Squonk

Squonk Platform
Squonk Computational Notebook
Current Application domains
ChemAxon functionality

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The Squonk Platform

Services

calculate

predict

transform

data

Runtime

kubernetes

keycloak

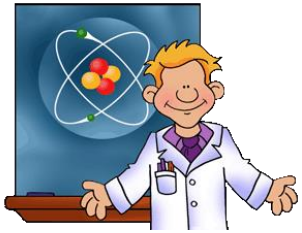
Hardware

Cloud
Virtual Private Cloud
Bare metal
Laptop

Vendor agnostic
Commercial + Open Source
Interoperable
Pluggable
Containerised

Performant
Scaleable
Resilient
Flexible
Secure
Cost effective
Cloud enabled

Squonk Computational Notebook



Computational Notebook

workflows | analysis | collaboration | provenance

Services

Democratise cheminformatics & computational chemistry (and beyond)

Make complex tools accessible to all

Break down barriers to access

Provide traceability and reproducibility

Application Domains

1: Chemical Safety Assessment
2: Drug Design

1: Chemical Safety Assessment

OpenRiskNet H2020 program (more)

Commenced Dec 2016

e-Infrastructure for chemical safety assessment

Is driving:

Platform development

Data and predictive models for toxicology, metabolism

OpenRiskNet

HORIZON 2020

Commissione europea

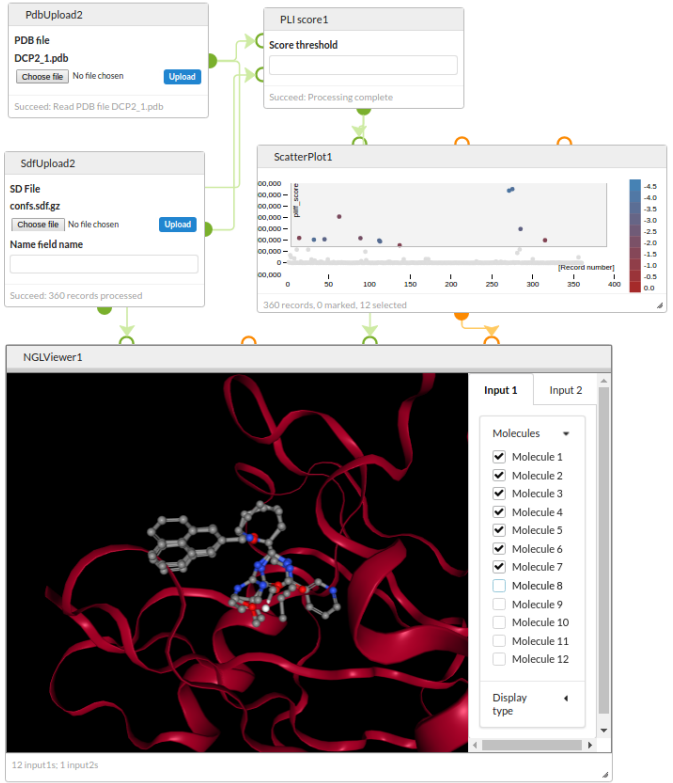
2: Drug Design

Fragment Based Drug Design Collaboration with:

- XChem at the Diamond Light Source
- SGC and Statistics at Oxford University

Is driving techniques for turning fragments into leads:

- 3D visualisation and analysis
- Chemical enumeration techniques



ChemAxon Functionality

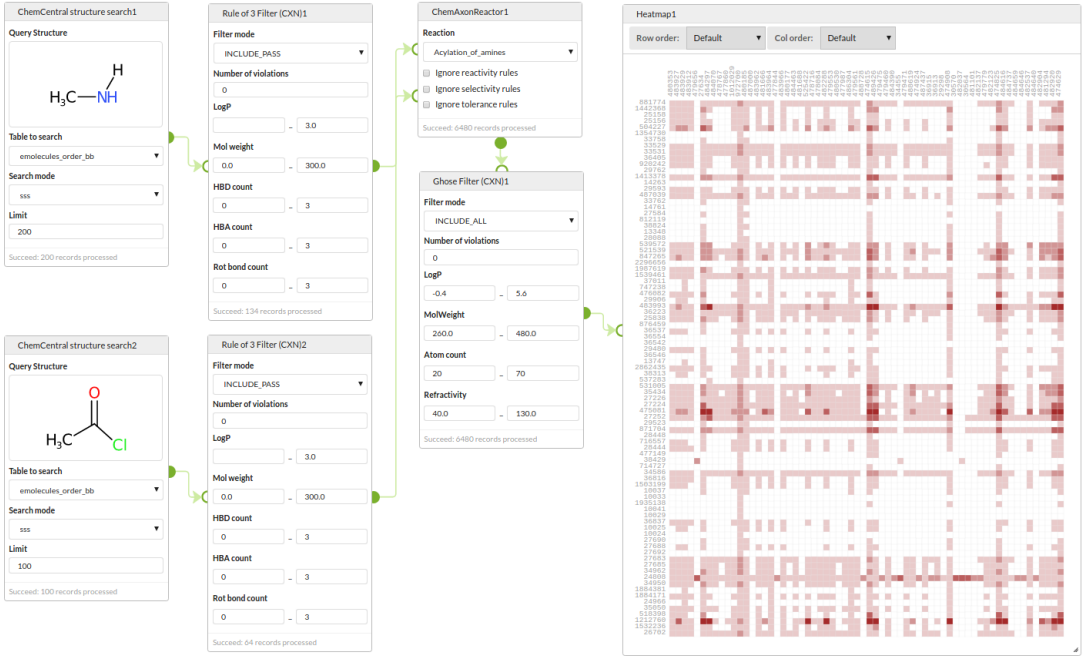
Visual
Marvin JS

Predictions
Property Calculators
Filters

Library Enumeration
Reactor

Screening
Fingerprint screening
Pharmacophore screening
Clustering

Database
JChem search



Looking for users wanting to use ChemAxon functionality

The Squonk Says:

Thank you for listening, come and see us to find out more

We are hiring

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