

ChemBioNavigator

Chemically-Aware Visualizations of Chemical & Biological Spaces

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The ChemBioNavigator

A compound-centric data browser that is easy

- ✦ .. to set up & run the application
 - standard (HTML5) web application
 - minimal intrusion on the client side
 - agile development: Ruby on Rails, CSS, JavaScript, AJAX
- ✦ .. to use for non-technical scientists
 - intuitive/responsive GUI with optimum user-guidance
 - allow “jumping” between Exemplars
 - extensive “linking” into related data sources





Navigate Chemically-Aware

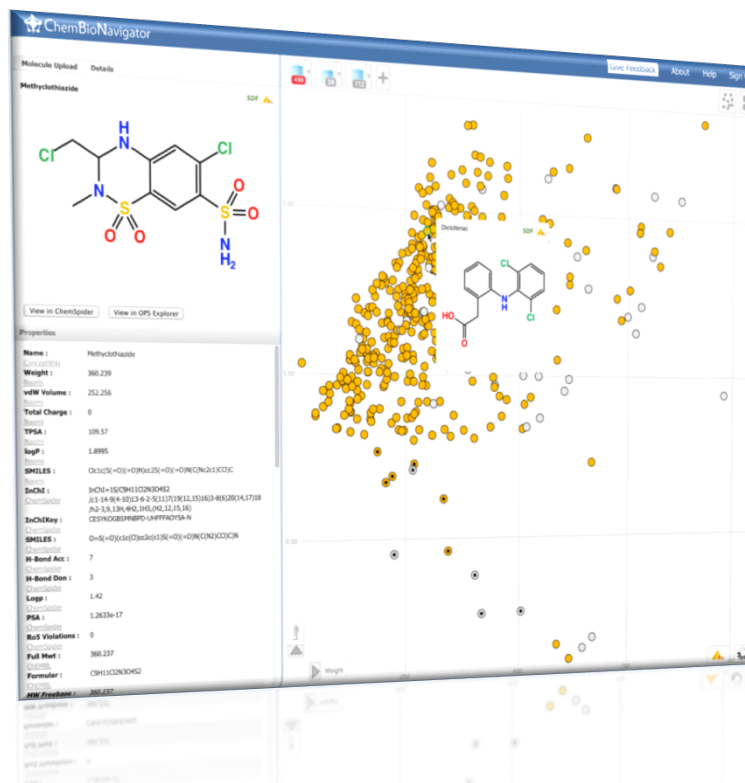
- ✦ **Use Case:** What do we know about similar molecules to a given query?"





“1-Stop Shopping”

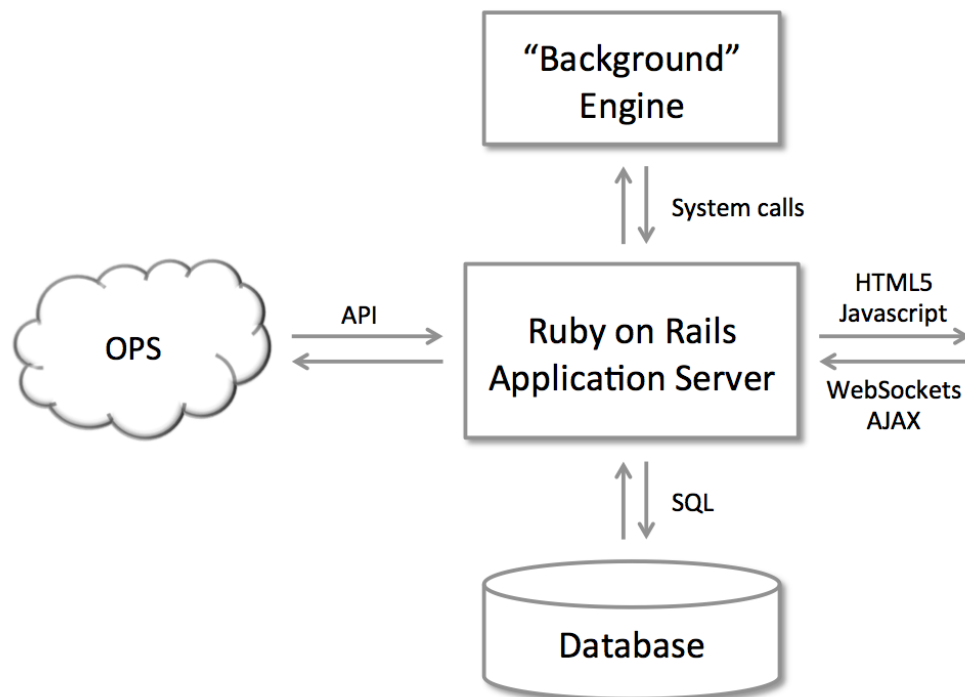
- ❖ **Use Case:** Combine my private and public knowledge!”





Behind the Scenes

- ✦ Building a modern web application with Rails and Open PHACTS





OPS Gem

- ❖ Standard Ruby way of sharing code
- ❖ Freely available under MIT licenses
- ❖ Wraps most API calls in a convenient interface



```
gem "ops", :git => "git://github.com/openphacts/ops_gems.git"
```

```
73
74 linked_data_cache_client = OPS::LinkedDataCacheClient.new(OPS_LINKED_DATA_CACHE_URL)
75
76 # Note: Takes some time
77 linked_data_cache_client.compound_info("http://rdf.chemspider.com/187440")
78 linked_data_cache_client.compound_pharmacology_count("http://rdf.chemspider.com/187440")
79 # Note: Takes some time
80 linked_data_cache_client.compound_pharmacology("http://rdf.chemspider.com/187440")
81
82 # Note: Takes some time
83 linked_data_cache_client.target_info("http://www.conceptwiki.org/concept/00059958-a045-4581-9dc5-e5a08bb0c291")
84 linked_data_cache_client.target_pharmacology_count("http://www.conceptwiki.org/concept/00059958-a045-4581-9dc5-e5a08bb0c291")
85 # Note: Takes some time
86 linked_data_cache_client.target_pharmacology("http://www.conceptwiki.org/concept/00059958-a045-4581-9dc5-e5a08bb0c291")
```




Open PHACTS to Go

- ✦ **Use Case:** How would I profit from all this in a mobile environment?"





<http://www.chembionavigator.org>

Please use the feedback form extensively or contact us at cbn@zbh.uni-hamburg.de