Open PHACTS
Open Pharmacological Space

imi

The Open Pharmacological Concepts Triple Store

www.openphacts.org

efpia

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Public Domain Drug Discovery Data:

Pharma are accessing, processing, storing & re-processing

Literature
Patents
PubChem
Genbank

Databases

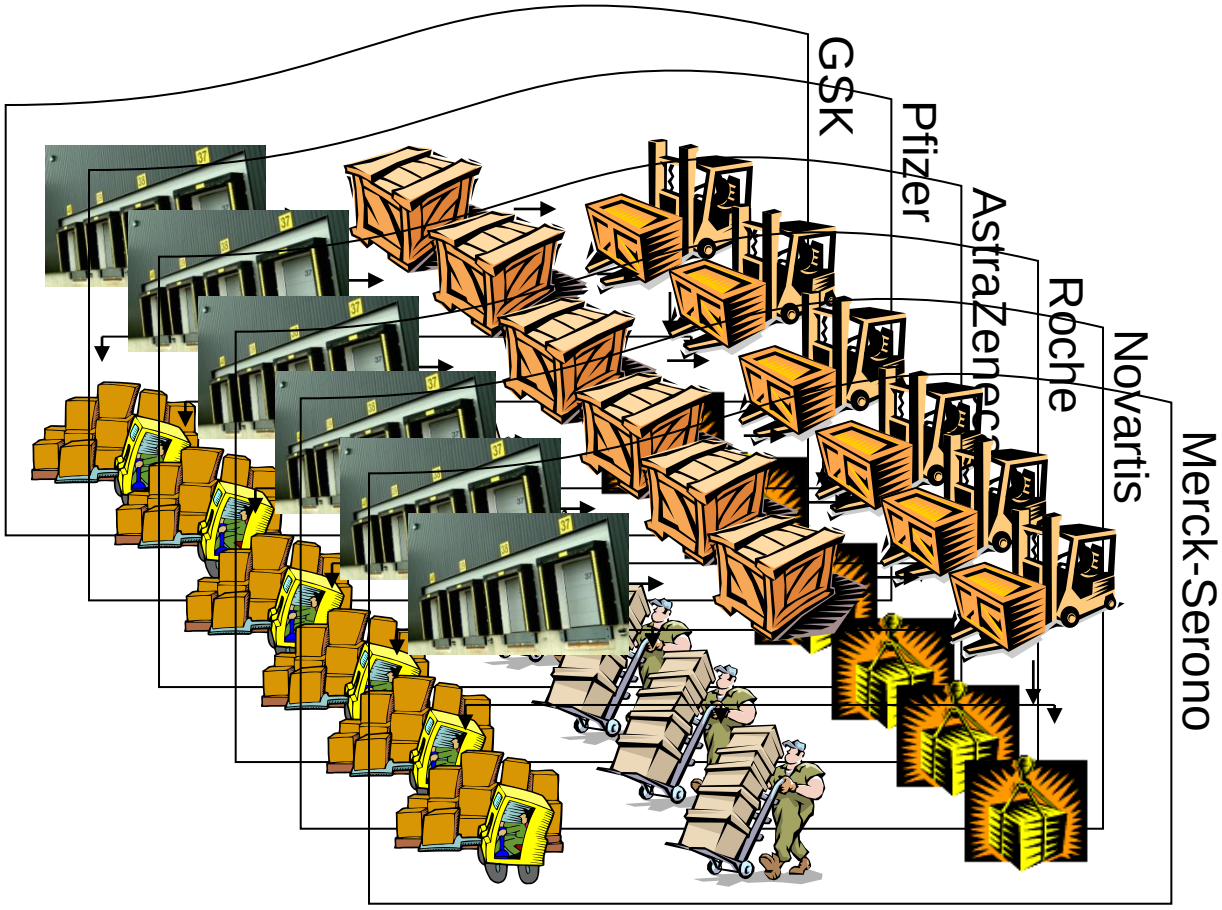
Downloads

Data Integration

Data Analysis

Firewalled Databases

We are all doing this many times……



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A user-friendly, full featured interface that allows scientists to explore and interrogate integrated biological and chemical data

What will users see?

OPS Services should allow to

- integrate data on target expression, biological pathways and pharmacology to identify the most productive points for therapeutic intervention
- investigate the *in vitro* pharmacology and mode-of-action of novel targets to help develop screening assays for drug discovery programmes
- compare molecular interaction profiles to assess potential off-target effects and safety pharmacology
- analyse chemical motifs against biological effects to deconvolute high content biology assays

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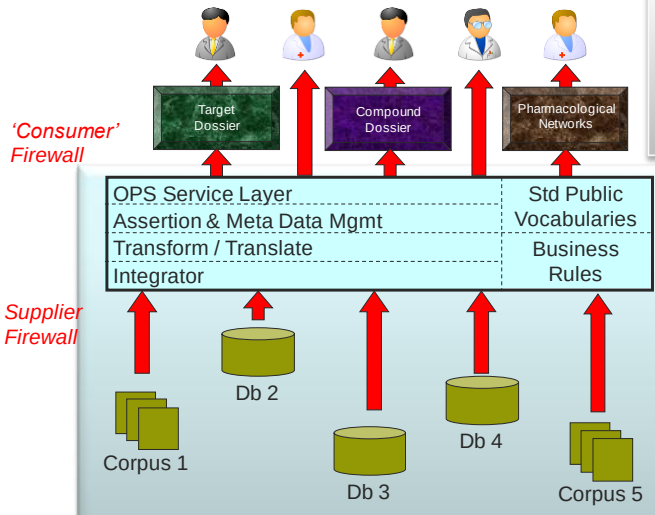
Major Work Streams:

- "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

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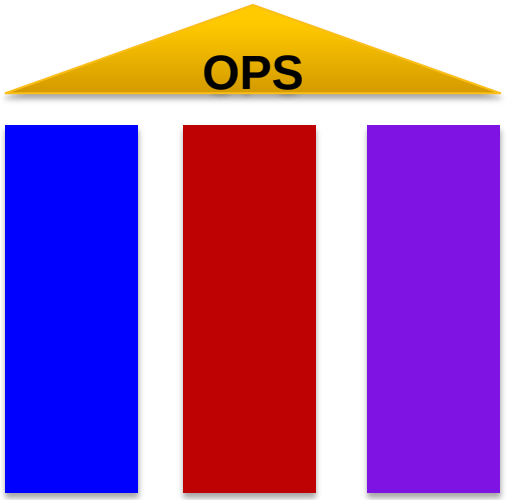
- **A Precompetitive Infrastructure**
  - Begin the task of creating an environment that can also power future collaborative efforts (public & industry)
  - **Expose Industry Experience:** Create drug-discovery focused tools outside of the firewall, influenced by decades of practical experience
- **A Pharmacology Use Case**
  - Showcase one application of this technology: a stable, responsive, user-orientated system for Pharmacology Analysis
- **A Data Publishing Methodology**
  - Develop standards and methodologies to promote good data sharing and interoperability
  - An exemplar project for the use of the Nanopublication concept
  - A technical approach that can be repeated in other areas



OPS 3 Pillars

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Current Status

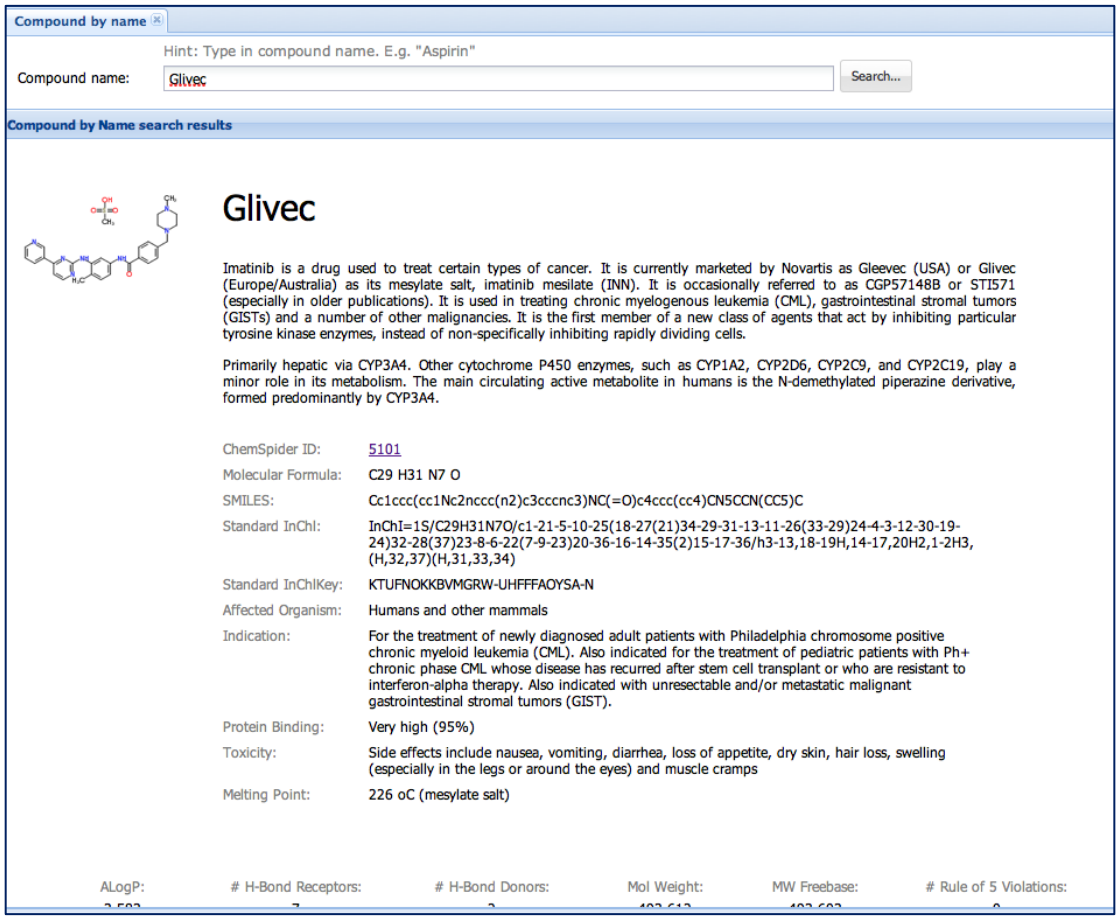
Prototype released to the consortium for broad testing

Datasets in this release

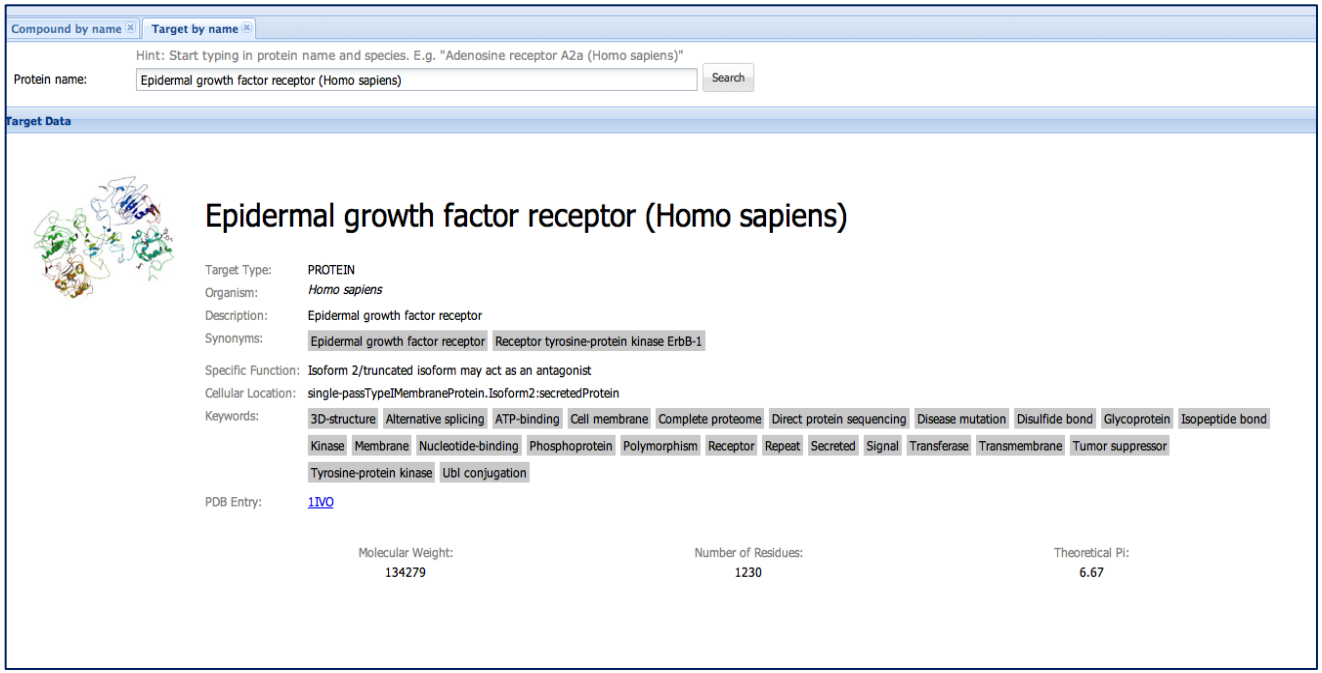
- **Enzyme**: Necessary for the enzyme classifications
- **ChEMBL v2**: Essential SAR database (**soon updated to v13**)
- **Drugbank v3**: Provides additional information on known drugs
- These are connected through **ConceptWiki IDs** (which contains **Uniprot mappings**) and **ChemSpider Ids** (chemistry resolution service)

The following queries are possible:

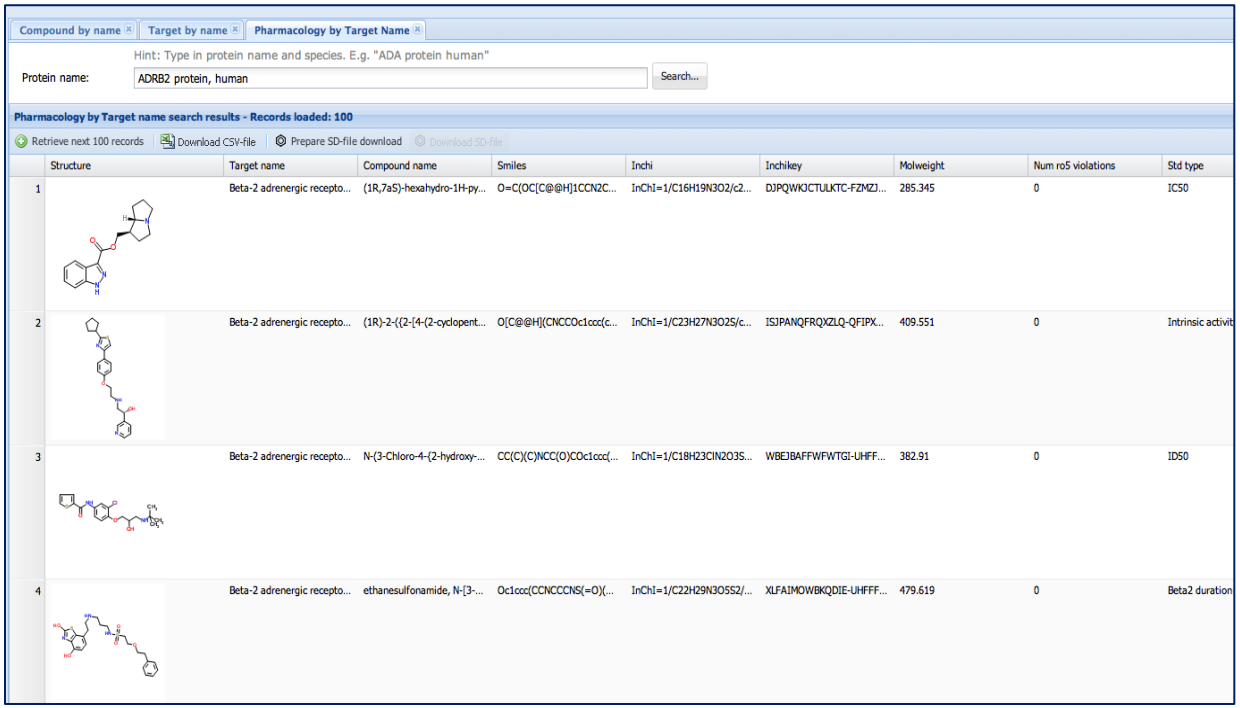
- Query pharmacology data by target (via target name search)
- Query pharmacology data by compound (via compound name search)
- Query pharmacology data by target family (via Enzyme hierarchy)
- Structure searches to identify compounds in the system (which can then be used in pharmacology searches)
- Text search to identify targets/proteins



Compound Information. As the user types, ConceptWiki uses ChemSpider validated synonyms to map text entry to a Concept. This is then linked to a Chemspider ID which is used to retrieve data from both ChemSpider and the DrugBank database



Target Information. As with compounds, ConceptWiki is used to translate entered text to an OPS Concept, using Uniprot as the main protein information system



Pharmacology search for the B2-adrenergic receptor

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Associated partners

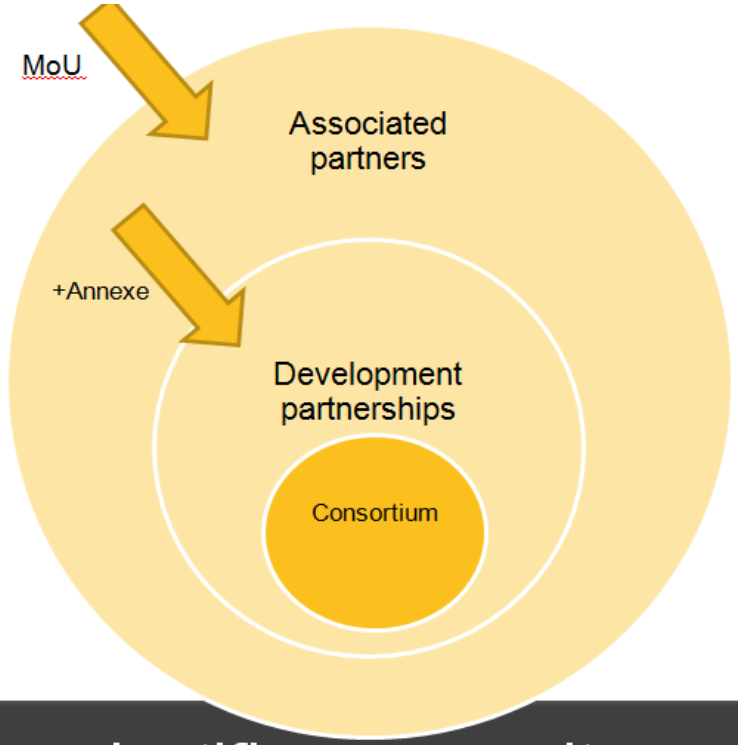
Organisations, most will join here
Support, information
Exchange of ideas, data, technology
Opportunities to demo at community webinars
Need MoU

Development partnerships

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

Consortium

22 current members



Open PHACTS and the scientific community

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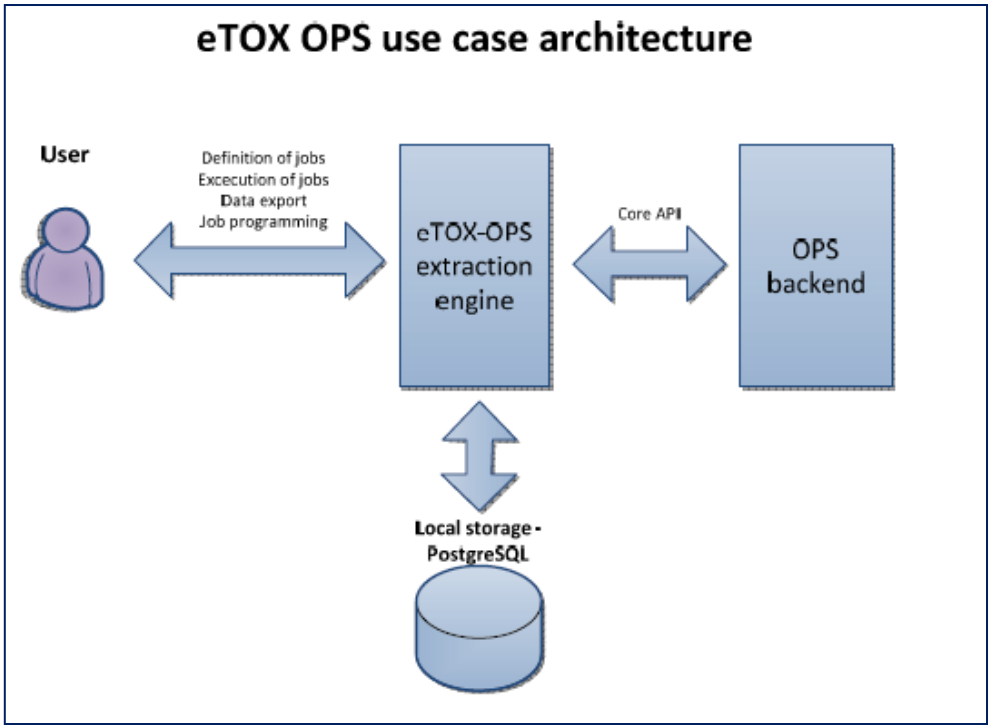
Build an automated tool to obtain the data needed to build eTOX predictive models with the following goals:

- Use the OpenPHACTS platform to extract relevant data to build toxicity models in eTOX.
- Develop a data crawler to extract the data needed to build toxicity models
- Develop a data curation platform that will filter the data extracted from OpenPHACTS
- Develop a web tool to browse the results obtained



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Next Steps

- Get licensing done
- complete call for professional hosting
- Go public
- Start 2nd wave pilots

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Open PHACTS Project Partners

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Pfizer– Coordinator
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Universität Wien – Managing entity of IMI JU funding *(Gerhard Ecker)*
Technical University of Denmark
(Sören Brunak)
University of Hamburg, Center for Bioinformatics
(Mattias Rarey)
BioSolveIT GmbH
(Christian Lemmen)
Consorci Mar Parc de Salut de Barcelona
(Ferran Sanz)
Leiden University Medical Centre
(Barend Mons)
Royal Society of Chemistry
(Richard Kidd, Antony Williams)
Vrije Universiteit Amsterdam
(Paul Groth, Frank van Harmelen)

Spanish National Cancer Research Centre
(Alfonso Valencia)
University of Manchester
(Carole Goble, Steve Pettifer)
Maastricht University
(Chris Evelo)
AQnowledge
(Jan Velterop)
University of Santiago de Compostela
(Mabel Loza)
Rheinische Friedrich-Wilhelms-Universität Bonn
(Martin Hofmann-Apitius)
AstraZeneca
(Niklas Blomberg)
GlaxoSmithKline
(Andrew Leach)
Esteve
(Leo Salgado)

Novartis
(Edgar Jacoby)
Merck Serono
(Thomas Grombacher)
H. Lundbeck A/S
(Askjaer Sune)
Eli Lilly
(Hans Constandt)
Stichting Netherlands Bioinformatics Centre
(Barend Mons)
Swiss Institute of Bioinformatics
(Christine Chichester)
Connected Discovery
(Bryn Williams-Jones)
European Bioinformatics Institute
(John Overington)
Janssen Pharmaceutica
(Herman van Vlijmen)