



Open PHACTS

Open Pharmacological Space



Mobile semantic technologies using Open PHACTS

iPharm

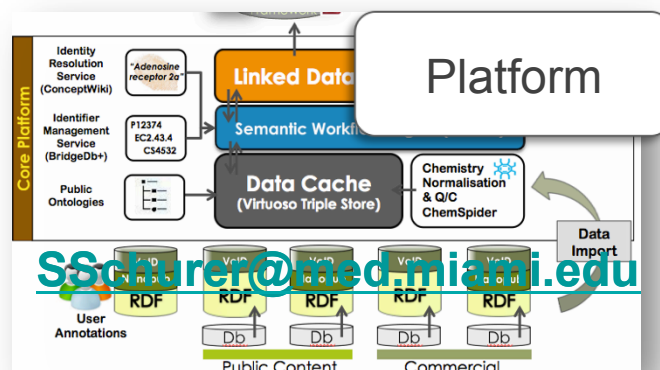
ChemBioNagivator

10/17/13

NETTAB Conference on Mobile
Semantic Technologies



Components of Open PHACTS



SScience@med.miami.edu

API

```

w_uri .
equiv_target .
get_name ;
void:inDataset <http://www.conceptwiki.
?equiv_target dc:title ?target_name;
ops:target_organism ?target_organism ;
ops:targetOfAssay ?equiv_assay ;
void:inDataset <http://data.kasabi.com/
ops:targetOfAssay owl:inverseOf chembl:hasTarget
?equiv_assay chembl:organism ?assay_organism ;
chembl:hasDescription ?assay_descriptio
ops:assayOfActivity ?activity_uri .
ops:assayOfActivity owl:inverseOf chembl:onAssa
?activity_uri chembl:type ?std_type ;

```

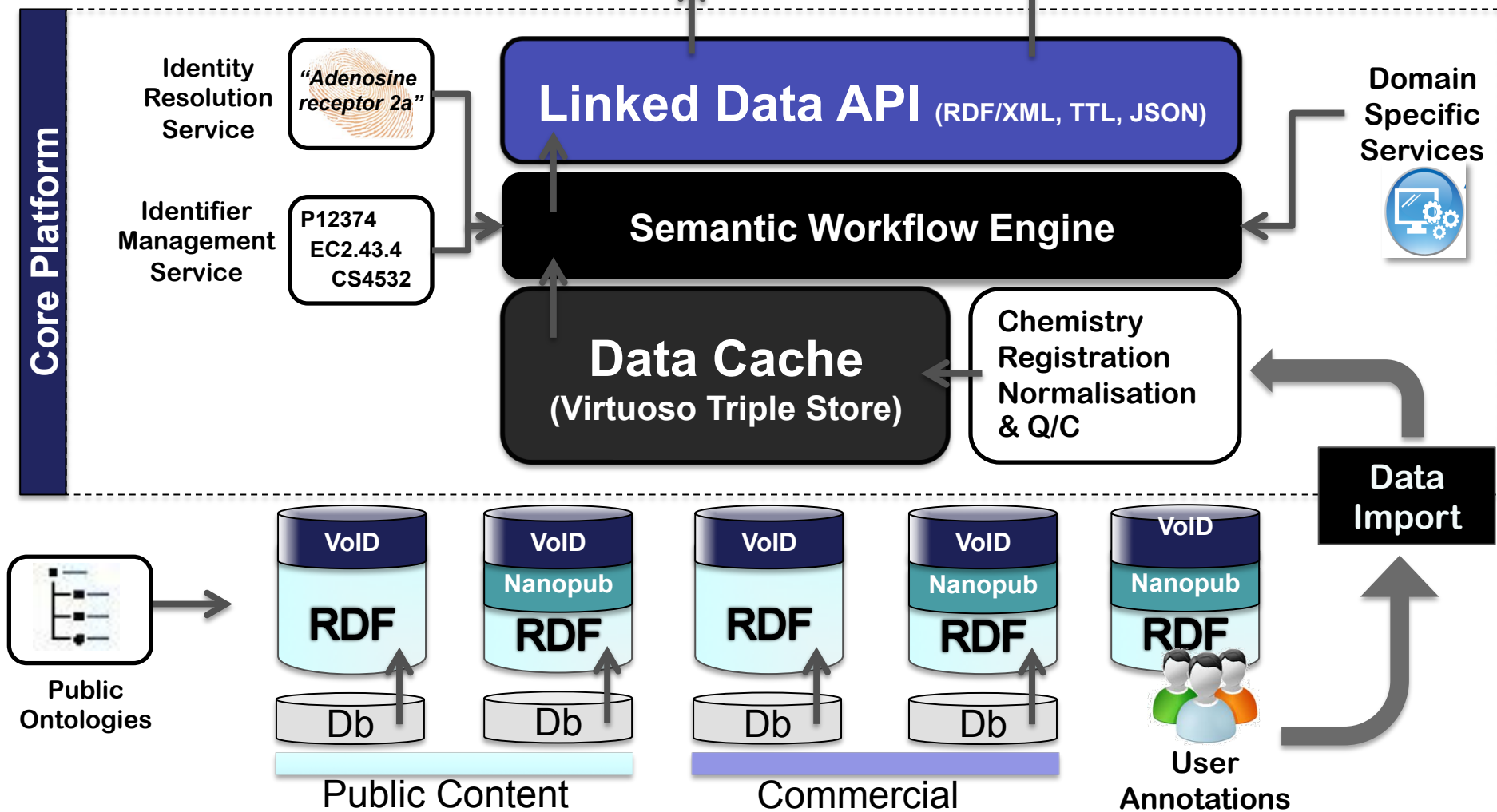
Apps

Standards





Applications





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Premise

Did you see that
new cancer drug
on the news?

Oh yeah, I definitely
did.

How does it
work?

Erm.....



Pharmacology on your phone

- ❖ Many complex data-rich websites
- ❖ Some apps replicate complex workflows on a phone or tablet
- ❖ Leave the complexity to the desktop and other apps
 - Instead, deliver data that can be useful for on-the-fly lookup
- ❖ Aim not to produce an app that provides deep SAR tables
 - But, produce an app that provides high-level summaries & key facts



How is it done?

- ✦ For iPharm app development kits used:
 - jQuery Mobile
 - Phonegap
 - Open PHACTS jsSDK
 - TestFlight



jQuery mobile

- Standards-based development with HTML5 – means you don't need to learn iOS/Objective C
- HTML/CSS/Javascript – means it works in a web browser too – easy to test
- Cross-platform compatibility
- Accepted by app stores (Apple, Google) as an approved application framework



[Demos](#) [API](#) [Download](#) [Platforms](#) [Themes](#) [Resources](#) [Blog](#)

JQUERY MOBILE 1.4.0 BETA RELEASED!

jQuery Mobile: Touch-Optimized Web Framework for Smartphones & Tablets

A unified, HTML5-based user interface system for all popular mobile device platforms, built on the rock-solid jQuery and jQuery UI foundation. Its lightweight code is built with progressive enhancement, and has a flexible, easily themeable design.

Latest stable version - 1.3.2

Legacy versions: [1.2.1](#) - [1.1.2](#) - [1.0.1](#)

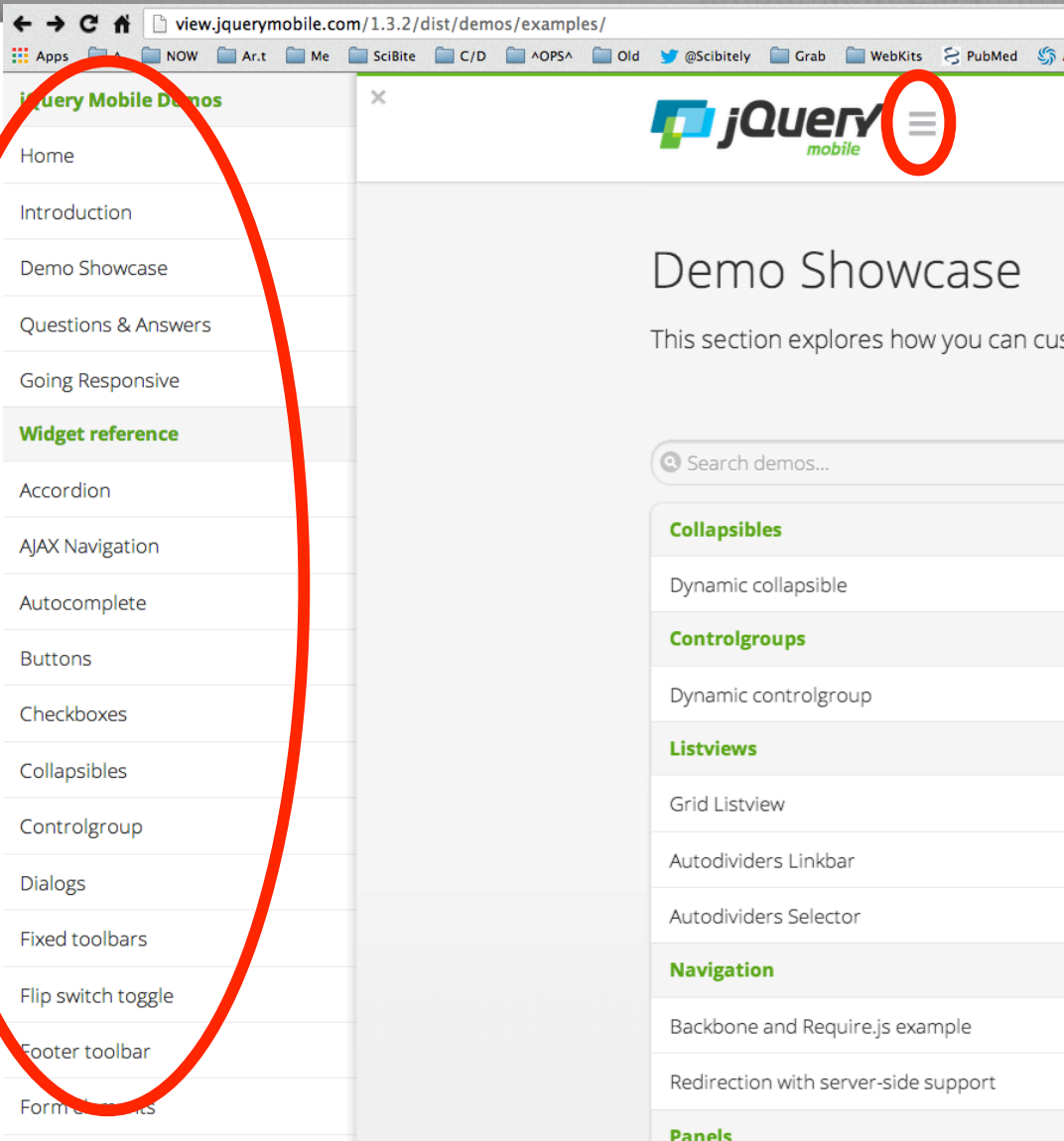


Seriously cross-platform with HTML5

jQuery mobile framework takes the "write less, do more" mantra to the next level: Instead of writing unique apps for each mobile device or OS, the jQuery mobile framework allows you to design a single highly-branded web site or application that will work on all popular smartphone, tablet, and desktop platforms. [Device support](#)



Help us support all platforms: [Donate test devices](#) to the jQuery Mobile project



view.jquerymobile.com/1.3.2/dist/demos/examples/

jQuery Mobile Demos

- Home
- Introduction
- Demo Showcase
- Questions & Answers
- Going Responsive
- Widget reference**
- Accordion
- AJAX Navigation
- Autocomplete
- Buttons
- Checkboxes
- Collapsibles
- Controlgroup
- Dialogs
- Fixed toolbars
- Flip switch toggle
- Footer toolbar
- Form elements

jQuery mobile

Demo Showcase

This section explores how you can cus

Search demos...


- Collapsibles**
 - Dynamic collapsible
- Controlgroups**
 - Dynamic controlgroup
- Listviews**
 - Grid Listview
 - Autodividers Linkbar
 - Autodividers Selector
- Navigation**
 - Backbone and Require.js example
 - Redirection with server-side support
- Panels**

jQuery Mobile Demos

- Menu icon expands a left hand option menu with popular UI choices for today's mobile apps
 - e.g., buttons, checkboxes, etc.



Phonegap



PhoneGap About Developer Community Apps Support [Install](#)

Easily create apps using the web technologies you know and love:
HTML, CSS, and JavaScript

PhoneGap is a free and open source framework that allows you to create mobile apps using standardized web APIs for the platforms you care about.

[Install PhoneGap](#) [Getting Started Guides](#)

[Watch Intro](#)

JS CSS HTML → Wrap your app with PhoneGap → Deploy to mobile platforms! → Mobile Apps



Phoneygap creates “app store ready” applications


- ❖ Development Workflow:
 - Code the app in jQuery Mobile
 - Compile it to native code for your source deployment platform using Phoneygap (e.g. iOS or Android)
 - Test
 - Deploy
 - Sell (not quite that easy!)
- ❖ In practice:
 - Can take some time to set everything up correctly, esp with iOS, but works pretty well
 - Probably not as fast/responsive as a full native app, but for many use-cases is more than adequate



Ops.js

JavaScript SDK on top
of the Open PHACTS
API.

Means you don't need
to manually code all of
the web-service calls



This screenshot shows the GitHub repository page for `openphacts / ops.js`. The repository has 73 commits, 5 branches, 0 releases, and 2 contributors. The latest commit is by `egonw` 5 days ago. The repository contains a `lib` directory, a `spec` directory, a `src` directory, a `.gitignore` file, a `README.md` file, a `SpecRunner.html` file, and a `create_combined_js.sh` script. The `README.md` file is expanded, showing the title `OPS.js` and the following text:

OPS.js is a javascript based library for accessing the OpenPHACTS Linked Data API (LDA). It uses jquery to handle the asynchronous nature of the requests. OPS.js can also be used to parse responses from the LDA.



Concept Wiki compound search

```
var searcher = new Openphacts.ConceptWikiSearch("https://beta.openphacts.org", appID, appKey);
var callback=function(success, status, response){
  searcher.parseResponse(response);
};
// success is 'true' or 'false', status is the http status code, response is the raw result which the parser function accepts
// response will be null in the case of errors
// limit to 20 results, species human (branch 4), no uri for the type is required
searcher.findCompounds('Aspirin', '20', '4', callback);
```

Search for aspirin as a text query, get a UID, get all of aspirin's pharmacology ***in a couple of lines of JavaScript!***

Compound Pharmacology

```
var searcher = new Openphacts.CompoundSearch("https://beta.openphacts.org", appID, appKey);
var callback=function(success, status, response){
  var compoundResult = searcher.parseCompoundPharmacologyResponse(response);
};
// success is 'true' or 'false', status is the http status code, response is the raw result which the parser function accepts
// response will be null in the case of errors
// compound uri is for Aspirin, page 1, 20 results per page
searcher.compoundPharmacology('http://www.conceptwiki.org/concept/38932552-111f-4a4e-a46a-4ed1d7bdf9d5', 1, 20, callback);
```



The banner features the TestFlight logo (a blue square with a white starburst) and the tagline "Beta Testing On The Fly". Navigation links include "SDK", "Android", "Desktop App", "Support", "Blog", "About", "Jobs", "Log In", and a green "Sign Up" button. The main visual is a blue background with white chalk-like drawings of a rocket and a person, and several mobile app icons (a green one, a blue one, and a white one with a camera). The text "Try it Free!" with an arrow points to the "Sign Up" button. At the bottom, it says "The freedom to build better apps" in large white letters, followed by "A free testing service for mobile developers, managers and testers." and a blue ribbon with "iOS & Android".

Test Flight

Deploying to official Apple store is a very lengthy and complex process. Need a “production level” app before you go anywhere near

TestFlight is a free deployment framework that allows you to give your app to others

**** Deploying the app on a phone that is not yours is a hideously time consuming and frustrating process. People will think you’re being lazy for not “sending the app right now” – takes a lot of time & effort to even add ONE more person to the developer list ****



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[iPharm video](#)

Featured Apps

The following applications use the Open PHACTS Discovery Platform.

Open PHACTS Explorer

<https://explorer.openphacts.org>

The Open PHACTS Explorer is the web-based interface to the Open PHACTS Discovery Platform and allows the user to intuitively search and browse the data within the platform. Compounds or targets can be searched by common name, systematic name, chemical structure and SMILES. The provenance (origin) of the resulting data can be displayed and the original source easily assessed.

ChemBioNavigator

<http://www.chembionavigator.org/>

The ChemBioNavigator allows the user to visualize the chemical and biological space of a set of molecules in a chemically-aware manner. The physicochemical properties of sets of molecules can be plotted against each other and each individual data point investigated further via direct links to original data sources. The ChemBioNavigator allows searching for structurally related molecules via a substructure pattern or general similarity search.

PharmaTrek

<http://www.pharmatrek.org>

PharmaTrek, developed at the [Parc de Salut Mar \(PSMAR\)](#) in Barcelona, allows pharmacological space to be navigated in a flexible and interactive way, by accessing the content of ChEMBL via the Open PHACTS Discovery Platform. The results of a target search are highly filterable and easily linked with ligand chemical structure.



✦ **Use Case:**

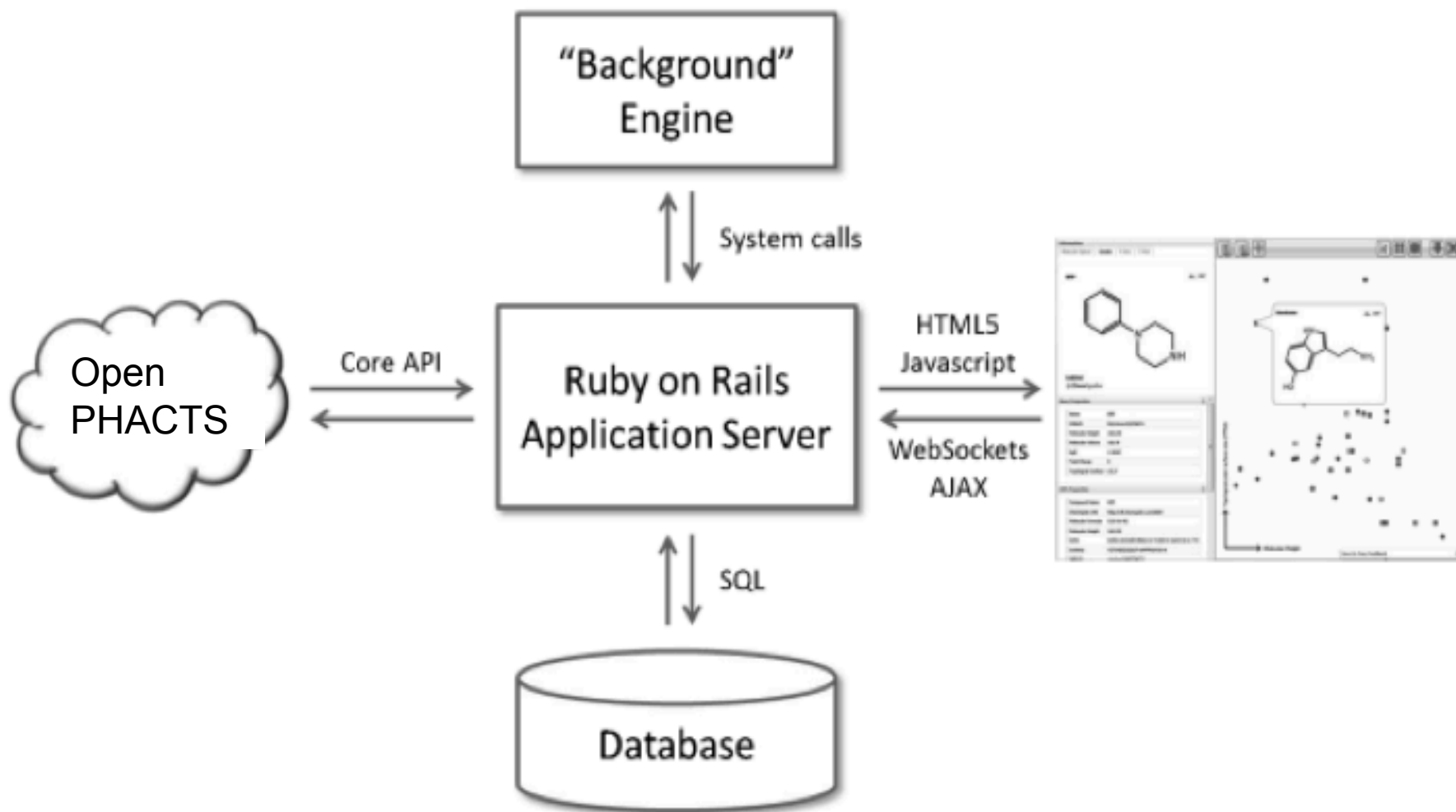
“Compare public and private compound data on the go”





Open PHACTS

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11:30

Friday, November 16



slide to unlock





Future

iPharm

- ❖ Waiting for the 1.3 Open PHACTS API before release
 - 1.3 contains a huge amount of new functionality and up-to-date data
- ❖ Will implement some of the more modern looking UI paradigms seen increasingly in apps
- ❖ Public release sometime early 2014

ChemBioNavigator

- ❖ Already available
- ❖ Extend a compound set based on similarity searches
- ❖ Further development will be the inclusion of target- and biological data



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 - ❖ Matthias Rarey
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ChemBioNavigator

cbn.zbh.uni-hamburg.de

Give Feedback About Help Sign Out

ChemBioNavigator

Type in a molecule name or a SMILES ..

Search/Upload Upload a molecule file

