



Drug Discovery FAQ

Lilly

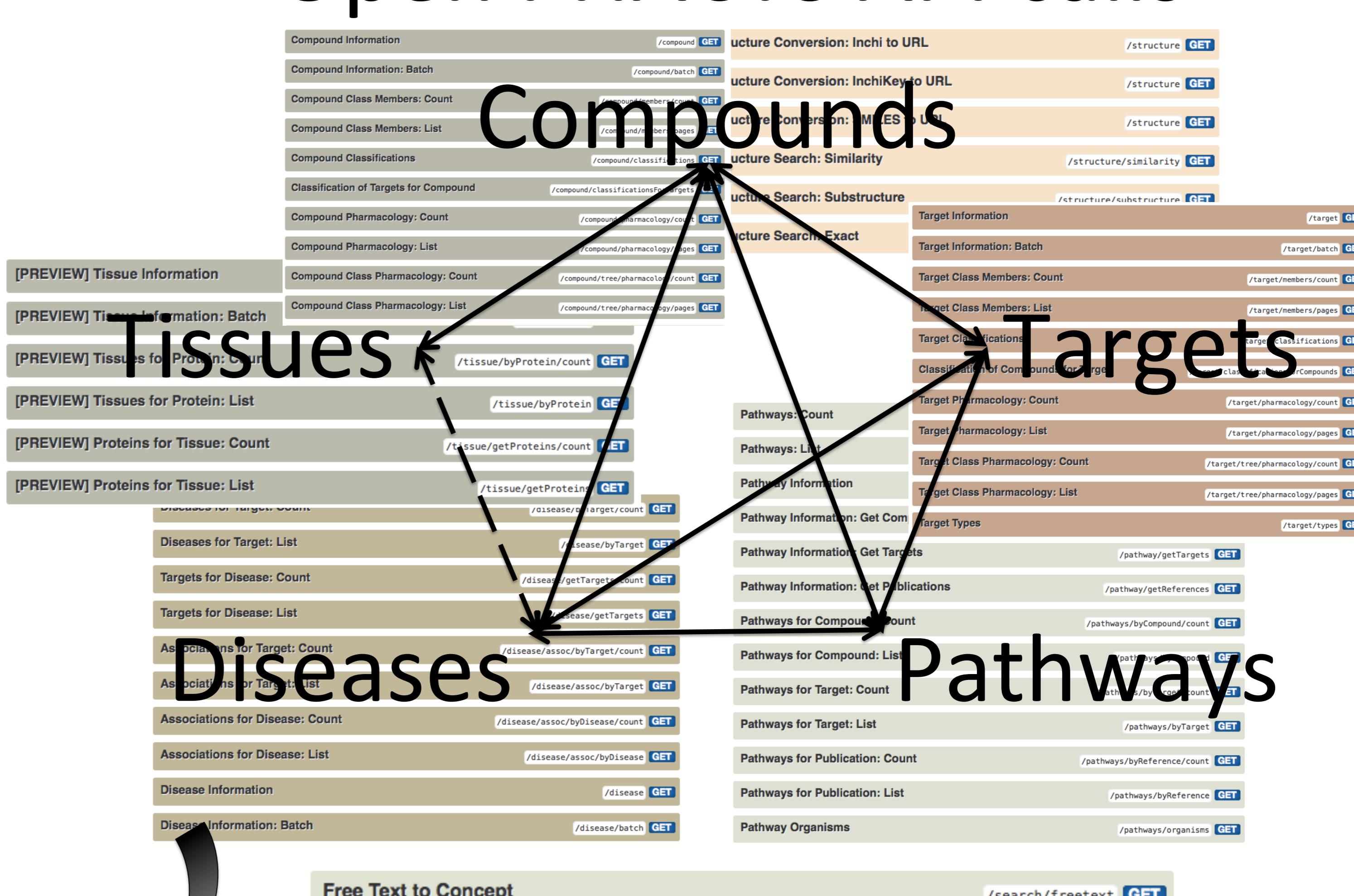
Open PHACTS API and KNIME have the answers!

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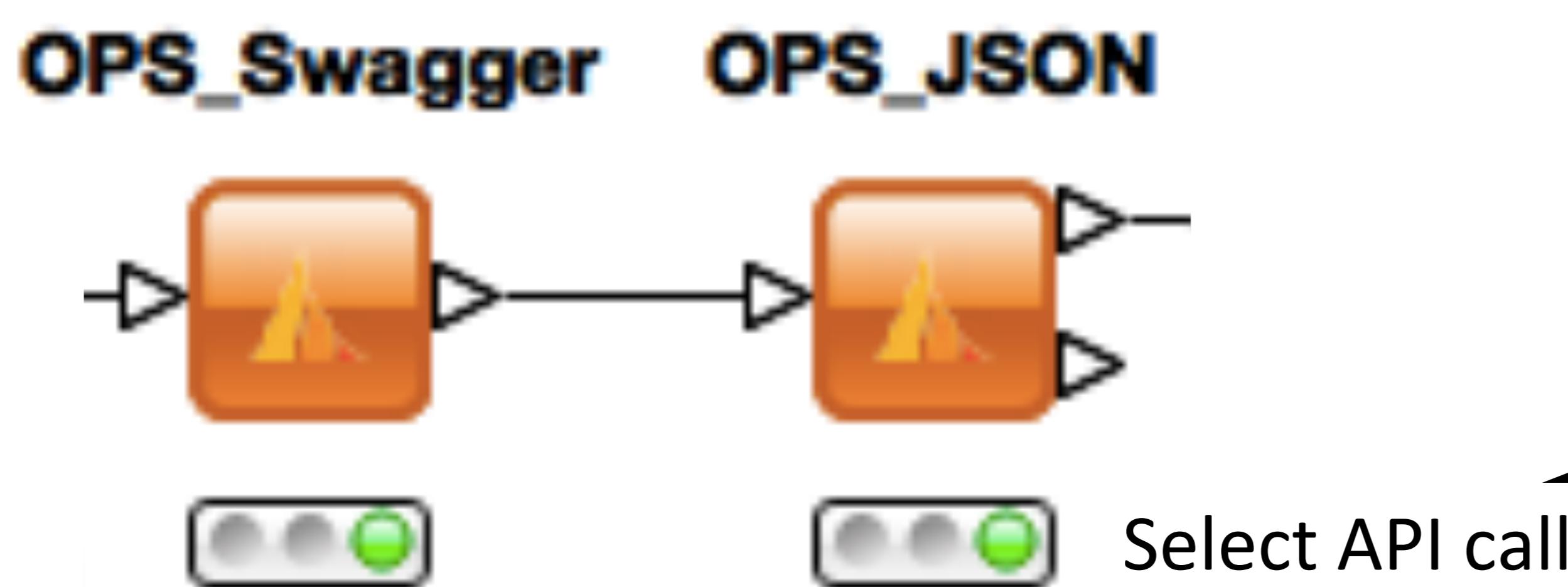
Drug Discovery Questions

Example Drug Discovery FAQs	Open PHACTS API calls needed
Give me all oxidoreductase inhibitors active <100 nM in human and mouse	Target Class Pharmacology (filters)
Given a target find me all actives against that target. Find/predict polypharmacology of actives.	Target Pharmacology (filters) > Compound Pharmacology
For a given interaction profile, give me similar compounds	Compound Information > Chemical Structure Search:Similarity
For molecules that contain substructure X, retrieve all bioactivity data in serine protease assays	Chemical Structure Search: Substructure > Compound Pharmacology (filters), Target Class Members
For a specific target family, retrieve all compounds in specific assays	Target Class Members > Target Pharmacology
Retrieve diseases associated with all approved drugs	Free Text to Concept > Compound Pharmacology > Disease Associations for Target

Open PHACTS API calls



Two nodes for all API calls



OPS_SWAGGER

This node parses a SWAGGER file to generate the **list of API calls** available from the Open PHACTS web service. After the user selects a call from the list, a **parameter panel** allows the addition of specific parameter settings.

OPS_JSON

OPS_JSON transforms the nested JSON results into columns that can be selected and renamed by the user. Two outputs are available; one that corresponds to the JSON paths as specified by the user, and the second table is the complete JSON result.

The screenshot shows three dialog boxes. The top-left box is 'Dialog - 2:100 - OPS_Swagger' with a dropdown menu 'Select service' containing various API endpoints like 'Target Information (/target)', 'Target Information: Batch (/target/batch)', etc. The top-right box is 'Dialog - 2:100 - OPS_JSON' with a section 'Default URL parameters' and a 'Add filter options' button. The bottom box is 'Dialog - 3:6 - OPS_JSON' titled 'select JSON Columns and optional new name', showing a list of JSON paths with checkboxes for selecting columns, and checkboxes for '..result..primaryTopic..about' and '..result..primaryTopic..exactMatch' are checked.

Nodes: <https://github.com/openphacts/OPS-Knime>

API: <https://dev.openphacts.org>

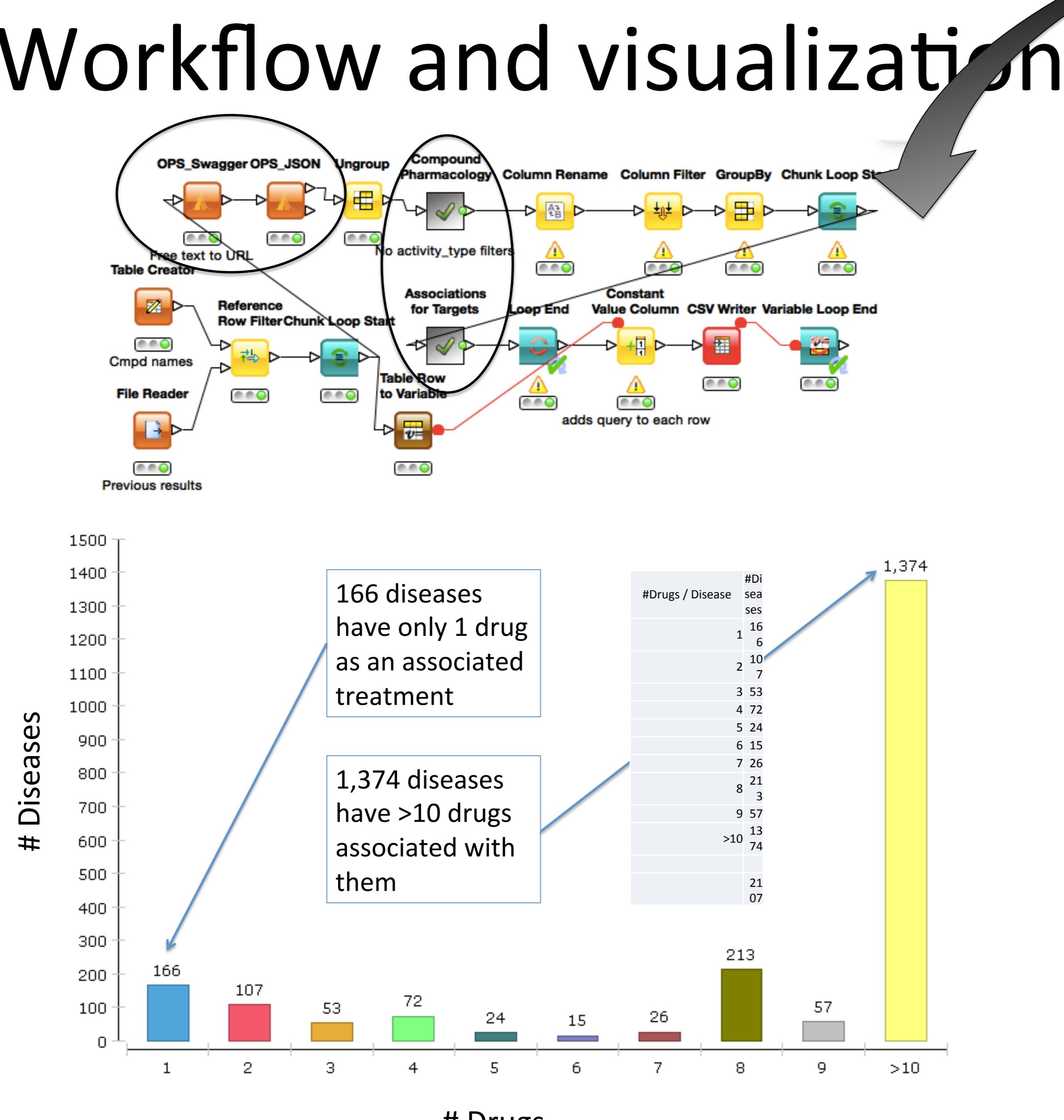
Support: <http://support.openphacts.org>

Open PHACTS Drug Discovery FAQ Workflows:
<http://www.myexperiment.org/packs/676.html>

Drug discovery FAQs: Workflows for answering multidomain drug discovery questions.

Drug Discovery Today, 2014:

<http://dx.doi.org/10.1016/j.drudis.2014.11.006>



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