

Mashing Up Drug Discovery

There's an API for that....

Lee Harland July 2013

Open PHACTS <http://openphacts.org>

SciBite <http://scibite.com>

ConnectedDiscovery <http://connecteddiscovery.com>

@Scibitely

What does an
Application Program
Interface look like?

```

<application xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://wadl.dev.java.net/2009/02" xmlns:ops="http://ops.epo.org"
xmlns:xs="http://www.w3.org/2001/XMLSchema" xsi:schemaLocation="http://wadl.dev.java.net/2009/02 ../schema/wadl.xsd">
  <grammars>
    <include href="../schema/ops.xsd"/>
  </grammars>
  <resources base="http://ops.epo.org/3.0/rest-services">
<!-- GET Published data search -->
<resource path="published-data/search/{publishedConstituents}/" id="publishedDataSearch">
  <doc xml:lang="en" title="Published document search"/>
  <param name="publishedConstituents" type="xs:string" required="true" style="template" default="biblio">
    <option value="biblio"/>
    <option value="abstract"/>
    <option value="full-cycle"/>
    <option value="abstract,full-cycle"/>
    <option value="biblio,full-cycle"/>
  </param>
  <method name="GET" href="#wpdSearchGET"/>
<!-- search query -->
</resource>
    <!-- GET Published data biblio -->
    <resource path="published-data/{ref-type}/{ref-format}/{number}/{publishedConstituents}" id="publishedDataRetrieval">
      <doc xml:lang="en" title="Published document retrieval GET interface"/>
      <param href="#ref-type"/>
      <param href="#ref-format"/>
      <param name="number" type="xs:string" required="true" style="template" default="EP1000000">
        <doc xml:lang="en">Reference number</doc>
      </param>
      <param name="publishedConstituents" type="xs:string" required="true" style="template" default="biblio">
        <option value="biblio"/>
        <option value="abstract"/>
        <option value="full-cycle"/>
        <option value="abstract,full-cycle"/>
        <option value="biblio,full-cycle"/>
      </param>
      <method name="GET" href="#wpdGETPOST"/>
    </resource>
<!--Published data fulltext availability inquiry GET -->
<resource path="published-data/{ref-type}/{ref-format}/{number}/fulltext" id="publishedDataFulltextRequest">
  <doc xml:lang="en" title="Published document fulltext availability inquiry"/>
  <param href="#ref-type"/>
  <param href="#ref-format"/>
  <param name="number" type="xs:string" required="true" style="template" default="EP1000000">
    <doc xml:lang="en">Reference number</doc>
  </param>
  <method name="GET" href="#wpdGETPOST"/>
</resource>
<!--Published data claims retrieval GET -->
<resource path="published-data/{ref-type}/{ref-format}/{number}/claims" id="publishedDataClaimsRequest">
  <doc xml:lang="en" title="Published document claims"/>
  <param href="#ref-type"/>
  <param href="#ref-format"/>
  <param name="number" type="xs:string" required="true" style="template" default="EP1000000">
    <doc xml:lang="en">Reference number</doc>
  </param>
  <method name="GET" href="#wpdGETPOST"/>
</resource>
<!--Published data description retrieval GET -->
<resource path="published-data/{ref-type}/{ref-format}/{number}/description" id="publishedDataDescriptionRequest">

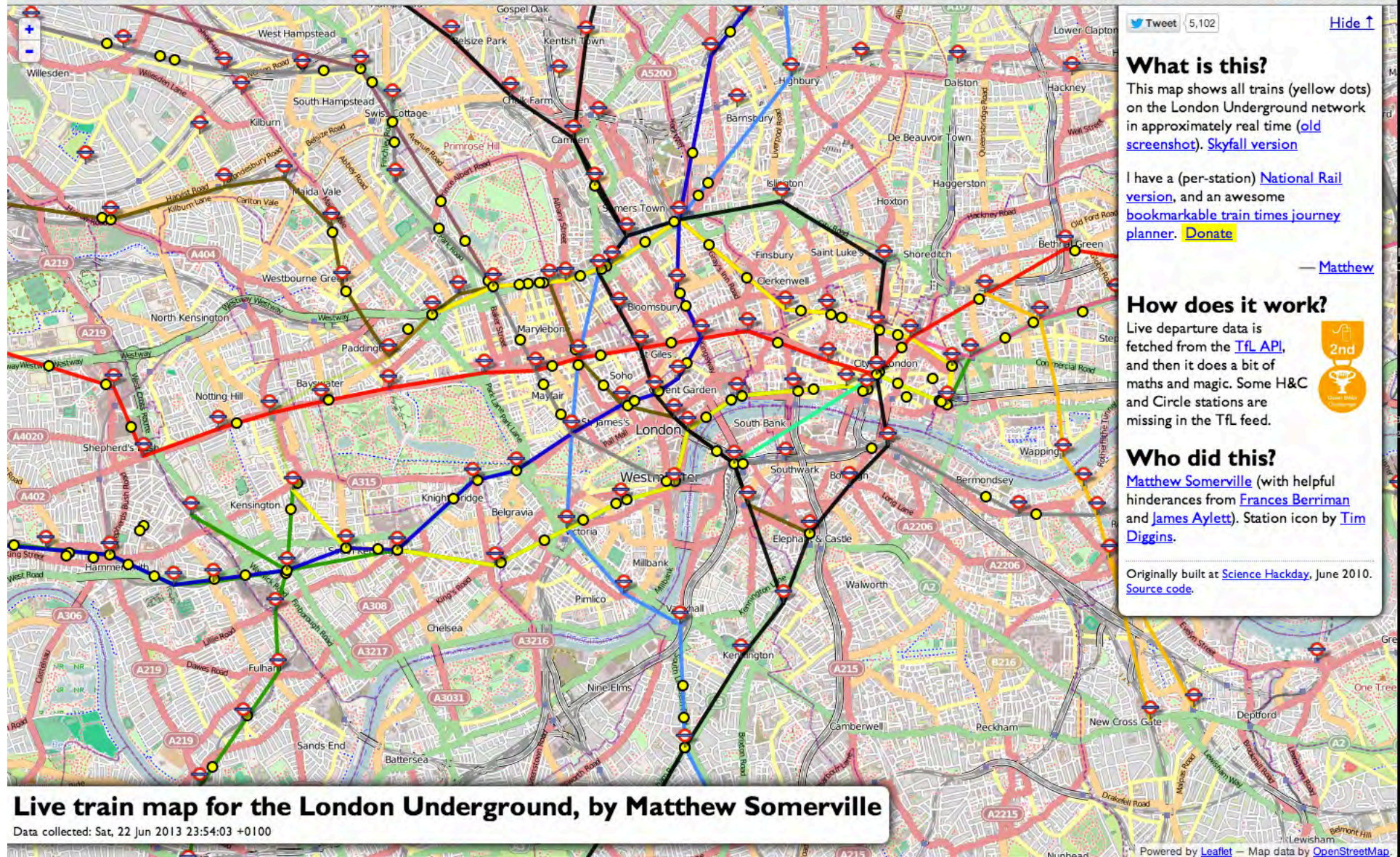
```


<http://traintimes.org.uk/map/tube/>

traintimes.org.uk/map/tube/

Click to go forward, hold to see history

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Live train map for the London Underground, by Matthew Somerville

Data collected: Sat, 22 Jun 2013 23:54:03 +0100

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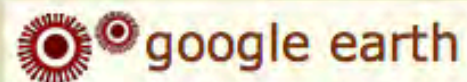
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Discovery](#)

[Naturejobs](#)



Track the spread of the H5N1 virus worldwide since 2003 with our award-winning animated Google Earth Mash-Up.



View the time-enabled maps



Are There Any Bio/Chem/Med?

API Directory - ProgrammableWeb

www.programmableweb.com/apis/directory/1?apicat=Medical

Hot APIs » Twitter YouTube Facebook Google Maps Flickr LinkedIn More » Latest news Today in APIs: Twitter adds Six New Ads API Partners, Microsof...

Home API News API Directory Mashups Community How-to Contests Subscribe: RSS Email Twitter Facebook

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Keywords: Category: Medical Company: Protocols / Styles:

Date: Date: All Managed By:

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Viewing 1 to 117 of 117 APIs

API	Description	Category	Updated
Access Plans USA	Health care insurance directory service	Medical	2013-02-04
Aetna CarePass	Health and drug information portal	Medical	2012-06-05
AIDSinfo	Government info on HIV/AIDS treatment	Medical	2011-07-26
Allen Brain Atlas	Neuroscience information resource directory	Medical	2012-04-05
Assay Depot	Pharmaceutical research service catalog	Medical	2012-08-17
Beddit	Sleep monitoring service	Medical	2012-12-19
Biilite	Health data graphing service	Medical	2013-02-04
BioLabeler	Library of Medicine text extractor and indexing engine	Medical	2011-12-23
bioNMF	Biomedical data analysis service	Medical	2012-02-24
Biosemantics	Clinical record annotation service	Medical	2013-02-08
ACCCA			
Boliven	Online repository of medical device information	Medical	2012-01-19
Byomei	Japanese disease reference service	Medical	2012-10-16
CDC Wonder	CDC health statistics retrieval service	Medical	2011-11-15
Centers for Disease Control (CDC) Content Syndication	Health information content syndication service	Medical	2011-09-27
ChemBank	Biomedical database	Medical	2012-01-17
China Cancer Database	Chinese cancer information database	Medical	2012-01-31

MASHERY
The Premier API Management Solution

MuleSoft
Connect APIs Learn more

Beyond APIs: Mobile-Enabling Developer Ecosystems
On-Demand Webinar FORRESTER anypresence

FREE API MANAGEMENT SOLUTION
BY 3SCALE SIGNUP NOW!
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Extend your Enterprise with IBM API Management
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#1 Data loader for Salesforce
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http://programmableweb.com/

Good Examples

- NLM/NCBI/PubChem - <http://www.ncbi.nlm.nih.gov/>
- EBI (inc ChEMBL, ChEBI etc) – <http://ebi.ac.uk>
- NCI Cactus - <http://cactus.nci.nih.gov/>
- ChemSpider - <http://www.chemspider.com/>
- ChemAxon – e.g. Chemicalize
<http://www.chemicalize.org/>
- OpenTox -
<http://www.opentox.org/dev/apis/api-1.2/structure>
- Altmetric & ImpactStory
- .. Many more web services out there...

Free

vs

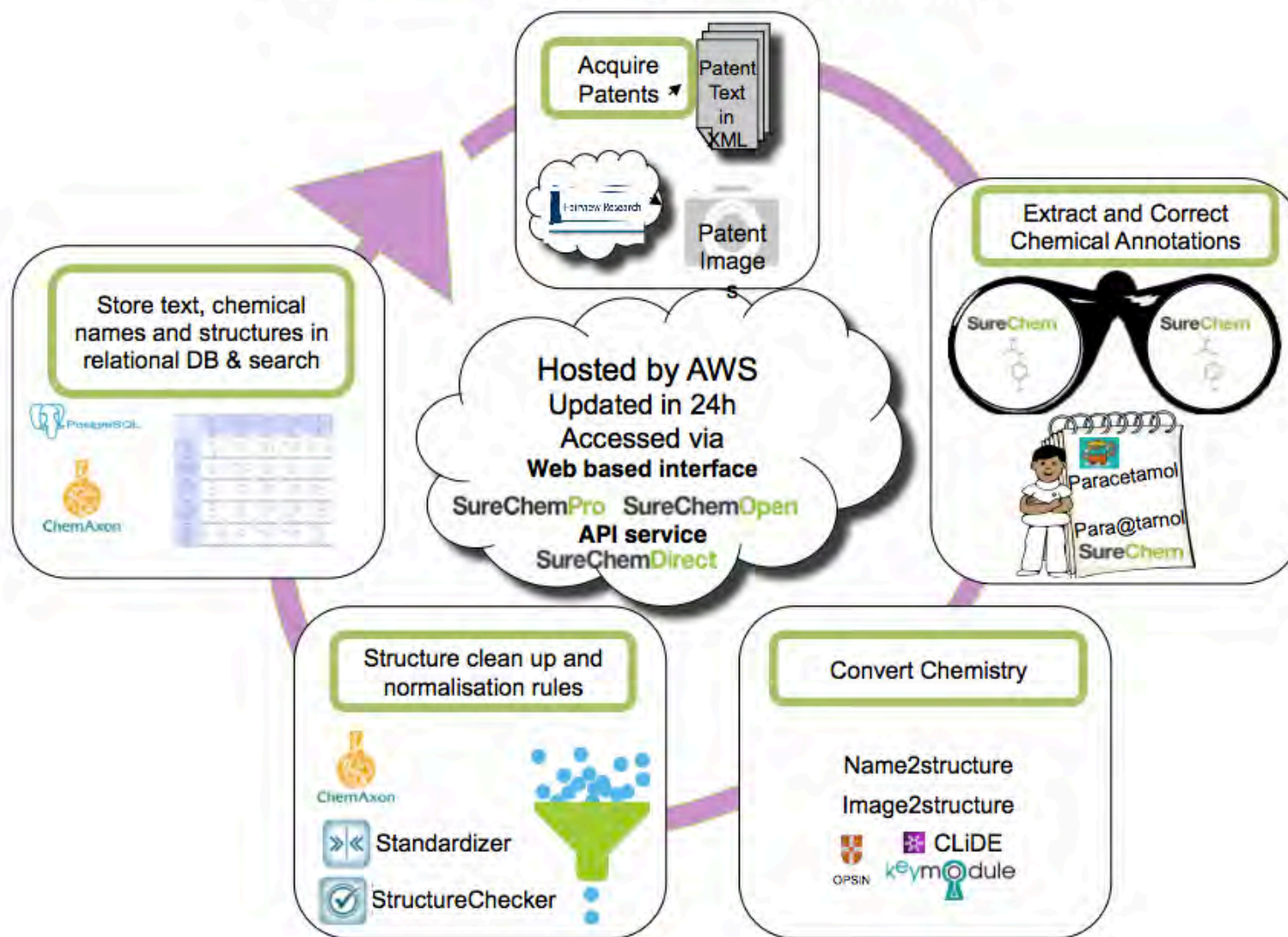
Accessible

Case Studies

1. SureChem

Patent Chemistry

SureChem Chemistry Mining Workflow



SureChemOpen

- ✦ **Free** patent chemistry searching for **all**
- ✦ **Early** access to newly published structures
- ✦ **Easy navigation** through the relevant chemistry in the full text of patent documents
- ✦ Search, View, Print
- ✦ Links to ChemSpider and RSC journals
- ✦ A free viewer for SureChemDirect users

Secured by 128-bit encryption providing same level of security as online banking and other proprietary chemistry searching tools!

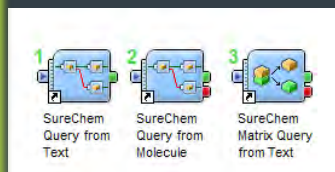
SureChemDirect

API

- ✦ Direct access to **chemistry & full text** patent data
- ✦ Data and search hosted on SureChem AWS instance
 - ✦ Dedicated AWS instances available
 - ✦ Secure https line, 128-bit encryption
- ✦ **Next day indexing** of chemistry
- ✦ **Integration** with internal databases and workflow tools (SharePoint, Seurat, SpotFire etc)
- ✦ **Rapid deployment** using **Pipeline Pilot package**
- ✦ Easy manipulation of large volumes of patent chemistry
- ✦ Full support and documentation
 - ✦ <http://docs.surechem.com/direct/>

Data Feed

- ✦ Direct access to **chemistry & patent metadata in csv** format
- ✦ Access via secure ftp
- ✦ Batch screening & analysis behind your firewall
- ✦ Daily updates



The screenshot shows the SureChemDirect API documentation page. It includes a navigation bar with links like 'View Pipeline Pilot user guide', 'View SureChemOpen documentation', and 'Submit support ticket'. Below this is a 'Getting Started' section with an 'Overview' subsection. The overview text describes SureChemDirect as an enterprise offering that integrates patent chemistry with internal research and analysis applications. It mentions that the API provides a set of protocols for retrieving patent documents, organized by family, sorted by chemical properties, or exported for full-text search. The page also lists supported HTTP verbs (POST, GET, PUT, DELETE) and provides a link to the full documentation.

2. SciBite

Drug Discovery, Right Now.

Therapeutic Intelligence

I care about asthma.

*What does the current
landscape of (Drugs,
Targets, Companies, Trials,
Collaborations...) look like?*

Where does TI come from?

The collage features several prominent websites:

- PubMed:** Displays search results for "Medical treatment ha EP 12621" with abstracts and download options.
- EMBL-EBI:** The European Bioinformatics Institute website, part of the European Molecular Biology Laboratory. It includes a search bar, a "Press releases" section, and a "Mapping metabolism" article.
- Other sites:** Includes a "ClinicalTrials.gov" search page, a "Nature" news section, and a "Tweets" sidebar.

Mapping metabolism

A comprehensive map of human metabolism has been produced by a large consortium including researchers from EMBL-EBI. Published in *Nature Biotechnology*, the model is freely available through EMBL-EBI's *BioModels Database*. It contains verified information on thousands of metabolites and reactions and represents a goldmine for systems biologists.

Something different

We've changed things a bit! On 4 March we re-launched the EMBL-EBI website, hoping to give all our visitors a warmer welcome. We've been working behind the scenes to give you a more consistent experience, because a big part of our mission is to make molecular data available – and accessible – to everyone.

Data storage in DNA becomes a reality

Researchers at the EMBL-European Bioinformatics Institute (EMBL-EBI) have created a way to store data in the form of DNA – a material that lasts for tens of thousands of years. The new method, published in the journal *Nature*, makes it possible to store at least 100 million hours of high-definition video in about a cup of DNA.

Twitter-like Newsfeed

SciBite³. Drug Discovery, Now.
Live Pharma/Biotech News. From Molecule To Merger.

HomeHot TrendsProductsCompanySearch

Latest News / GlaxoSmithKline Newsletter

Latest articles for **GlaxoSmithKline**, as of Thu Jan 31. Use the toolbox on the right to get updates and filter these articles to find the companies, targets, indications and drugs most interconnected.

Coloured tags show you key topics also mentioned in the article. Click a tag to see its own newsletter, or the link to create a newsletter that specifically mentions the two topics together.

AllPopularNewsLiteratureTrialsPatentsGrants

Trpv4 Antagonists (Glaxosmithkline Llc)
Patent #EP2549872 (GLAXOSMITHKLINE LLC) (Today)
[transient receptor potential c...](#) [GlaxoSmithKline](#)
Patent: [Expand](#) | [View \[This Window\]](#) [[New Window](#)]

Vertex Sales Lag As Hep C Patients Pass On Incivek
FiercePharma (Today)
[Hepatitis C](#) [Cystic Fibrosis](#) [Ribofluranosyl Carboxamide](#) [VX-950](#) [PSI 7977](#) [Ivacaftor](#)
[Gilead](#) [Vertex](#) [GlaxoSmithKline](#) [Abbott Laboratories](#) [interferon](#) [New Drug](#)
Web/News Item: [Expand](#) | [View \[This Window\]](#) [[New Window](#)]

Boehringer Gets Fda Panel's Thumbs Up On 'modest' New Copd Treatment
FierceBiotech (1 day ago)
[Lung Diseases](#) [Chronic Obstructive Pulmonary ..](#) [Olodaterol](#) [Boehringer-Ingelheim](#)
[GlaxoSmithKline](#) [Novartis](#) [Theravance](#) [glycogen synthase kinase](#) [Pharmacovigilance](#)
Web/News Item: [Expand](#) | [View \[This Window\]](#) [[New Window](#)]

A Dose Escalation Study Of Omp-52m51 In Subjects With Solid Tumors
ClinicalTrials.gov Trial Updates Record#NCT01778439 [Sponsor:OncoMed P... (1 day ago)
[GlaxoSmithKline](#) [OMP-52M51](#)
Clinical Trial: [Expand](#) | [View \[This Window\]](#) [[New Window](#)] | [Read by 3 scibite.com users](#)

The Purpose Of This Study Is To Evaluate The Spirometric Effect (Trough Fev1) Of Umeclidinium/Vilanterol 62.5/25 Mcg Once Daily Compared With Tiotropium 18 Mcg Once Daily

Articles per day [last 90 days]

Analysis Tools
Daily Updates
Everything (except grants) [RSS] [eMail]
NIH Grants only [RSS]
[Need Help With RSS?]
About This Topic
Quick Help
Geographical View
Connected Topics
Filters & Analysis

Kinase Inhibitors
www.selleckchem.com
Novel & Potent Kinase Inhibitors Oncology & Cell

Operations

SciBite Main API Methods (v3.1)

EntityBooleanQueryService: Get News For One Or More Entities

/EntityBooleanQueryService **GET**

EntityNewsService: Get recent news articles for an input entity

/EntityNewsService **GET**

EntitySearchService: Find ID for an entity

/EntitySearchService **GET**

EntityWebLinksService: Get HTML Links for interesting sites

/EntityWebLinksService **GET**

EntityTextToNewsService: Entity news by text query

/EntityTextToNewsService **GET**

DocumentToNewsService: Get news for entities in a document

/DocumentToNewsService **GET**

DocumentEntitiesService: Get entities in a document

/DocumentEntitiesService **GET**

ListEntitiesService: List all entities

/ListEntitiesService **GET**

TermiteService: Run termite NER on a piece of text

/TermiteService **GET**

InsightLinksService: Get entities most correlated with an input entity

/InsightLinksService **GET**

InsightTopTypesService: Top entities in the news

/InsightTopTypesService **GET**

InsightJointInSourceService: Co-occurring entities in a source

/InsightJointInSourceService **GET**

InsightLitSpaceService: Co-occurring entities in historical medline abstracts

/InsightLitSpaceService **GET**

InsightLitSpacePairService: Co-occurring entity-entity data in historical medline abstracts

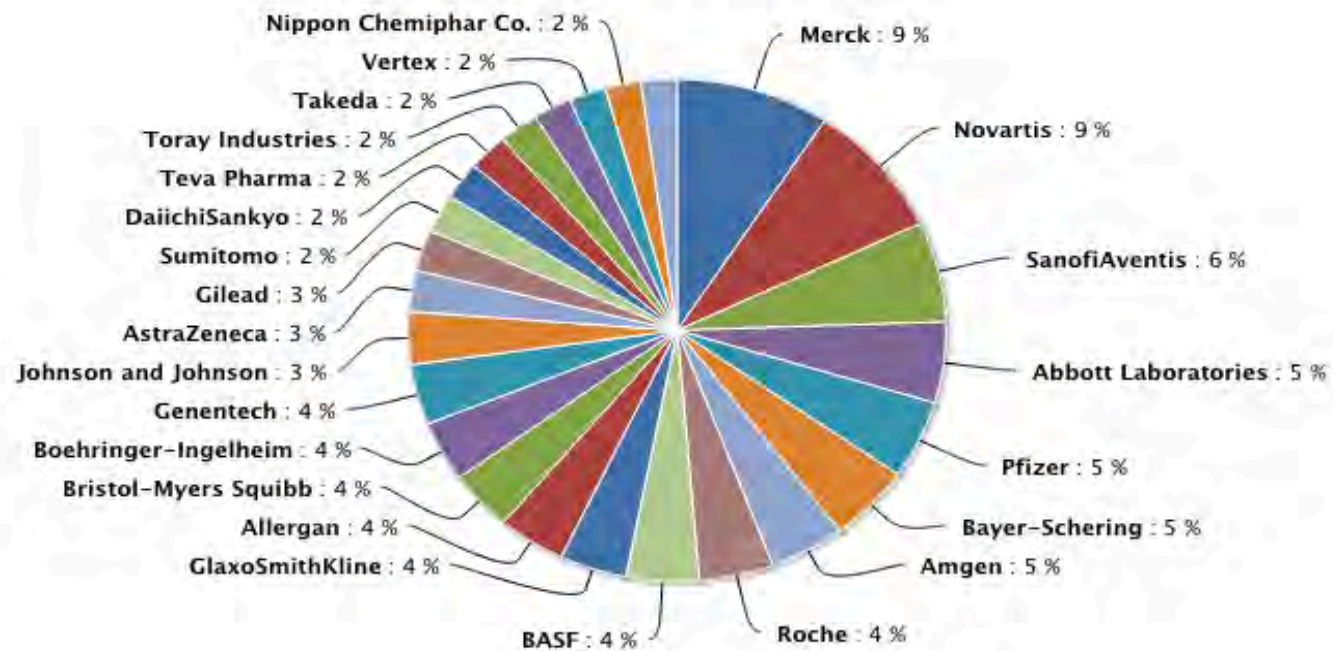
/InsightLitSpacePairService **GET**

Slice & Dice With The API



Which companies are filing the most patents?

Patents By Company (Last 6 Months)



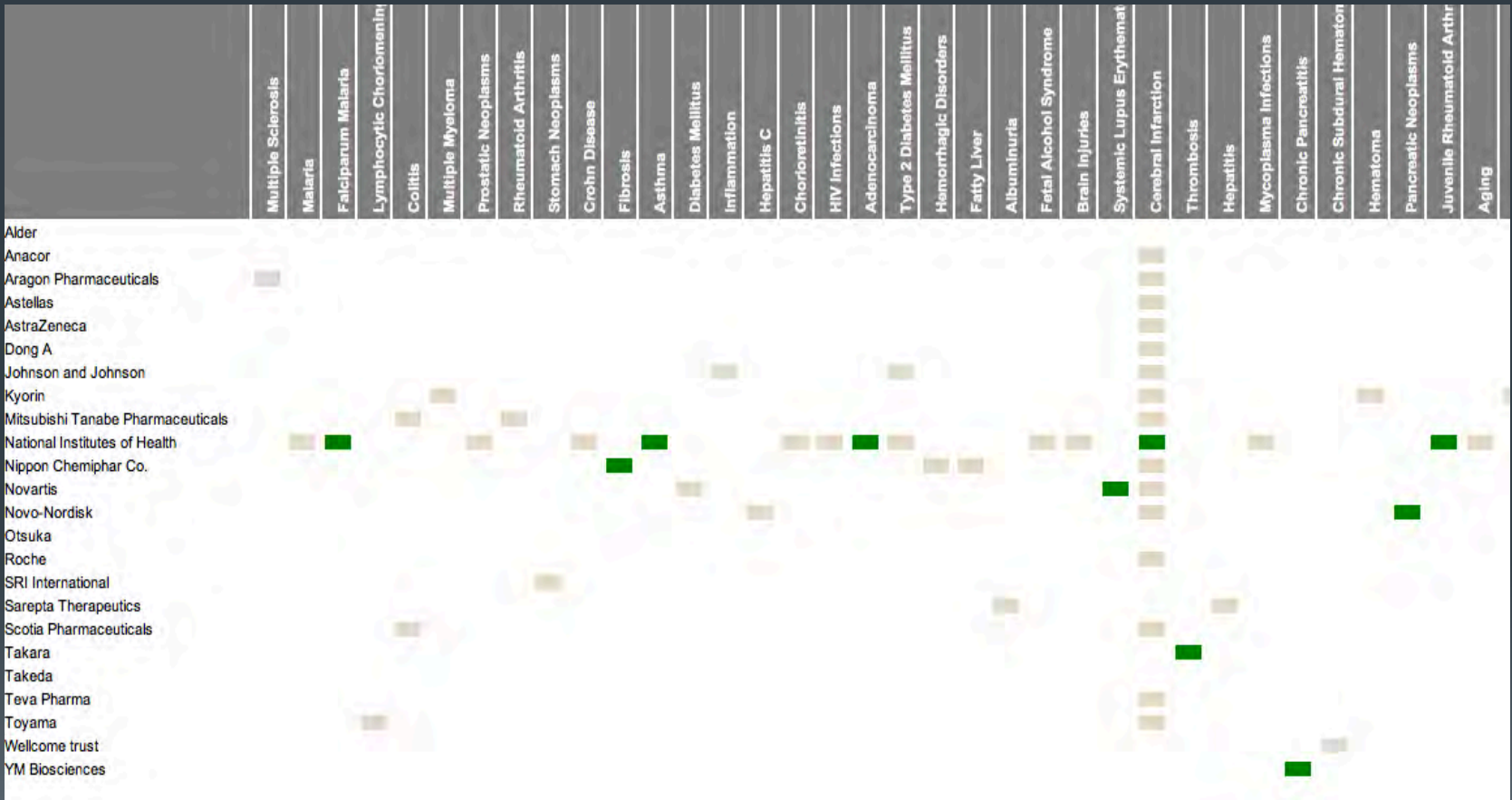
Hot Target Barcodes

ID	Name	2002-2013 Literature Significance Plot
CD4	CD4 molecule	
CD8A	CD8a molecule	
HLA-DRB1	major histocompatibility complex, class II, DR beta 1	
IFNB1	interferon, beta 1, fibroblast	
IFNG	interferon, gamma	
MMP9	matrix metalloproteinase 9 (gelatinase B, 92kDa gelatinase, 92kDa type IV collagenase)	
MOG	myelin oligodendrocyte glycoprotein	
IL10	interleukin 10	
IL4	interleukin 4	
APOE	apolipoprotein E	
IL6	interleukin 6 (interferon, beta 2)	
BDNF	brain-derived neurotrophic factor	
CCL2	chemokine (C-C motif) ligand 2	
CTLA4	cytotoxic T-lymphocyte-associated protein 4	
IL12A	interleukin 12A (interleukin 12 subunit alpha, interleukin 12 subunit alpha, interleukin 12 subunit alpha)	
IL1B	interleukin 1, beta	
CRYAB	crystallin, alpha B	
IL2	interleukin 2	
IL2RA	interleukin 2 receptor, alpha	
CCR5	chemokine (C-C motif) receptor 5	
ISG20	interferon stimulated exonuclease gene 20kDa	

CCR2	chemokine (C-C motif) receptor 2	
HLA-DRB5	major histocompatibility complex, class II, DR beta 5	
PON1	paraoxonase 1	
FASLG	Fas ligand (TNF superfamily, member 6)	
HMGCR	3-hydroxy-3-methylglutaryl-CoA reductase	
CAM1	intercellular adhesion molecule 1	
IL7	interleukin 7	

Organisations →

Organisations →



3. Open PHACTS

Navigating Pharmacological Space

Open PHACTS Project Partners

Pfizer Limited – Coordinator

Universität Wien – Managing entity

Technical University of Denmark

University of Hamburg, Center for Bioinformatics

BioSolveIT GmbH

Consorci Mar Parc de Salut de Barcelona

Leiden University Medical Centre

Royal Society of Chemistry

Vrije Universiteit Amsterdam

Spanish National Cancer Research Centre

University of Manchester

Maastricht University

Aqnowledge

University of Santiago de Compostela

Rheinische Friedrich-Wilhelms-Universität Bonn

AstraZeneca

GlaxoSmithKline

Esteve

Novartis

Merck Serono

H. Lundbeck A/S

Eli Lilly

Netherlands Bioinformatics Centre

Swiss Institute of Bioinformatics

ConnectedDiscovery

EMBL-European Bioinformatics Institute

Janssen

OpenLink



It **Should** be easy to ask...

"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 <1 μ M"



ChEMBL

DrugBank

Gene
Ontology

Wikipathways

GeneGo

ChEBI

UniProt

UMLS

GVKBio

ConceptWiki

ChemSpider

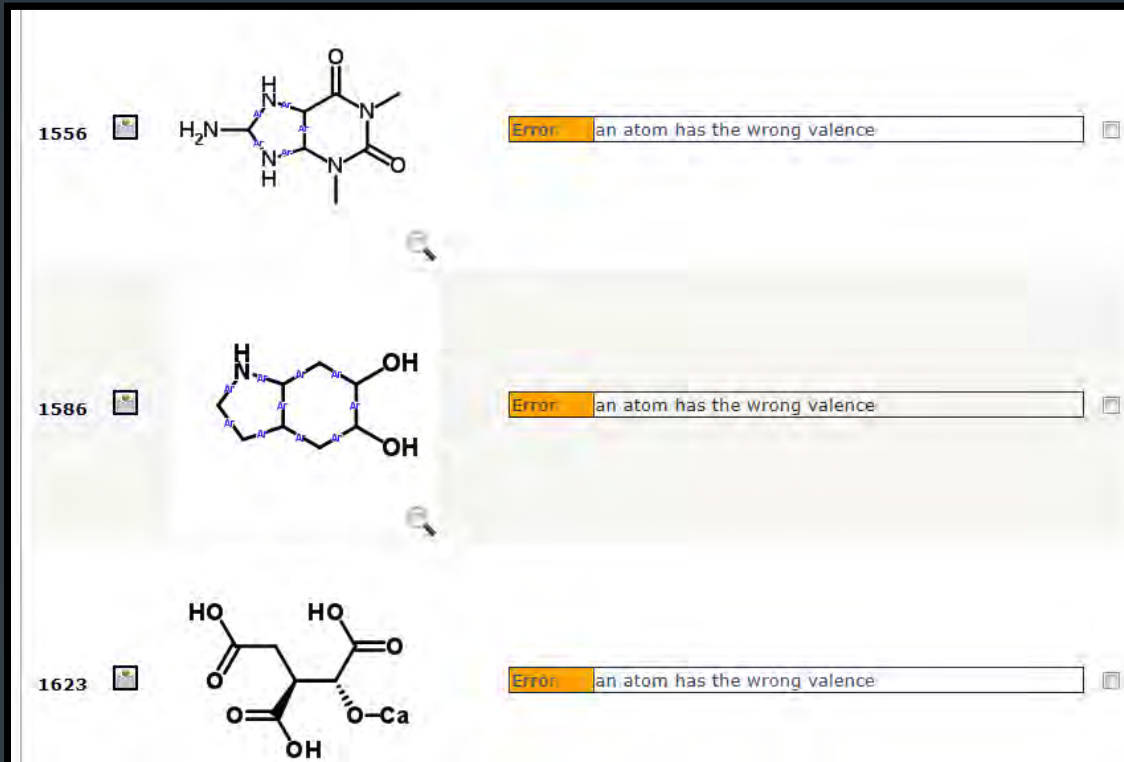
TrialTrove

TR Integrity

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. Determine ADMET profile of actives.
32	13	8	For a given interaction profile, give me compounds similar to it.
37	13	8	The current Factor Xa lead series is characterised by substructure X. Retrieve all bioactivity data in serine protease assays for molecules that contain substructure X.
38	13	8	Retrieve all experimental and clinical data for a given list of compounds defined by their chemical structure (with options to match stereochemistry or not).
41	13	8	A project is considering Protein Kinase C Alpha (PRKCA) as a target. What are all the compounds known to modulate the target directly? What are the compounds that may modulate the target directly? i.e. return all cmpds active in assays where the resolution is at least at the level of the target family (i.e. PKC) both from structured assay databases and the literature.
44	13	8	Give me all active compounds on a given target with the relevant assay data
46	13	8	Give me the compound(s) which hit most specifically the multiple targets in a given pathway (disease)
59	14	8	Identify all known protein-protein interaction inhibitors

... paper coming very soon in DDT



- Chemical Registration System
 - Utilizes ChemSpider Validation and Standardization platform including collapsing tautomers
 - Utilizes FDA rule set as basis for standardization (GSK lead)
 - All molecules get a CVSP report – helps us biologists!

dev.openphacts.org

OpenPHACTS API

Chemical Structure Exact Search

InchiKey to URL

Inchi to URL

Chemical Structure Similarity Search

SMILES to URL

Chemical Structure Substructure Search

Get concept description

Map free text to a concept URL based on semantic tag

Map free text to a concept URL

Map URL

Get ChEBI Ontology Class Members

Get ChEBI Ontology Root Classes

Get ChEBI Ontology Class

ChEBI Class Pharmacology Count /comp

ChEBI Class Pharmacology Complete (DEPRECATED)

ChEBI Ontology Class Pharmacology Paginated /comp

Compound Information

Compound Pharmacology Count

Compound Pharmacology Complete (DEPRECATED)

Compound Pharmacology Paginated

Data Sources

Get Enzyme Classification Root Classes

Get Enzyme Classification Class

Get Enzyme Classification Class Members

Enzyme Pharmacology Count

Enzyme Pharmacology Complete (DEPRECATED)

Enzyme Pharmacology Paginated

Pathway Information

Activity types

Units for activity type /pha

Target Information

Target Pharmacology Count

Target Pharmacology Complete (DEPRECATED)

PharmaTrek

The screenshot displays the PharmaTrek web application interface. The top navigation bar includes the 'PHARMATREK' logo and a search icon. The main content area is divided into three primary sections: 'TARGETS', 'LIGANDS', and an 'Interaction Map'.

TARGETS Section:

- Left Panel:** Lists two targets:
 - p38 alpha homo**: Mitogen-activated protein kinase 14 (Homo sapiens). Amino Acid, Peptide, or Protein.
 - alpha thalassemia/mental retardation syndrome X-linked homolog (human) protein, mouse**: Amino Acid, Peptide, or Protein.
- Right Panel:** Shows 'You have 1 targets selected' with a list containing 'Mitogen-activated protein kinase 14 (Homo sapiens)'. Amino Acid, Peptide, or Protein.
- Bottom:** Includes a 'connect' button.

LIGANDS Section:

- Displays three chemical structures with their corresponding names:
 - 2(1H)-quinazolinone, 5-(2-chloro-4-fluorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-7-(4-piperidinyl)-**
 - 2(1H)-quinazolinone, 5-(2-chloro-4-fluorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-7-(4-piperidinyl)-**
 - 2(1H)-quinazolinone, 5-(2-chlorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-7-(1-piperazinylmethyl)-**

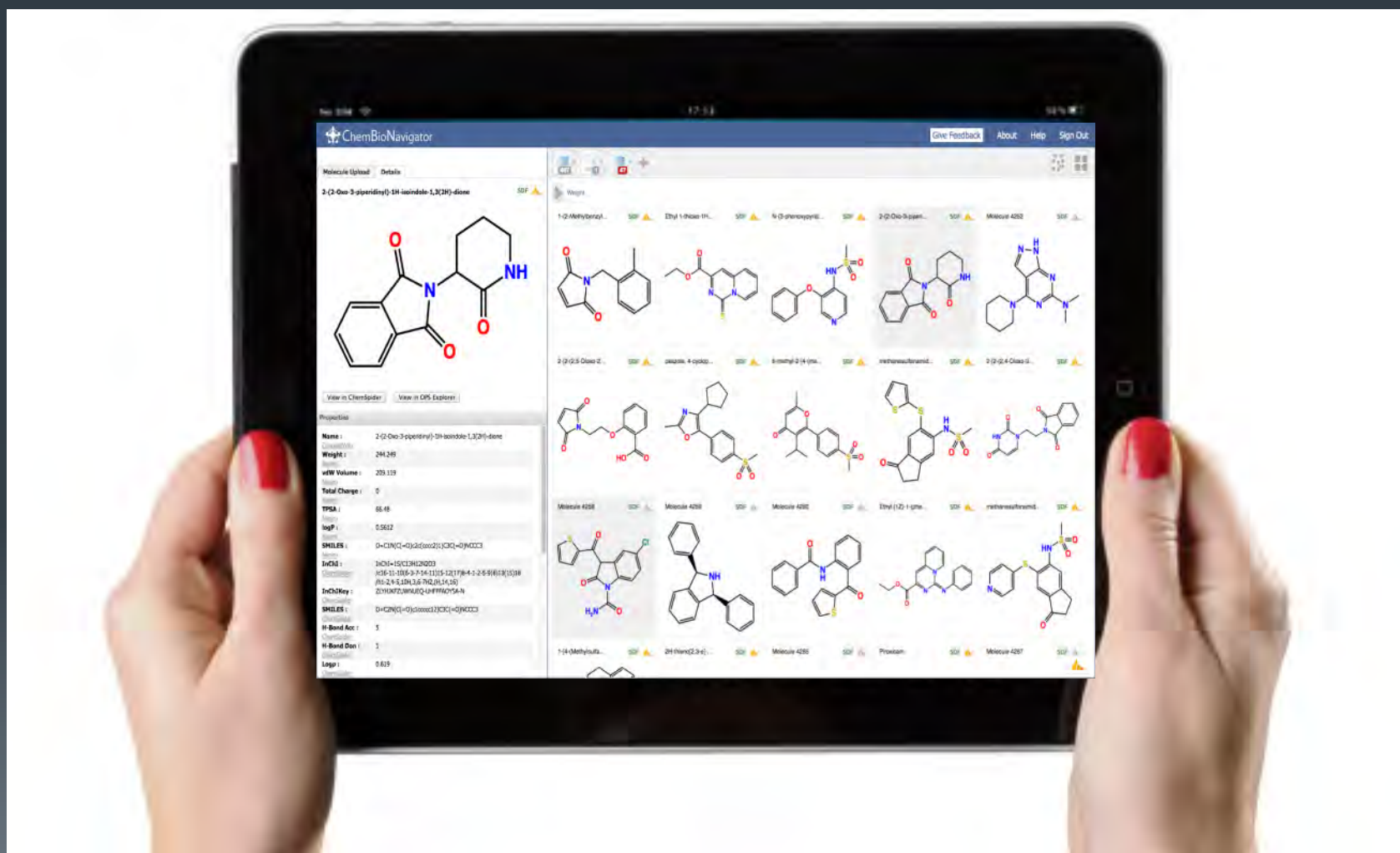
Interaction Map Section:

- Features a large, dark visualization area for target-ligand interactions.
- Summary Statistics:**
 - 35 TARGETS
 - 546 MOLECULES
 - Min annotation [8.00]
 - Max annotation [10.41]
- Controls:** Includes a checkbox for 'Expand target space' and a legend.

<http://pharmatrek.org>

The ChemBio Navigator

<http://chembionavigator.org/>



Utopia Documents - pcbl.1000976 1..16

Back to overview

acetolactate

2-acetolactate mutase

2-acetolactate mutase
In enzymology, a 2-acetolactate mutase is an enzyme that catalyzes the chemical reaction 2-acetolactate \rightleftharpoons 3-hydroxy-3-methyl-2-oxobutanoate. Hence, this enzyme has one substrate, 2-acetolactate, and one product, 3-hydroxy-3-methyl-2-oxobutanoate. This enzyme belongs to the family of isomerases, specifically those intramolecular transferases transferring other groups. The systematic name of this enzyme class is 2-acetolactate methylmutase.

[View Wikipedia web page...](#)

Acetolactate decarboxylase

Acetolactate decarboxylase
In enzymology, an acetolactate decarboxylase is an enzyme that catalyzes the chemical reaction (S)-2-hydroxy-2-methyl-3-oxobutanoate \rightleftharpoons (R)-2-acetoin + CO₂. Hence, this enzyme has one substrate, (S)-2-hydroxy-2-methyl-3-oxobutanoate, and two products, (R)-2-acetoin and CO₂. This enzyme belongs to the family of lyases, specifically the carboxy-lyases, which cleave carbon-carbon bonds.

[View Wikipedia web page...](#)

ACETOLACTSYNI-CPXL

ACETOLACTSYNI-CPXL
Bifunctional aceto-hydroxybutanoate synthase / acetolactate synthase (IlvB/N) carries out both the first step in valine biosynthesis and the second step in isoleucine biosynthesis. The IlvB/N protein complex catalyzes the conversion of pyruvate and oxobutanoate into 2-aceto-2-hydroxy-butyrate and the conversion of pyruvate into 2-acetolactate. Both reactions generate carbon dioxide as a product [CITS: [4608700][370104][7009323][6181375][3011751][16326011]]. This enzyme has a wide substrate range *in vitro* [CITS: [15538598]]. This bifunctional enzyme is a tetramer comprising two IlvB subunits and two IlvN subunits. Its apparent molecular weight rises above the expected weight for this configuration when pyruvate is added *in vitro* [CITS: [6360995]]. The IlvB large subunit can catalyze the reaction in isolation and is not inhibited by valine in the manner of the holoenzyme. However the V_{max} for the reaction as catalyzed by only IlvB is

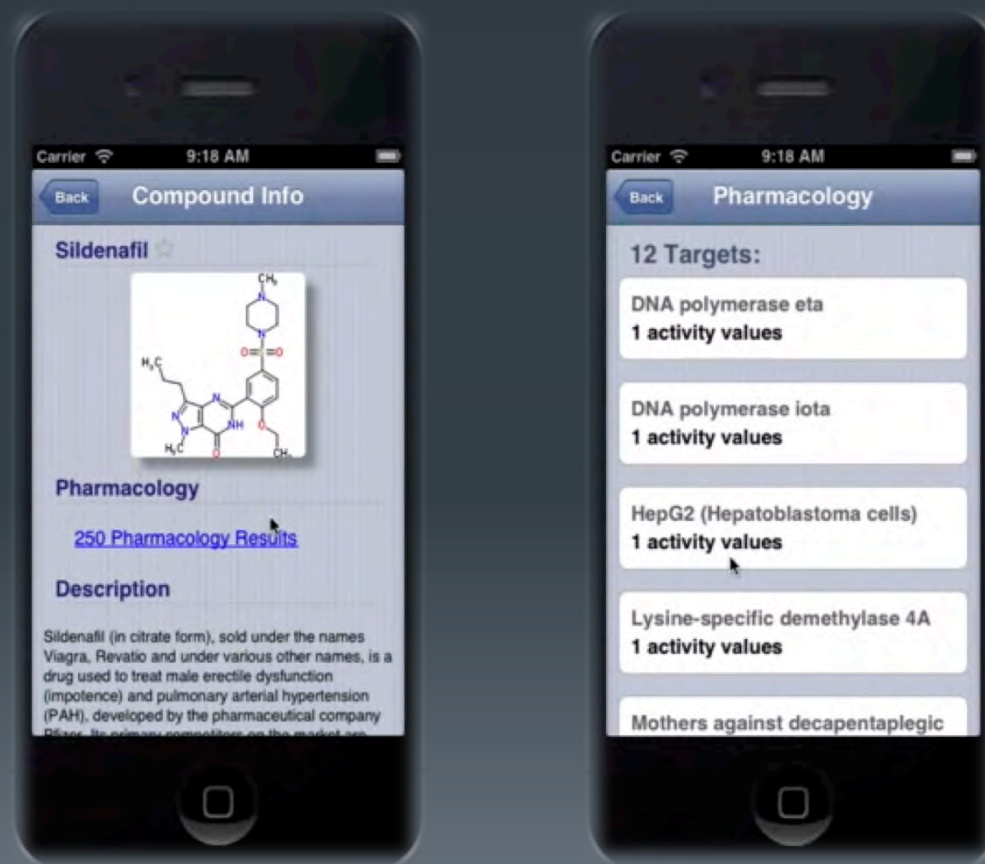
[Look up](#)

Table 4: The 10 most highly connected drug and Mtb proteins

Drug	Intended Targets	Total Number of Connections	Connected Mtb proteins with Solved Structures
Alendronate	Receptor, acid receptor, ROR-α, ROR-β, ROR-γ, ROR-δ, ROR-ε, ROR-ζ, ROR-η, ROR-θ, ROR-ι, ROR-κ, ROR-λ, ROR-μ, ROR-ν, ROR-ξ, ROR-ο, ROR-π, ROR-ρ, ROR-σ, ROR-τ, ROR-υ, ROR-φ, ROR-χ, ROR-ψ, ROR-ω, ROR-1, ROR-2, ROR-3, ROR-4, ROR-5, ROR-6, ROR-7, ROR-8, ROR-9, ROR-10, ROR-11, ROR-12, ROR-13, ROR-14, ROR-15, ROR-16, ROR-17, ROR-18, ROR-19, ROR-20, ROR-21, ROR-22, ROR-23, ROR-24, ROR-25, ROR-26, ROR-27, ROR-28, ROR-29, ROR-30, ROR-31, ROR-32, ROR-33, ROR-34, ROR-35, ROR-36, ROR-37, ROR-38, ROR-39, ROR-40, ROR-41, ROR-42, ROR-43, ROR-44, ROR-45, ROR-46, ROR-47, ROR-48, ROR-49, ROR-50, ROR-51, ROR-52, ROR-53, ROR-54, ROR-55, ROR-56, ROR-57, ROR-58, ROR-59, ROR-60, ROR-61, ROR-62, ROR-63, ROR-64, ROR-65, ROR-66, ROR-67, ROR-68, ROR-69, ROR-70, ROR-71, ROR-72, ROR-73, ROR-74, ROR-75, ROR-76, ROR-77, ROR-78, ROR-79, ROR-80, ROR-81, ROR-82, ROR-83, ROR-84, ROR-85, ROR-86, ROR-87, ROR-88, ROR-89, ROR-90, ROR-91, ROR-92, ROR-93, ROR-94, ROR-95, ROR-96, ROR-97, ROR-98, ROR-99, ROR-100, ROR-101, ROR-102, ROR-103, ROR-104, ROR-105, ROR-106, ROR-107, ROR-108, ROR-109, ROR-110, ROR-111, ROR-112, ROR-113, ROR-114, ROR-115, ROR-116, ROR-117, ROR-118, ROR-119, ROR-120, ROR-121, ROR-122, ROR-123, ROR-124, ROR-125, ROR-126, ROR-127, ROR-128, ROR-129, ROR-130, ROR-131, ROR-132, ROR-133, ROR-134, ROR-135, ROR-136, ROR-137, ROR-138, ROR-139, ROR-140, ROR-141, ROR-142, ROR-143, ROR-144, ROR-145, ROR-146, ROR-147, ROR-148, ROR-149, ROR-150, ROR-151, ROR-152, ROR-153, ROR-154, ROR-155, ROR-156, ROR-157, ROR-158, ROR-159, ROR-160, ROR-161, ROR-162, ROR-163, ROR-164, ROR-165, ROR-166, ROR-167, ROR-168, ROR-169, ROR-170, ROR-171, ROR-172, ROR-173, ROR-174, ROR-175, ROR-176, ROR-177, ROR-178, ROR-179, ROR-180, ROR-181, ROR-182, ROR-183, ROR-184, ROR-185, ROR-186, ROR-187, ROR-188, ROR-189, ROR-190, ROR-191, ROR-192, ROR-193, ROR-194, ROR-195, ROR-196, ROR-197, ROR-198, ROR-199, ROR-200, ROR-201, ROR-202, ROR-203, ROR-204, ROR-205, ROR-206, ROR-207, ROR-208, ROR-209, ROR-210, ROR-211, 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Hacking The iPhone

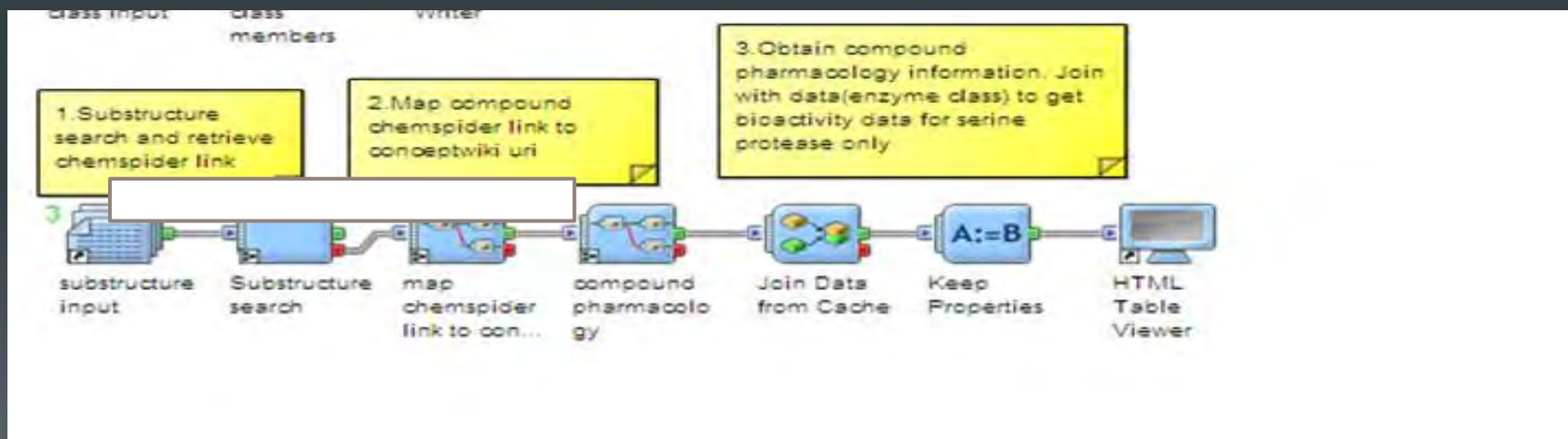
<http://www.youtube.com/watch?v=0aGB6YqtuQ0>



Workflow Tools

The screenshot shows the KNIME software interface. On the left is the 'Workflow Projects' pane with a tree view of the 'KNIME_project' containing nodes like 'Column Filter (#27)', 'Column Rename (#30)', 'File Reader (#3)', 'Interactive Table (#19)', 'Java Snippet (#1)', 'Java Snippet (#25)', 'Java Snippet (#28)', 'JsonArray_2_Rows (#26)', and 'Split Collection Column (#29)'. Below this is the 'Node Repository'. The main workspace shows a workflow with the following nodes: 'File Reader' (description: 'Simply gets the URL [I dont know how to get it to start otherwise!]'), 'Java Snippet' (description: 'Fetch JSON from web'), 'Get Name and Inchi' (description: 'Name & Inchi Grabber'), 'Get Activity' (description: 'Now turn the activity JSON into rows'), 'Activity Parser' (description: 'For each activity row, extract the columns we want'), 'Column Filter' (description: 'Tidy Up: Remove Processing Columns Now'), and 'Interactive Table' (description: 'Node 31'). A 'Table View' window is open, displaying a table with 7 columns: Name, Inchi, Activity, Units, Relation, and Target. The table contains 6 rows of data for 'Sorafenib' with various activity values and targets.

Name	Inchi	Activity	Units	Relation	Target
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	3400	nM	=	Serine/threonine-protein kinase PLK4
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	250	nM	=	MAP kinase signal-integrating kinase 2
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	5.4	uM	=	HCT-116 (Colon carcinoma cells)
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	1700	nM	=	Ephrin type-B receptor 1
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	3300	nM	=	Dual specificity mitogen-activated protein kinase kin.
.. Sorafenib	MLDQJTXFUGDVEO-UHFFFAOYSA...	6200	nM	=	Cyclin-dependent kinase 5

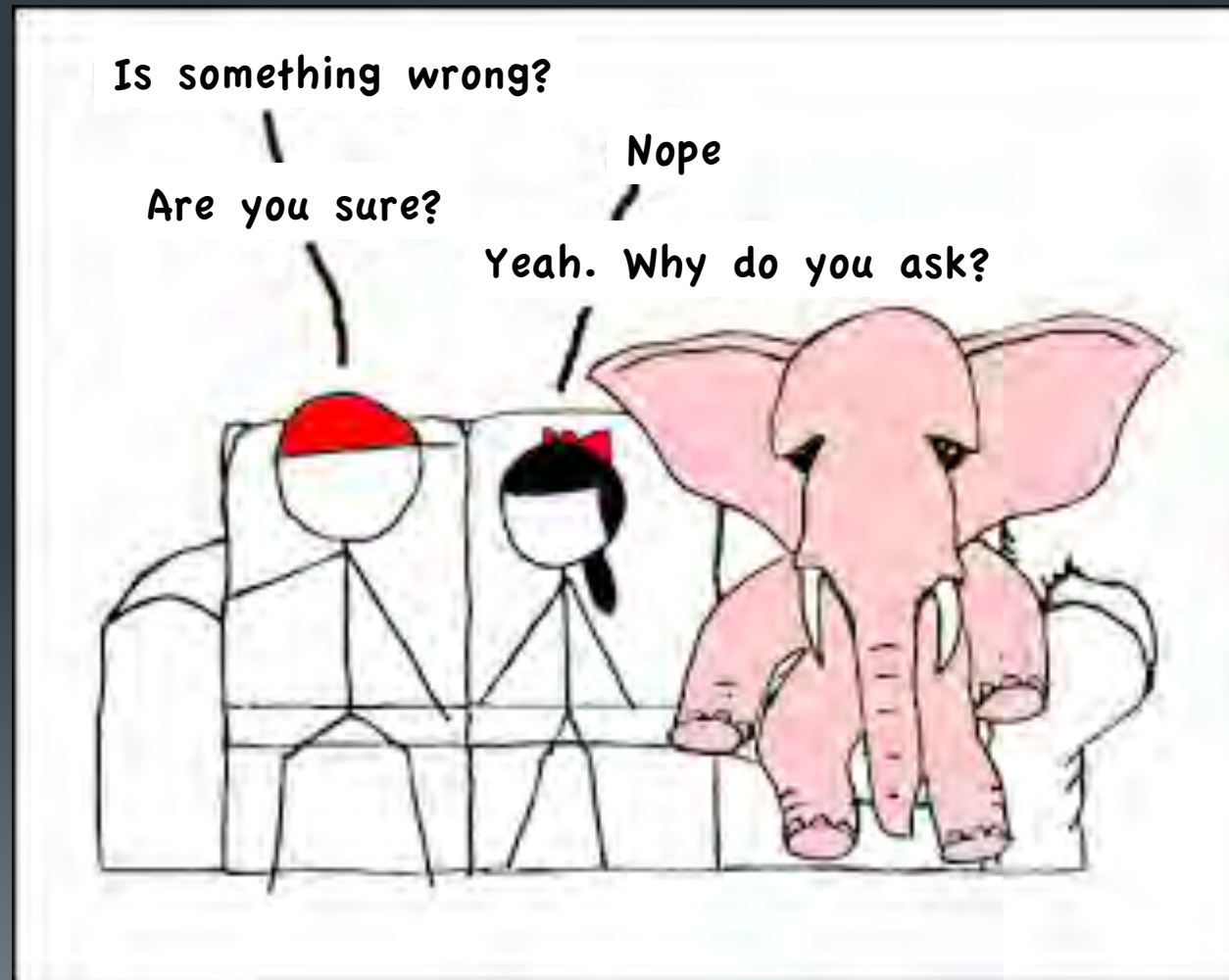


+ Google Refine, Helium For Excel, Taverna

Anyone can now ask...

- Who's working on what targets for what indications?
- What chemical matter has been tested against those targets?
- What does that chemical space look like?
- What's been patented in that area?
- What other targets do those compounds hit?
- Who's working on those targets for what indications...?

Security?



Security: Still A Concern For Some

- But more companies moving to cloud externalisation
- Starting to see emergence of security principles (Pistoia, Open PHACTS)
- VM's (local, remote)
- Clever workflows
- Will opportunity overtake fear?

Conclusions

- Accessible API's increasing
- Let people explore, they'll find new use cases
- Can't build a big interface on big data
- Usability, Discovery & Security key challenges

Acknowledgements

- SureChem Limited: <http://surechem.com>
- SciBite Limited: <http://scibite.com>
- Open PHACTS Consortium: <http://openphacts.org> | <http://dev.openphacts.org> | <http://explorer.openphacts.org>