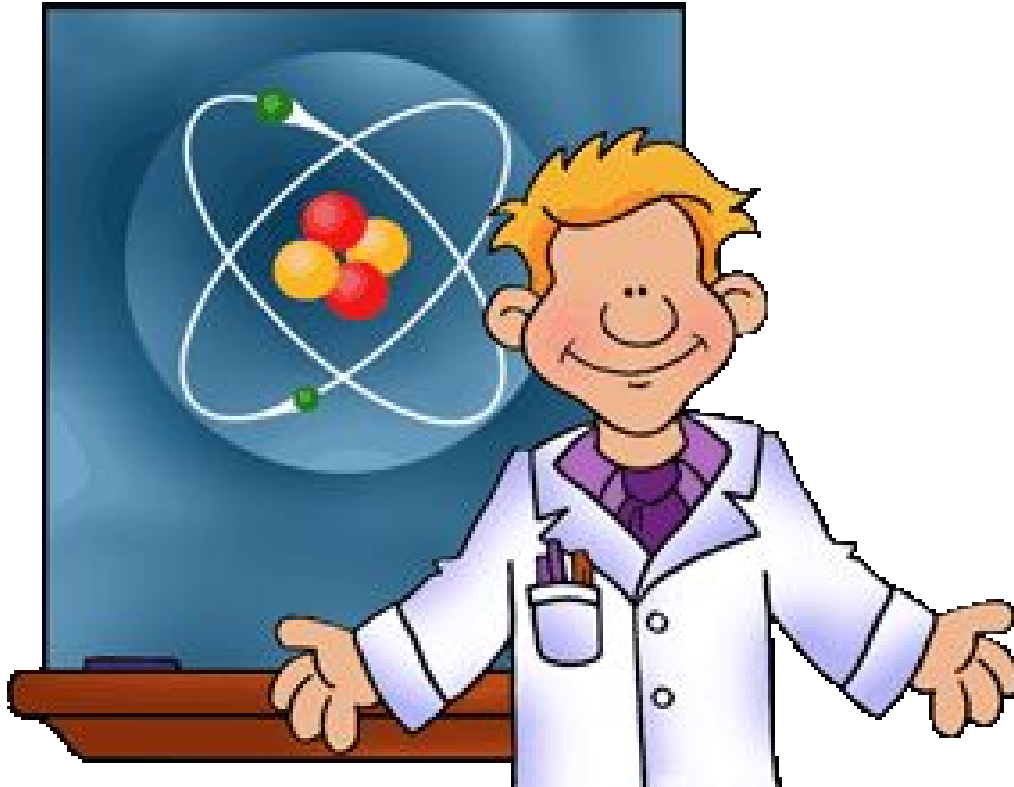


The Squonk Computational Notebook

Making cheminformatics and comp chem accessible to normal people!

Tim Dudgeon
tdudgeon@informaticsmatters.com

The Target Audience



Cameras - a metaphor



- Very Powerful
- Pretty Complex
- Incompatible

Cameras - a metaphor

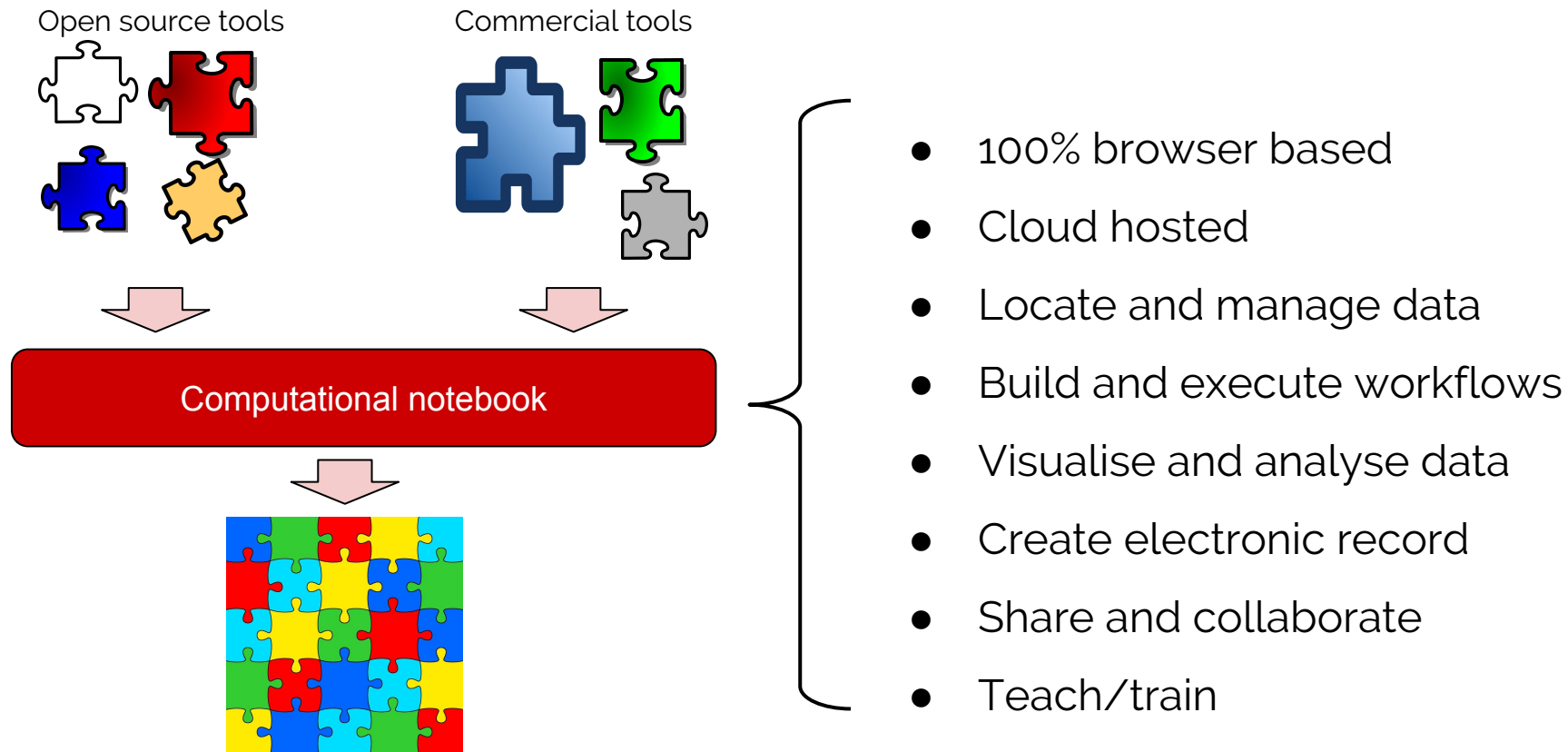


Cameras - a metaphor

- Simple
- Convenient
- Compatible
- But Still Powerful



An Open platform for scientific workflows



Computational Notebook

Your notebooks + those shared with you

Name	Owner
HTS data analysis	user2
notebook 2	user2
pains2	user1

Filter

Cell palette

Drag n Drop

Input

cxn pharmacophore screening1

Similarity Cutoff

0.8

Query Structure

CN1C=NC2=C1C(=O)N(C)C(=O)N2C

Output

Notebook Canvas

History and versions

Id: 447
Created: 20160711 10:54:04
Updated: 20160711 15:54:04

Predict And Visualise

sdfupload1

SD File
dhfr_st
Choose
Name f
Succeed: 756 records processed

1. SD File Upload

lipinski (rdkit)1

Succeed

2,3. Predict using RDKit

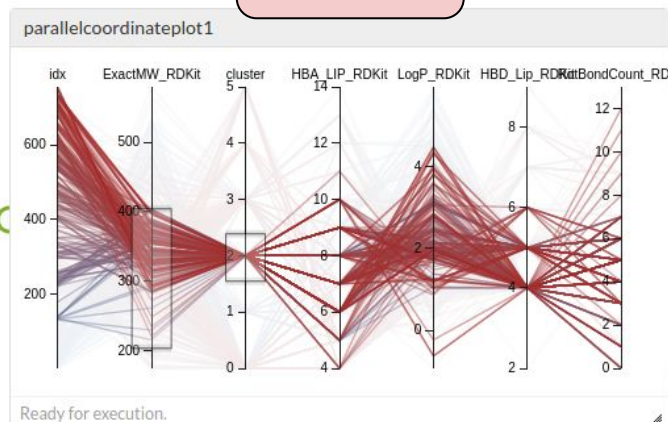
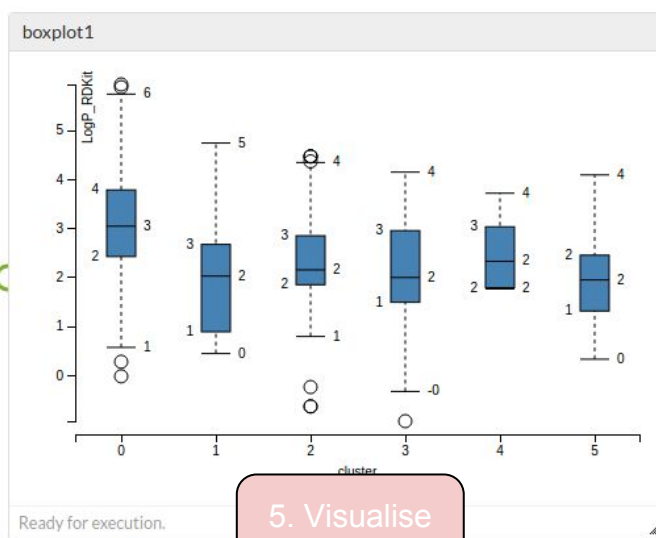
rotat

Succeed: 756 records processed

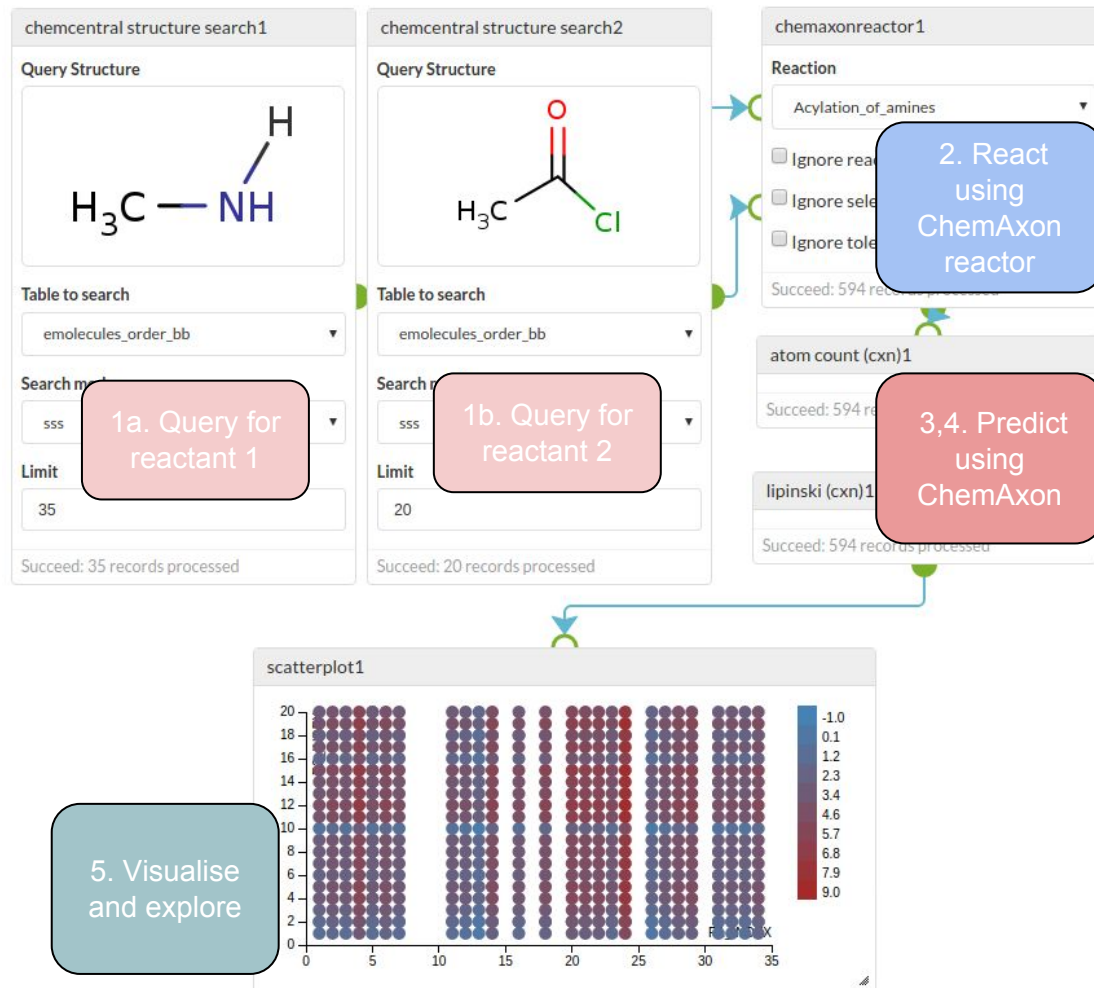
sperex clustering (cxn)1

Min clu
5
Max clu
12
Succeed: 756 records processed

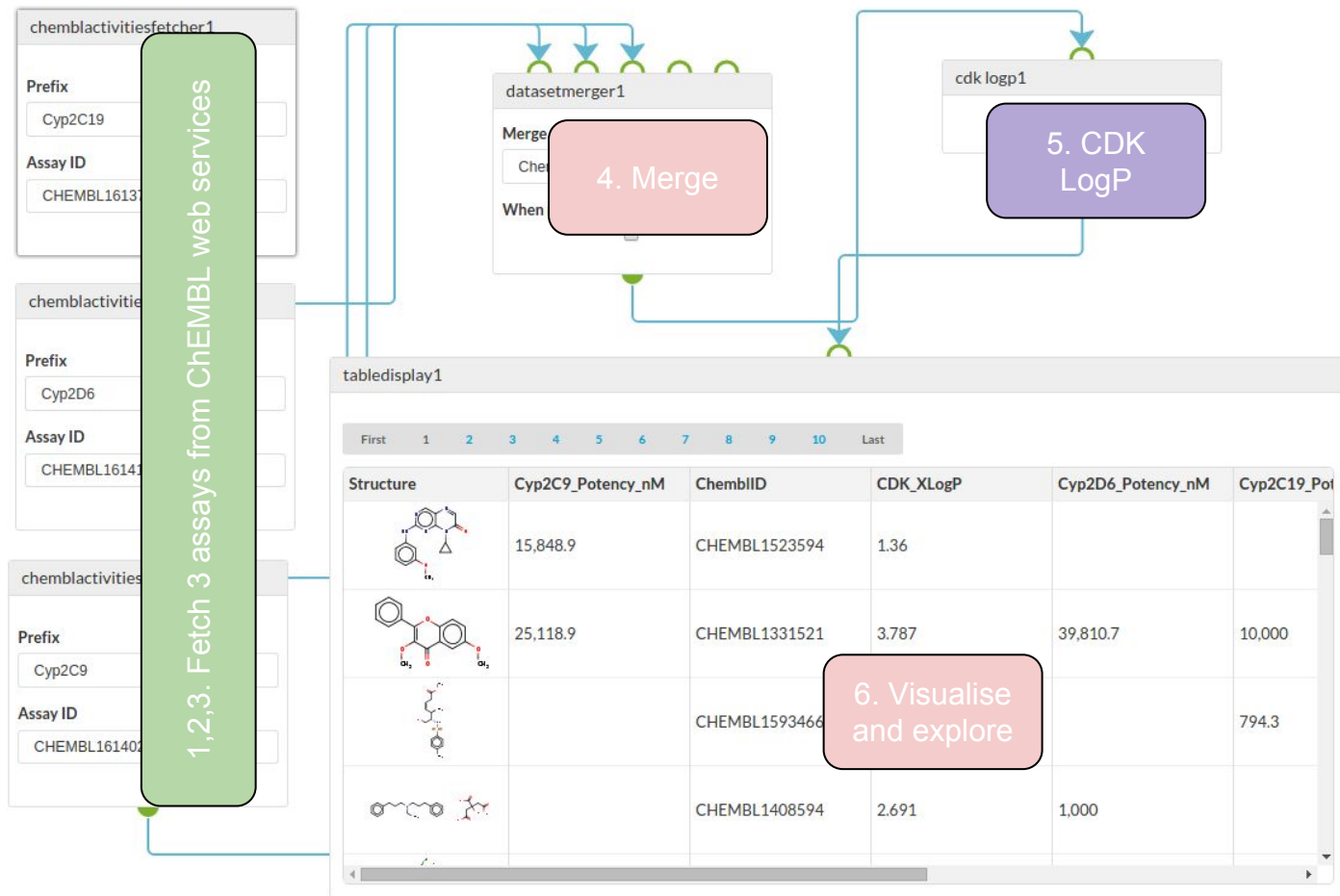
4. Cluster using ChemAxon



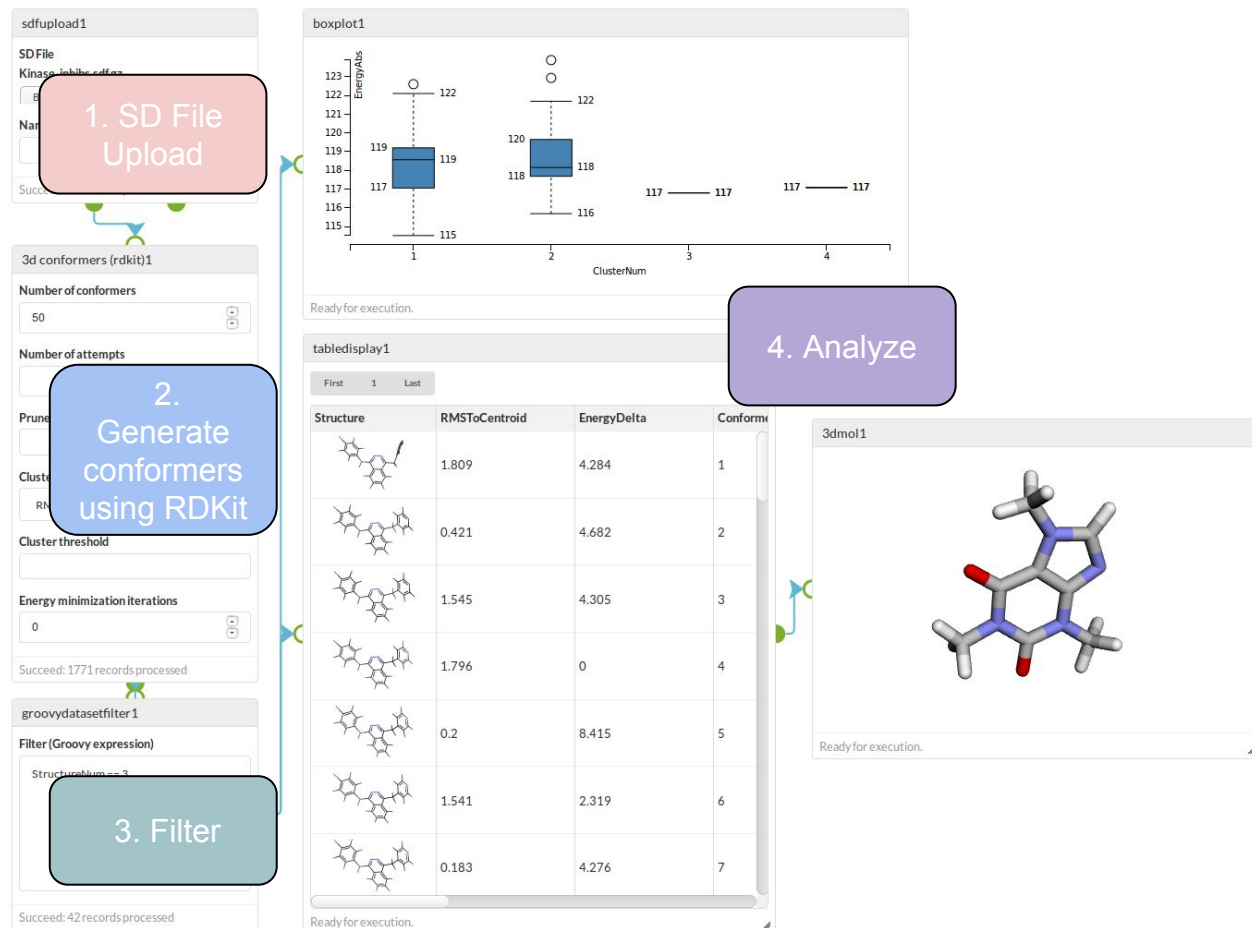
Combichem Library Generation



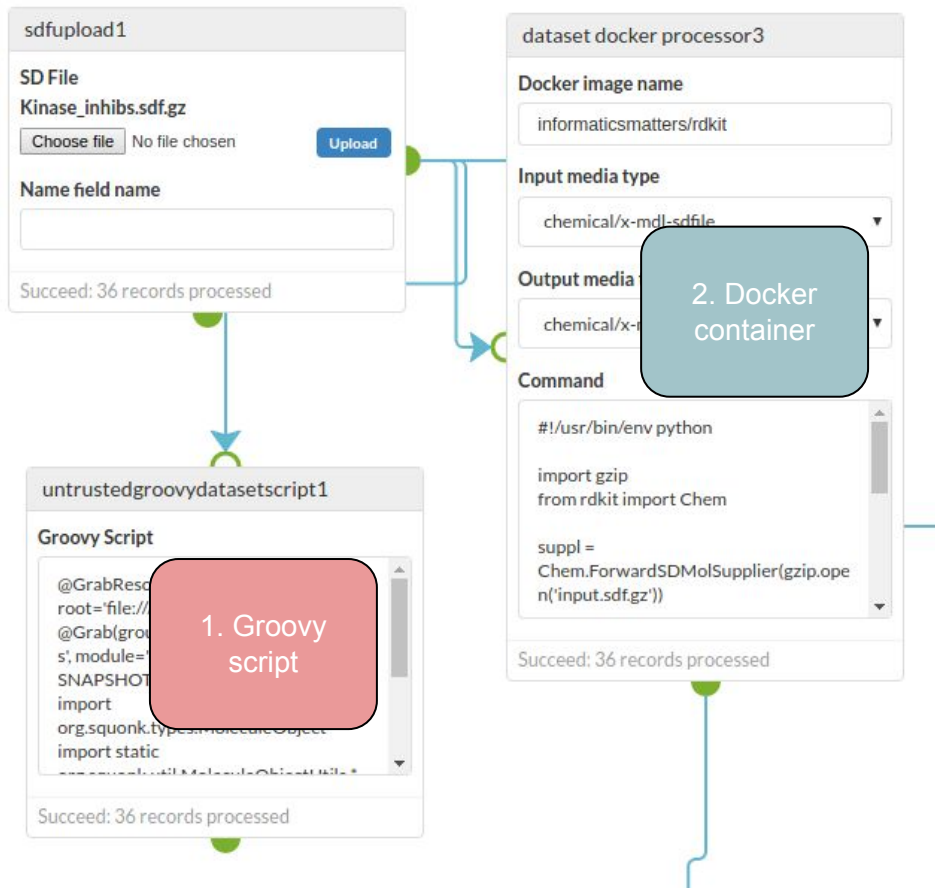
Data Curation



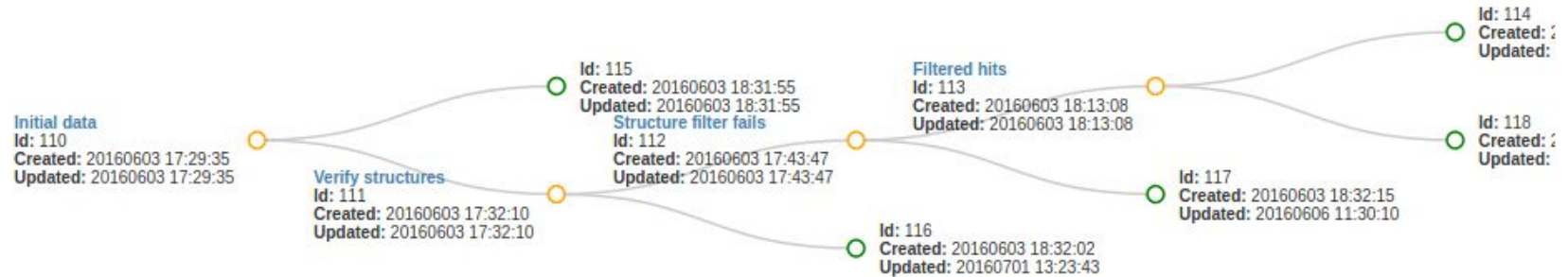
Conformer Generation and Analysis



Programming And Containers



Workflow Versioning and Branching



Interested?

Currently in alpha
testing stage

**Seeking users to
provide feedback**

Seeking tool providers
who have tools to
make available to a
wider audience

Current domains:

- Cheminformatics
- Comp Chem

Next domains

- Predictive models (esp. Tox prediction)
- Bioinformatics
- Genomics

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