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Using Open PHACTS with KNIME

Daniela Digles
daniela.digles@univie.ac.at

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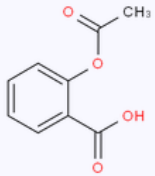
Accessing the data (for non-developers)

- eApps (Explorer, ChemBioNavigator, …)

Open PHACTS Explorer | aspirin | Search | Search for structure | Draw Molecule | Browse by Ontology | Help

Home / Aspirin / Compound Pharmacology



Aspirin (50 of 2882 results loaded)

Filter Results | Create TSV | Show provenance | Hide provenance

Target		Assay		Activity					
Name	Organism	Organism	Description	Type	Relation	Value	Units	PubMed Article	pChembl
PC-3	Homo sapiens		PUBCHEM_BIOASSAY: NCI human tumor cell line growth inhibition assay. Data for the PC-3 Prostate cell line. (Class of assay: confirmatory)	GI50		100000	nM		
MCF7	Homo sapiens		PUBCHEM_BIOASSAY: NCI human tumor cell line growth inhibition assay. Data for the MCF7 Breast cell line. (Class of assay: confirmatory)	GI50		100000	nM		
SK-OV-3	Homo sapiens		PUBCHEM_BIOASSAY: NCI human tumor cell line growth inhibition assay. Data for the SK-OV-3 Ovarian cell line. (Class of assay: confirmatory)	GI50		100000	nM		
			PUBCHEM_BIOASSAY: NCI human tumor cell line						

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Accessing the data (for developers)

- Programming interface (API)

Open PHACTS API development version

Assay — Show/Hide | List Operations | Expand Operations

Chemical structure search — Show/Hide | List Operations | Expand Operations

Compound — Show/Hide | List Operations | Expand Operations

GET	/compound	Compound Information
GET	/compound/batch	Compound Information: Batch
GET	/compound/classifications	Compound Classifications
GET	/compound/classificationsForTargets	Classification of Targets for Compound
GET	/compound/members/count	Compound Class Members: Count
GET	/compound/members/pages	Compound Class Members: List
GET	/compound/pharmacology/count	Compound Pharmacology: Count
GET	/compound/pharmacology/pages	Compound Pharmacology: List

Implementation Notes

Returns a variety of pharmacological data, including assay and activity information, for a user specified compound. Filtering of results is possible via a variety of options such as: target organism, activity type, activity value, etc.

KNIME

- KNIME Analytics Platform
- Available from www.knime.org
- Open source data analytics, reporting and integration platform
- Workflows can be built by connecting „Nodes“
- Open PHACTS KNIME nodes developed by Ronald Siebes (VU Amsterdam) available from github: https://github.com/openphacts/OPS-Knime

Open for Innovation
KNIME

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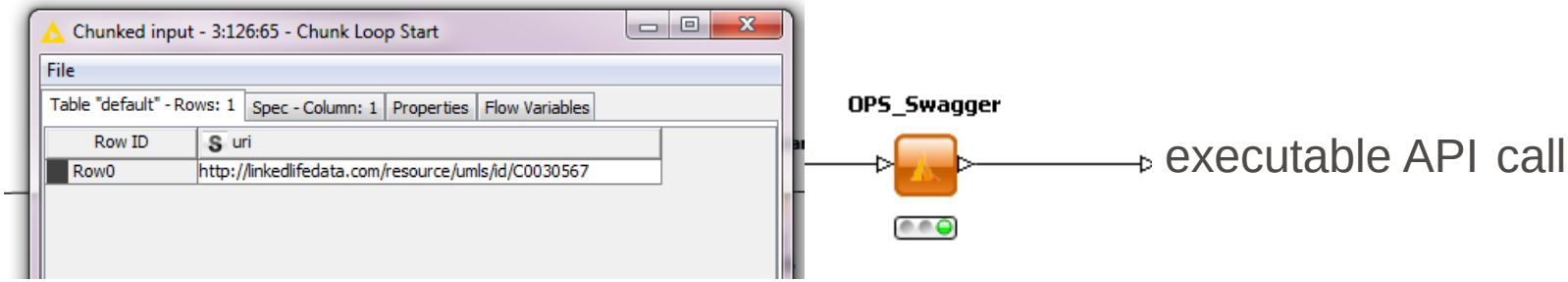
Open PHACTS KNIME node



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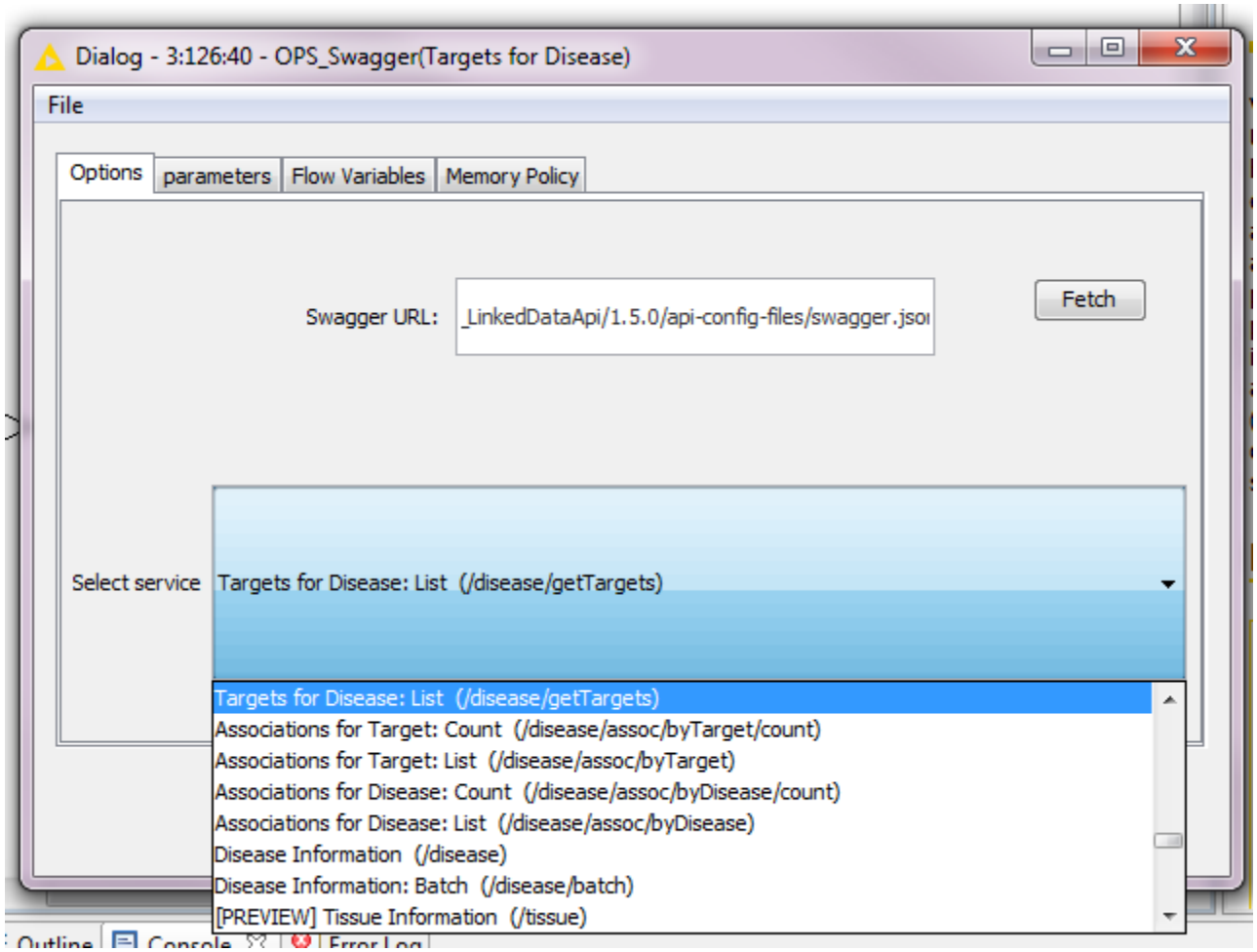
Open PHACTS KNIME node



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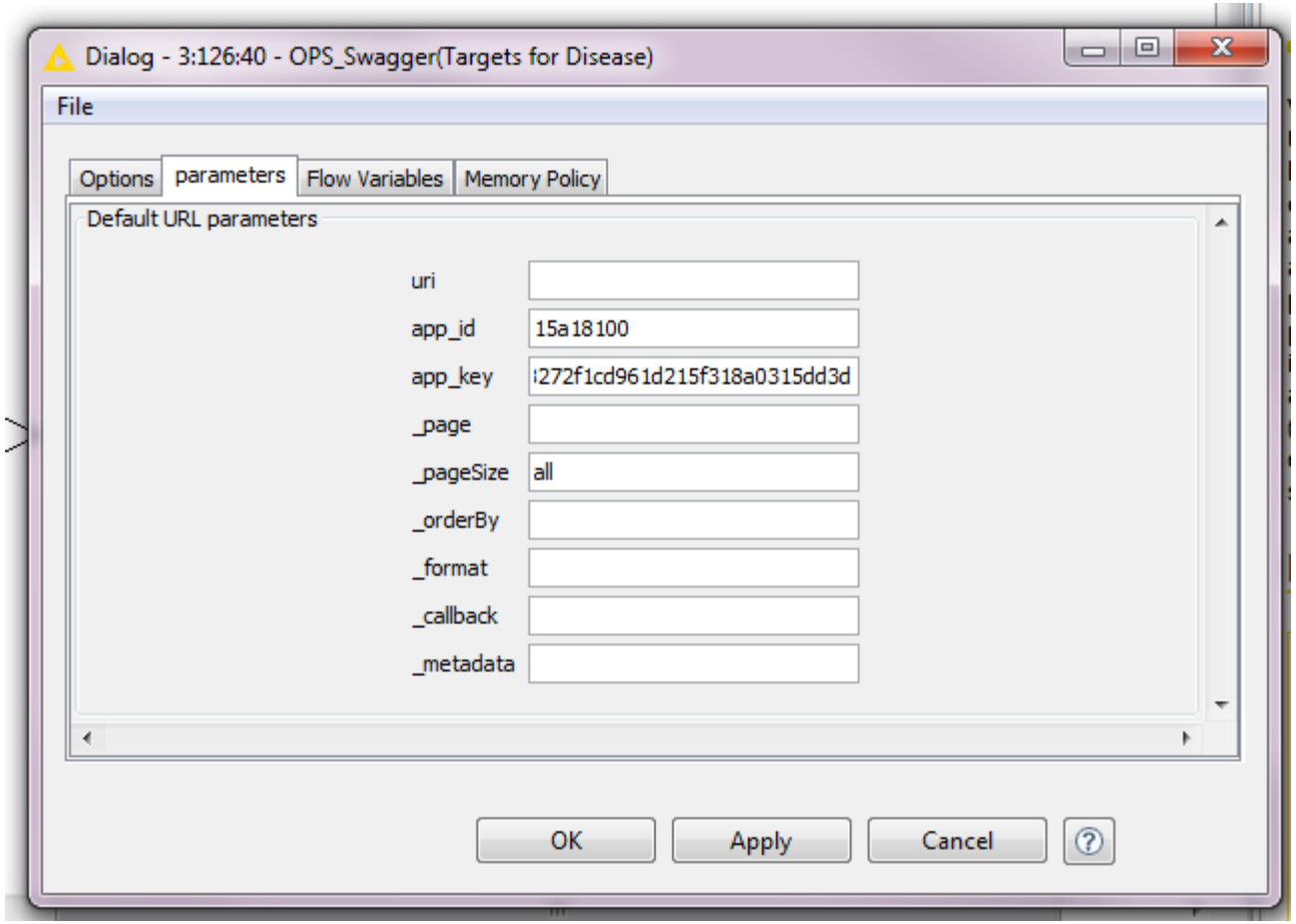
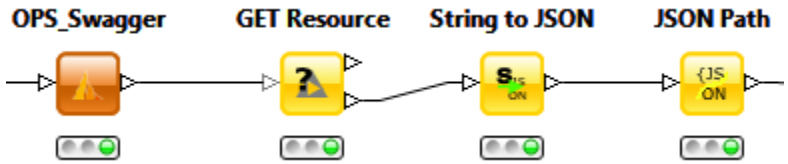
Open PHACTS KNIME node



Parsing the results

- Either use OPS_Json (deprecated) or the REST and JSON nodes available as add-in from KNIME.
- GET Resource: retrieves the actual data from the server. Configure the node to use the column url as input. Response representation cell type: Autodetection.
- String to JSON: transforms the result to a JSON column type.
- JSON Path: allows the individual selection of the data which is transformed into a tabular structure.
- XML/XPath users: set the parameter _format in OPS_Swagger to xml.



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JSON path details


```
{
    "format":"linked-data-api",
    "version":"1.5",
    "result":{
        "_about":"https://beta.openphacts.org/1.5/compound/pharmacology/count?app_id=15a18100&app_ke
        "definition":"https://beta.openphacts.org/api-config",
        "extendedMetadataVersion":"https://beta.openphacts.org/1.5/compound/pharmacology/count?app_i
        "linkPredicate":"http://www.w3.org/2004/02/skos/core#exactMatch",
        "activeLens":"Default",
        "primaryTopic":{
            "_about":"http://rdf.ebi.ac.uk/resource/chembl/molecule/CHEMBL1945801",
            "compoundPharmacologyTotalResults":4,
            "isPrimaryTopicOf":"https://beta.openphacts.org/1.5/compound/pharmacology/count?app_id=1
        }
    }
}
```


Row ID	count	url
Row 1	4	https://beta.openphacts.org/1.5/compound/pharmacology/count?app_id=15a18100&app_key=52

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JSON path configuration

Dialog - 0:106:121 - JSON Path

File

Settings | Flow Variables | Memory Policy

Input

Representation

☑ Remove source column

Outputs

Output column	JSONPath	List	Paths
S count	$['result']['primaryTopic']['compoundPharmacologyTotalResults']		
S url	$['result']['_about']		

Add single query | Add collection query | Add JSONPath | Edit JSONPath | Remove JSONPath

JSON-Cell Preview

```
1 {
2   "format" : "linked-data-api",
3   "version" : "1.5",
4   "result" : {
5     "_about" : "https://beta.openphacts.org/1.5/compound/pharmacology/count?app_id=15a18100&app_key=528a8272f1cd961d
6     "definition" : "https://beta.openphacts.org/api-config",
7     "extendedMetadataVersion" : "https://beta.openphacts.org/1.5/compound/pharmacology/count?app_id=15a18100&app_key=
8     "linkPredicate" : "http://www.w3.org/2004/02/skos/core#exactMatch",
```

OK | Apply | Cancel

Example JSON path queries

- To easily generate a query, click on the wanted property in the JSON-Cell Preview and click on Add single query. If the data is actually a list, and you want to retrieve all entities, click on Add collection query instead.
- Simple query:

  $['result']['primaryTopic']['compoundPharmacologyTotalResults']

  OR

  $.result.primaryTopic.compoundPharmacologyTotalResults

  OR

  $..compoundPharmacologyTotalResults

- Be aware that the path might change depending on the used query. The last version is therefore the preferred one.

Example JSON path queries – advanced queries

- Retrieving one property, while filtering for another one
  - Example for compound classification API call: retrieve the labels of the classification, but only when the classification is of the type “has role”.

$..hasChebiClassification[?(@.classificationType.prefLabel=='has role')].prefLabel

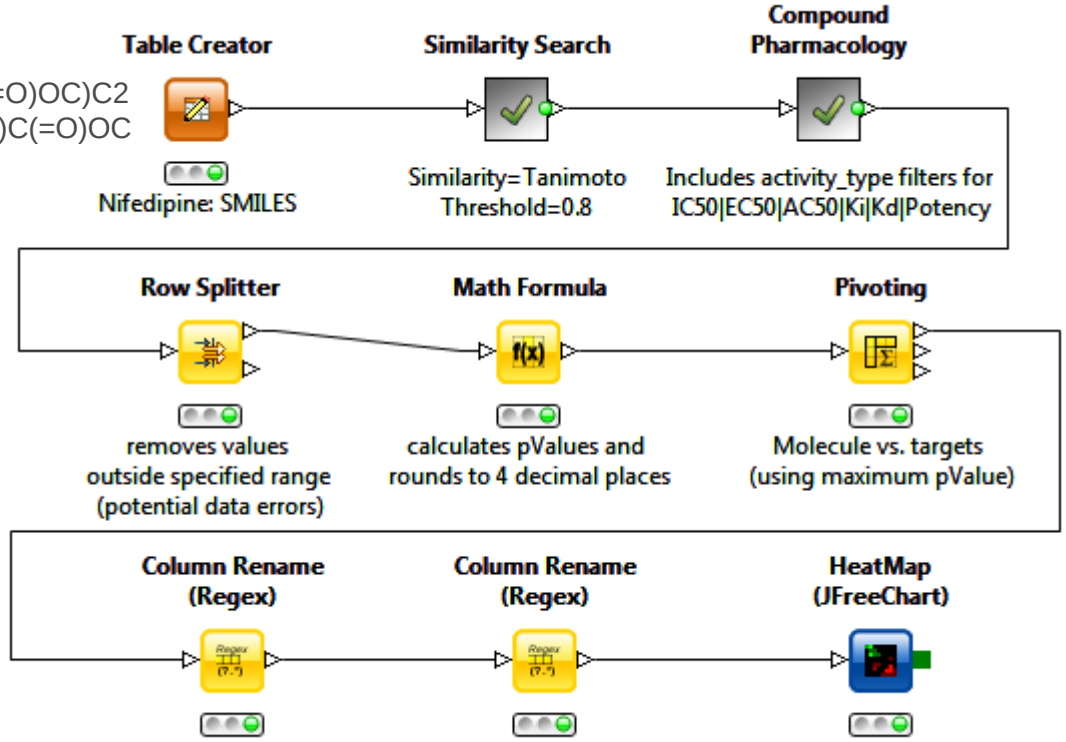
  - Example for any API call returning data from Concept Wiki: retrieves the URI from Conceptwiki.

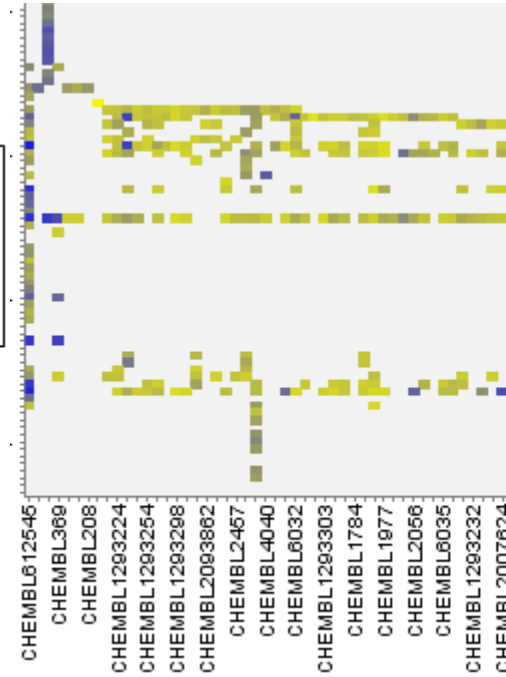
$..[?(@.inDataset== 'http://www.conceptwiki.org')]._about

Example workflow

- Q10: For a given compound, summarize all similar compounds and their activities

CC1=C(C(C(=C(N1)C)C(=O)OC)C2
=CC=CC=C2[N+](=O)[O-])C(=O)OC





Conclusions

- KNIME workflows allow the individual solution of research questions.
- All available Open PHACTS call can be accessed (if specified in the Swagger documentation).
- JSON Path or Xpath nodes allow individualized extraction of the data.
- But: not really user-friendly yet.

Outlook

- Next steps (by Evan Tzanis, QMUL):
- Open PHACTS Connector node: creates the API call and returns the results (JSON or XML)
- 1 node per API call (or API call group): returns tabular result

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Thank you for your attention!

- Open PHACTS – KNIME

Developers:

- Ronald Siebes, VU Amsterdam
- Evan Tzanis, QMUL

Testers:

- Christine Chichester, SIB
- Daniela Digles, UNIVIE
- Nick Lynch, Open PHACTS Foundation
- George Papadatos, EBI

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