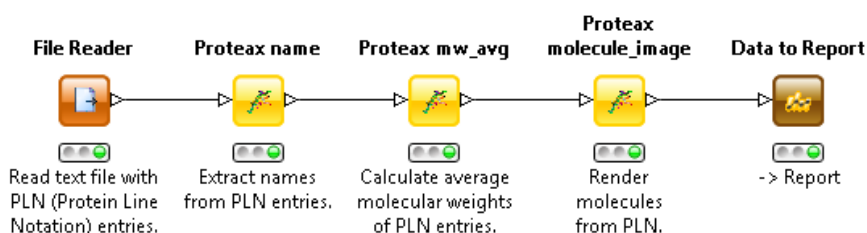


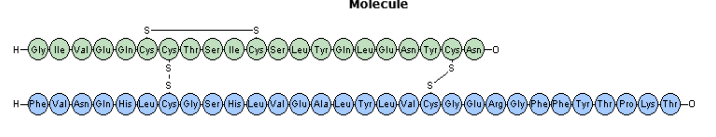
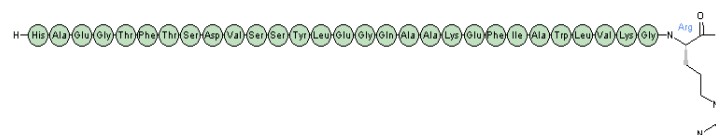
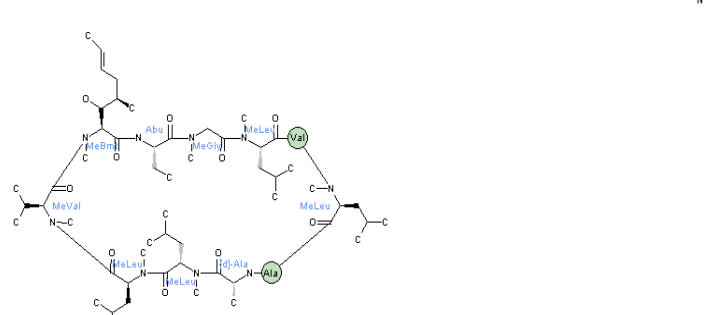
Proteax for KNIME

Biochemfusion introduces **Proteax® for KNIME** nodes - protein chemistry nodes for analyzing, manipulating, and visualizing peptides and proteins inside KNIME™.

- Supports protein sequences with modified residues, terminals, disulfide bridges and lactam cyclizations.
- On-the-fly translation from chemical structure to sequence and generation of chemical structure from sequence.
- Protein comparison and naming for readable protein SAR tables.
- Generate protein derivatives via naming expressions.
- Supports mass-spec analysis via import/export to Lighthouse Data's GPMW format.

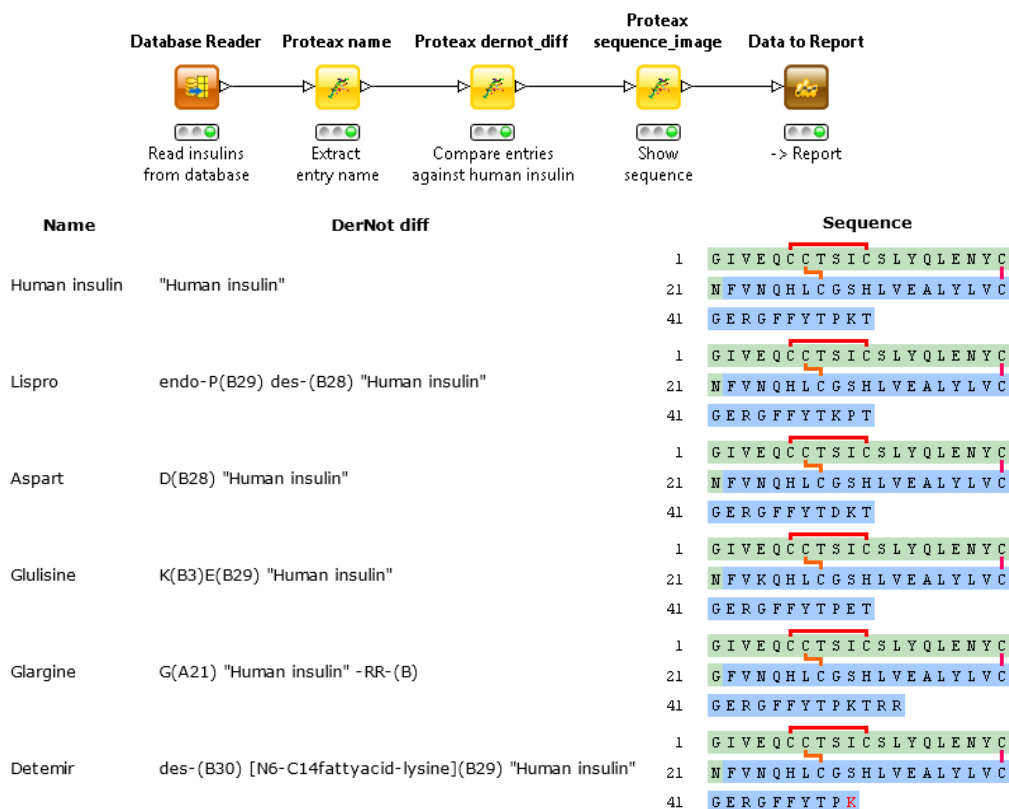


KNIME workflow that reads in three well-known biological molecules from a PLN (Protein Line Notation) file. The chemical structure is generated on-the-fly from the PLN and used to calculate the average molecular weight of the peptides/proteins and render the molecule graphically.

PLN	Name	Avg. MW	Molecule
H-GIVEQC(1)C(2)TSIC(1)SLYQLENYC(3)N-OH.H-FVNQHL(2)GSHLVEALYLVC(3)GERGFYTPKT-OH name="Human insulin"	Human insulin	5807.57	
H-HAEGFTSDVSSYLEGQAAKEFIAWLVKGR-[NH2] name="GLP-1 sequence (7-36)"	GLP-1 sequence (7-36)	3297.63	
(cyclo1)-[MeBmt][Abu][Sar][MeLeu]V[MeLeu]A{d}A[MeLeu][MeLeu][MeVal]- (cyclo1) name="Cyclosporin CsA"	Cyclosporin CsA	1202.61	

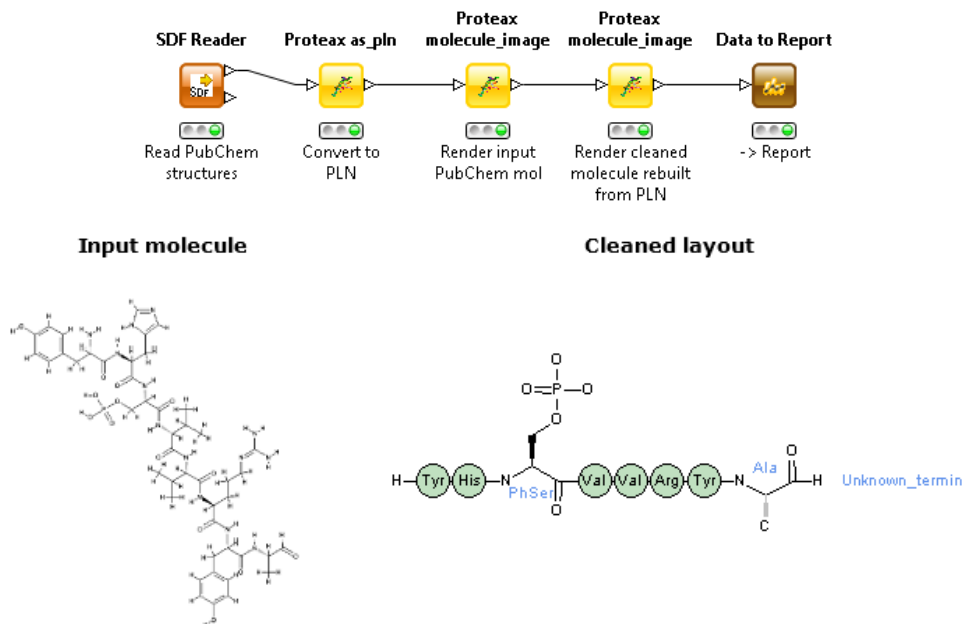
Above workflow data shown in the KNIME Report Designer.

Protein SAR table example



KNIME workflow that reads insulin entries from a database, calculates the difference between the insulins, and displays the result in a report.

Peptide structure cleaning example



KNIME workflow that reads PubChem molecules from an SD file, reformats them to PLN (Protein Line Notation) and displays Proteax's cleaned version of the molecules. The first record of the report is shown.

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 KNIME™ is a registered trademark of KNIME.com GmbH, <http://www.knime.org>
 GPMaw is a 3rd party product by Lighthouse Data, <http://www.gpmaw.com>

Learn more about Proteax at <http://www.biochemfusion.com/products/>
 Contact info@biochemfusion.com or call +45 3048 0050 to obtain a free trial license.

May 2013