

Open PHACTS

Open Pharmacological Space

Hangout session Nov 2015

Drug discovery is extremely complex and relies on data ranging from chemistry properties and genomic maps to clinical trials and patient records.

Even addressing just the combination of curated medicinal chemistry and molecular biology databases can address up to a 100 different databases.

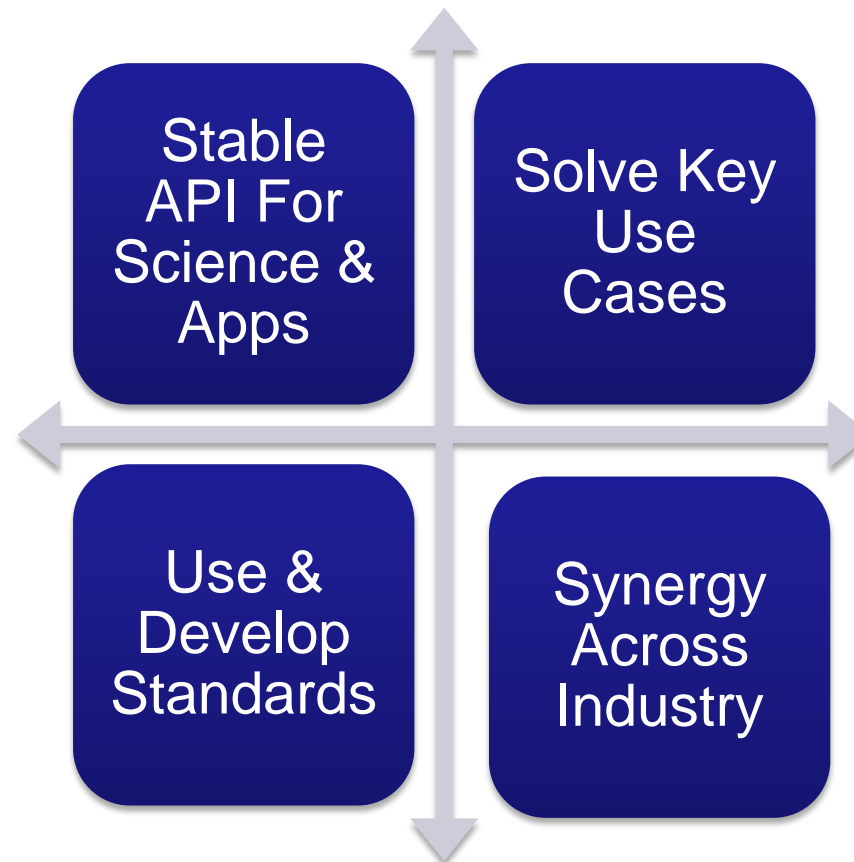
Open PHACTS helps!

The key challenges in processing data include the variety of the data involved in terms of representations, schemas, and semantics.



The Mission

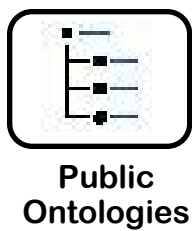
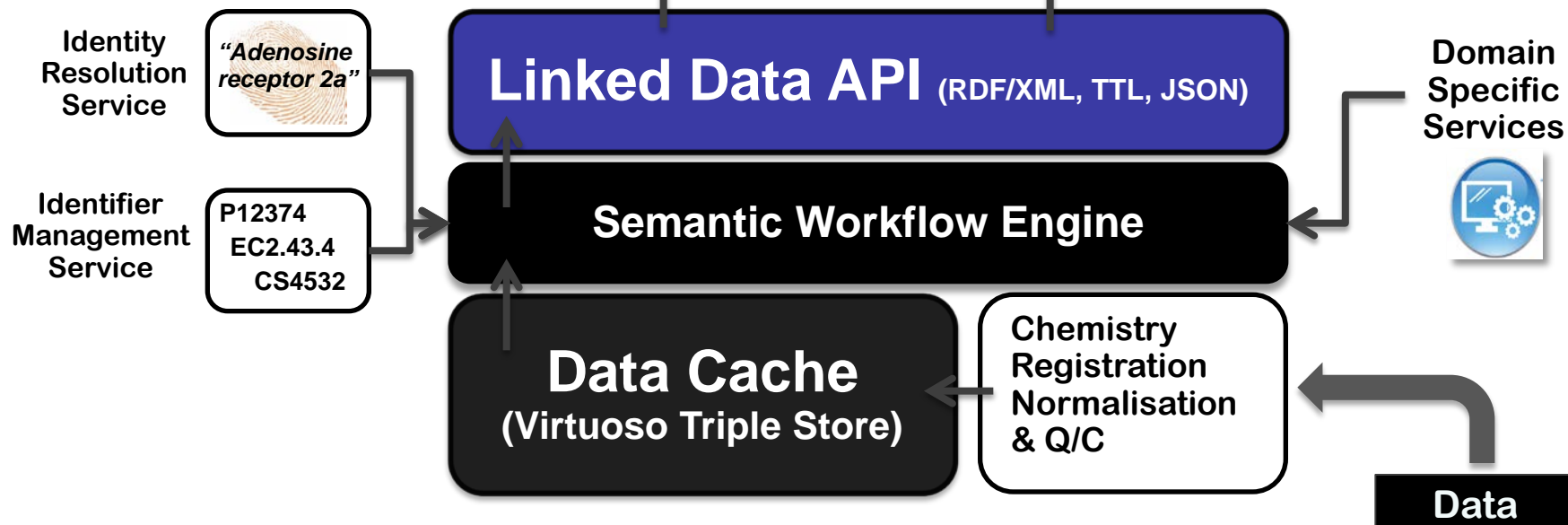
A shared infrastructure for data integration; promoting best practice and facilitating collaboration



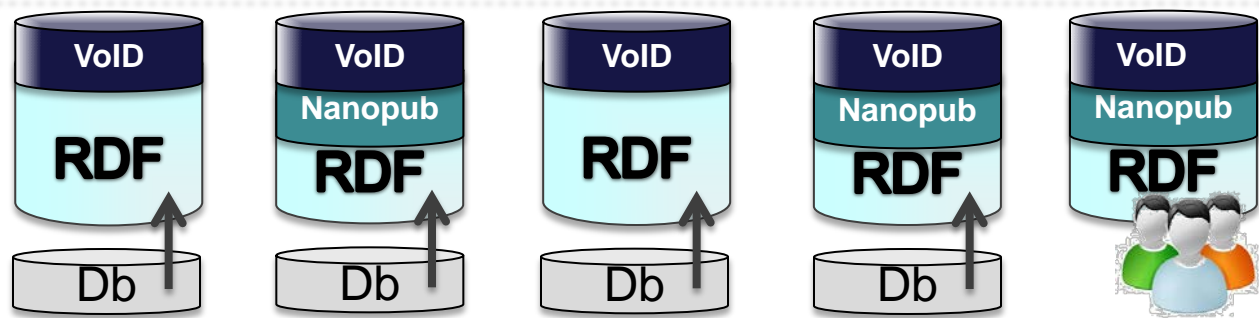


Apps

Core Platform



Public Ontologies



Public Content

Commercial

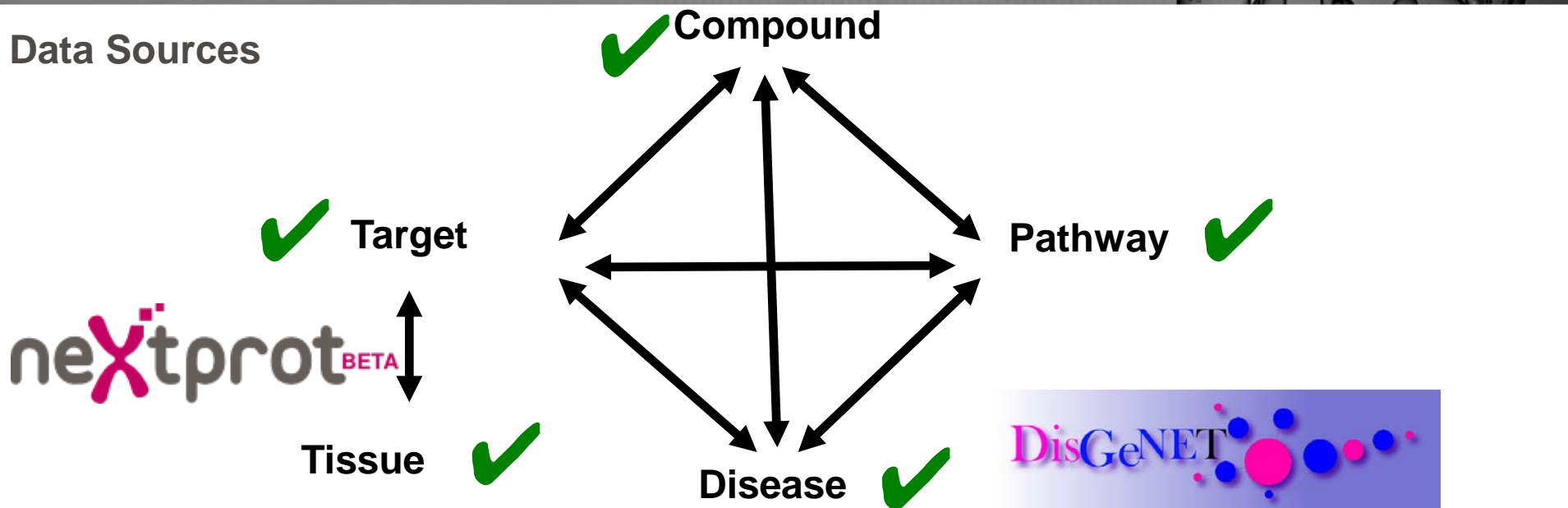
User Annotations



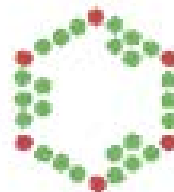
Data Import



Data Sources



ChEMBL



WIKIPATHWAYS
Pathways for the Brave



GENEONTOLOGY
Unifying Biology



OpenPHACTS v1.4 API Active Docs

The response template for each operation colour coded as follows:

- Required elements that always return a **single value**.
- Required elements that return **either a single value or an array**.
- Optional elements that always return a **single value**
- Optional elements that return **either a single value or an array**.

Operations

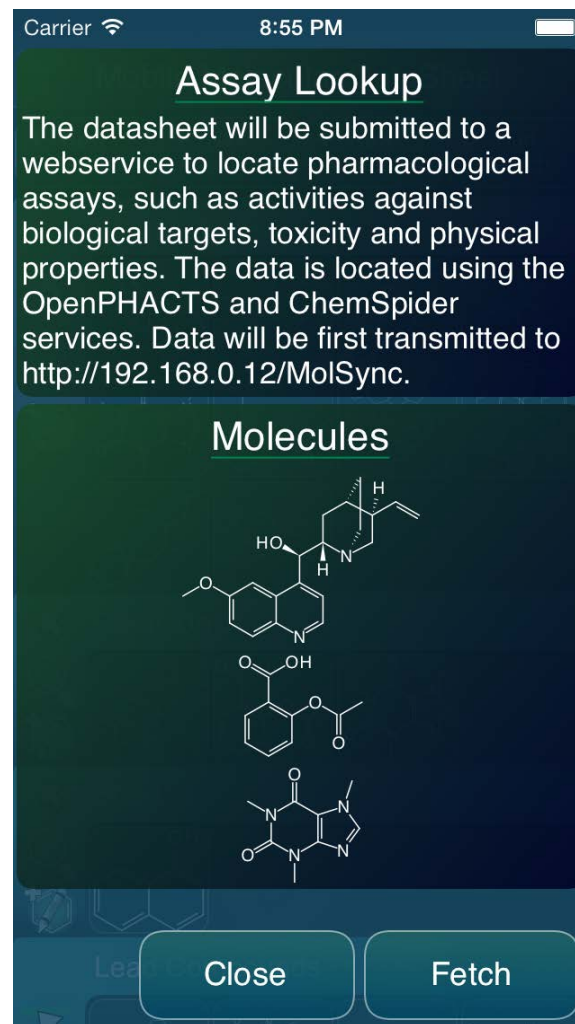
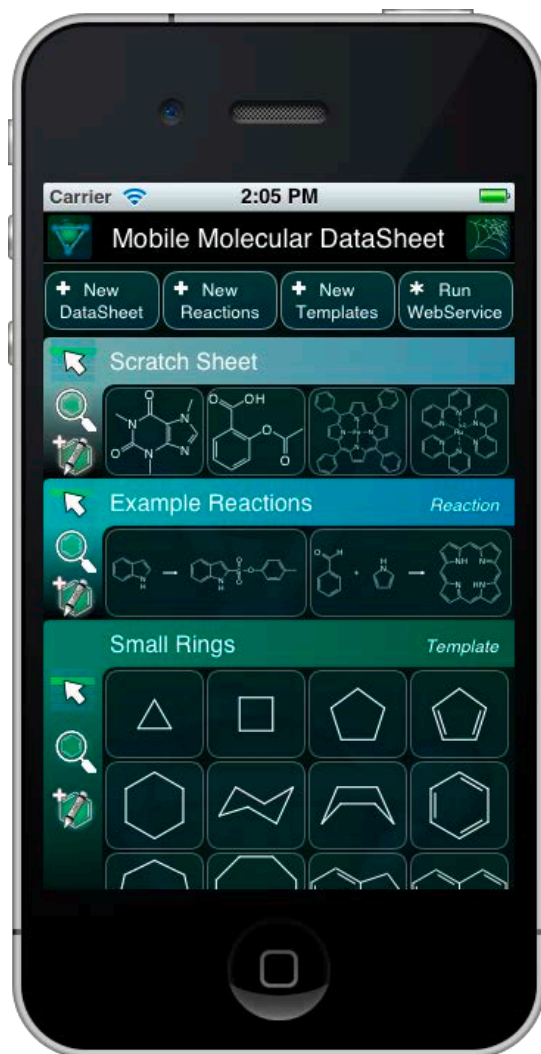
OpenPHACTS API v1.4

Compound Information	<code>/compound</code>	GET
Compound Information: Batch	<code>/compound/batch</code>	GET
Compound Class Members: Count	<code>/compound/members/count</code>	GET
Compound Class Members: List	<code>/compound/members/pages</code>	GET
Compound Classifications	<code>/compound/classifications</code>	GET
Classification of Targets for Compound	<code>/compound/classificationsForTargets</code>	GET
Compound Pharmacology: Count	<code>/compound/pharmacology/count</code>	GET
Compound Pharmacology: List	<code>/compound/pharmacology/pages</code>	GET
Compound Class Pharmacology: Count	<code>/compound/tree/pharmacology/count</code>	GET
Compound Class Pharmacology: List	<code>/compound/tree/pharmacology/pages</code>	GET

What's new in 1.5

- Adverse events (FDA)
- Disease data
- Tissue data

Associations for Target: Count	<code>/disease/assoc/byTarget/count</code>	GET
Associations for Target: List	<code>/disease/assoc/byTarget</code>	GET
Associations for Disease: Count	<code>/disease/assoc/byDisease/count</code>	GET
Associations for Disease: List	<code>/disease/assoc/byDisease</code>	GET
Disease Information	<code>/disease</code>	GET
Disease Information: Batch	<code>/disease/batch</code>	GET
[PREVIEW] Tissue Information	<code>/tissue</code>	GET





ANSWERED 18/20

- **Generalized and then answered**
 - Provide all activities for a given compound X, with targets annotated by gene (Compound -> target)
 - Provide all compounds assayed for target Y with target indicated by a gene (Target -> Compound)
 - For target X provide target family. (Gene -> Gene family)
 - Retrieving Pharmacology for all proteins with a given classification
 - Filter annotation results by activity cutoffs
 - Substructure and similarity search
 - For a target Y, find pathway Z
 - For a pathway Z, find target Y