

Open PHACTS impact at Janssen

Herman van Vlijmen, 19 Feb 2016

Pictured left: Pancreas tissue

Open PHACTS: Impact in multiple ways

- Access to integrated biomedical and chemical databases
 - Maximising the value of internal data by integration with public data
 - Create information workflows that were very difficult before, such as:
 - Searching for compounds across protein families, pathways, diseases
 - Target validation
 - Phenotypic screen analysis
- Changing the mindset of Pharma IT
 - At start of project Relational Databases was the only game in town
 - Now a strong realisation of the value of semantic databases, and actual efforts to integrate internal databases. This would not have been done in the pre Open PHACTS situation. Value for the pharma scientists!
- Changing the mindset of scientists
 - Semantic querying opens up new ways of using existing data
 - Target annotation, Assay ontology (BAO)
 - Sky is the limit, especially when additional domains are added, such as patent data (SureChEMBL), ADME, (pre)-clinical data
- Changing the mindset of public and commercial databases

Chem³ is here

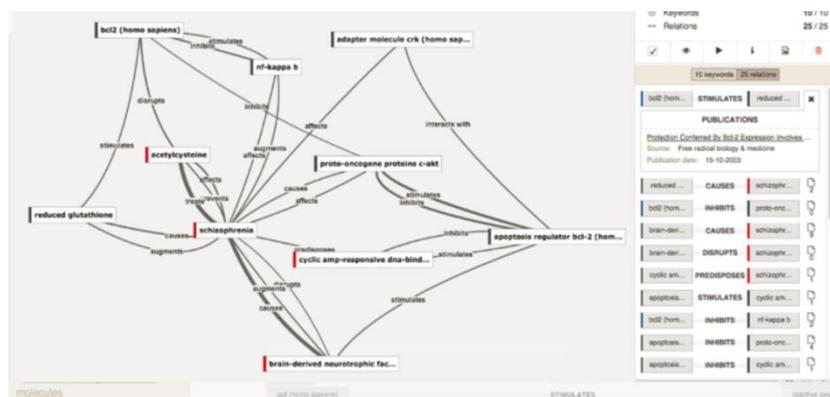
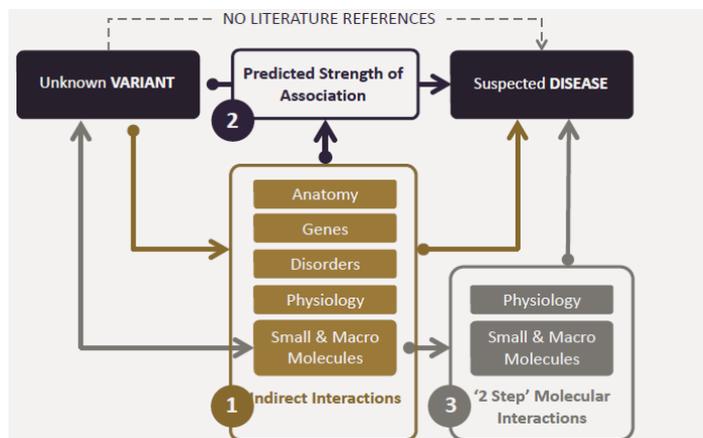
In 3DX and in Pipeline Pilot

The screenshot displays the Chem3 software interface. The menu bar includes File, Edit, Select, View, Data, Chemistry, Query, Request, Reports, Sequence, Abcd2, PDS, Tools, and Help. The 'Abcd2' menu is open, showing 'Database' and 'Research' options. The 'Database' submenu is further open, listing 'EZ SPARQL', 'EMolecules', 'Abcd2 (Target, Compound)', and 'ABCD and ChEMBL Compound Act'. A large white arrow points from the 'EZ SPARQL' menu item to a table below. Another white arrow points from the 'PDS' menu item to the right side of the interface.

	Concept
465	http://purl.uniprot.org/core/Alternative Promoter Usage Annotation
466	http://purl.uniprot.org/core/Unknown Sequence
467	http://purl.uniprot.org/core/Pharmaceutical Annotation
468	http://purl.uniprot.org/core/Alternative Initiation Annotation
469	http://purl.uniprot.org/core/Toxic Dose Annotation
470	http://purl.uniprot.org/core/Ribosomal Frame Shifting
471	http://biohackathon.org/resource/faldo#OneOfPosition
472	http://purl.uniprot.org/core/Redox Potential Annotation

Additional interface elements include a toolbar with various icons, a status bar at the bottom showing 't.eu.jnj.com' and '9.2.0', and a partially visible 'Excel Viewer' window on the right.

Exploring Linked Data analysis tools



FILTER ON TYPE DISCOVER > DRUG OR CHEMICAL (560)

Drug or chemical 560 results

Finetune your results

Drug type (56)

growth X hormone X

42 small molecule

14 biotech

Affected organism (55)

54 Humans and other mammals

1 Enteric bacteria and other eubacteria

Bromocriptine

Type: Drug or chemical

Sources: drugbank chembl additional_drugbank_atc sameas search_terms_chembl search_terms_drugbank labels_drugbank additional_drugbank_dirtargets

1,2-Propanediol

Type: Drug or chemical

BRAIN (Euretos www.euretos.com)

Discover (Ontoforce www.ontoforce.com)

Time and €€ savings

- Certain queries were possible before but were tedious work and took a lot of time (days). These can now be done in less than an hour
- Semantically integrated databases allow for completely new ways of analysing the data
- Integration of different databases is difficult, costly, and time consuming, and probably would not have been done at this level of quality without Open PHACTS
- Conclusion: Without Open PHACTS, pharma companies would not have access to this valuable resource
 - Sharing the cost and effort in precompetitive project saved millions
 - Accelerated research using integrated data
 - Involvement in the project sparked internal innovation in this area