



Squonk update

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The Squonk Platform



Services



calculate



predict



transform



data

Vendor agnostic
Commercial + Open Source
Interoperable
Pluggable
Containerised

Runtime



docker



kubernetes



keycloak

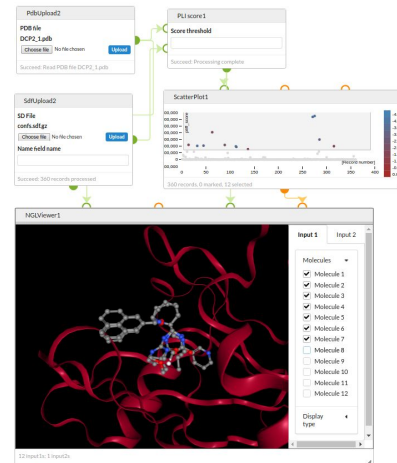
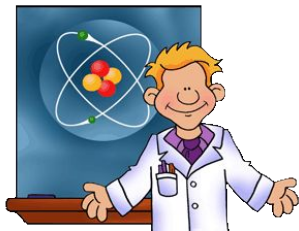
Performant
Scaleable
Resilient
Flexible
Secure
Cost effective
Cloud enabled



Hardware

Cloud
Virtual Private Cloud
Bare metal
Laptop

Squonk Computational Notebook



Computational Notebook



workflows



analysis



collaboration



provenance

Services



- Democratisise cheminformatics & computational chemistry (and beyond)
- Make complex tools accessible to all
- Break down barriers to access
- Provide traceability and reproducibility
- Facilitate secure collaboration

Status Update



- Work continues on OpeRiskNet preproject, mostly related Squonk Platform
 - Resilience and (auto-)scaling
 - Flexible Deployment using Kubernetes & OpenShift
 - Orchestration of services
- Collaboration with Diamond/XChem has been positive
 - 3D visualisation
 - Protein & ligand preparation
 - Docking, scoring
 - Proven interoperability
 - Extensibility through containers
 - Planning how to integrate into Diamond's XChem offerings
- Awaiting outcome of Innovate UK grant proposal
 - Will provide significant developer resource to work on architecture and content

Open Source Status



- Core part of Squonk Platform and Computational Notebook have just been open sourced under Apache 2.0 license
 - <https://github.com/InformaticsMatters/squonk>
- The Web front end (portal app) will follow once it is better integrated
- Pipelines repository that provides many of the XChem related services has been under Apache 2.0 license since it was created 6 months ago
 - <https://github.com/InformaticsMatters/pipelines>
- Other [InformaticsMatters](#) public repos of note:
 - jsviztools - Javascript components (NGL, D3) for visualisation
 - Various Docker images (e.g. RDKit) also available from [DockerHub](#)

Objective is to provide an open and sustainable platform with commercial support for those who want it