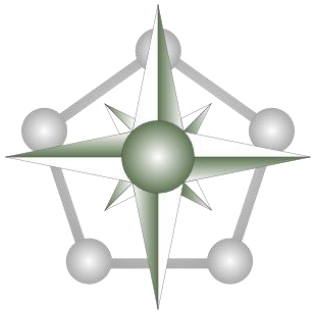


CBN

ChemBioNavigator

Universität Hamburg

Open PHACTS

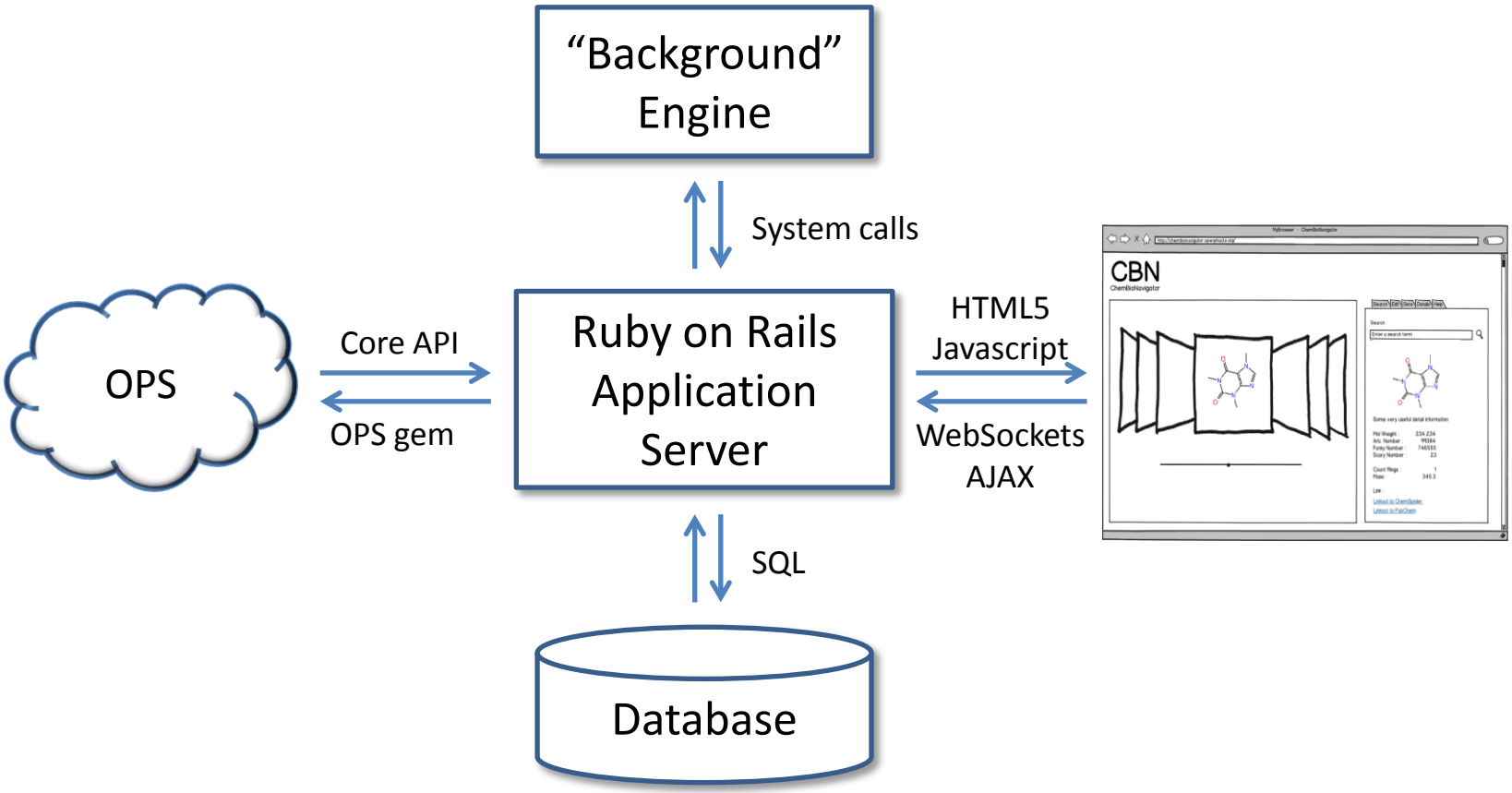
Open Pharmacological Space

CBN Design Goals

… 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
- easy to … use for non-technical scientists
  - intuitive/responsive GUI with optimum user-guidance
  - allow “jumping” between Exemplars
  - extensive “linking” into related data sources

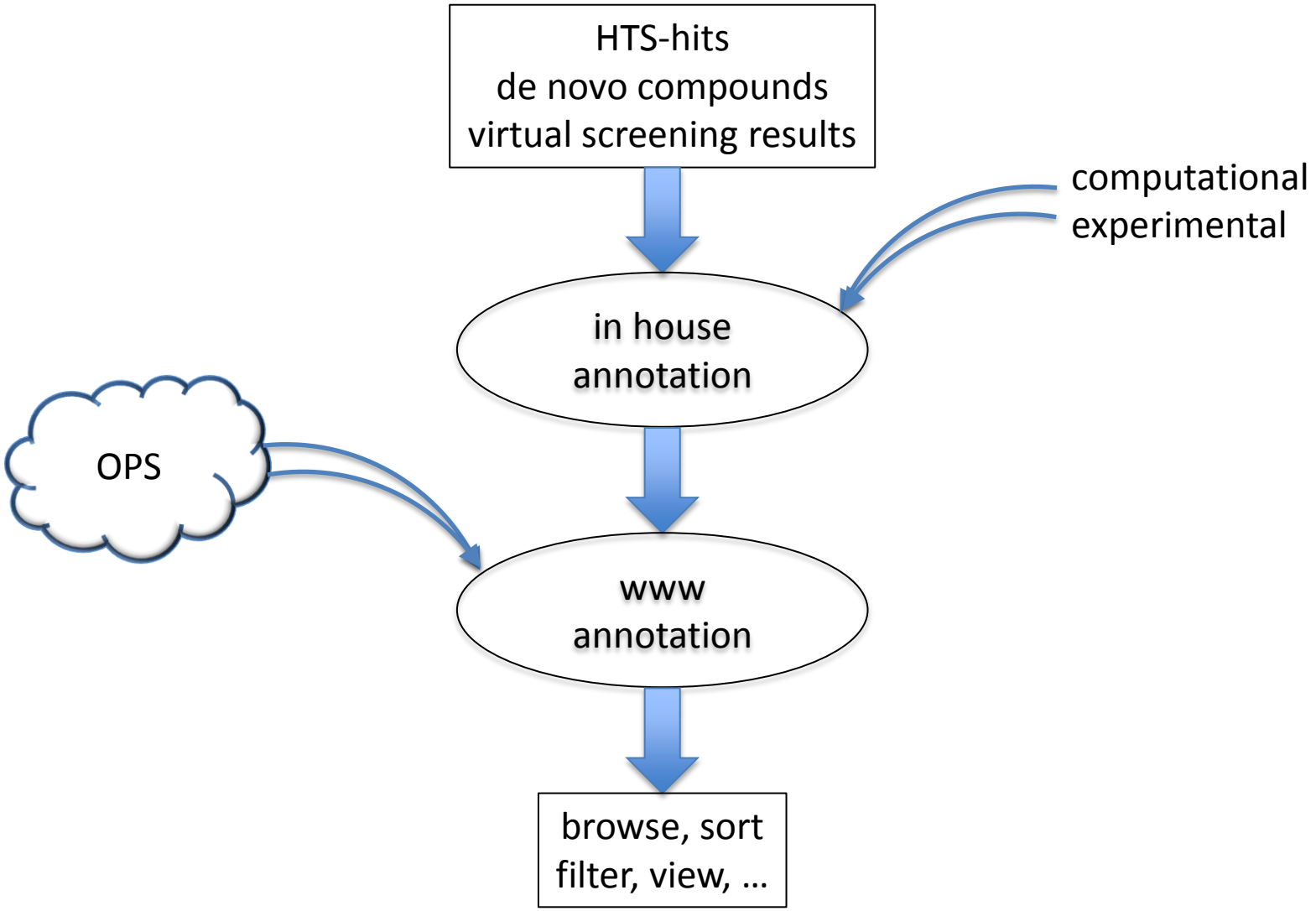
Architecture



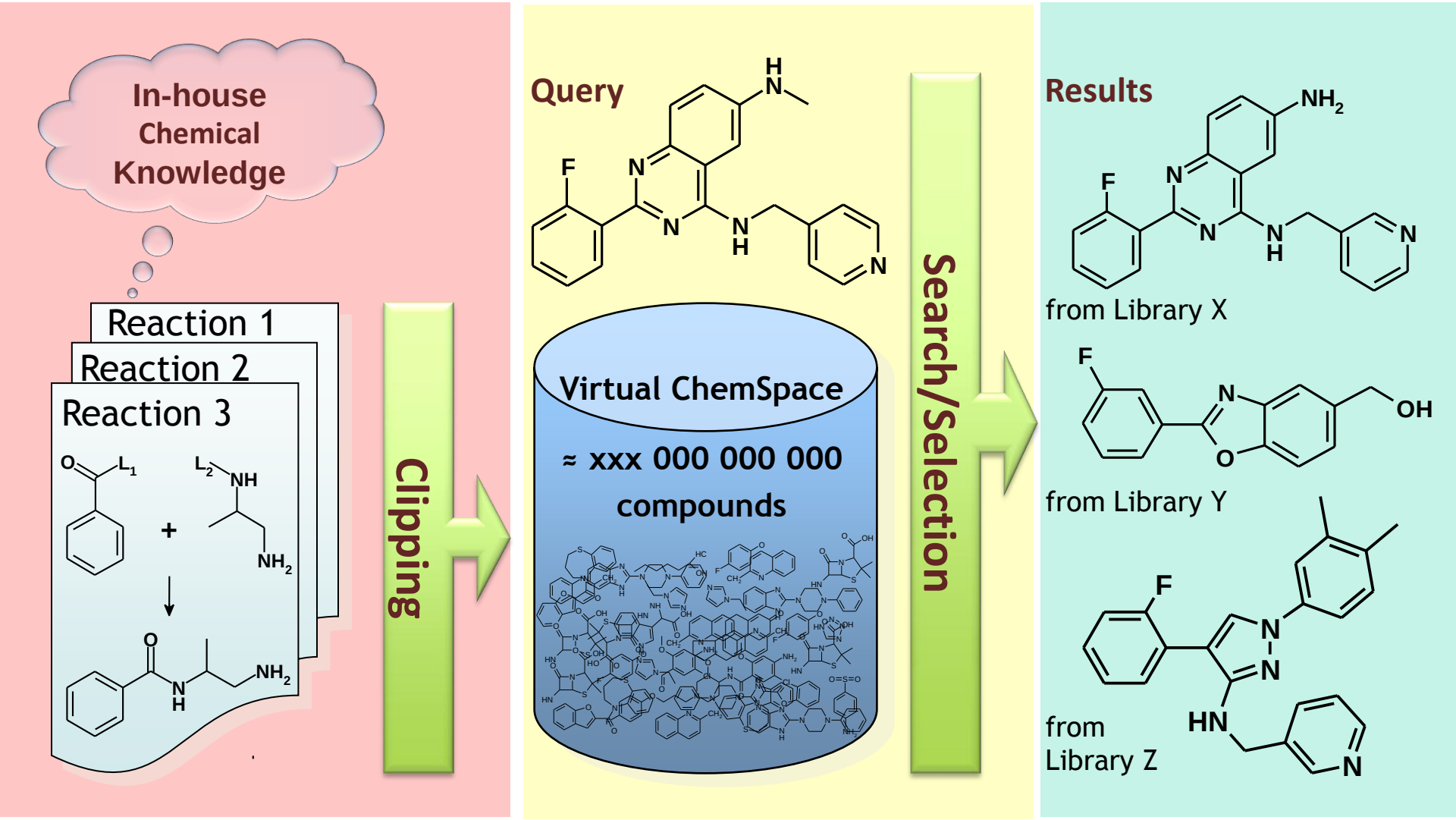
User Centric Design

- Release 1: Goals & Use Cases
  - upload and browse molecules
  - connect to OPS-framework
  - merge external and internal data
  - display molecules / browse data
  - getting an overview of what is currently loaded
  - export combined data

Primary Workflow



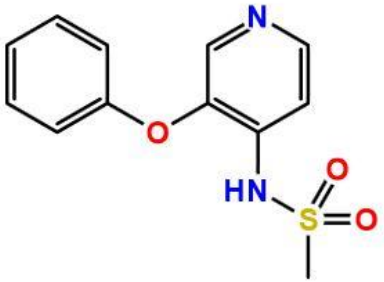
Virtual Screening



Information

Molecule Upload | Details | X Axis | Y Axis

N-(3-phenoxypyridin-4-yl)methanesulfonamide SDF



LinkOut:
ChemSpider

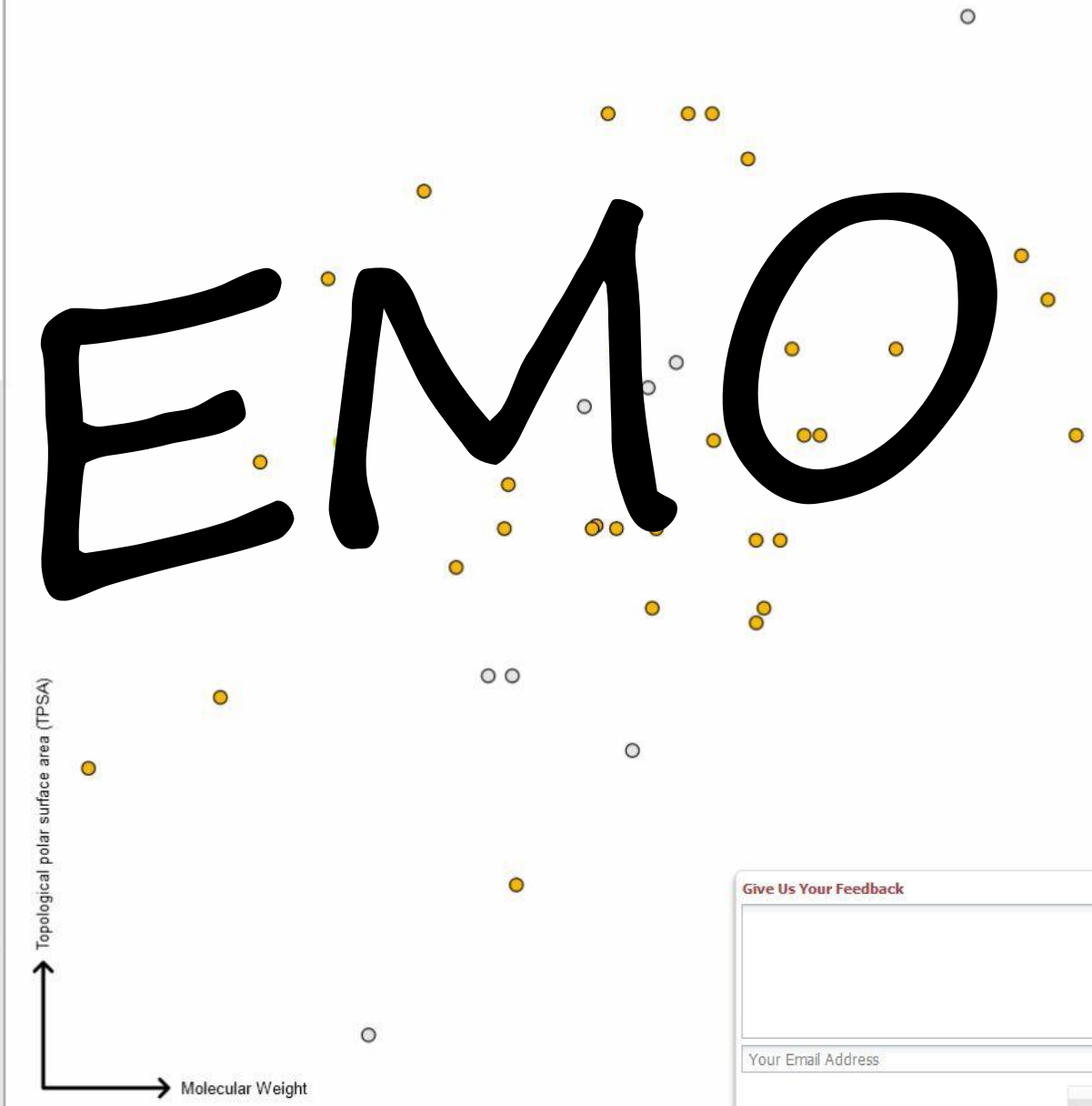
DEMO

Base Properties

Name	N-(3-phenoxyp -4-yl)methanesulfonamide
SMILES	S(=O)(=O)(Nc 2ccccc2)cncc1)C
Molecular Weight	264.303
Molecular Volume	219.068
logP	1.90882
Total Charge	0
Topological Surfac...	68.29

OPS Properties

Compound Name	N-(3-phenoxypyridin-4-yl)methanesulfonamide
ChemSpider URI	http://rdf.chemspider.com/8420030
Molecular Formular	C12 H12 N2 O3 S
Molecular Weight	264.304
InChi	InChI=1S/C12H12N2O3S/c1-18(15,16)14-11-7-8-1...
InchiKey	CQEDUEBRINEBGP-UHFFFAOYSA-N
SMILES	O=S(=O)(Nc2ccncc2Oc1ccccc1)C
ALogP	1.15
Hydrogen Bond A...	4
Hydrogen Bond D...	1
Molecular Weight ...	264.3
Rule of 5 Violations	0
Polar Surface Area	76.67



Give Us Your Feedback

Your Email Address

Send

Status

- Prototype ready for testing
- Official release towards the end of the year

Limitations

- Max 500 molecules per session
- Anonymous users -> no storage

Outlook

- Similarity searches to expand sets
- Inclusion of target information
- Suport of tablet PCs

Availibility

Early testers are welcome

email: cbn@zbh.uni-hamburg.de

Please provides us with lots of feedback!