

JChem Extensions for KNIME



Takahiro Ohshima



ChemAxon



Tímea Polgár

*2011 March, Zurich
4th KNIME User Group Meeting*

ChemAxon's Support



ChemAxon

Technical Support Forum

Access ChemAxon scientists and developers here. For confidential or other support please [email](#).

[FAQ](#) [Search](#) [Usergroups](#) [Digests](#)

[View posts since last visit](#)
[View your posts](#)
[View unanswered posts](#)

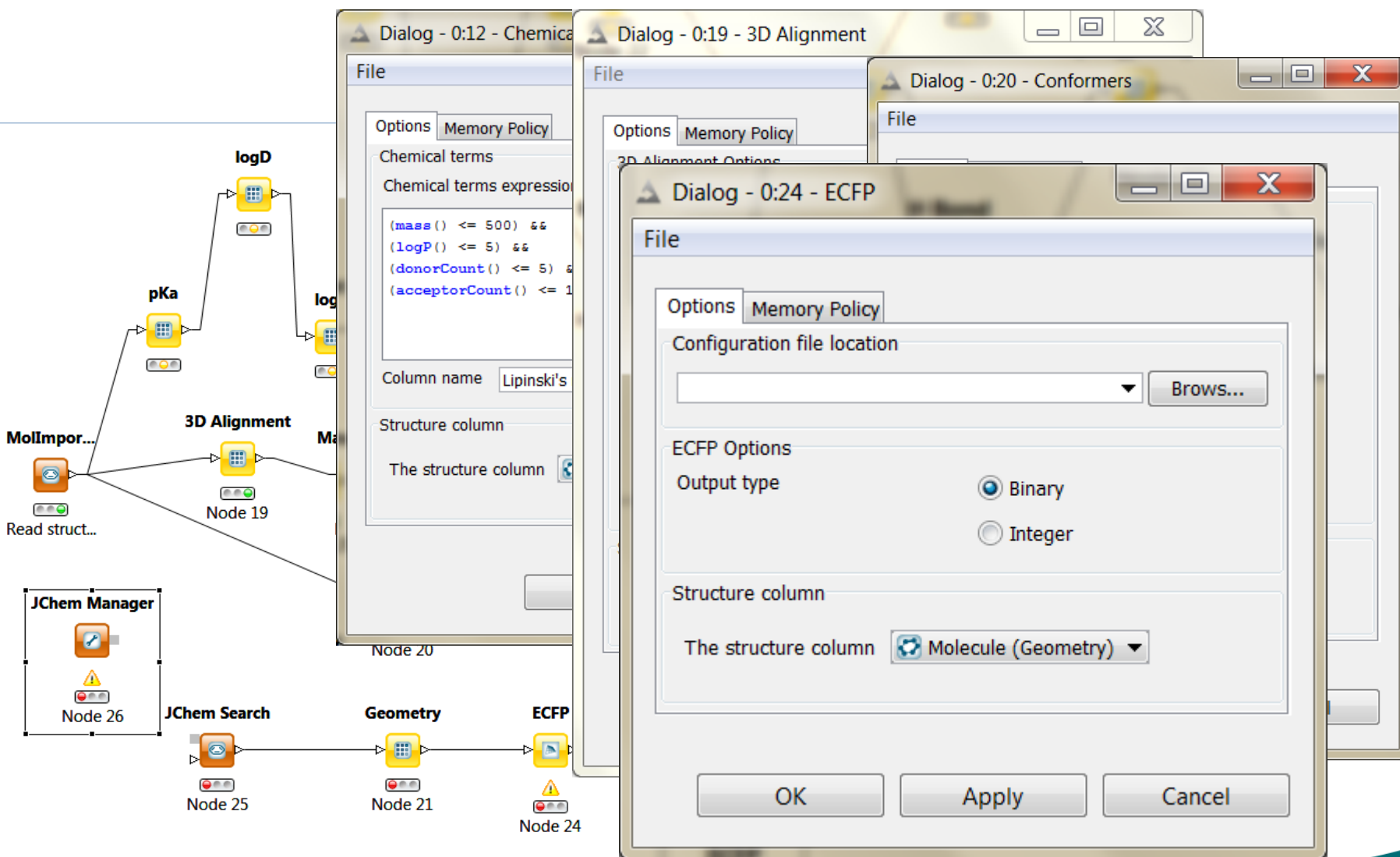
[My Forum Profile](#)

[Log out \[tpolgar\]](#)

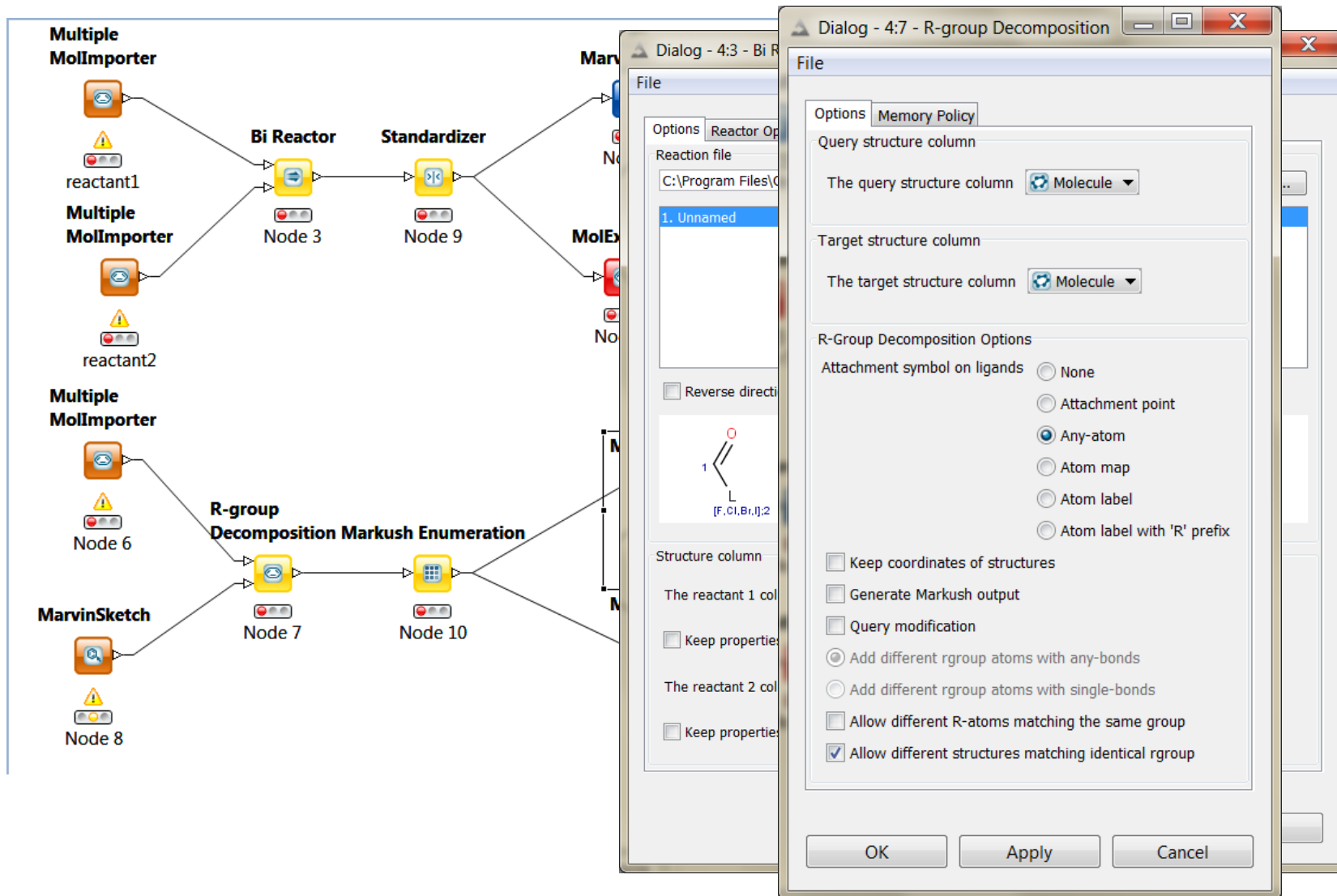
ChemAxon.com > Forums

Support	Topics	Posts	Status	Last Post
Drawing & visualization: Marvin/Sketch /View /Space Support for MarvinSketch, MarvinView, MarvinSpace, file formats and image generation	1635	8494	Open	Fri Jul 09, 2010 3:28 pm bobor ↗
Storage & search: JChem Base /Cartridge Support for JChem Base and JChem Cartridge.	1001	5802	Open	Fri Jul 09, 2010 1:24 pm vmltsev ↗
Storage & search: Instant JChem Support for Instant JChem (Structure database GUI, batch Calculator Plugin processor etc)	461	2013	Open	Mon Jul 12, 2010 8:28 am tudqeen ↗
Storage & search: Markush search & enumeration Support for Markush search & enumeration, in Marvin, JChem Base, JChem Cartridge & Instant JChem	26	97	Open	Thu Jun 17, 2010 5:36 pm Nora ↗
Storage & search: JChem for Excel JChem for Excel support forum	77	295	Open	Sat Jul 10, 2010 12:10 pm proximity4 ↗
Structure based predictions: Calculation Plugins & Chemical Terms Support for structure based prediction/calculations, such as lopP, pKa, tautomers, conformers, etc.	346	1878	Open	Mon Jul 12, 2010 12:14 pm Zsolt ↗
Library profiling: Virtual screening, clustering & molecular descriptors Support for Screen & JKlustor	173	762	Open	Wed Jul 07, 2010 5:46 pm adrian ↗
Structure manipulation: Canonicalization / standardization Support for Standardizer and Structure Checker	122	535	Open	Fri Jul 09, 2010 9:36 am Gyuri ↗
Structure manipulation: Reactor & Fragmenter Support for Reactor & Fragmenter	188	1052	Open	Mon Jul 12, 2010 9:36 am mvarqvas ↗
Integration: KNIME Support for ChemAxon's KNIME (Konstanz Information Miner) nodes	3	4	Closed	Mon Jul 12, 2010 3:47 am tohshima ↗
Integration: Pipeline Pilot Support for ChemAxon's Pipeline Pilot component collection	17	61	Open	Fri Jul 02, 2010 2:28 am Szilard ↗
Integration: .NET Support for Marvin and JChem .NET API	40	209	Open	Thu Jan 01, 1970 1:00 am ↗
Integration: Web Services and AJAX Support for ChemAxon's JChem Web Services Server, SOAP Interface. Usage from AJAX, Python and other languages	43	295	Open	Tue Jul 06, 2010 10:46 am ilee ↗
Other: Naming topics & chemicalize.org Support for name <-> structure & the chemicalize.org web service	25	94	Open	Mon Mar 01, 2010 5:02 pm nrcrci ↗
Other: License issues Support for the technical questions related to license handling	75	368	Open	Sat Jul 10, 2010 3:01 am wucy ↗

Example workflow 1



Example workflow 2



www.chemaxon.com

Thank you for your attention