Open PHACTS

Open Pharmacological Space

INTERNATIONAL ASSOCIATION OF SCIENTIFIC, TECHNICAL & MEDICAL PUBLISHERS

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stm


In vivo
Safety
Pipeline
Patents
Literature
SAR
News

data integration

data integration

data integration

data integration

data integration

data integration

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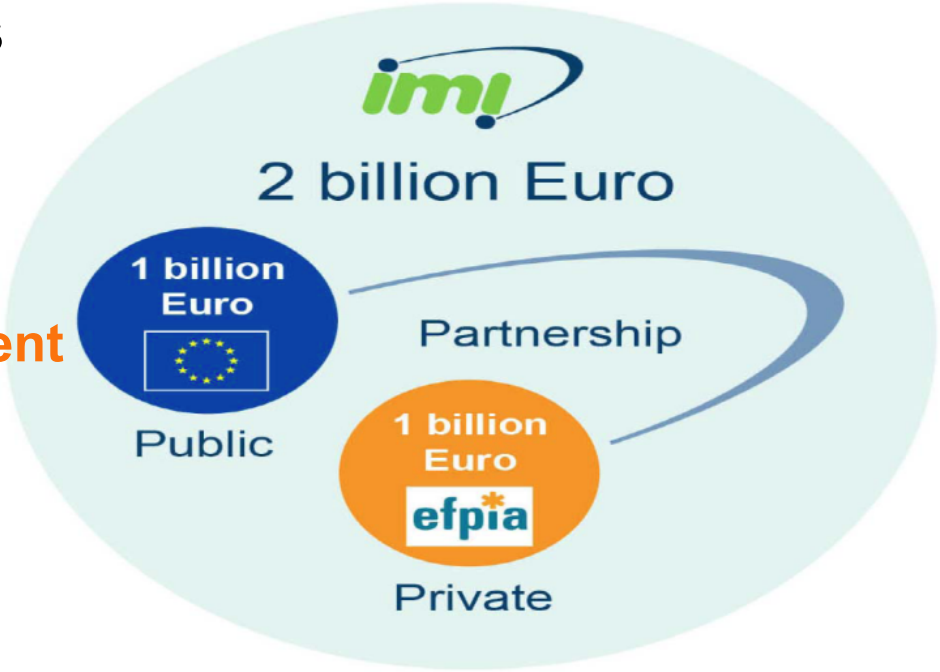
data integration

The Innovative Medicines Initiative

EC funded public-private partnership for pharmaceutical research

Focus on key problems

- Efficacy
- Safety
- Education & Training
- **Knowledge Management**



Open PHACTS
an infrastructure project

Develop / apply a set of robust **standards**…

Implementing the standards in a **semantic integration platform** *("Open Pharmacological Space")…*

Delivering **services** to support on-going drug discovery programs in pharma and public domain

Mix ideal with the pragmatic. Build open that can accommodate non-open components in the real world.

23 partners

9 pharma

14 academic/SME/society

5 new partners in the process

Pharma bring...

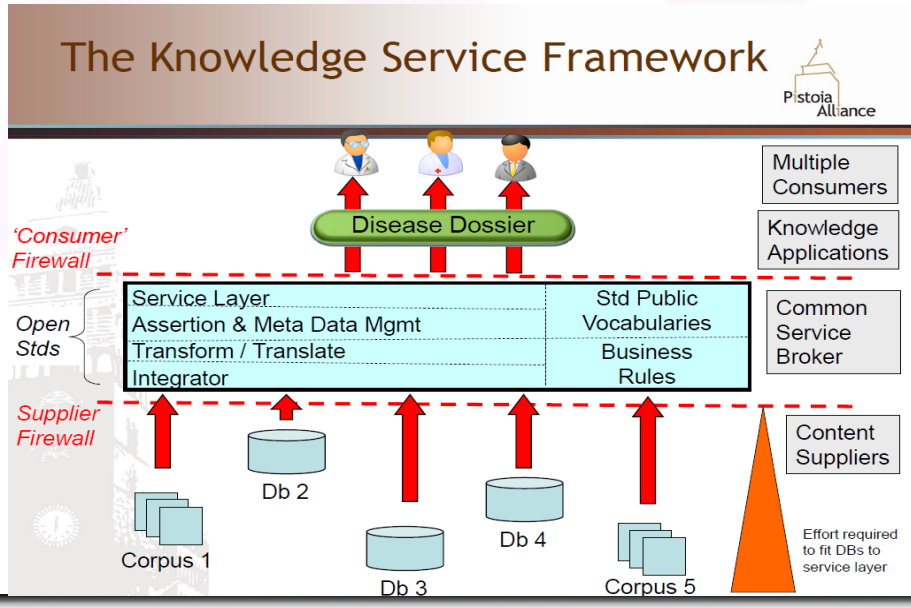
Pre-competitive collaboration

Agreement on standards, approaches

Research questions drive development

Clear use cases

Drive and direction



Example research questions

Give all compounds with IC50 < xxx for target Y in species W and Z plus assay data

What substructures are associated with readout X (target, pathway, disease, …)

Give all experimental and clinical data for compound X

Give all targets for compound X or a compound with a similarity > y%

73 questions identified across consortium

What does ‘Open’ mean?

OPS Open - open access to all

OPS Consortia - data sets licensed just to the consortia

OPS Academia - fully open to academia

“My OPS”

Open Source

Open Access Infrastructure. GUI and back-end platform, online or download both + data for local setup

Open Services: for example, RSC services

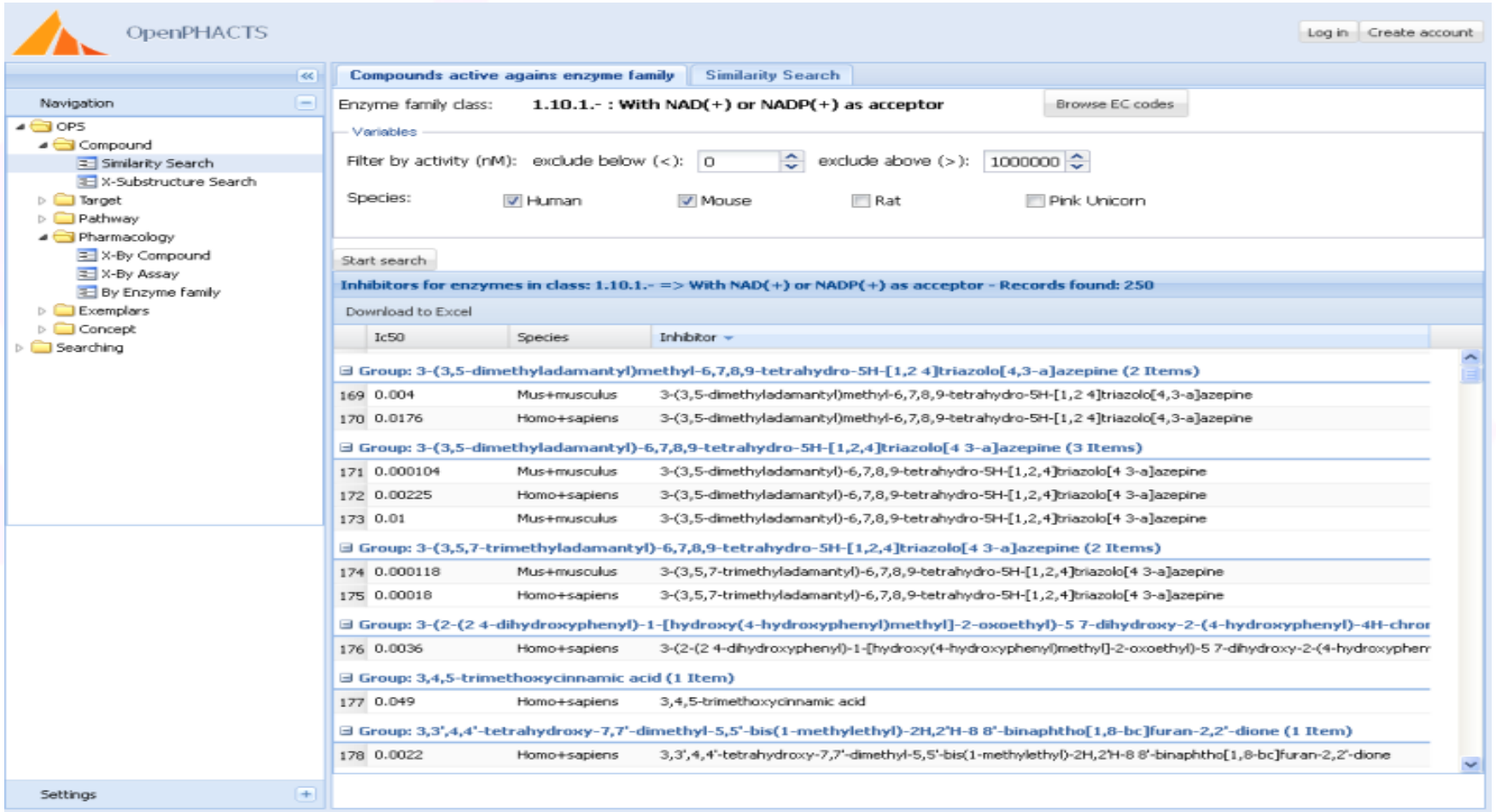
Open Data + Private Data: licensing fun for all the family

Commercial providers: abstract service interface to swap in commercial and open source platforms

Agile Development: 6 month 'lash up'

- Produce a working 'lash up' system
- Constrained to technologies in consortium + a few data sources
- Focused on 2 prioritized research questions
  - All oxidoreductase inhibitors active <100nM in both human and mouse
  - For a given compound [clozapine], give me the interaction profile with [human or mouse] targets
- Minimum requirements: two data sources (one targets, one compounds) and able to produce answers in 'manual time'.

‘lash-up’: youtube.com/openphacts



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Discovery and functional evaluation of diverse novel human CB_1 receptor ligands

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ABSTRACT

Ligand-based virtual screening with a 3D pharmacophore led to the discovery of 30 novel, diverse and drug-like ligands of the human cannabinoid receptor 1 (hCB_1). The pharmacophore was validated with a hit rate of 16%, binding selectivity versus hCB_2, and expected functional profiles. The discovered compounds provide new tools for exploring cannabinoid pharmacology.

The cannabinoid system was initially identified as mediating the effects of the major psychoactive components of *Cannabis sativa*, Δ^9-tetrahydrocannabinol. To date, this system includes at least two receptors, CB_1 and CB_2, the biology of which has been extensively reviewed.[1–3] CB_1, a GPCR coupled to inhibitory G-proteins $G_{i/o}$, is expressed in the central nervous system where it is found on presynaptic terminals, serving to modulate neurotransmitter release. It is also found in peripheral tissue. CB_1 is primarily found

Endocannabinoids like anandamide and 2-arachidonoyl glycerol are elevated in the plasma, adipose tissue and pancreas of obese humans and animals.[10] In genetically obese rodents endocannabinoid levels are elevated in the hypothalamus, an area of the brain that modulates feeding behavior.[11] Centrally, endocannabinoids elicit feeding behavior via activation of CB_1 receptors.[7] Peripheral CB_1 activation causes lipogenesis in adipose tissue and liver, and reduces the oxidation of free fatty acids (FFA).[12] Also

Back to overview

10.1016/j.bmcl.2009.05.114

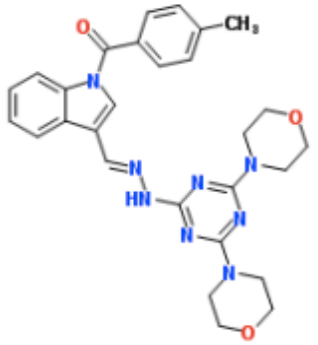
(3-((2-(4,6-...yl)methanone

(3-((2-(4,6-dimorpholino-1,3,5-triazin-2-yl)hydrazono)methyl)-1H-indol-1-yl)(p-tolyl)methanone

[More...]

Ki Value : 2299

Ki of 2299 in 19520572



1-(4-(3-(2,4...-yl)ethanone

1-(4-(3-(2,4-dimethoxyphenyl)-1-m-tolyl-1H-pyrazole-5-carbonyl)piperazin-1-yl)ethanone

[More...]

Ki Value : 1943

Ki of 1943 in 19520572

Look up

Sustainability and community

Data in and data out

Consortium (pharma) members

Public and commercial databases

Publishers

Services built on OPS

Sustainability $

After 3 years?

Pharma customers

Public funders

Services built on top

Publishing data in

Focus and future

One area - **pharmacology**
"Production Level" software
Semantic pragmatics: everyday use by scientists not informaticians

Developers
(Builders)

An **infrastructure** that can be built upon, to provide a stable foundation for further pre-competitive informatics collaboration

End users
(Drivers)

Nanopublications

Capturing scientific information in the Triple Store

nature genetics

nature.com ▸ journal home ▸ archive ▸ issue ▸ commentary ▸ full text

NATURE GENETICS | COMMENTARY

The value of data

Barend Mons, Herman van Haagen, Christine Chichester, Peter-Bram 't Hoen, Johan T den Dun
Gertjan van Ommen, Erik van Mulligen, Bharat Singh, Rob Hooft, Marco Roos, Joel Hammond, E
Kiesel, Belinda Giardine, Jan Velterop, Paul Groth & Erik Schultes

Affiliations | Contributions | Corresponding author

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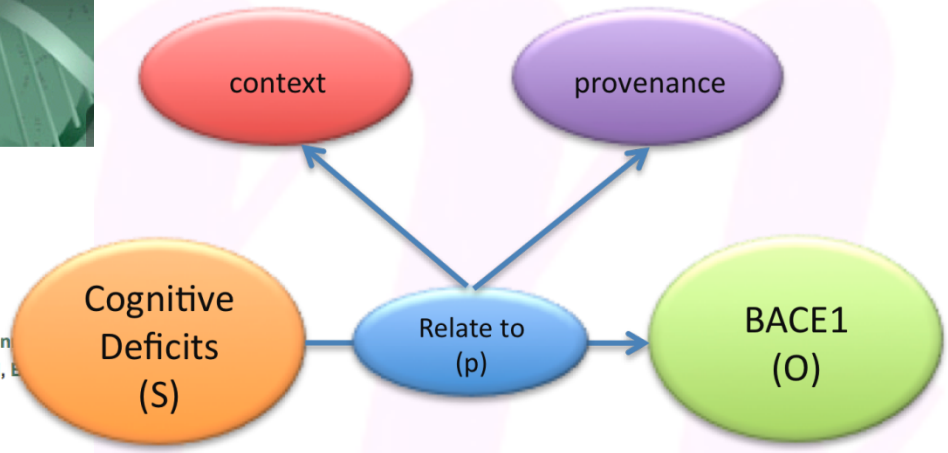

Nano-Publication in the e-science era

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The Anatomy of a Nano-publication

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ABSTRACT

Newer standards like RDFa also facilitate this and integrate with

Onwards and Upwards

Connection between developers and users
Architecture
Services: e.g. entity identification and resolution and representing similarity, ORCID, DataCite
Models: RDF / Nanopublication model spec and guidelines

Prototype

March 2012: Internal Prototype Delivery
September 2012: Release 1st Prototype

Why should you care?

Will be first real large scale semantic data integration project – a pilot that can be extended

Provides a single delivery format and pipeline to your customers?

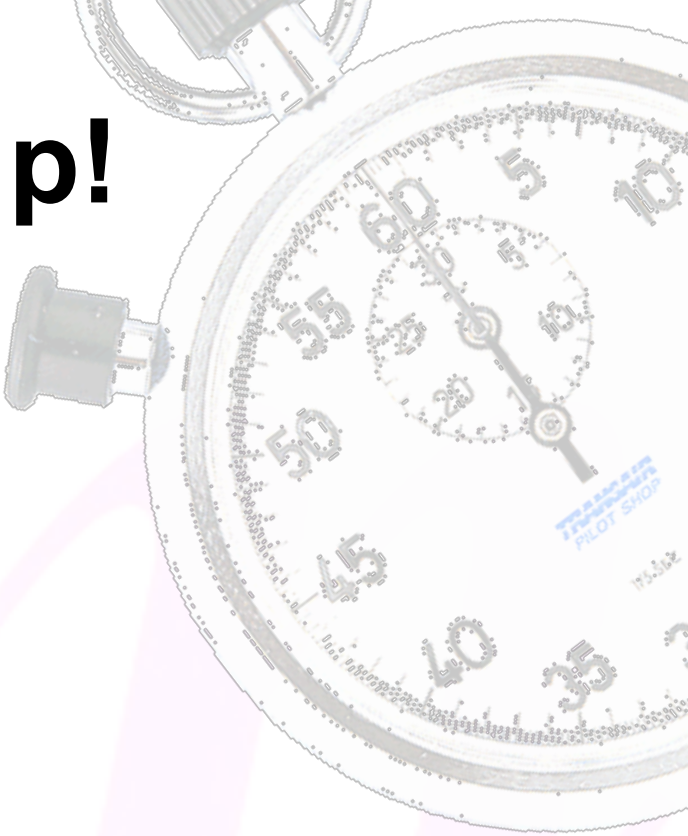
Find out more?

Email me

Apr/May 2012 - a workshop and intro for publishers

also for data providers/vendors

Time's Up!



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