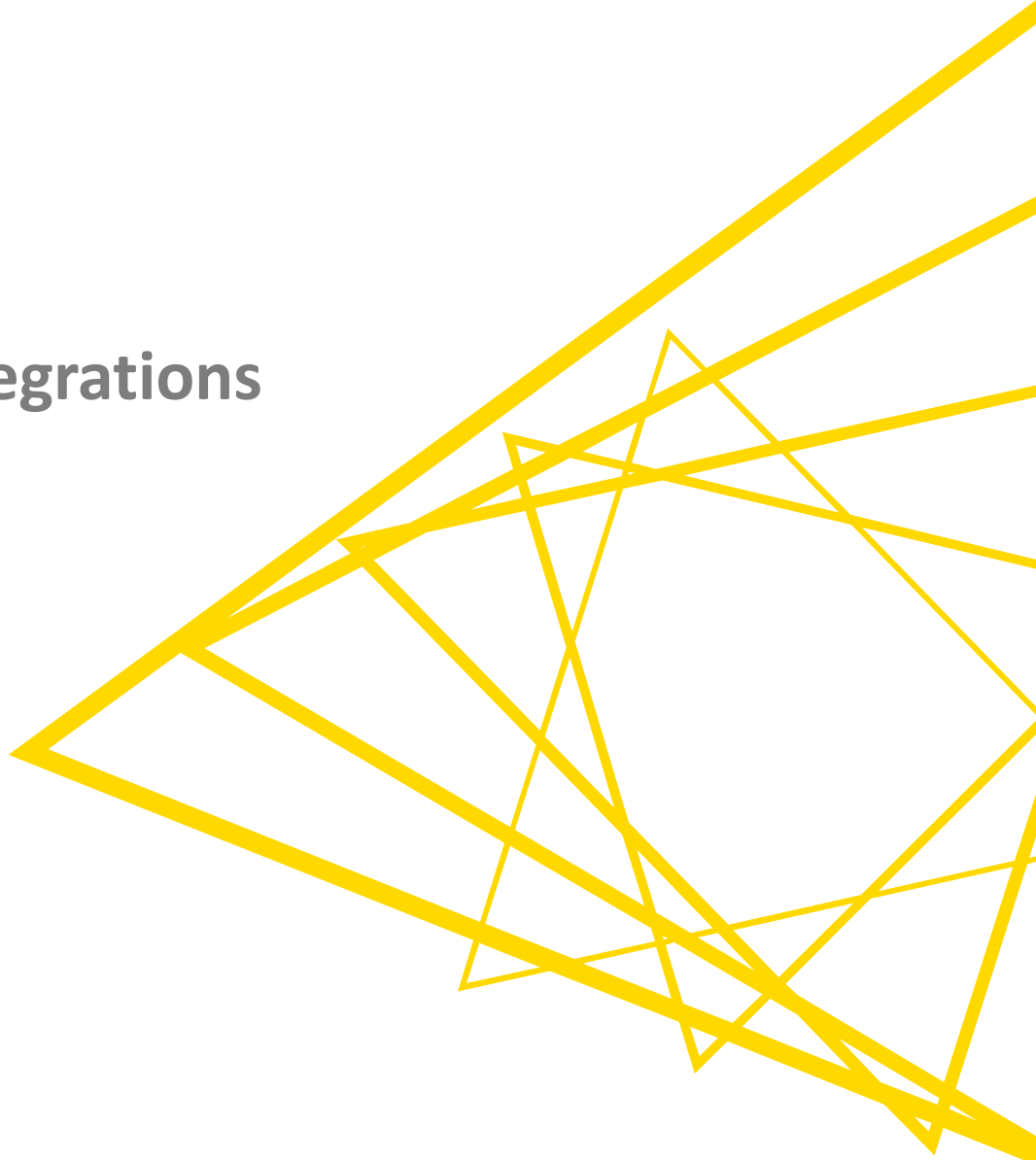
Open for Innovation ®
KNIME

# ChemAxon & KNIME integrations

Medzi, KNIME AG

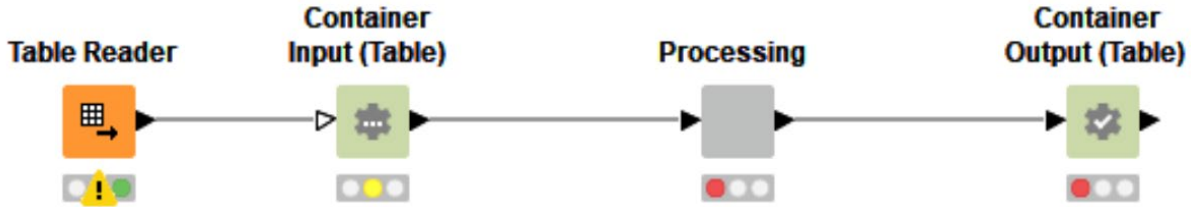
ChemAxon User Meeting Europe 2019

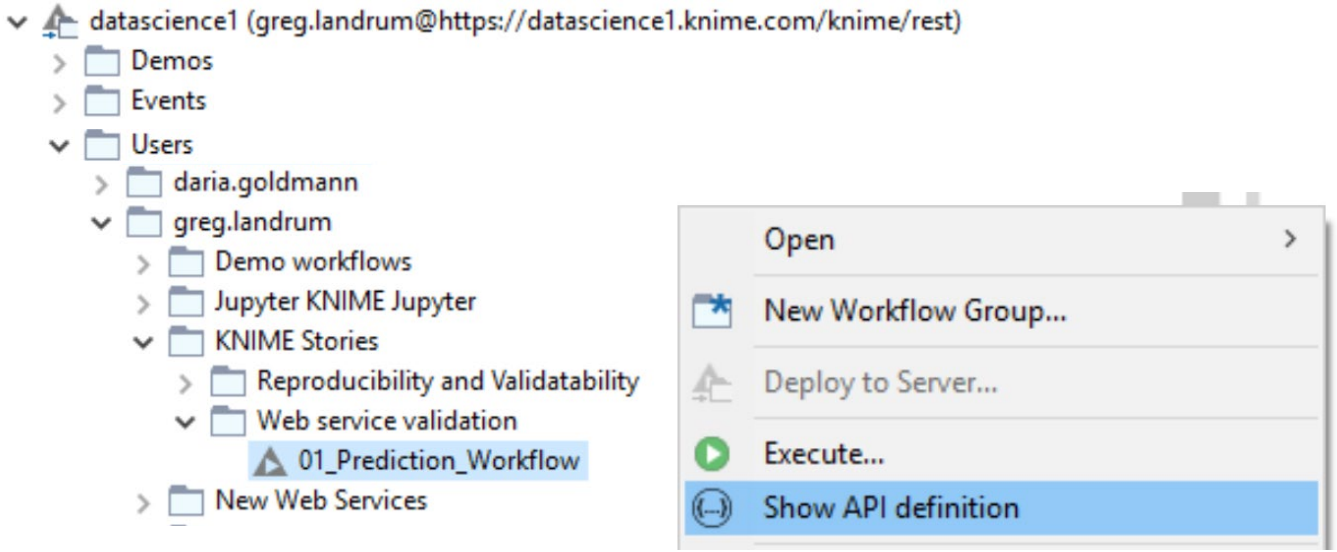


# ChemAxon & KNIME integrations

- 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?



# Input spec in Swagger UI

Request body | application/json

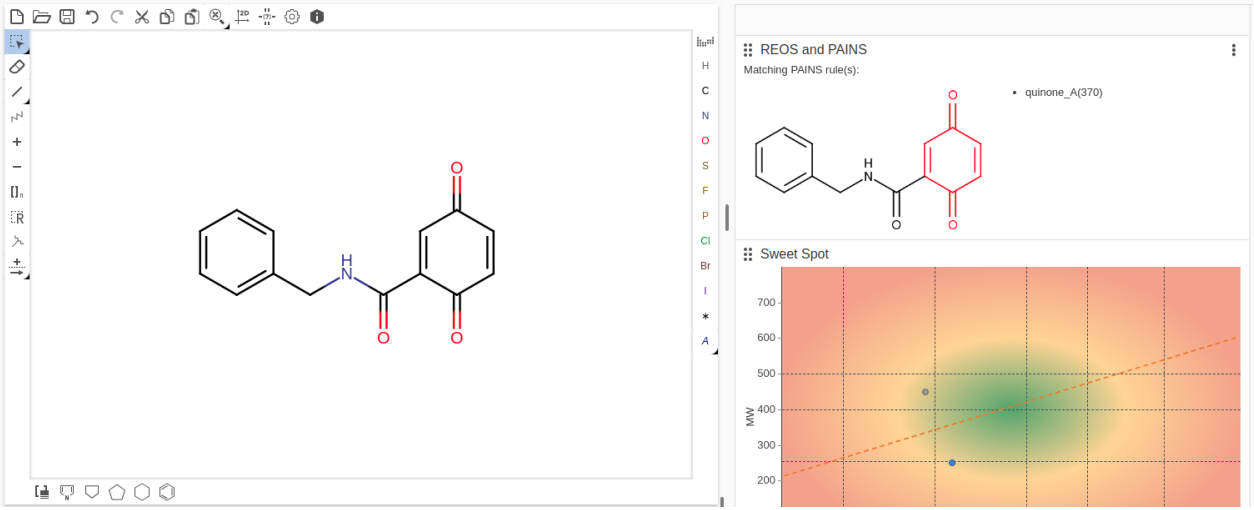
Inline input parameters for the job

**Example Value** | Schema

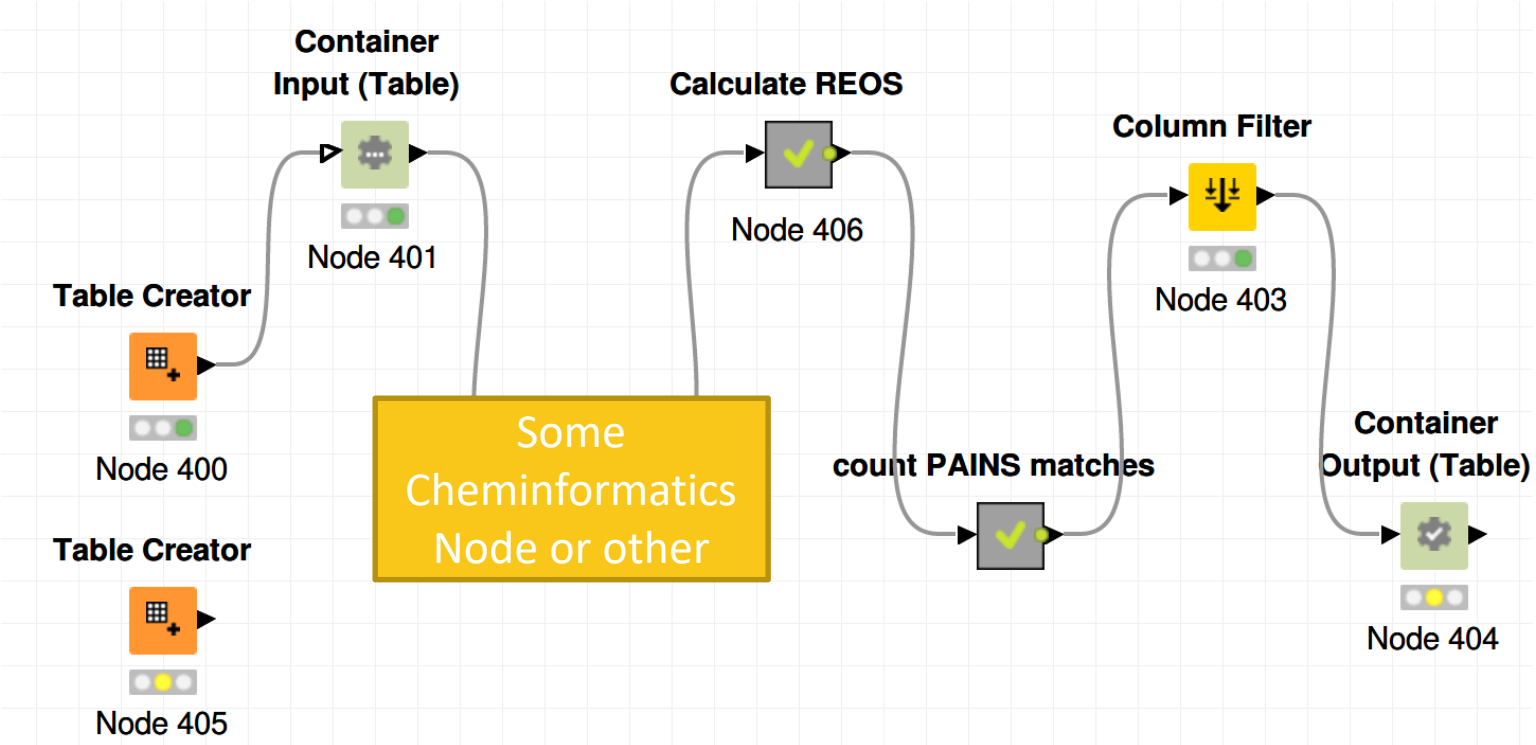

```
{
  "molecule_input-250": {
    "table-spec": [
      {
        "compound_id": "string"
      },
      {
        "smiles": "Smiles"
      }
    ],
    "table-data": [
      [
        "ChEMBL_36_A_1",
        "CN(C)c1ccc(C2CC3(C)C(CCC3(O)C#Cc3ccc(C(C)(C)C)cc3)C3OCC4=CC(=O)CCC4=C23)cc1"
      ],
      [
        "ChEMBL_36_A_2",
        "CCc1cn(CCN)c(CC)c1Oc1ccc(C#N)cc1"
      ]
    ]
  }
}
```

# KNIME in Marvin (Live)

Rules — KNIME — KNIME Server — Plugin



# KNIME Workflow (courtesy of Greg Landrum)



# Architecture: KNIME Server – Distributed Executors