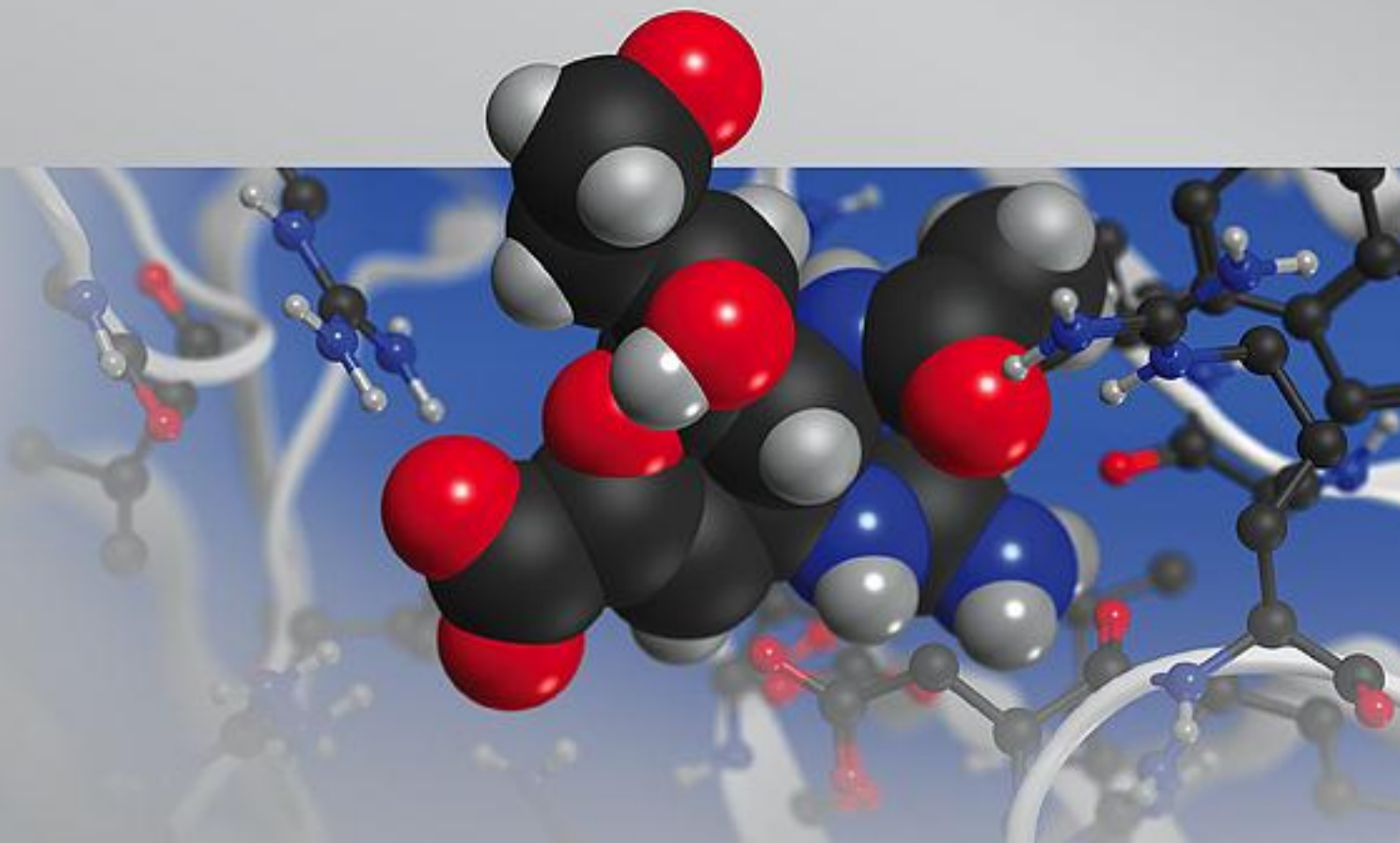
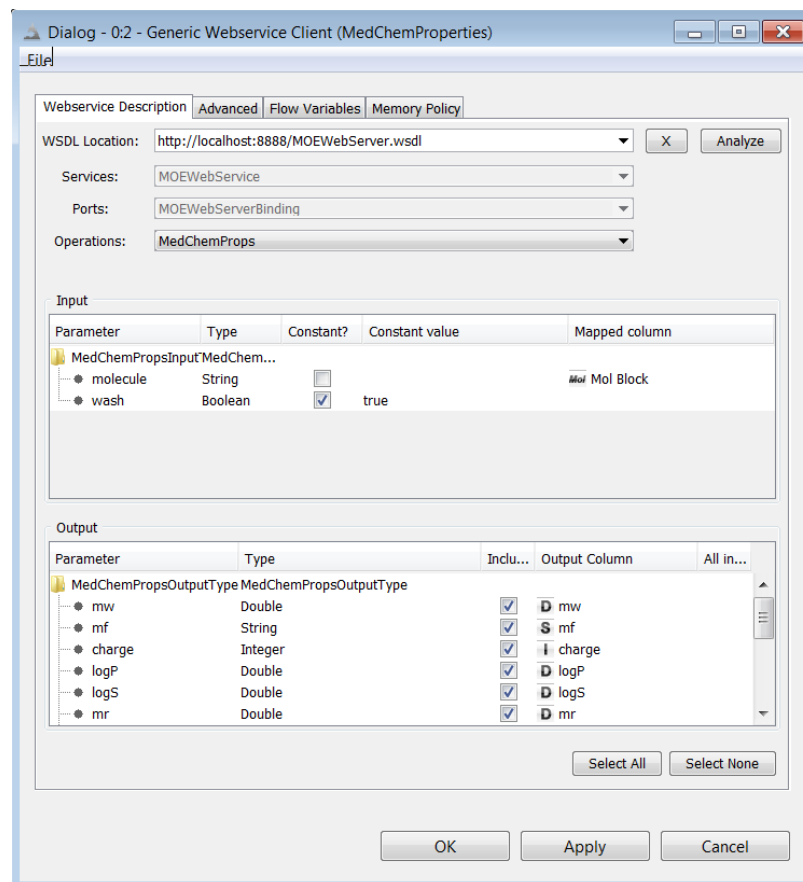
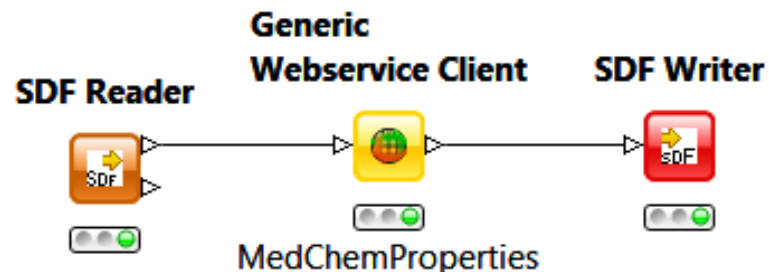


Bringing MOE and KNIME together



MOE SOAP Server

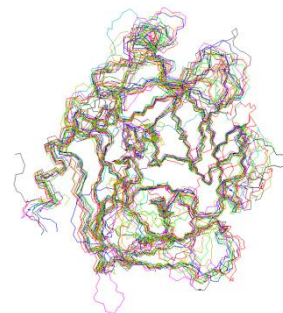
- **SOAP Server is part of MOE Release**
 - Standardized protocol can be accessed by many different clients
 - Runs MOE/batch sessions
- **Four Applications included**
 - Depiction Layout
 - MedChem Properties
 - Mol To SMILES
 - SMILES To Mol
- **Add custom SOAP functionality with SVL programs**
 - Full documentation available
- **KNIME Web service Client**
 - Analyzes the WSDL file
 - Runs on MolCells



MOE Extensions for KNIME

- **Extensions available free of charge from CCG Support**

- 100+ Nodes included
- Renderers for Molecules, Sequences and Plots
- MOE/batch like speed



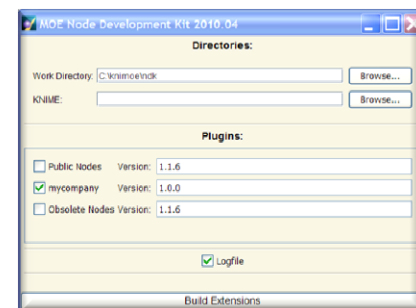
- **Full Support of KNIME features**

- File Drag and Drop
- Optional, Model and Image Ports
- 18+ Data Types supported including 6 for molecules
- Improved compatibility with 3rd party nodes

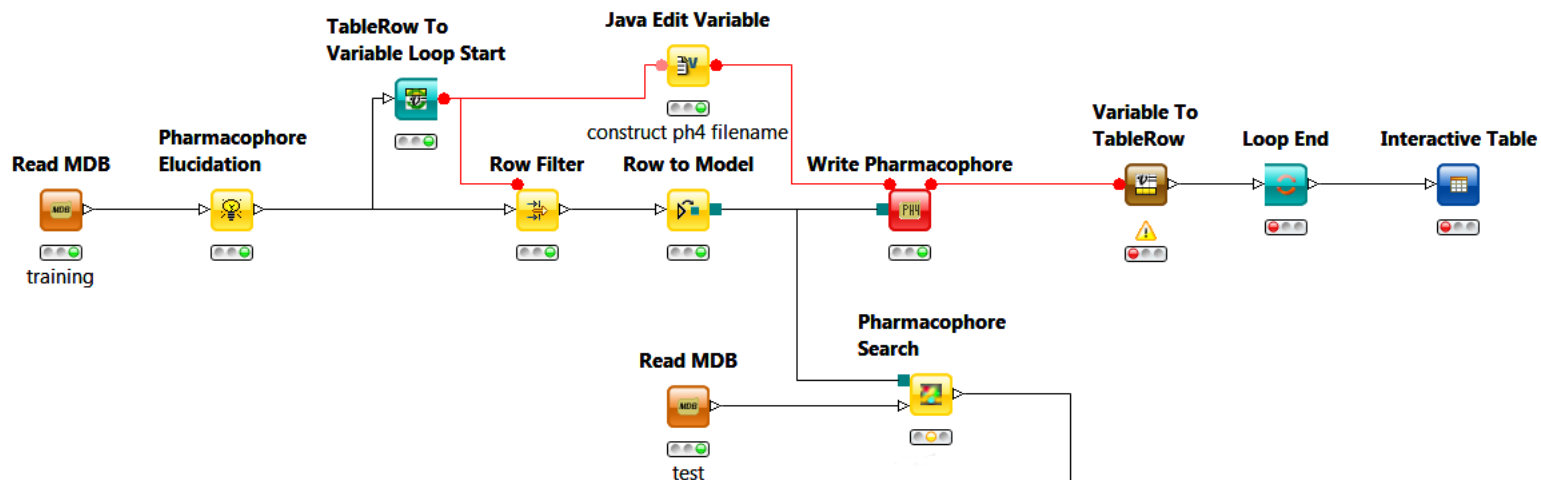


- **Node Development Kit**

- Compile custom nodes from SVL sources
- Open source (readable and editable by user)
- Easy Installation and Deployment



Workflow Example: Pharmacophore Elucidation



- Multiple Pharmacophore Models are created
- KNIME Loop Nodes can be used to access the individual models or vary the configure options
- Fast method to create 3D alignments

see also:

Pradon, Juliette

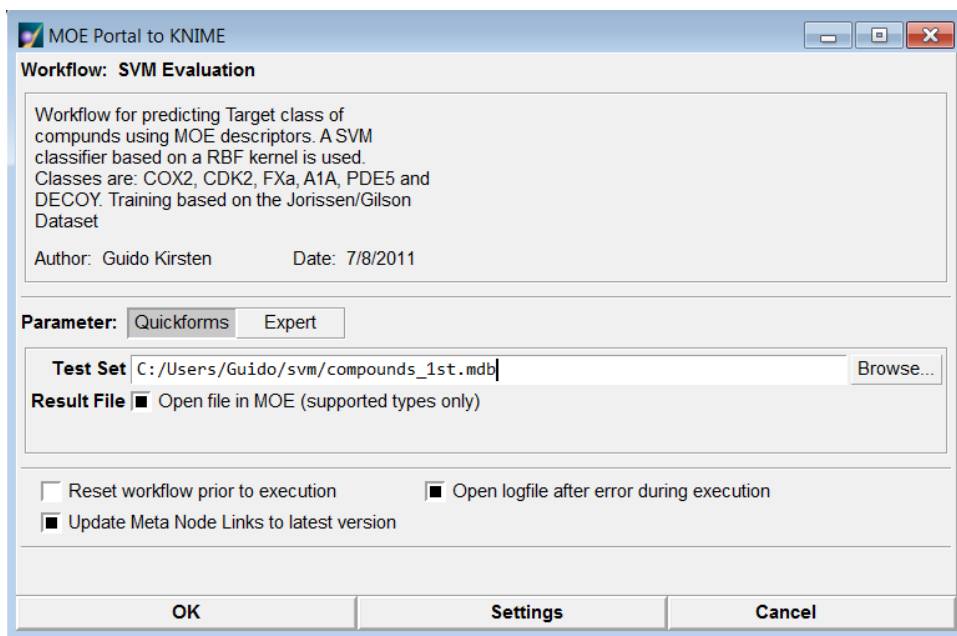
A New Approach for Chemotype Enrichment in Ligand Based Design

UK-QSAR Meeting Autumn 2010

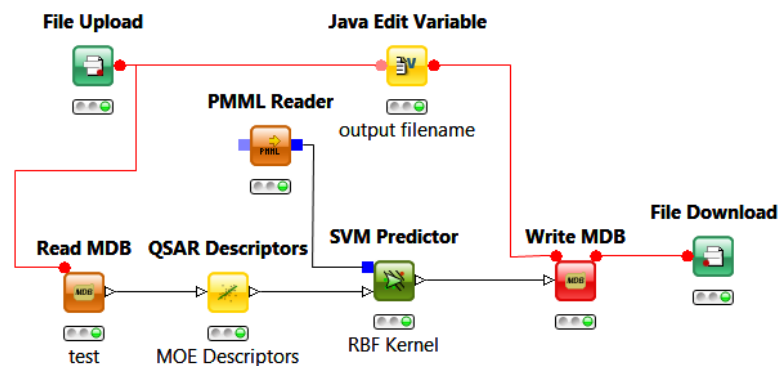
www.ukqsar.org/slides/JuliettePradon_A2010.pdf

MOE Portal for KNIME

- **SVL available from SVL Exchange**
 - Graphic user interface to run KNIME batch jobs from MOE
 - All workflow options can be adjusted
- **Quickform Nodes**
 - Quickforms can be used to influence panel layout
- **Visualize Results in MOE**
 - Result files can be opened automatically



SVM Classification Workflow



MOE / KNIME Interfaces

▪ MOE SOAP Server access for KNIME

- Java based server allows easy installation
- Easy deployment of MOE/batch applications
- Access through Web Service Client Node



▪ MOE Extensions for KNIME

- 100+ Nodes
- MOE/batch like speed
- Supports KNIME 2.4 features
(File Drag & Drop, URI's, Flow Variables, Types, ...)
- Node Development Kit



▪ MOE Portal for KNIME

- Batch execution of KNIME workflows in MOE
- Support for Quickform Nodes
- Visualize results in MOE

