- Uses standard InChI to compare chemical structures across databases

UniChem



[Currently querying: 'unichemx' on 'chempro'.]

Current UniChem sources...

SRC_ID	Name	Name_long	Description	src_details	Number or Date release type	SRC latest release number	SRC latest release date	records loaded
1	chembl	ChEMBL	A database of bioactive drug-like small molecules and associated bioactivities abstracted from the scientific literature	Standard InChIs and Keys provided on ftp site for each release.	number	11		1059477
2	drugbank	DrugBank	A database that combines drug (i.e. chemical, pharmacological and pharmaceutical) data with drug target (i.e. sequence, structure, and pathway) information.	Standard InChIs and Keys provided within sd file on ftp site for each release.	date		02-NOV-11	6391
3	pdb	PDBe (Protein Data Bank Europe)	The European resource for the collection, organisation and dissemination of data on biological macromolecular structures, including structures of small molecule ligands for proteins.	Standard InChIs and Keys provided by direct querying of Oracle DB.	date		05-OCT-11	12616
4	iuphar	International Union of Basic and Clinical Pharmacology	A resource for representing the interests of pharmacologists around the world. DB contains structures of small molecule ligands of pharmacological significance.	Standard InChIs and Keys provided by email on request.	date		07-OCT-11	1714
5	pubchem_dot	PubChem ('Drugs of the Future' subset)	A subset of the PubChem DB: from the original depositor 'drugs of the future' (Prous).	Mol files for SIDs downloaded manually, via PubChem interface, and Standard InChIs and Keys generated by InChI software. SIDs used as identifiers.	date		01-OCT-11	5487
6	kegg_ligand	KEGG (Kyoto Encyclopedia of Genes and Genomes) Ligand	KEGG LIGAND database: DRUGS, DRUGS, COMPOUND, GLYCAN, REACTION, PATHWAY	Standard InChIs and Keys generated by InChI software. SIDs used as identifiers.	date		01-JUN-11	14123
7	chebi	ChEBI (Chemical Entities of Biological Interest).		Standard InChIs and Keys generated by UniChem. SIDs used as identifiers.	date		25-NOV-11	17707

[Back to UniChem Home and Query page.](#)

Query UniChem...

To query UniChem, first select a data type, then enter a list of such data in the text box, and then hit 'search'...

Select a data type...

- ☐ Standard Inchi
☐ Standard InchiKey
☒ Database identifiers ...

(NB: Database identifiers listed below must all be from a single source, as specified above)

Enter a list of this type of data...

CHEMBL1

(NB: Enter

Search

Query UniChem for identical structures to these chembl Ids: 'CHEMBL1086445'...

Results...

Database	Database Id	UniChemId	Assignment*	Last release current**	Standard Inchi Key	Standard Inchi
chembl	CHEMBL1086445	330113	1		MLUCVPASIODCQM-NSCUHMNNSA-N	InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3/b3-2+
drugbank	DB04381	330113	1		MLUCVPASIODCQM-NSCUHMNNSA-N	InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3/b3-2+
pdb	CRD	330113	1		MLUCVPASIODCQM-NSCUHMNNSA-N	InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3/b3-2+

* Assignment of Id to structure (1 = Assigned in the current release from this source, 0 = This assignment was valid in a previous data release from this source, but not the current one)

** The last release that this Assignment was made (null if currently assigned). NOTE: This field is currently under development. The release number currently shown in this field is the UniChem release tracking id (which is meaningless to the user), and not the release number or release date as declared by the source database. The field needs to be changed to display the latter.

[Back to UniChem Home and Query page.](#)

Summary

- ChEMBL is publicly available database of drugs, drug-like small molecules and their bioactivity data
- Useful resource for anyone involved in drug discovery particularly those in academia or SMEs
- As well as enabling users to access ChEMBL data they can link to other resources where information about common chemical structures (or targets) exists
- Standardising chemical structures and comparing across databases is challenging
- Standard InChi is a simple method to reference compounds across different databases

Acknowledgements

ChEMBL Group

John Overington

Anne Hersey

Anna Gaulton

Mark Davies

Jon Chambers

Louisa Bellis

Kazuyoshi Ikeda

Patricia Bento

Shaun McGlinchey

Yvonne Light

Felix Krueger

Ben Stauch

Ruth Akhtar

Francis Atkinson

Rita Santos

EMBL-EBI

Samuel Kerrien, Sandra Orchard,
Bruno Aranda, Rafael Jimenez,
Reactome, UniProt and ChEBI teams

Collaborators

Imperial Cancer Research, University
of Dundee, University of Cambridge,
Sanger Centre, University of
Maryland, NCBI, TDR, IUPHAR,
Bayer-Schering, Pfizer, GSK,
Schering-Plough, MMV, Novartis, St
Jude Children's Research Hospital

Former Inpharmatica colleagues

wellcometrust

EMBL

