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Open Pharmacological Space

ChEMBL supplementary bioactivity data – A step towards sharing more bioactivity data

EMBL-EBI

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What is Open PHACTS trying to achieve?

Open PHACTS aims to reduce the barriers to Drug Discovery by building a freely available platform, integrating pharmacological data from a variety of sources and providing tools and services to question the integrated data to support pharmacological research.

To find out more, see http://www.openphacts.org

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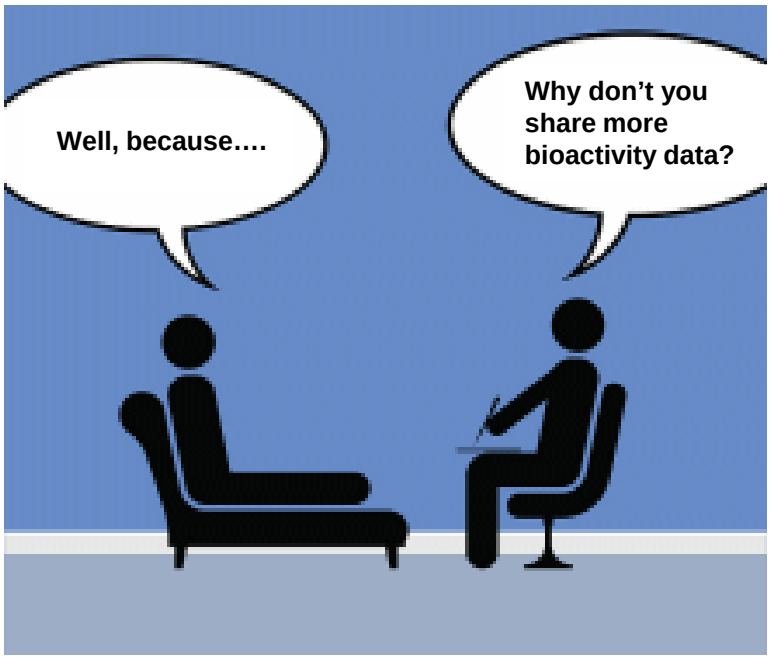
Stating the obvious: The more data is shared, the better

The vision: What can be shared, is shared



Let's look at some of our 'limiting beliefs'…

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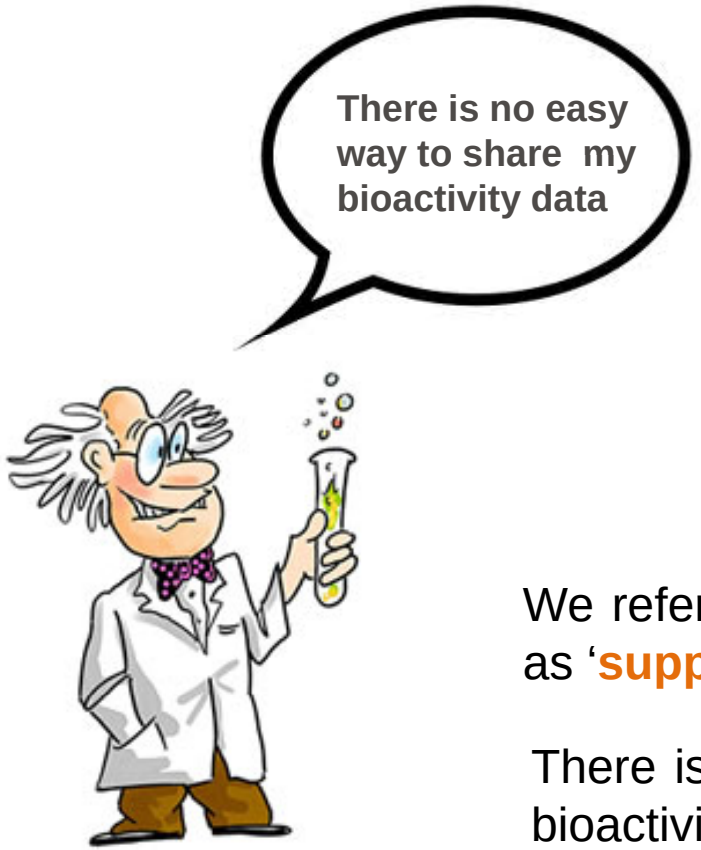

Well, now there is a way if...

… the bioactivity data was generated in an assay that has been described in a publication in a scientific journal.

We refer to bioactivity data that satisfies this criterion as '**supplementary bioactivity data**'

There is now a mechanism to deposit supplementary bioactivity data in ChEMBL.

A. Hersey, S. Senger, J. P. Overington "Open data for drug discovery: learning from the biological community" *Future Med. Chem.* **2012**, *4(15)*, 1865-1867 (http://dx.doi.org/10.4155/fmc.12.159)

Let‘s look at an example...

- In GSK, bioactivity data has been generated in an ethidium bromide release assay for a P2X7 project.
- The GSK ethidium bromide release assay is referenced in the publication *Bioorg. Med. Chem. Lett.* **2010**, *20*, 3161-3164.
- This publication is ‘in ChEMBL’. Hence, the assay has a ChEMBL assay ID. It is CHEMBL1103860.
- Supplementary bioactivity data (i.e. bioactivity data generated in the assay CHEMBL1103860 but not included in the publication CHEMBL1157114) for 54 compounds has been deposited in ChEMBL and is now available in ChEMBL_15.

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Let‘s look at the example...

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ChEMBL

Search ChEMBLdb... | Compounds | Targets | Assays | Activity Source Filter

Provides the option to include/exclude supplementary bioactivity data when searching

- ChEMBLdb
- Malaria Data
- ChEMBL-NTD
- Kinase SARfari
- GPCR SARfari
- DrugEBIlity
- ChEMBL Group
- Downloads
- Web Services
- FAQ

ChEMBLdb Statistics

- DB: ChEMBL_15
- Targets: 9,570
- Compound records: 1,434,432
- Distinct compounds: 1,254,575
- Activities: 10,509,572
- Publications: 48,735

ChEMBL Blog

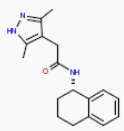
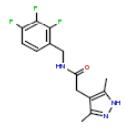
- GPCR Structure-based

ChEMBL Bioactivity Search Results: 54

Please select...

10 records per page

Show / hide

Ingredient	Molweight	AlogP	PSA	#RO5 Vio.	Standard Type	Relation	Standard Value	Standard Units	Assay Type	Description	Assay Src Description	Assay Organism	Target Type	Protein Accession	Target Name	Target Organism	Referen
 CHEMBL2094196	283.37	2.54	57.78	0	IC50	=	100	nM	B	SUPPLEMENTARY: Inhibition of human P2X7 receptor assessed as inhibition of ethidium bromide accumulation. Same assay as CHEMBL1103860	Deposited Supplementary Data	Homo sapiens	SINGLE PROTEIN	Q99572	P2X purinoceptor 7	Homo sapiens	CHEMBL
 CHEMBL2094197	297.28	2.15	57.78	0	IC50	=	63.1	nM	B	SUPPLEMENTARY: Inhibition of human P2X7 receptor assessed as inhibition of ethidium bromide accumulation. Same assay as CHEMBL1103860	Deposited Supplementary Data	Homo sapiens	SINGLE PROTEIN	Q99572	P2X purinoceptor 7	Homo sapiens	CHEMBL

Links to Assay Report Card

Links to Document Report Card

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Let‘s look at the example...

EBI > Databases > Small Molecules > ChEMBL Database

Document Report Card

Doc ID	CHEMBL2094195
Title	Structure-activity relationship data for a series of N-(phenylmehtyl)-2-(1H-pyrazol-4-yl)acetamide and N-(phenylmethyl)2-(4-isoxazolyl) acetamide antagonists of the P2X7 receptor (Supplementary Bioactivity Data for publication CHEMBL1157144)
Authors	Senger S, Beswick PJ, Chambers LJ, Davies DJ, DK, Demont EH, Roomann S, Walters DS
Abstract	Supplementary bioactivity data for the GlaxoSmithKline (GSK) publication Bioorg. Med. Chem. Lett. 2010, 20, 3161-3164 (ChEMBL Doc ID: CHEMBL1157144): pIC50 values for 54 compounds that have been tested in the ethidium bromide release assay (ChEMBL Assay ID: CHEMBL1103860) described in reference 24 of the aforementioned publication. All compounds have been tested at least four times and have been reported as being active in all test occasions.
DOI	http://dx.doi.org/10.6019/CHEMBL2094195

ChEMBL supplementary bioactivity data depositions get assigned a DOI, i.e. they are citable.

Example: http://dx.doi.org/10.6019/CHEMBL2094195

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Supplementary Bioactivity data: What's the benefit?

Bioactivity data can be shared outside the rigid publication framework. For example, if

- no further publications for a project are planned, or
- bioactivity data doesn't 'make it' into a publication, or
- bioactivity data is generated after the manuscript has been submitted and doesn't warrant a separate publication

it can still be shared*.

The vision: What can be shared, is shared

* The (obvious) added benefit is that the data is searchable.

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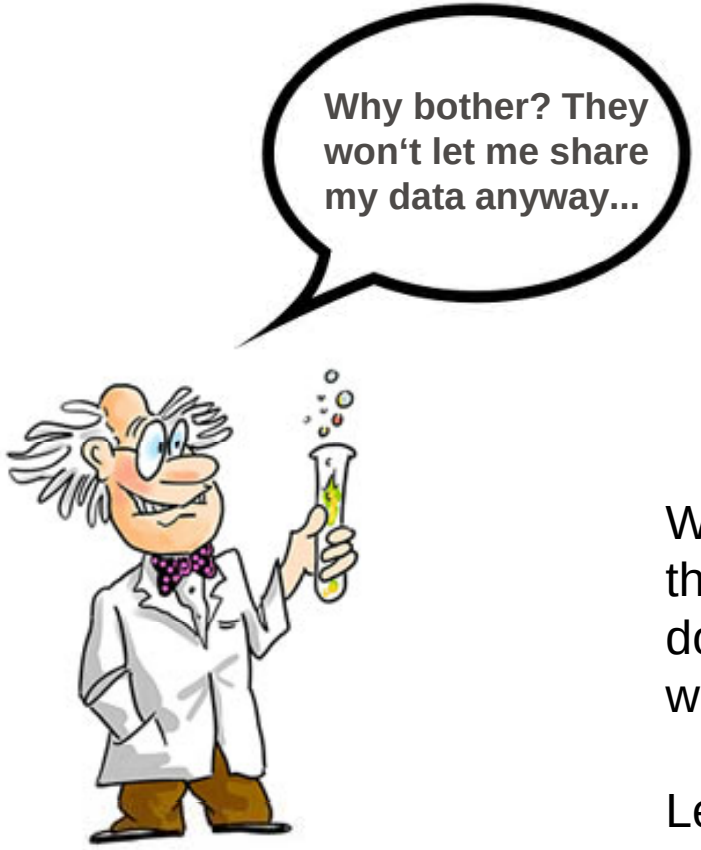
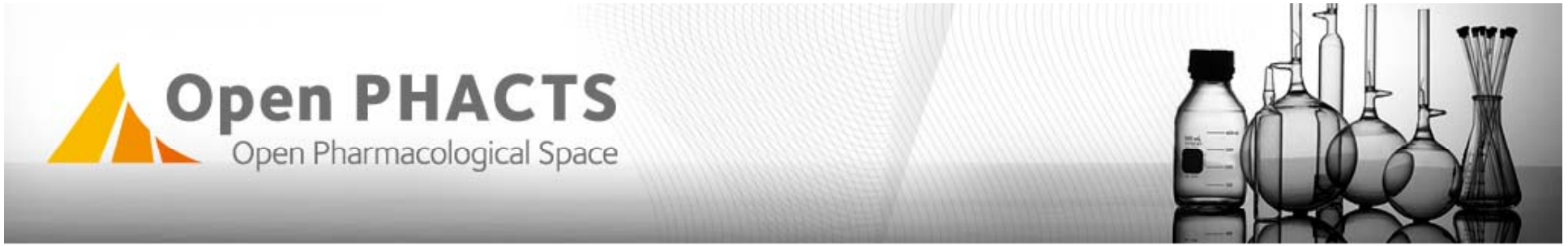
Back to the ‘limiting beliefs’: Let’s look at another one



Have you tried it? Have you? – if you don‘t try, you will never know

Why not start ‘small’, and take it from there. The more people/organisations do it, the easier it will get and the more we will all benefit from it.

Let’s get the ball rolling!



Let’s get the ball rolling…

To find out more and/or get the process started, please email chembl-help@ebi.ac.uk and put ‘**ChEMBL supplementary bioactivity data**’ in the subject of your email.

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