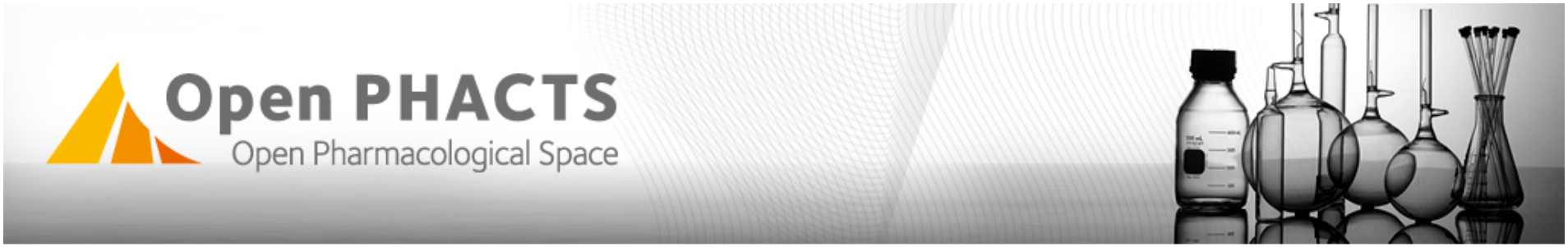


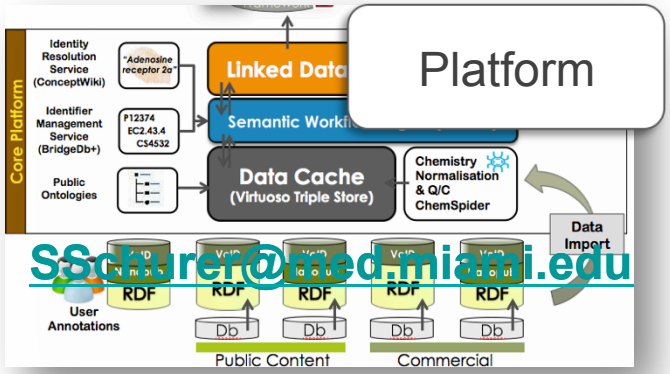
Mobile semantic technologies using Open PHACTS

iPharm

ChemBioNagivator

Open PHACTS
Open Pharmacological Space

Components of Open PHACTS

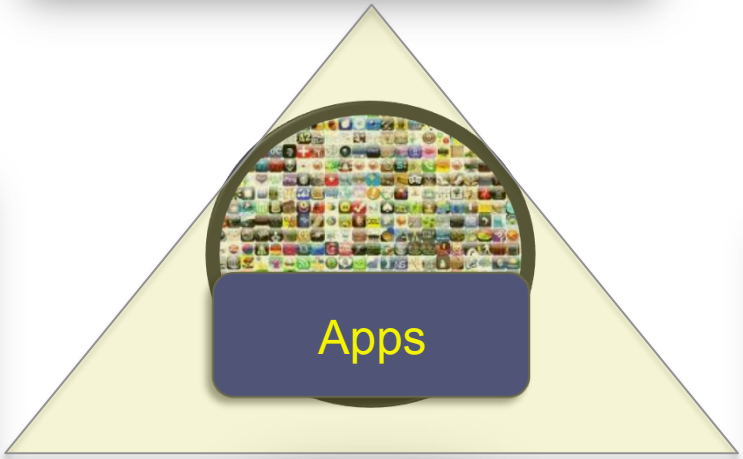


Platform

SSchurer@med.miami.edu

API

```
?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:hasTarge
?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 ;
```



Standards

Open PHACTS
Open Pharmacological Space

Applications

Core Platform

Identity Resolution Service

Identifier Management Service

P12374
EC2.43.4
CS4532

Linked Data API (RDF/XML, TTL, JSON)

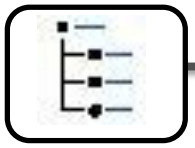
Semantic Workflow Engine

Data Cache
(Virtuoso Triple Store)

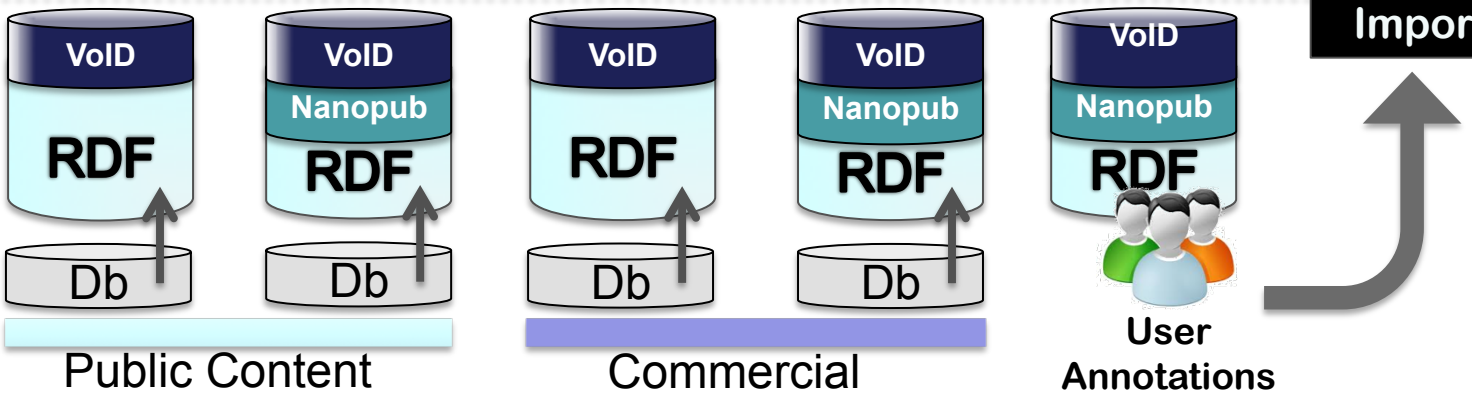
Domain Specific Services

Chemistry
Registration
Normalisation
& Q/C

Data Import



Public Ontologies



Public Content

Commercial

User Annotations

Open PHACTS
Open Pharmacological Space

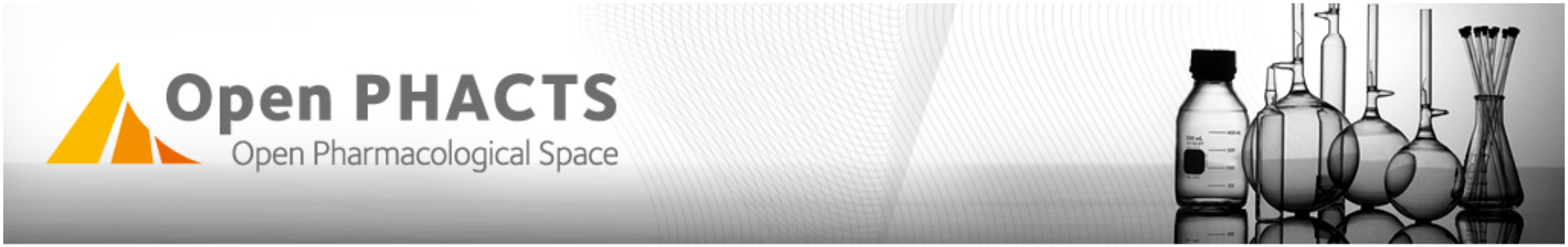
Premise

Did you see that new cancer drug on the news?

Oh yeah, I definitely did.

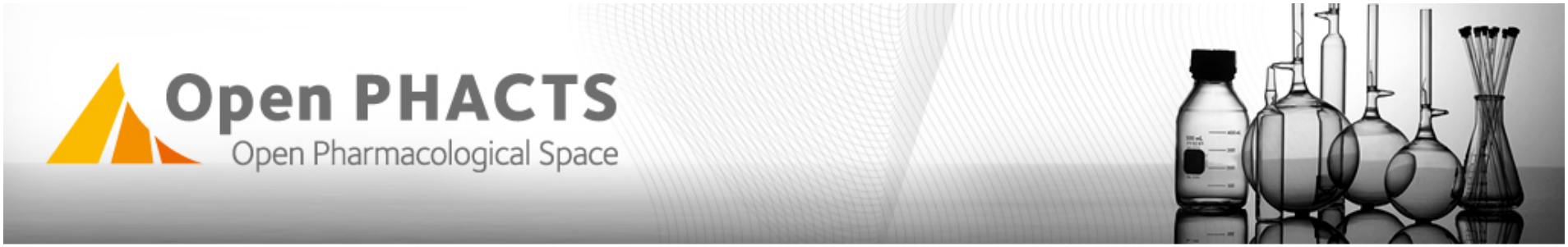
How does it work?

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



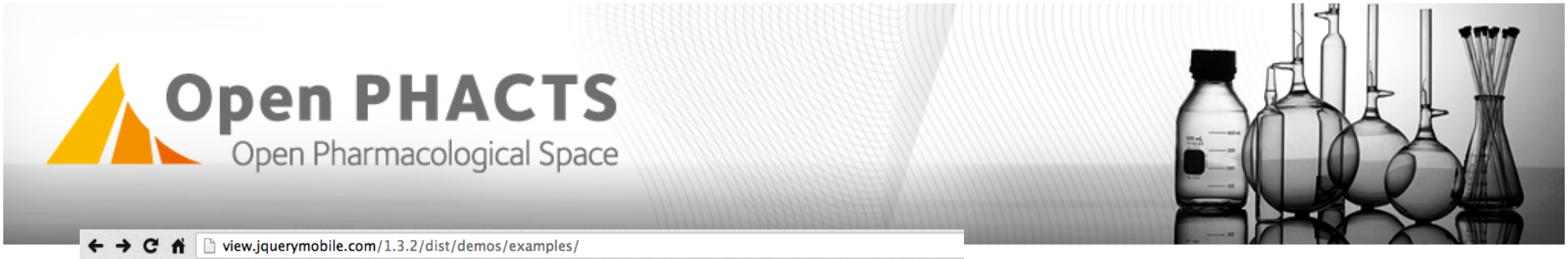
How is it done?

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

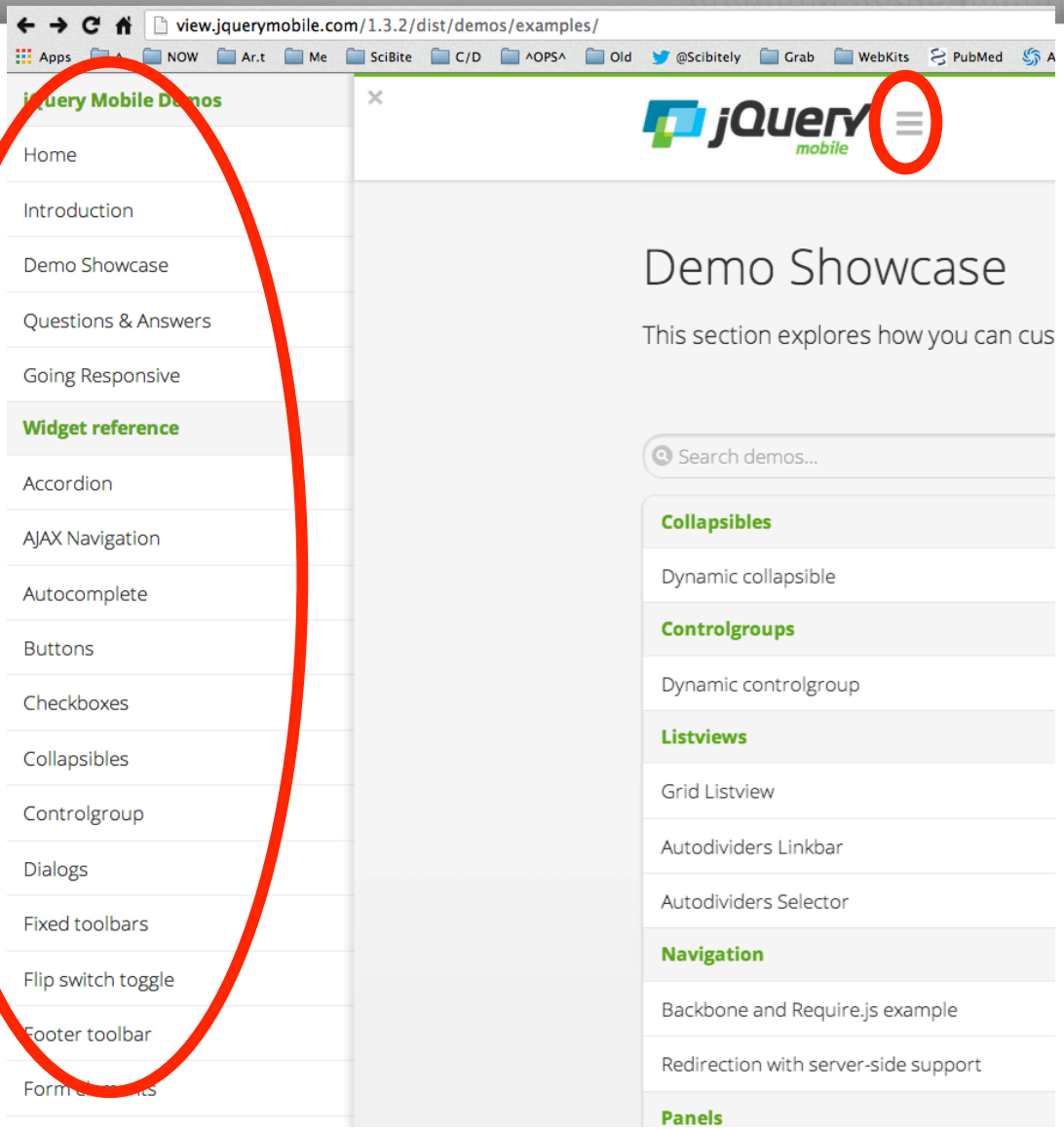
Open PHACTS
Open Pharmacological Space

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



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.

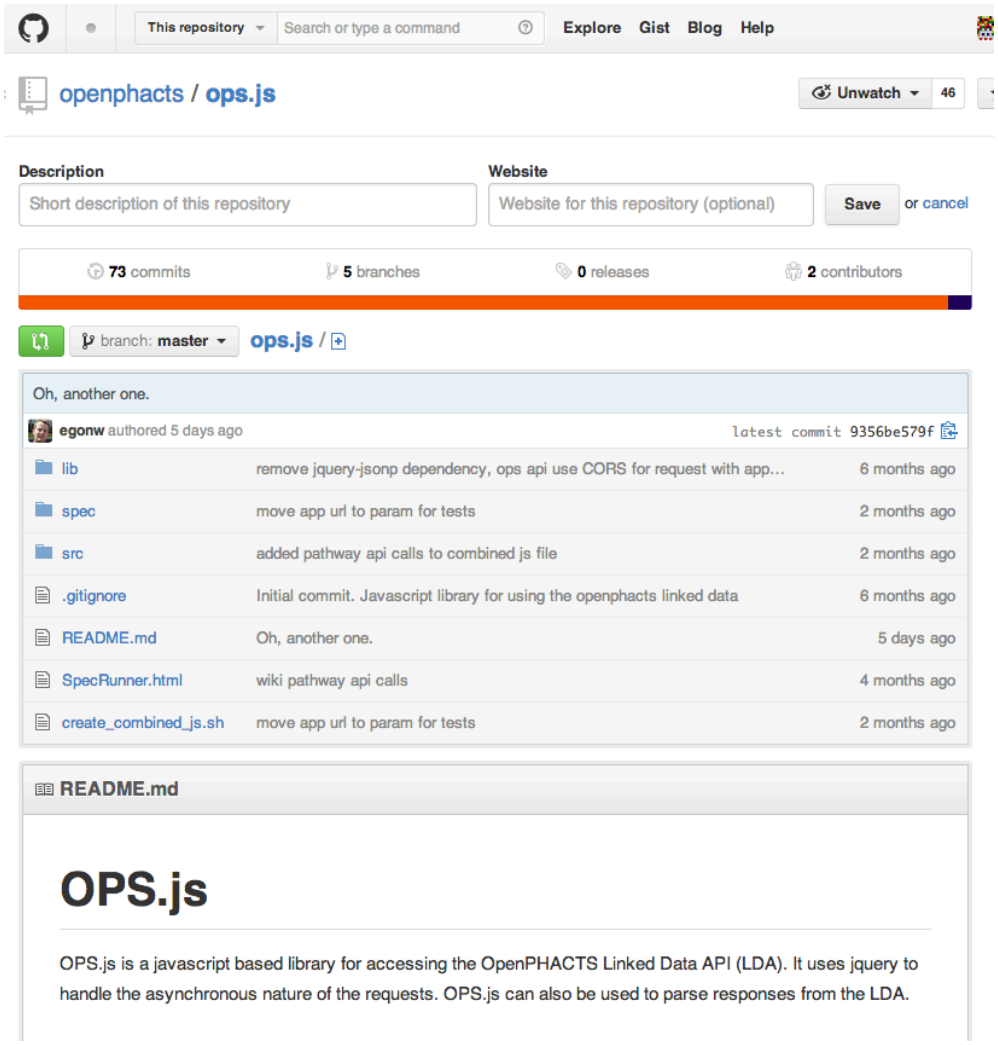
Phonegap


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
Wrap your app with PhoneGap
Deploy to mobile platforms!

Phonegap creates “app store ready” applications

- Development Workflow:
  - Code the app in jQuery Mobile
  - Compile it to native code for your source deployment platform using Phonegap (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

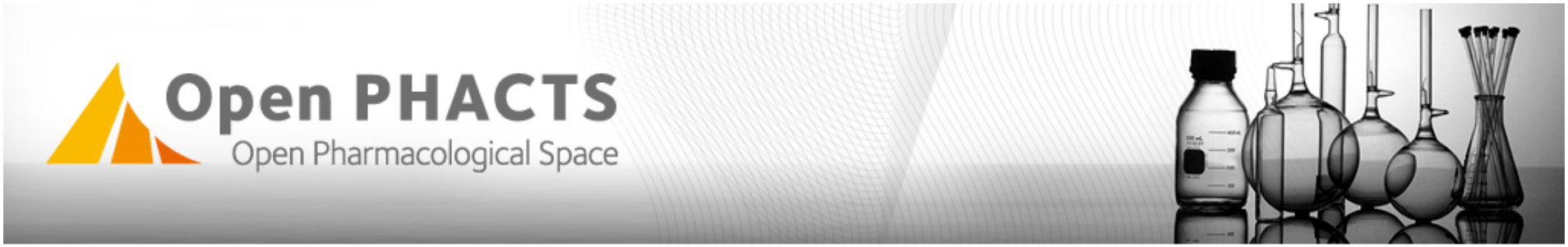
Open PHACTS
Open Pharmacological Space



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



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 th
e 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);
```

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 th
e 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-4ed1d7bdf9
d5', 1, 20, callback);
```

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

Open PHACTS
Open Pharmacological Space

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 *****

Open PHACTS
Open Pharmacological Space

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

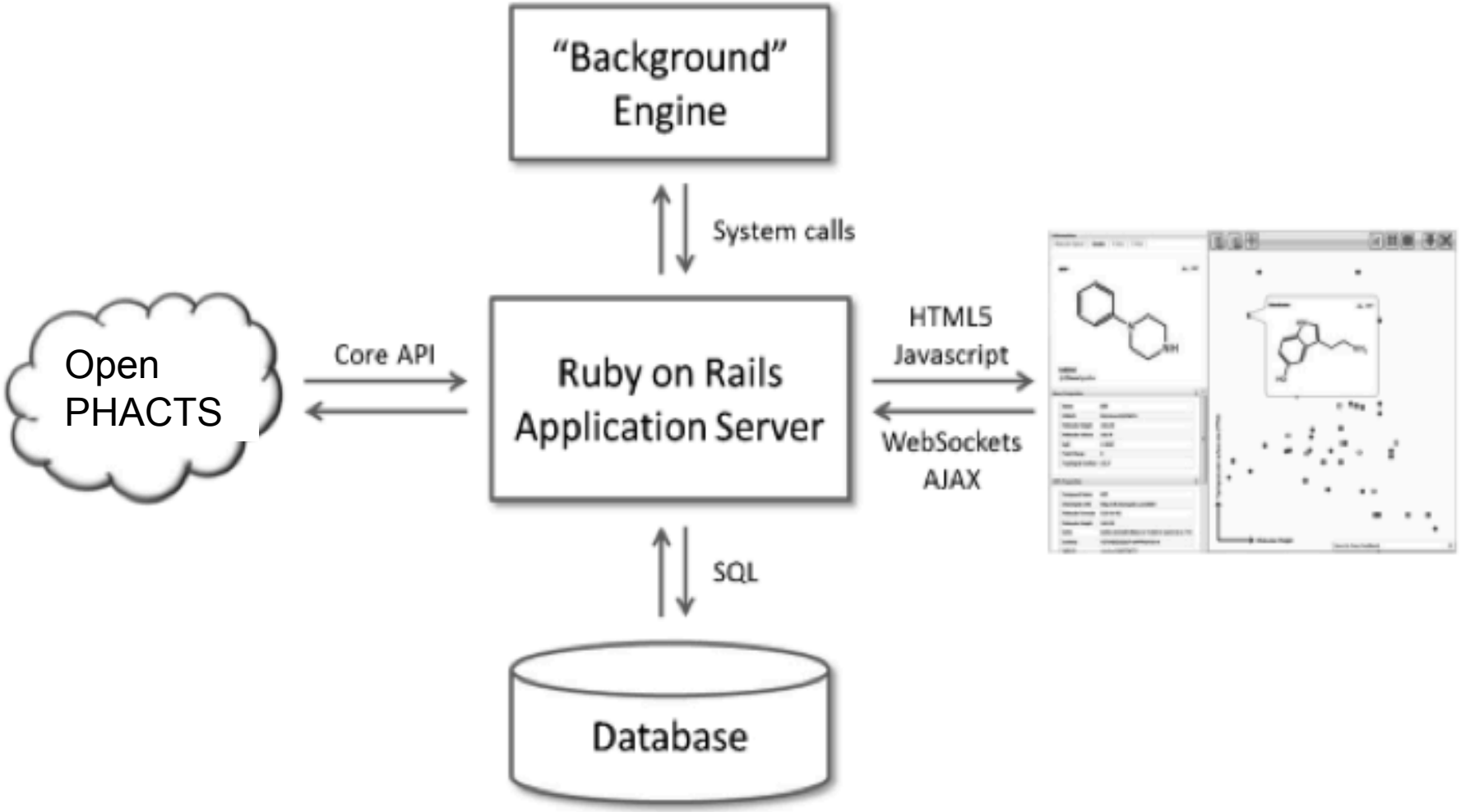
PharmaTrek, developed at the Parc de Salut Mar (PSMAR) in Barcelona, allows pharmacological space to be navigated in a flexible and interactive way, by accessing the content of ChEMBL via the Open PHACTS Discovery Platform. The results of a target search are highly filterable and easily linked with ligand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

Open PHACTS
Open Pharmacological Space

- **Use Case:**

  “Compare public and private compound data on the go”

Open PHACTS
Open Pharmacological Space




iPad
29%
11:30
Friday, November 16
slide to unlock

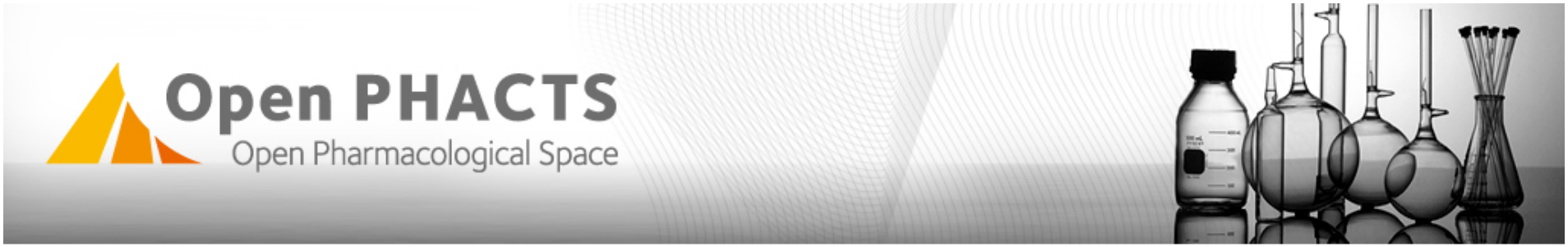
Future

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



Acknowledgements

- Lee Harland
- Ian Dunlop
- Rishi Ramgolam
- Tim Harder
- Christian Lemmen
- Matthias Rarey

- Innovative Medicines Initiative (IMI) for support of Open PHACTS


ChemBioNavigator
cbn.zbh.uni-hamburg.de
ChemBioNavigator
Give Feedback
About
Help
Sign Out
ChemBioNavigator
Type in a molecule name or a SMILES ..
Search/Upload
Upload a molecule file
UH
Bio Solve
Open PHACTS