



Christian Lemmen

BioSolveIT - KNIME Nodes



Current BioSolveIT KNIME Nodes

Molecular Similarity

Database



FTrees Similarity

Similarity Search



FlexX Docking

Fragment Spaces

Drug Design



FlexS Alignment



Naomi Filter Converter

Docking

De Novo Design



Interactive Table Viewer



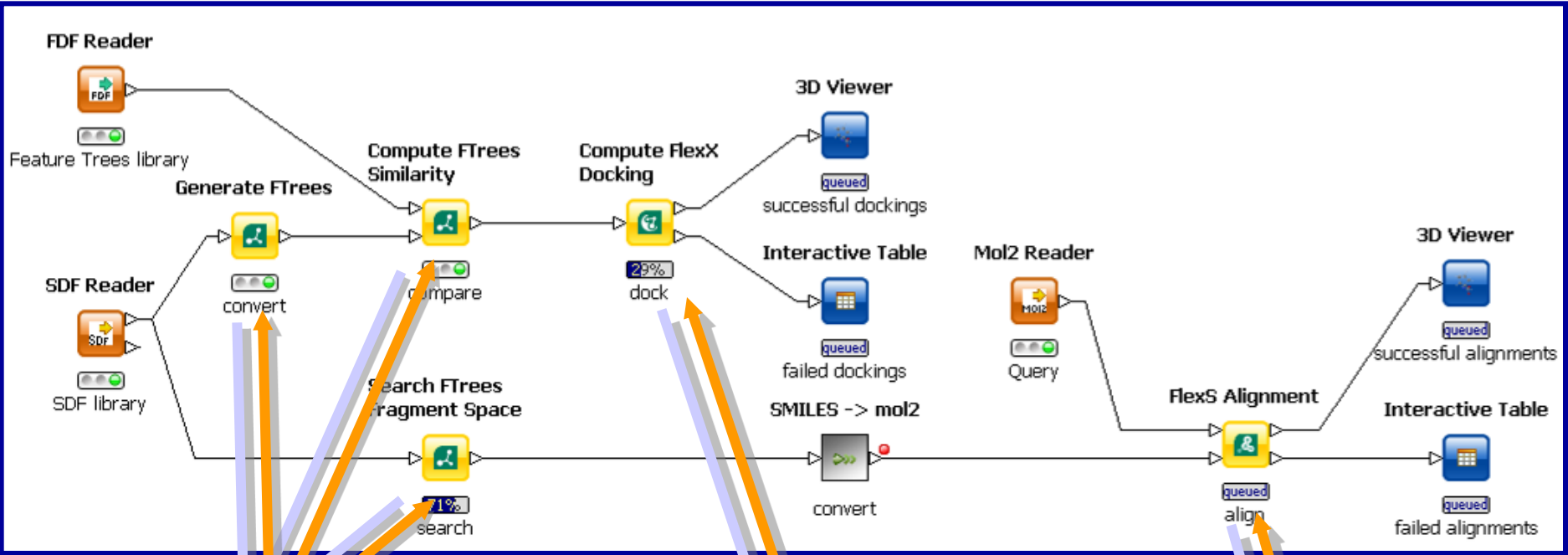
Interactive 3D Viewer

Scaffold

Molecular Alignment

Replacement

KNIME Interface Nodes



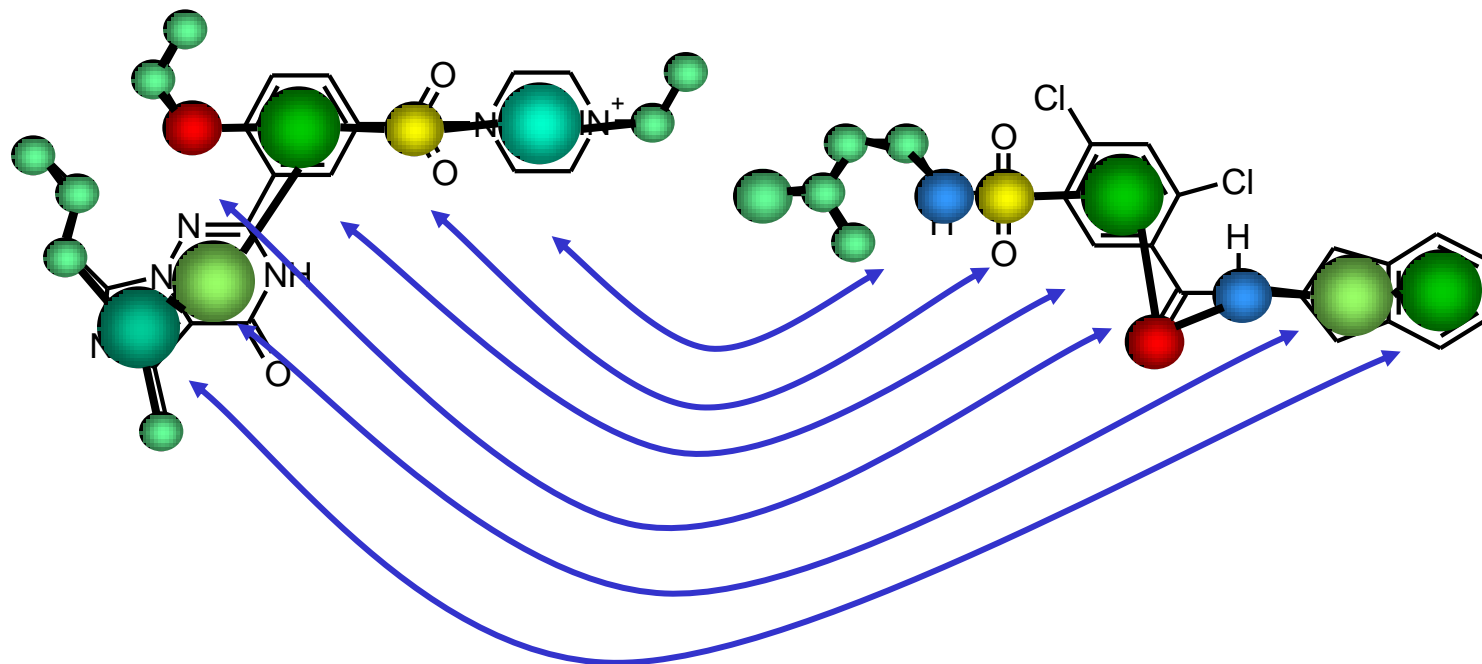
Similarity



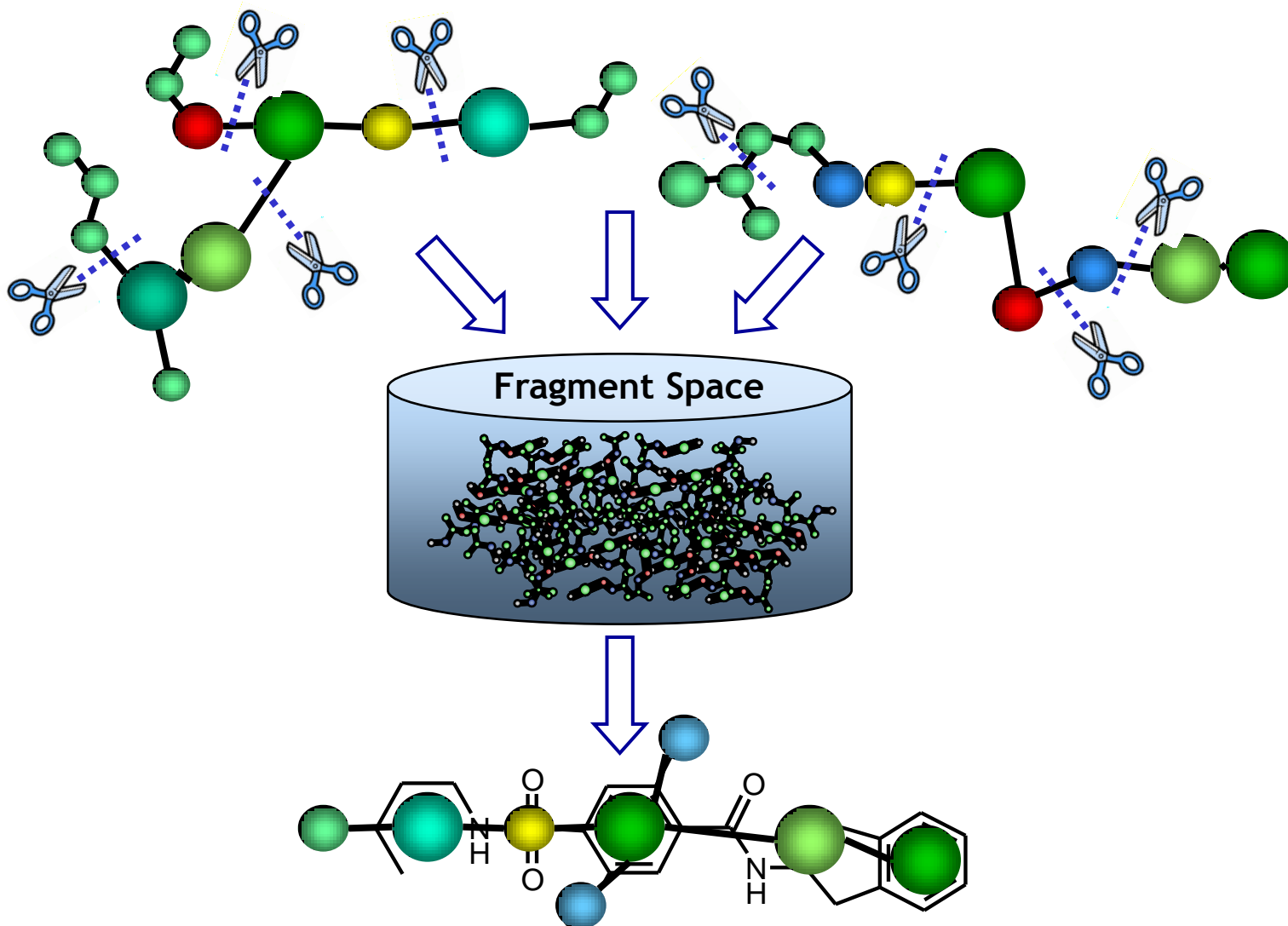
Docking



Alignment

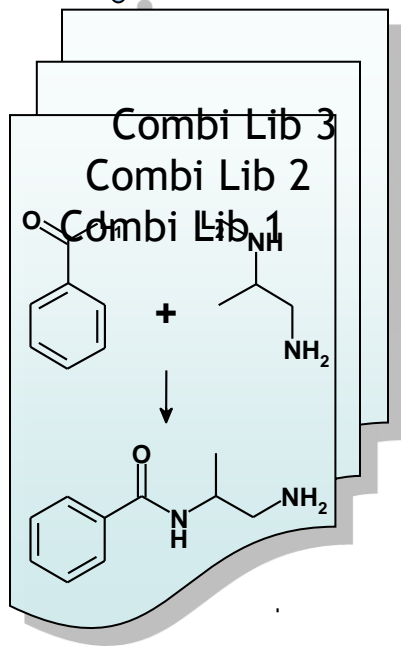


- FTrees Similarity: 0.85
 - global for whole molecule
 - local for each match
- Mapping of substructures

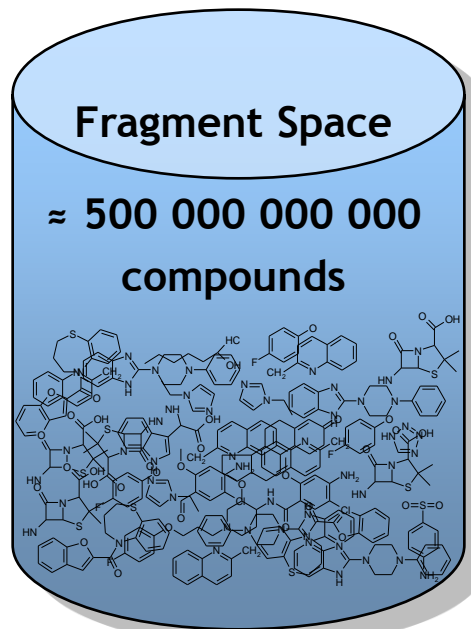
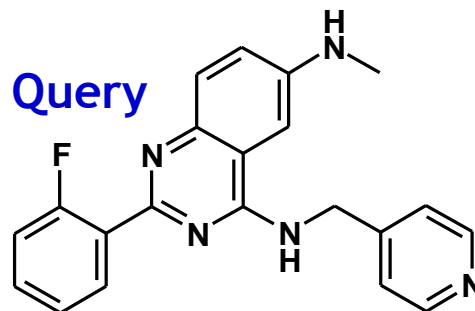


within a few minutes

In-house
chemical
knowledge

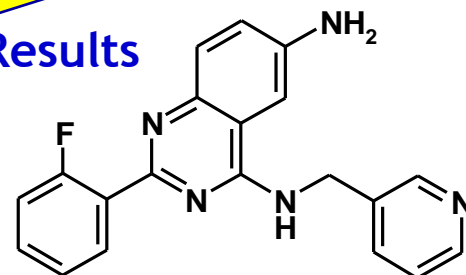


Encode & Unify

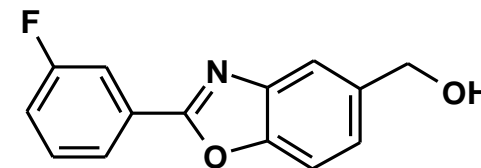


Search in Fragment Space

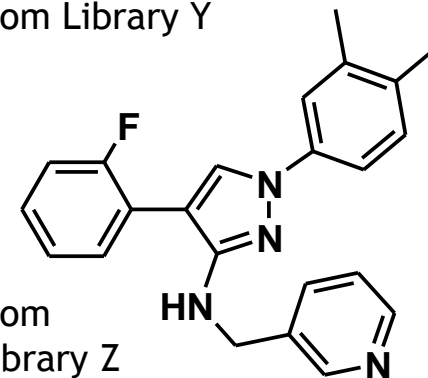
Results



from Library X



from Library Y



from
Library Z



4dfr* - LeadIT 1.0.0 (20.01.10)

LeadIT Receptor Docking ReCore Display Window Help

Receptor (4dfr)

Resolve Chemical Ambiguities

Use protonation from: FlexX default Input file

Assignments (O ↔ N), Protonation & Torsions (Θ)

AA-Chain	O ↔ N	Protonation	Θ1	Θ2
THR-35-A		thr	180	
THR-46-A		thr	180	
SER-49-A		ser	180	
ARG-52-A		arg+		
ARG-57-A		arg+		
TYR-100-A		tyr	0	
TYR-111-A		tyr	0	
THR-113-A		thr	180	

Water

Water	Type	Φ	Ψ	Θ
<input type="checkbox"/> HOH-4-*				
<input type="checkbox"/> HOH-72-*				
<input type="checkbox"/> HOH-219-*				

Show water with at least 2 interaction(s)

Assistant

Resolve Chemical Ambiguities

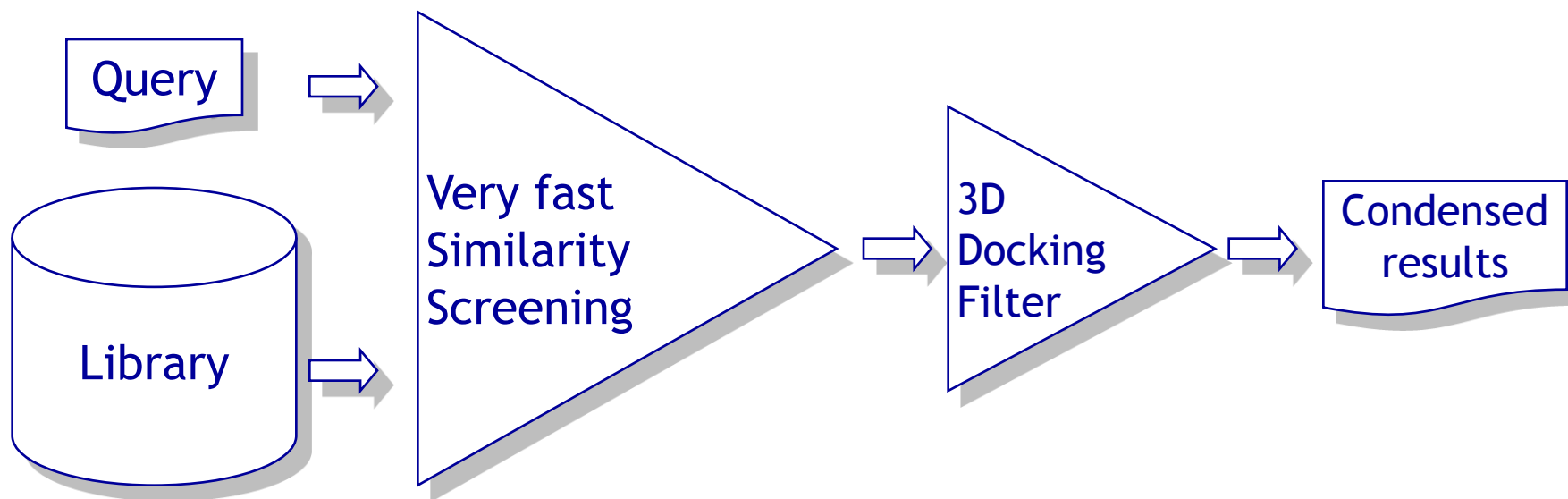
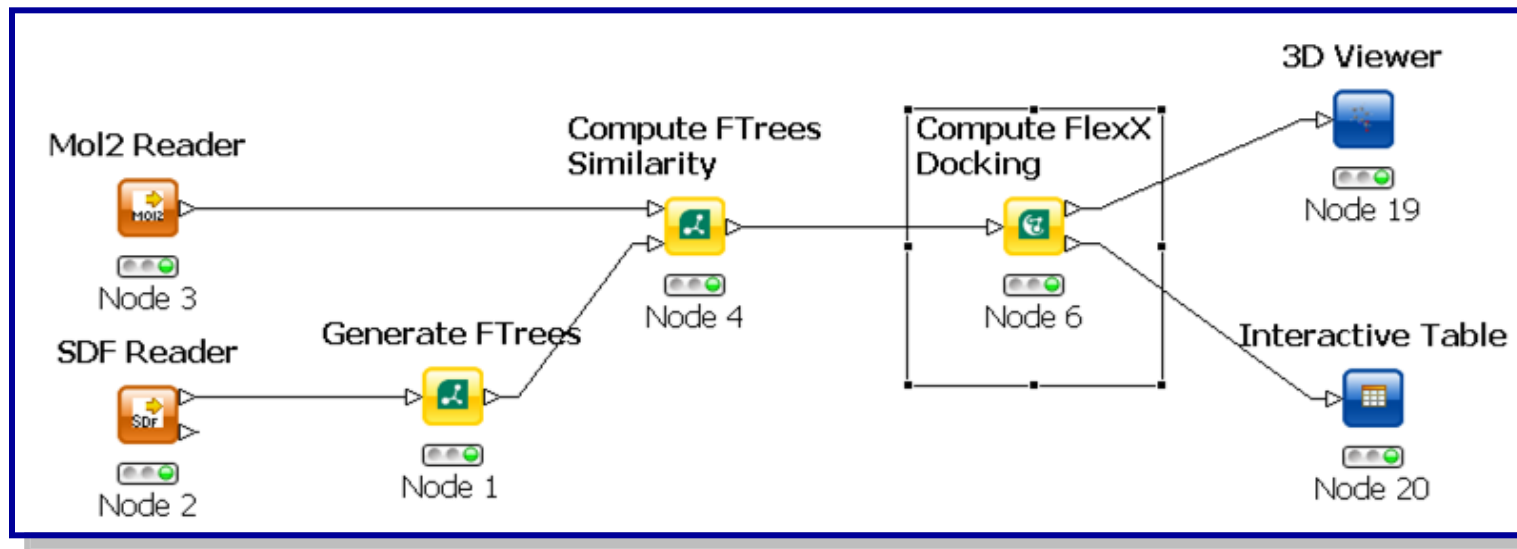
Here, protomers and tautomers are assigned (or adjusted if crystallography has left you with freedom). Also, water inclusions and specifications are made here.

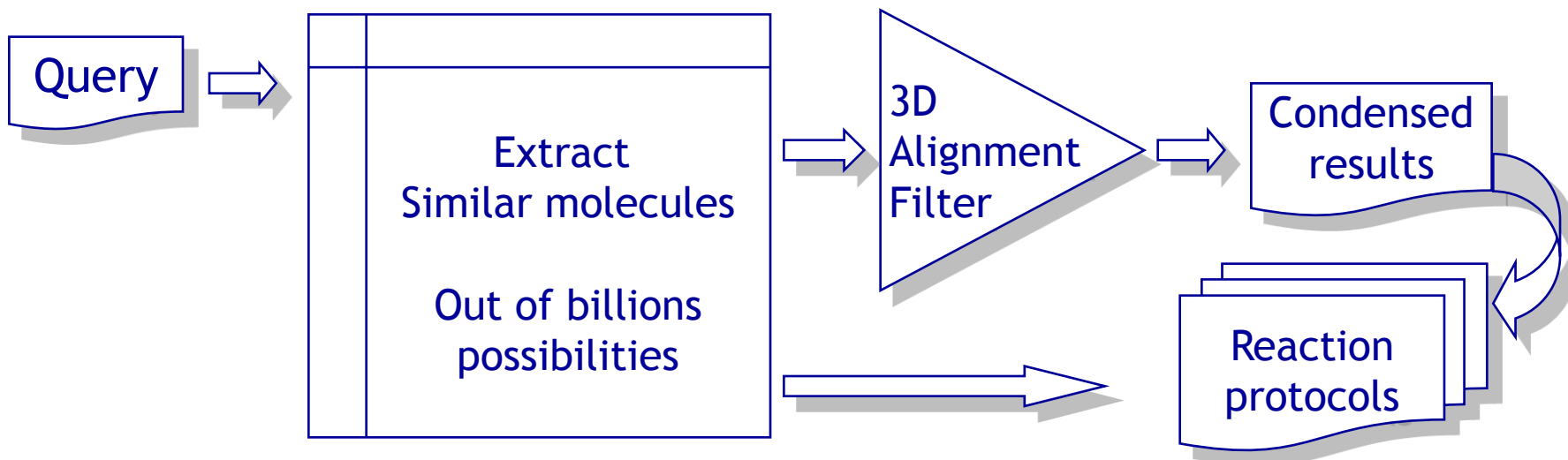
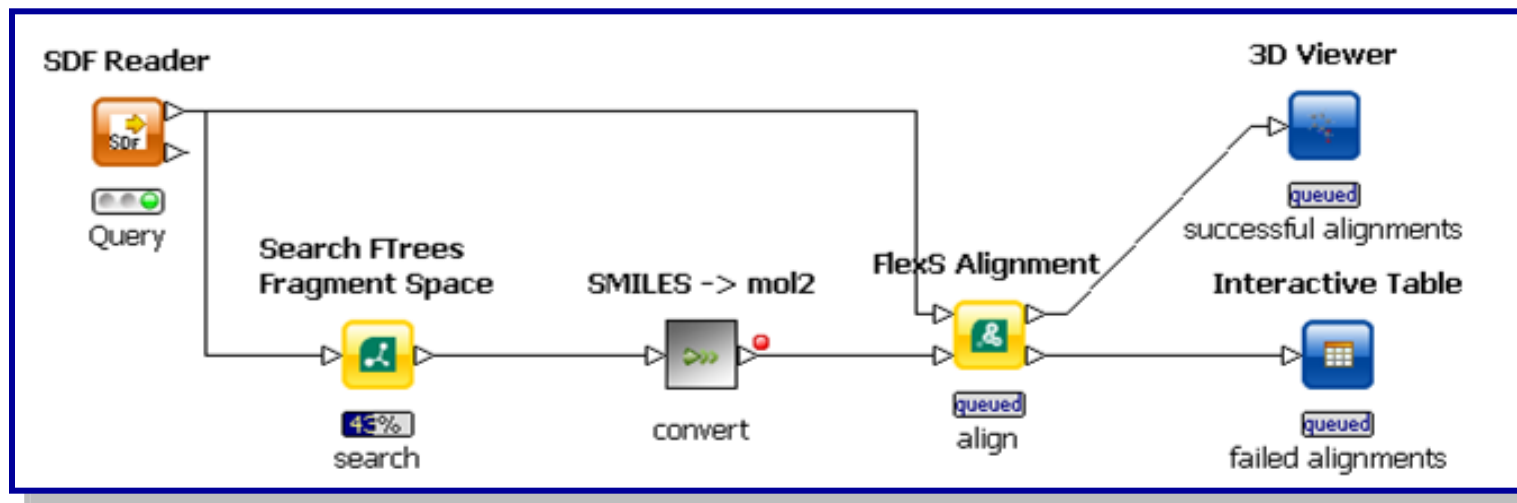
Orange entries denote that you must resolve an ambiguous state of a residue. As long as there are still orange entries, reaching the next step is blocked.

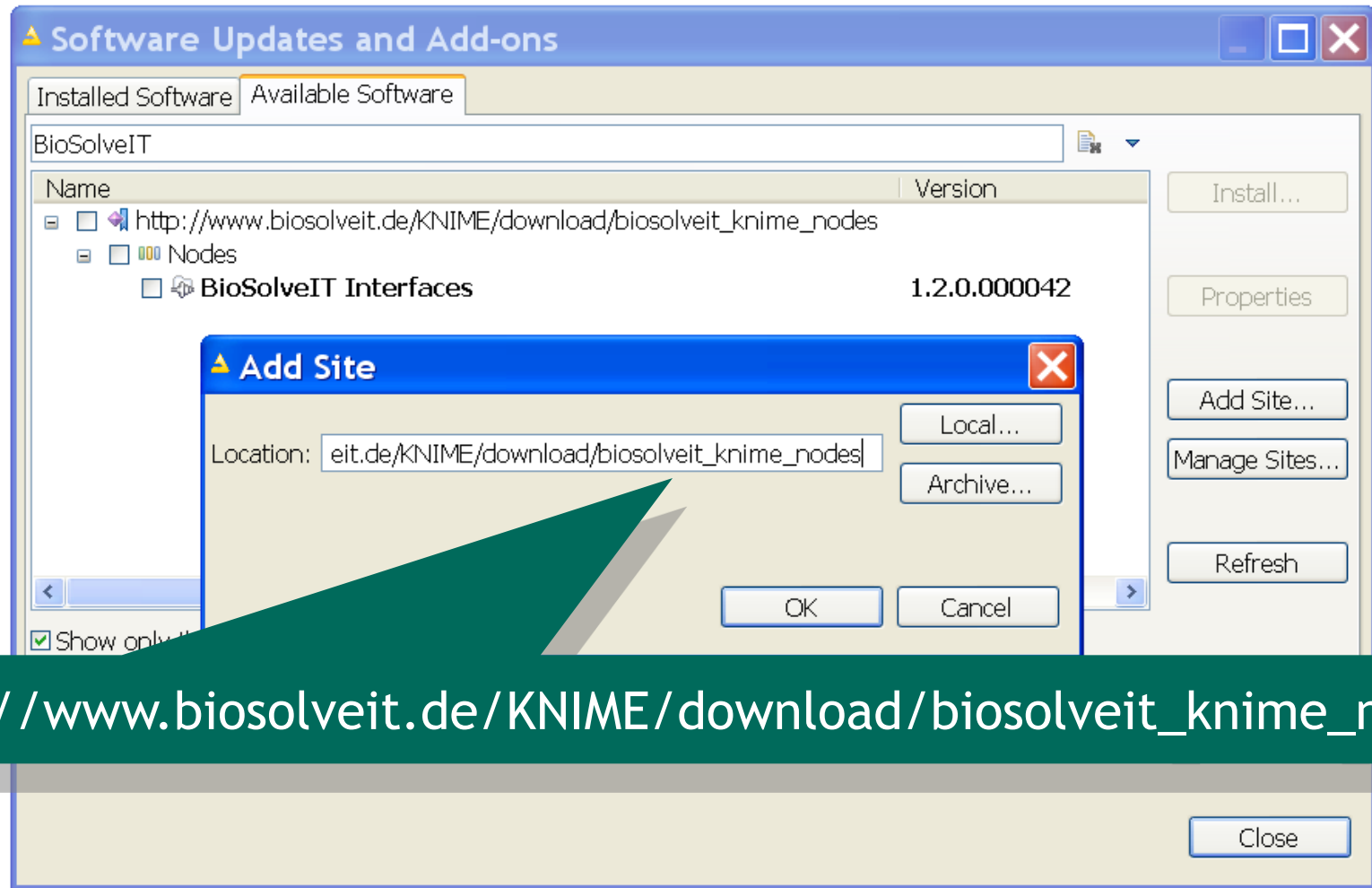
HINT for torsions adjustments:
Point your mouse above the orange entry, then use your mouse wheel to interactively turn γ H bonds around the respective torsion.

Colored lines may help to find sensible tautomers and/or H positions.

Project Tree Receptor (4dfr) Free Notes Area Assistant Information Stream







http://www.biosolveit.de/KNIME/download/biosolveit_knime_nodes

More Information on the Web



<http://www.biosolveit.de/KNIME/>

The screenshot shows the BioSolveIT website interface. At the top, the BioSolveIT logo and tagline "The Premier Scientific Solution Provider" are visible. A navigation menu on the left includes sections like HOME, LeadIT, APPLICATIONS (with sub-items like Docking, Alignment, Similarity, etc.), SUPPORT, SERVICES, DOWNLOAD, and COMPANY. The main content area is titled "KNIME® Interfaces" and features a sub-header "BioSolveIT software available in KNIME® now!". Below this, a workflow diagram is displayed with nodes such as "Search FTrees Fragment Space" (Node 14), "Histogram" (Node 18), "Compute FTrees Similarity" (Node 12), "Concatenate" (Node 11), "Compute FlexX Docking" (Node 15), "Molecule to CDK" (Node 20), "Generate FTrees" (Node 13), "Table Writer" (Node 19), "Histogram" (Node 17), and "Interactive Table" (Node 10). A sidebar on the right contains links for "documentation", "support", "installation for 2.1", "installation for 2.0", "source code", and "screenshot".

More Information on the Web



<http://www.biosolveit.de/KNIME/>

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