

**Open PHACTS**

Open Pharmacological Space

**The Open PHACTS**

**Discovery Platform**

**Collaborations in Semantic Data  
Integration for Life Sciences**

**Nick Lynch**

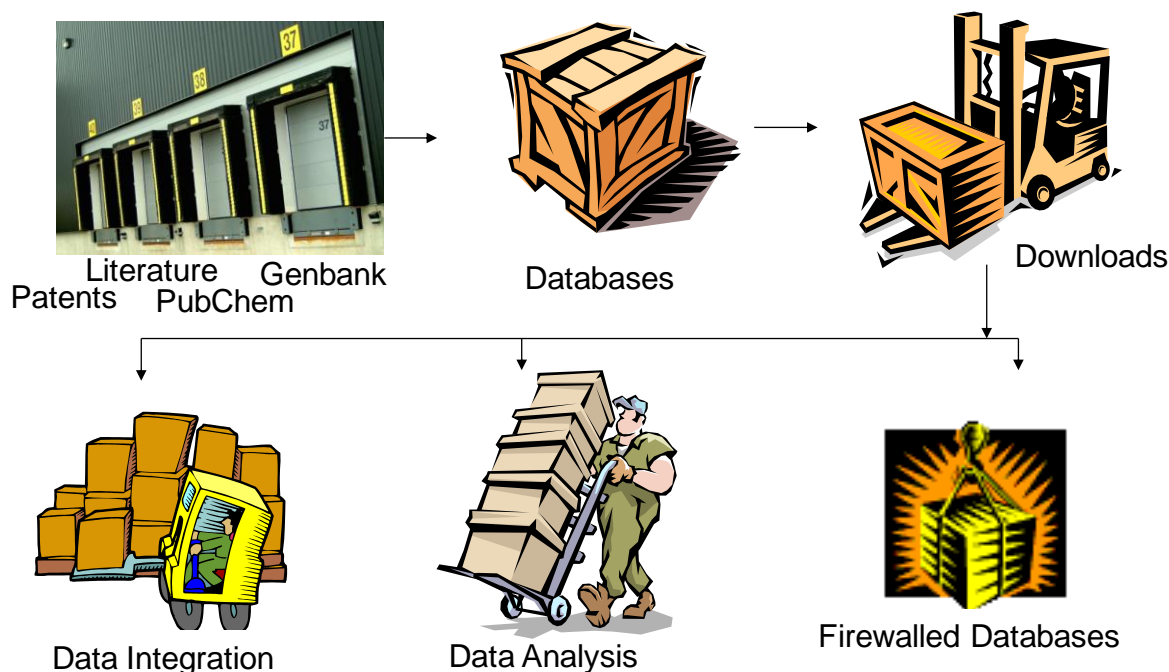


**Open PHACTS Mission:  
Integrate Multiple Research  
Biomedical Data Resources  
Into A Single **Open, Sustainable &  
Free**  
Access Point**



# Pre-competitive Informatics:

Pharma are all accessing, processing, storing & re-processing external research data



Repeat @  
X each  
company



"What is the selectivity profile of known p38 inhibitors?"



"Let me compare MW, logP and PSA for known oxidoreductase inhibitors"



"Find me compounds that inhibit targets in NFkB pathway assayed in only functional assays with a potency <math><1 \mu\text{M}</math>"



ChEMBL

DrugBank

Gene  
Ontology

Wikipathways

GeneGo

ChEBI

UniProt

UMLS

neXtProt

GVKBio

ConceptWiki

ChemSpider

DisGeNet

TrialTrove

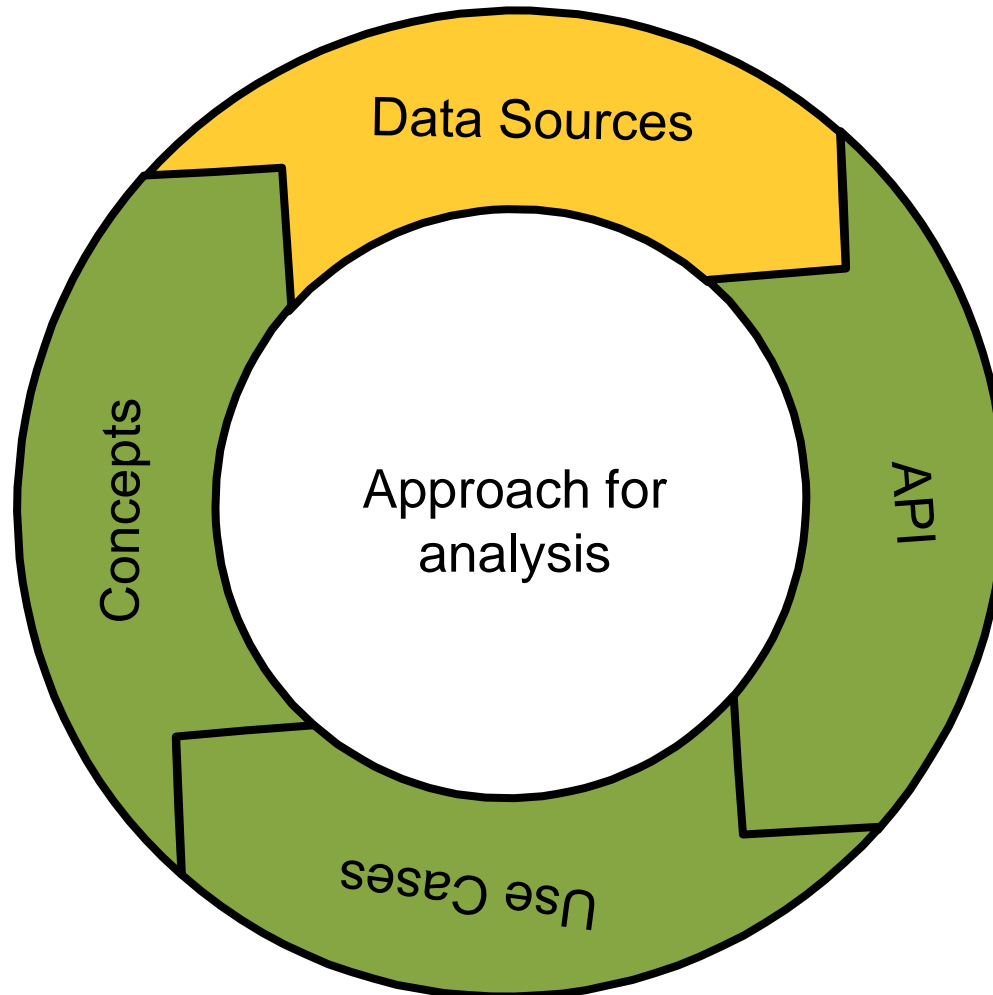
TR  
Integrity

ChEMBL  
Target Class

ENZYME

FDA adverse  
events

SureChEMBL





## Business Question Driven Approach

Number	sum	Nr of 1	Question
15	12	9	All oxidoreductase inhibitors active <100nM in both human and mouse
18	14	8	Given compound X, what is its predicted secondary pharmacology? What are the on and off, target safety concerns for a compound? What is the evidence and how reliable is that evidence (journal impact factor, KOL) for findings associated with a compound?
24	13	8	Given a target find me all actives against that target Find/predict polypharmacology of actives
32	13	8	For a give
37	13	8	The current data in se
38	13	8	Retrieve a chemical
41	13	8	A project i compound modulate least at the literature.
44	13	8	Give me a
46	13	8	Give me the compound(s) which hit most specifically the multiple targets in a given pathway (disease)



### Drug Discovery Today

Volume 18, Issues 17-18, September 2013, Pages 843-852



Review

### Scientific competency questions as the basis for semantically enriched open pharmacological space development

Kamal Azzaoui<sup>1</sup>, Edgar Jacoby<sup>14</sup>, Stefan Senger<sup>2</sup>, Emiliano Cuadrado Rodríguez<sup>3</sup>, Mabel Loza<sup>3</sup>, Barbara Zdrzil<sup>4</sup>, Marta Pinto<sup>4</sup>, Antony J. Williams<sup>5</sup>, Victor de la Torre<sup>6</sup>, Jordi Mestres<sup>7</sup>, Manuel Pastor<sup>7</sup>, Olivier Taboureau<sup>8</sup>, Matthias Rarey<sup>9</sup>, Christine Chichester<sup>10</sup>, Steve Pettifer<sup>11</sup>, Niklas Blomberg<sup>12</sup>. <sup>a</sup>, Lee Harland<sup>13</sup>, Bryn Williams-Jones<sup>13</sup>, Gerhard F. Ecker<sup>4</sup>.  



# The Open PHACTS Discovery Platform

- Cloud-Based “Production” Level System. Secure & Private

- Guided By Business Questions

- Uses Semantic Web Technology But provides a simple REST-ful API for everyone else



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<http://dx.doi.org/10.1016/j.drudis.2013.05.008>



## Web Semantics: Science, Services and Agents on the World Wide Web

Available online 8 April 2014

In Press, Accepted Manuscript — Note to users



API-centric Linked data integration: The open PHACTS discovery platform case study

Paul Groth<sup>a</sup>   , Antonis Loizou<sup>a</sup>, Alasdair J.G. Gray<sup>d</sup>, Carole Goble<sup>b</sup>, Lee Harland<sup>c</sup>, Steve Pettifer<sup>b</sup> <http://dx.doi.org/10.1016/j.websem.2014.03.003>



HELLO  
my name is

RS\_2353

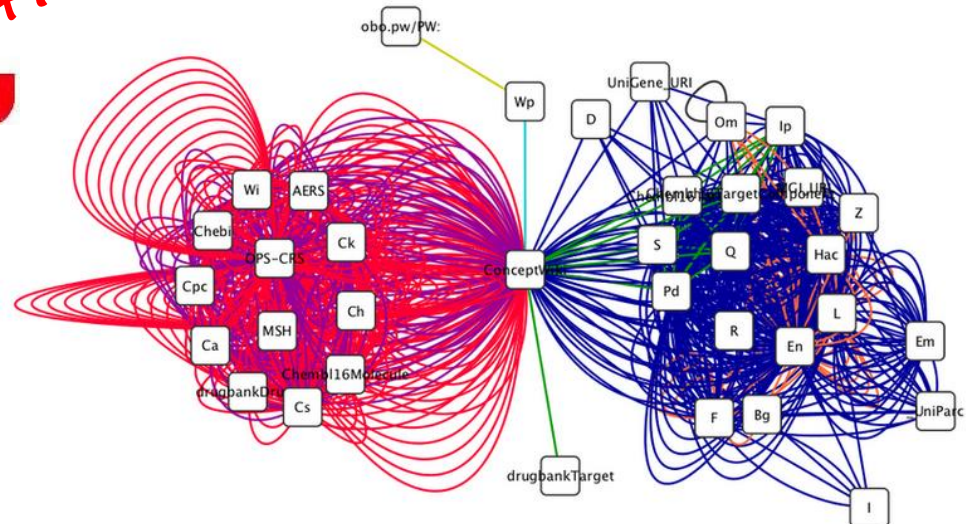
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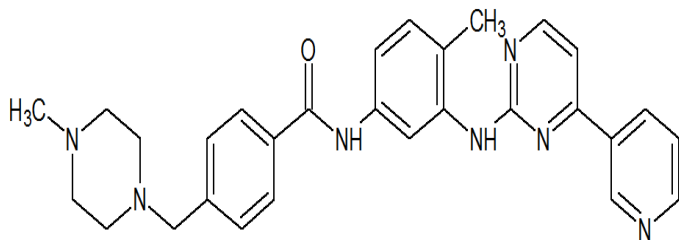
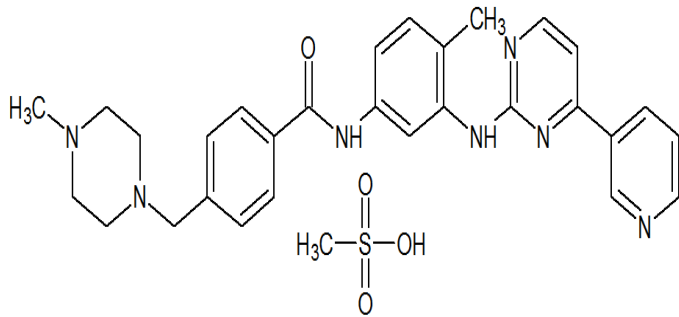
# Data Integration is key







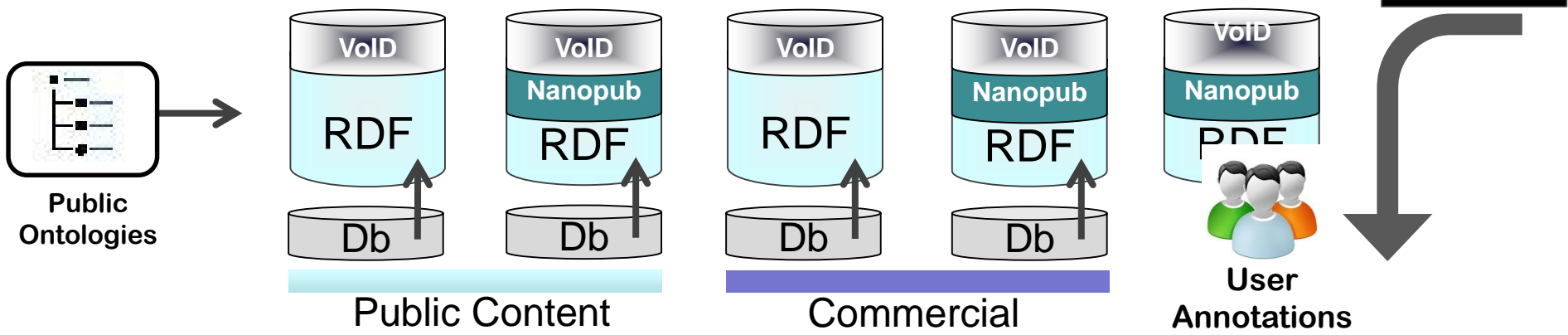
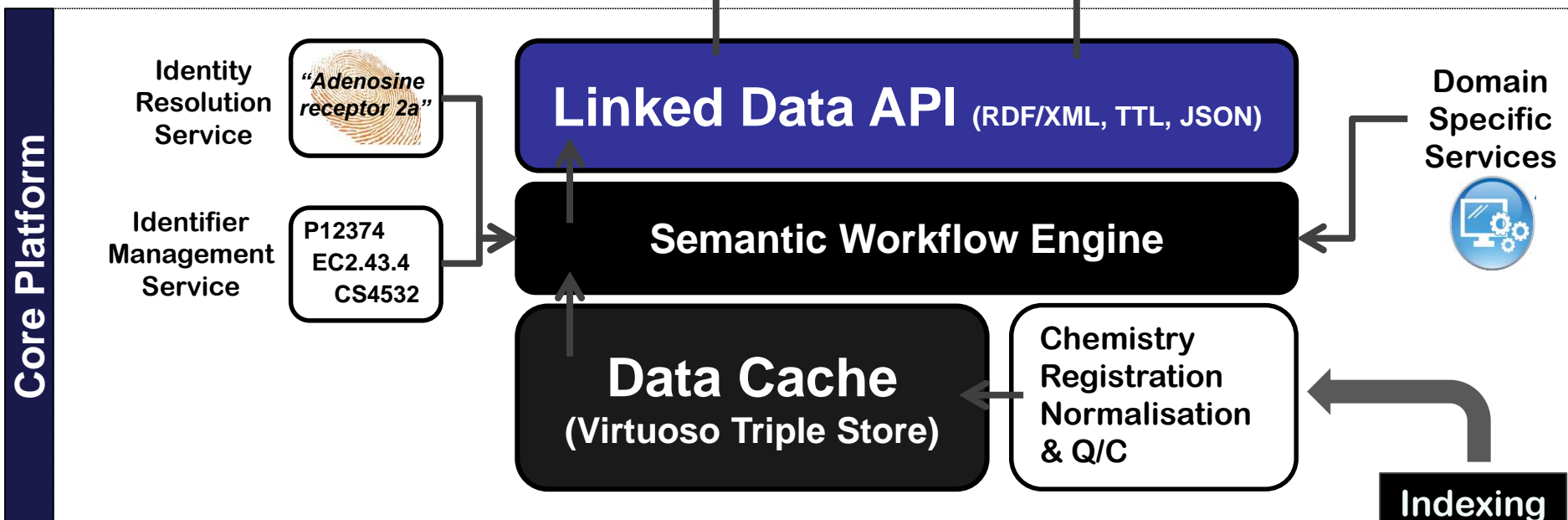
## Are These Two Molecules The Same(\*)



\*Really: Is it sensible to combine data associated with these two molecules?



# Apps





**> 1 billion triples**

Sources			
ChEMBL			
DrugBank			
UniProt			
ENZYME			
ChEBI			
GO/GOA			
ChemSpider/ACD			
ConceptWiki			
Disgenet			
WikiPathways			
SureChEMBL			

- ✦ Regular updates
- ✦ Future new sources planned based on business questions and interests
- ✦ Options for hosting commercial data ( e.g. GVKBio)
- ✦ Options for hosting private data
- ✦ Potential for Data update pipelines
- ✦ VM platform



Explorer

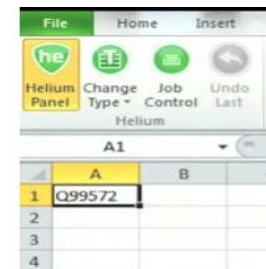
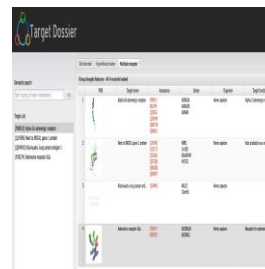
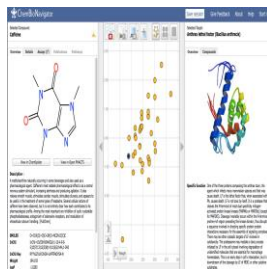
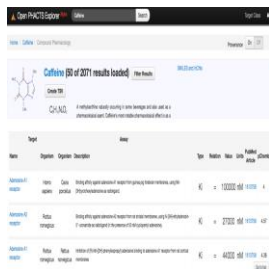
Explorer2

ChemBioNavigator

Target Dossier

Pharmatrek

Helium



MOE

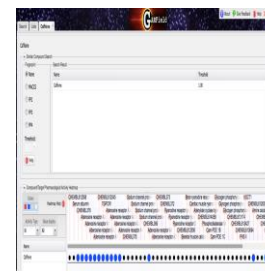
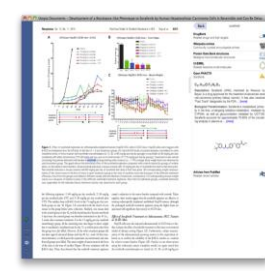
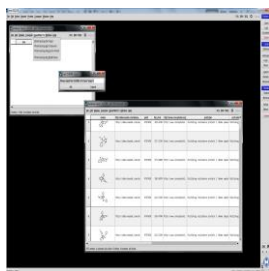
Collector

Cytophacts

Utopia

Garfield

SciBite



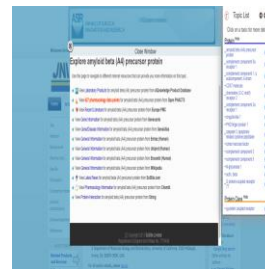
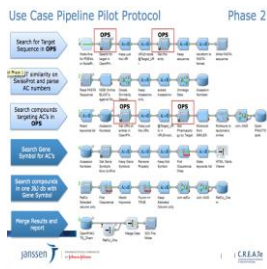
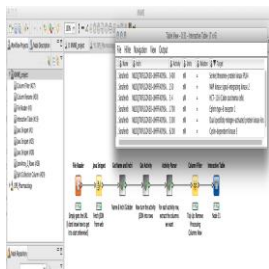
KNIME

Mol. Data Sheets

PipelinePilot

scinav.it

Taverna

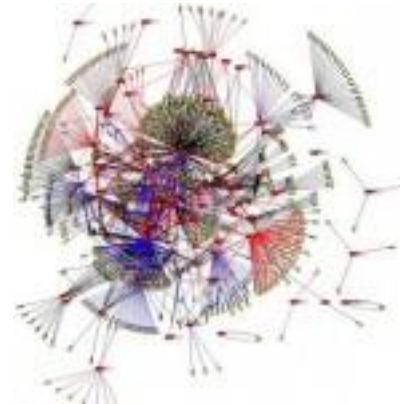




# Sustaining Impact

✦ “Software is free like puppies are free - they both need money for maintenance”

✦ ...and more resource for future development



# The Open PHACTS Foundation

*OPF is a not-for-profit membership organisation, supporting the Open PHACTS Discovery Platform:*

*A sustainable, open, vibrant and interoperable information infrastructure for applied life science research and development.*

To reduce the barriers to drug discovery in industry, academia and for small businesses, the **Open PHACTS Discovery Platform** provides tools and services to interact with multiple integrated and publicly available data sources. To integrate this data, extensive cross-referencing of scientific concepts is needed across all databases.

The Open PHACTS Foundation ensures the sustainability of the **Open PHACTS Discovery Platform** infrastructure and acts as a hub for relevant scientific research and development.



ChEMBL

ChemSpider  
The free chemical databaseDRUGBANK  
Open Data Drug & Drug Target DatabaseWIKIPATHWAYS  
Pathways for the People

## Key Resources

 [Open PHACTS API](#)

 [Open PHACTS Repository](#)

## Subscribe to the Foundation Newsletter

**Subscribe**

## Contact us

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# Acknowledgements



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H. Lundbeck A/S  
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AstraZeneca  
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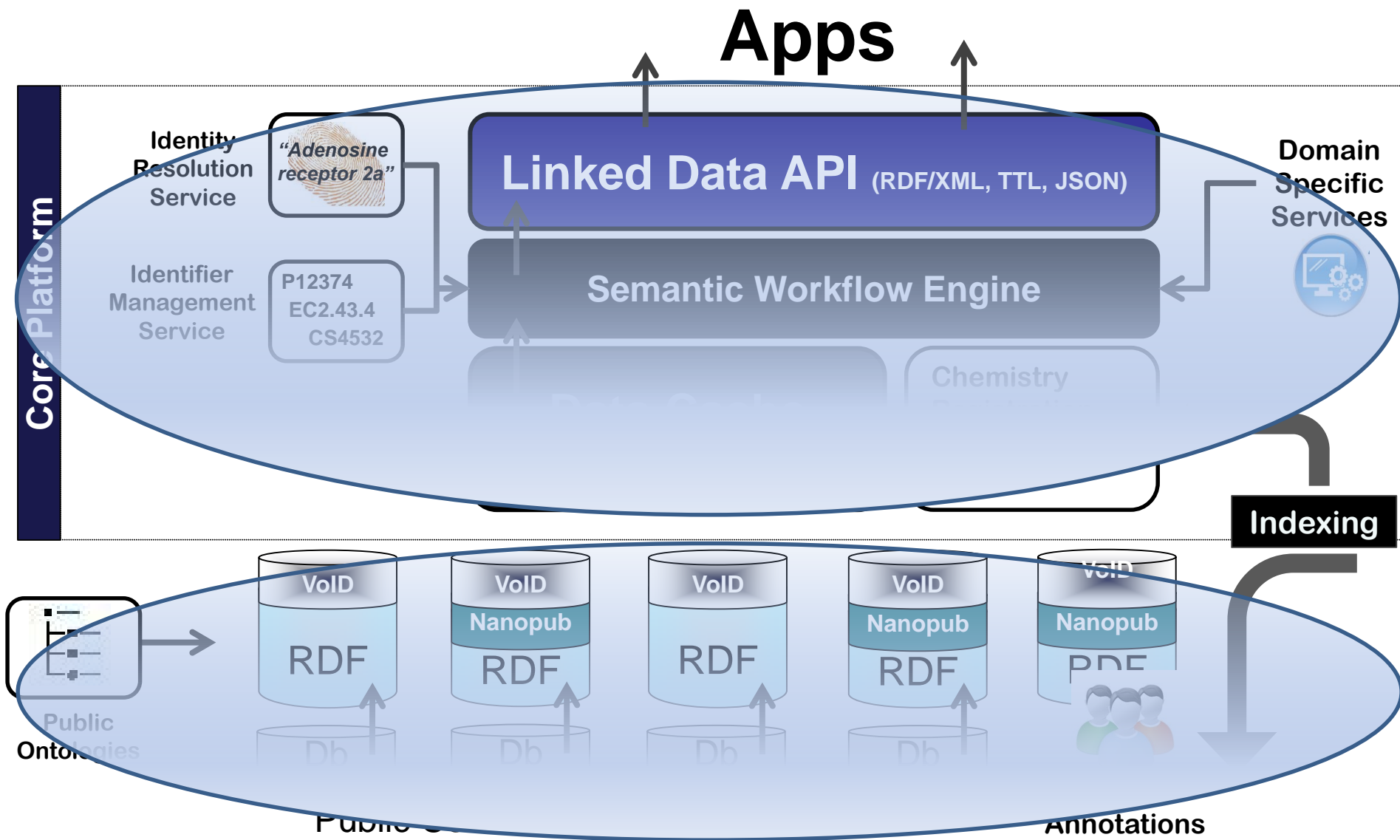
@Open\_PHACTS

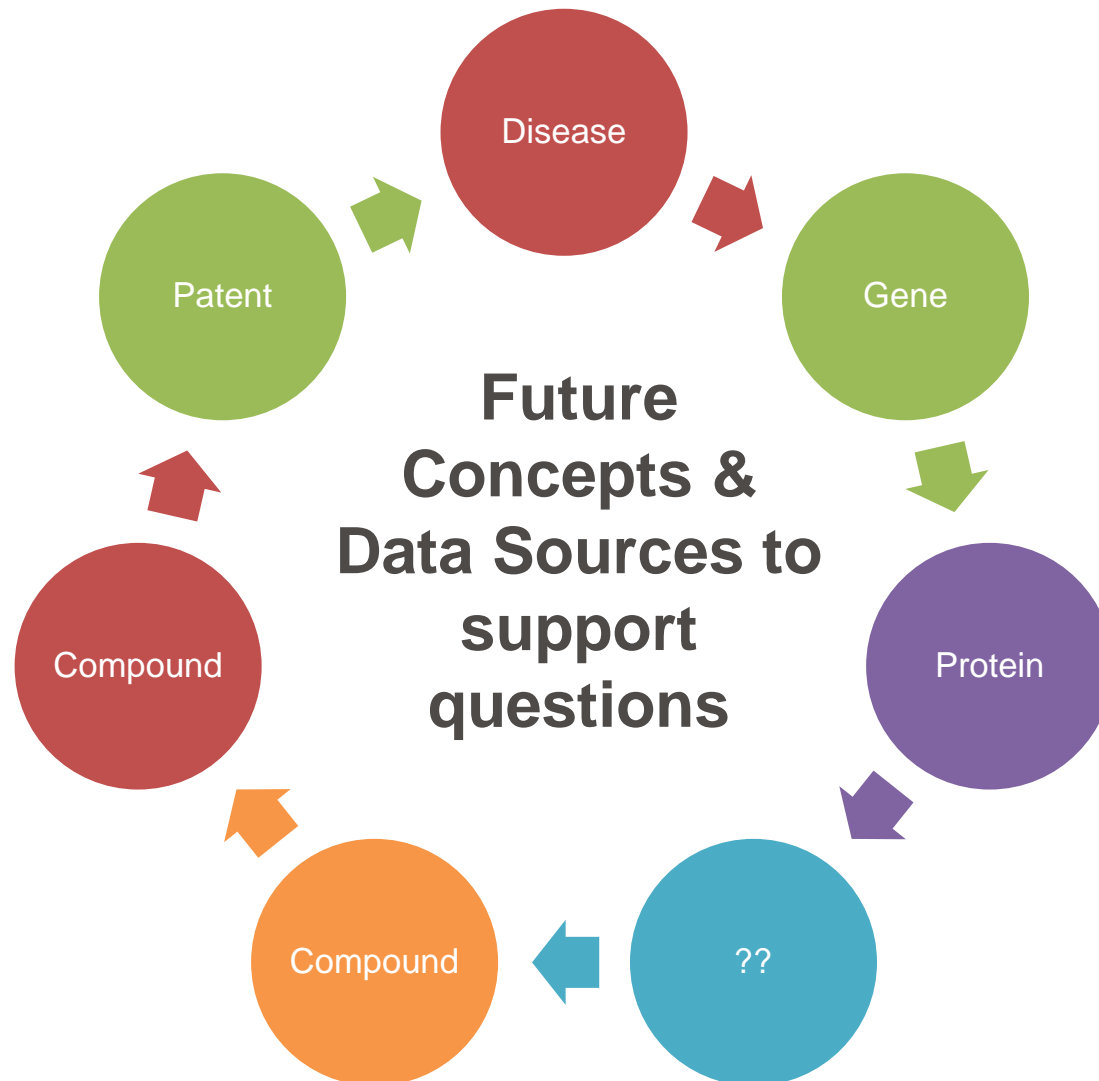
# Collaborations around Key Questions





# Platform, Data & Experience Tackling Big Data challenges







ANY  
QUESTIONS?



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