



ChemAxon & KNIME integrations

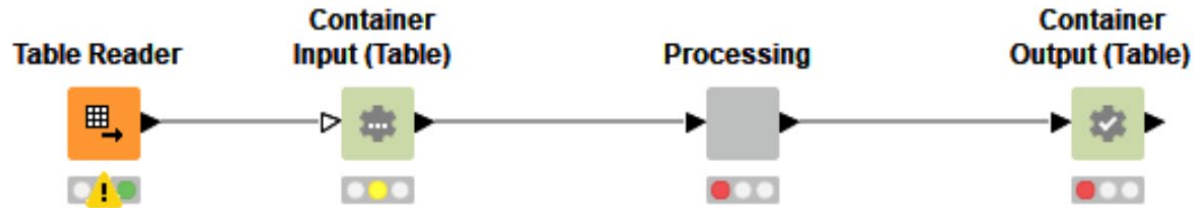
Medzi, KNIME AG

ChemAxon User Meeting Europe 2019

ChemAxon & KNIME integrations

- JChem Extensions for KNIME (including a few free ones)
 - Providing CXN tools in the usual KNIME node format, developed by Infocom
- MarvinJS in KNIME Server Web Portal
 - Versatile, familiar and friendly chemical sketcher for Guided Analytics Applications in the Browser
- Extending ChemAxon applications via KNIME Workflows
 - Choose best of breed components
 - Build workflows in KNIME AP
 - Deploy them via the KNIME Server REST API

How do I call the service?



▼ datascience1 (greg.landrum@https://datascience1.knime.com/knime/rest)

> Demos

> Events

▼ Users

> daria.goldmann

▼ greg.landrum

> Demo workflows

> Jupyter KNIME Jupyter

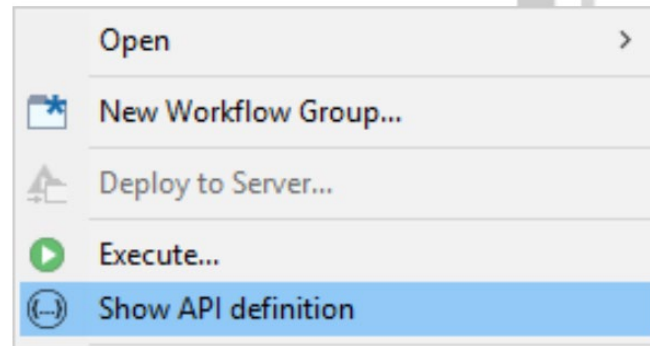
▼ KNIME Stories

> Reproducibility and Validatability

▼ Web service validation

01_Prediction_Workflow

> New Web Services



Input spec in Swagger UI

Request body application/json

Inline input parameters for the job

[Example Value](#) | [Schema](#)

```
{
  "molecule_input-250": {
    "table-spec": [
      {
        "compound_id": "string"
      },
      {
        "smiles": "Smiles"
      }
    ],
    "table-data": [
      [
        "ChEMBL_36_A_1",
        "CN(C)c1ccc(C2CC3(C)C(CCC3(O)C#Cc3ccc(C(C)(C)C)cc3)C3OCC4=CC(=O)CCC4=C23)cc1"
      ],
      [
        "ChEMBL_36_A_2",
        "CCc1cn(CCN)c(CC)c10c1ccc(C#N)cc1"
      ]
    ]
  }
}
```

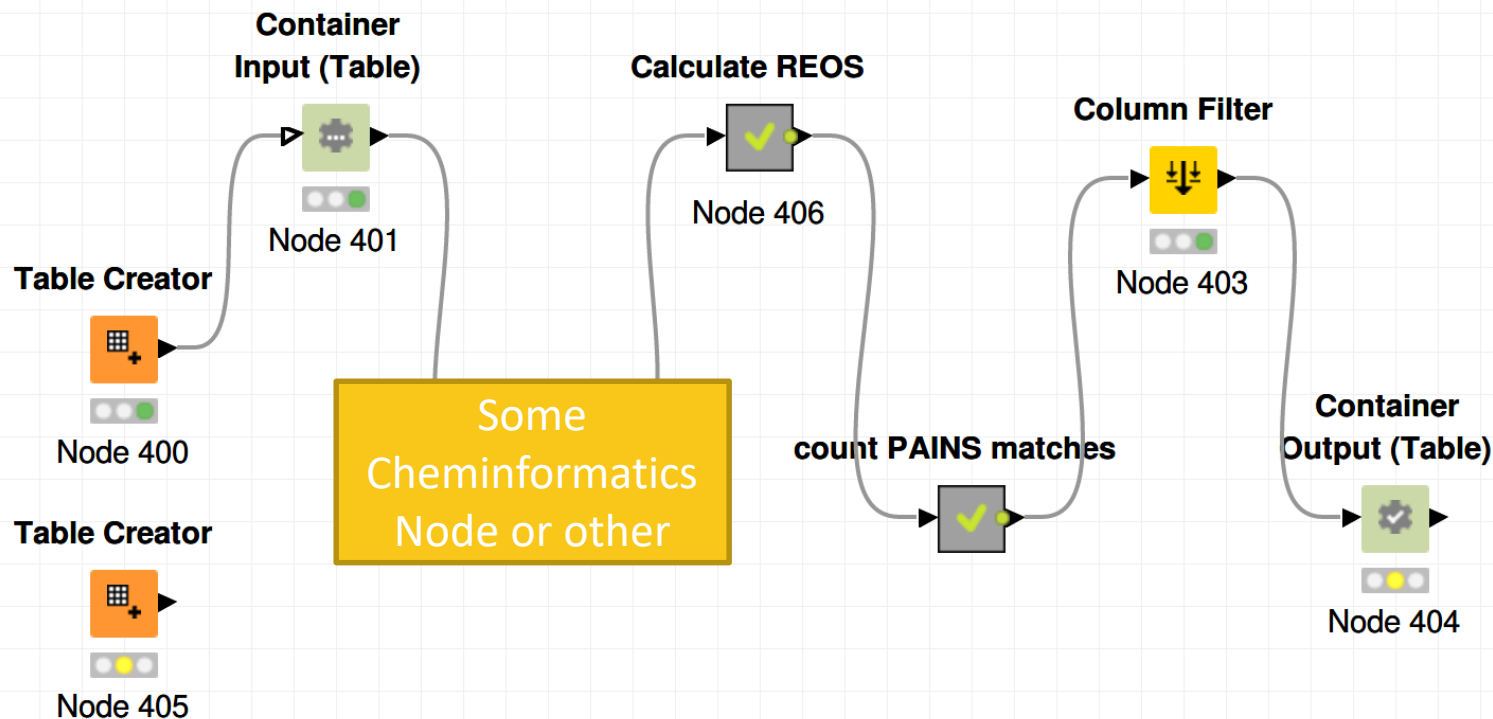
KNIME in Marvin (Live)



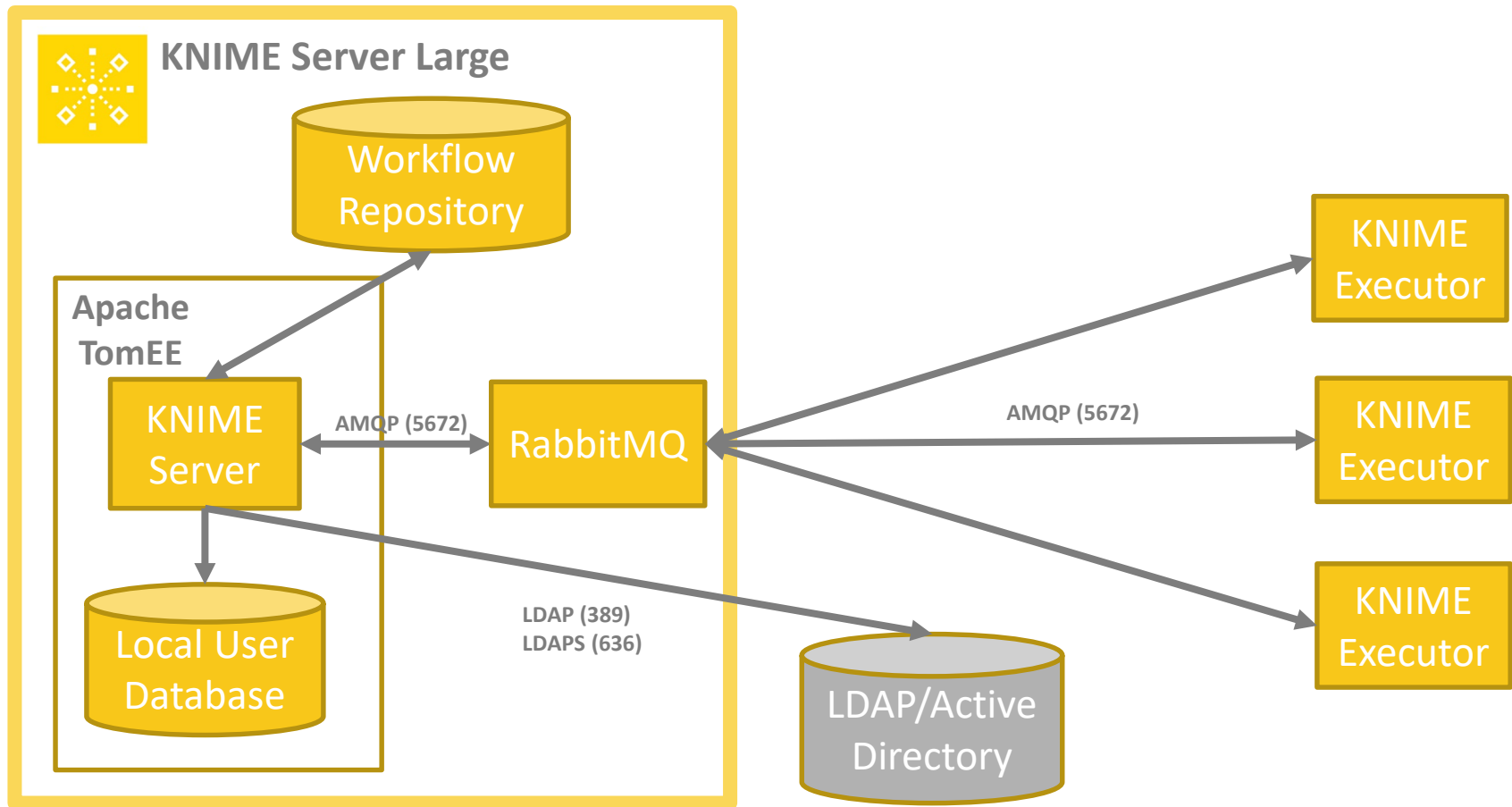
The screenshot displays the KNIME software interface. The main workspace shows a chemical structure of a benzamide derivative with a quinone ring system. The structure is O=C(NCc1ccccc1)C2=CC(=O)C=CC2=O. On the right side, there are two panels:

- REOS and PAINS**: This panel shows the matching PAINS rule(s) for the structure, which is `quinone_A(370)`. It includes a visual representation of the quinone ring system highlighted in red.
- Sweet Spot**: This panel displays a heatmap representing the Sweet Spot analysis. The y-axis is labeled **MW** (Molecular Weight) and ranges from 200 to 700. The heatmap shows a green region indicating a 'Sweet Spot' for the molecule, with a dashed orange line representing a trend line.

KNIME Workflow (courtesy of Greg Landrum)



Architecture: KNIME Server – Distributed Executors



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