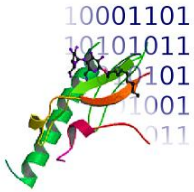
Sequence or structure

- ”You say tomaytoe, I say tomahto”

Gershwin, ca. 1937

Jan Holst Jensen
CEO, Biochemfusion



biochemfusion
- Enabling biochemformatics

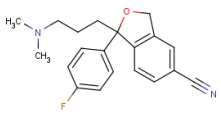
Dialects in representation

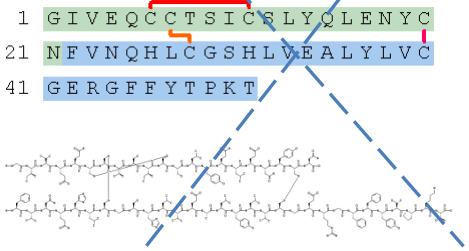
Cheminformatics

Bioinformatics

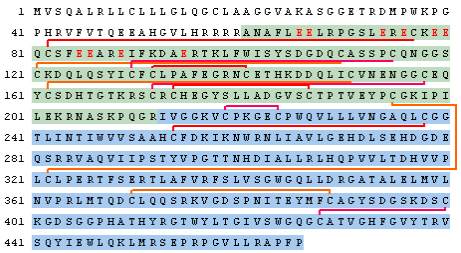
neither-nor / both-and

Molecule graphs





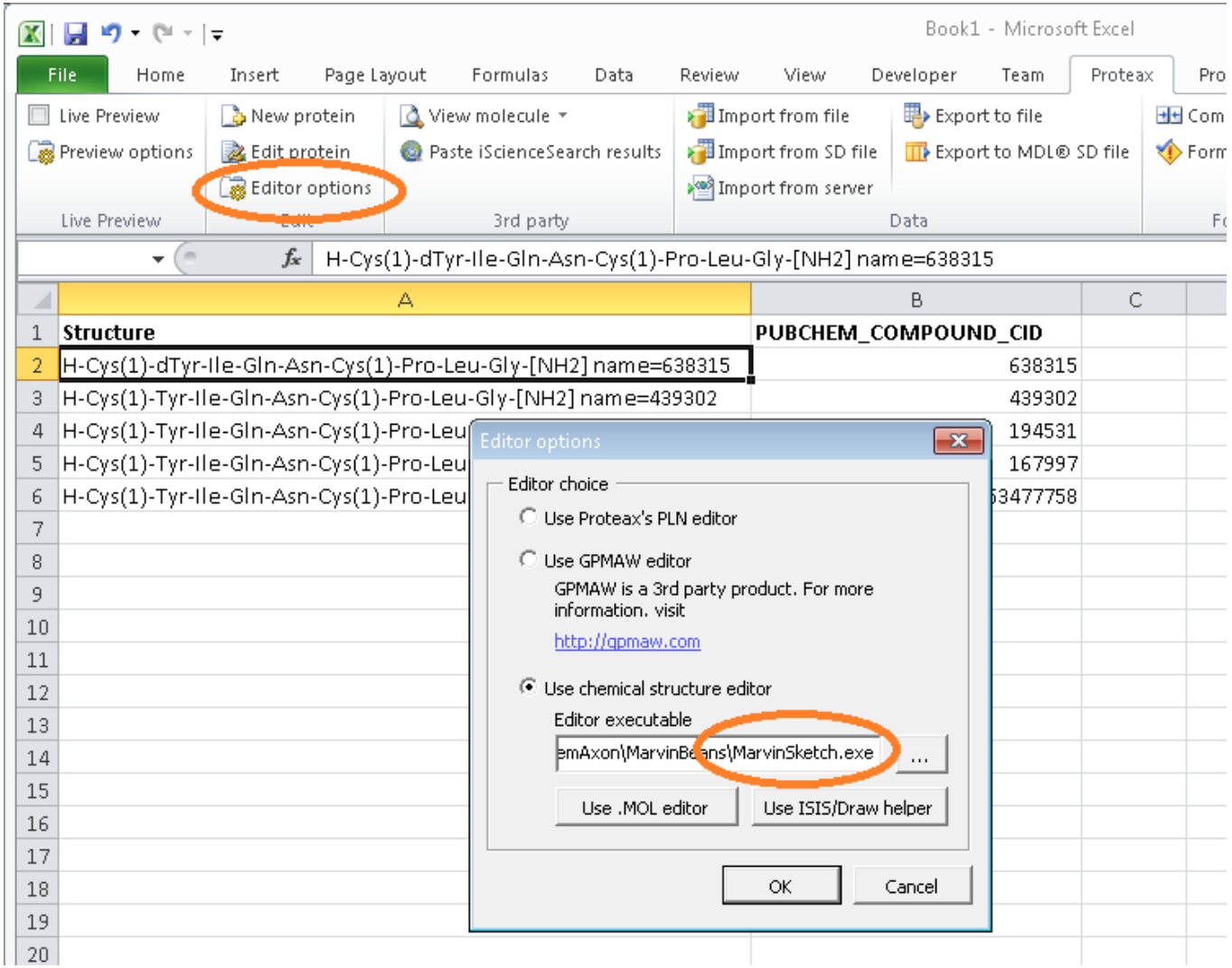
Sequences



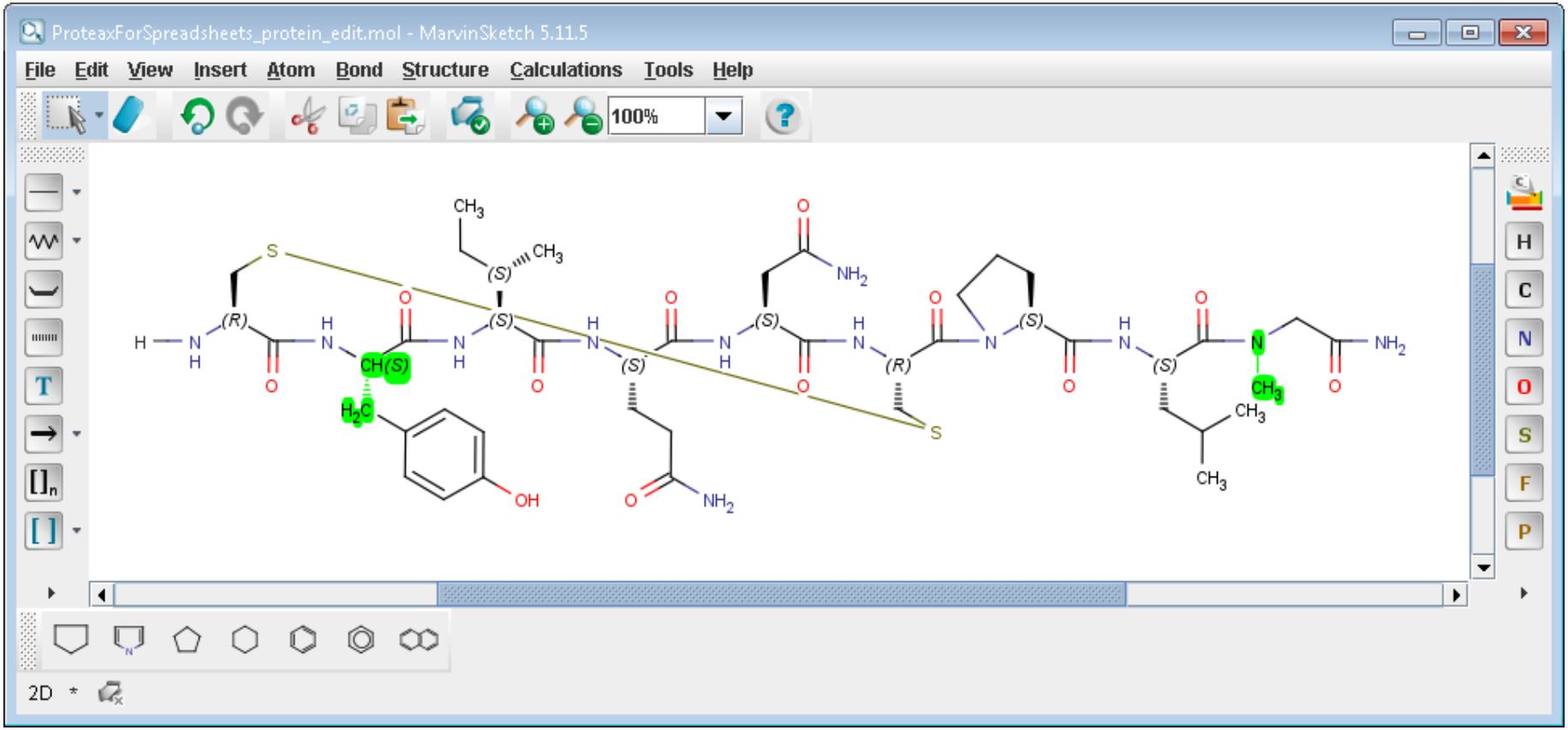
100 10k 1M MW Da

Two-way translation with Proteax®

PubChem structures imported from SD file into Proteax for Spreadsheets

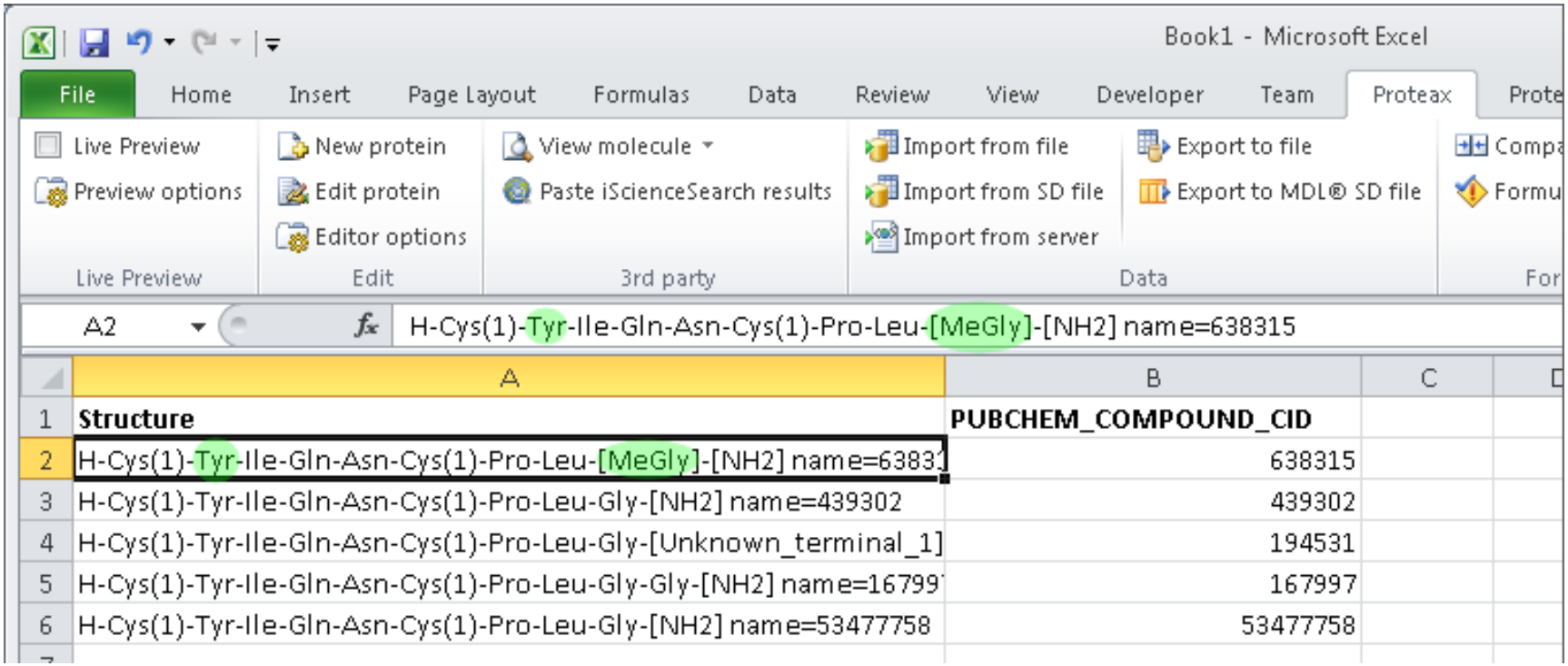


Edit Proteax-generated structure in MarvinSketch



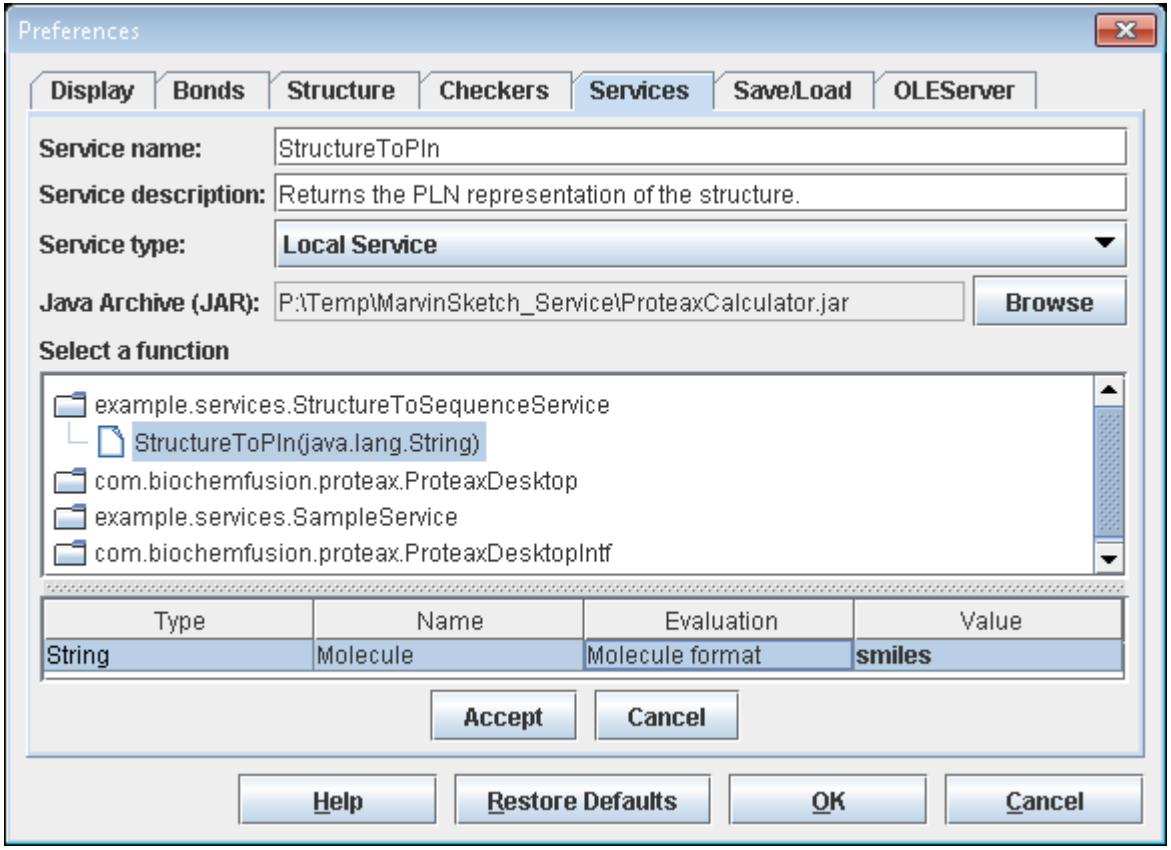
Change Tyr-2 back into its L-form and methylate the glysine.

File→Save in MarvinSketch detected: Proteax translates back to sequence

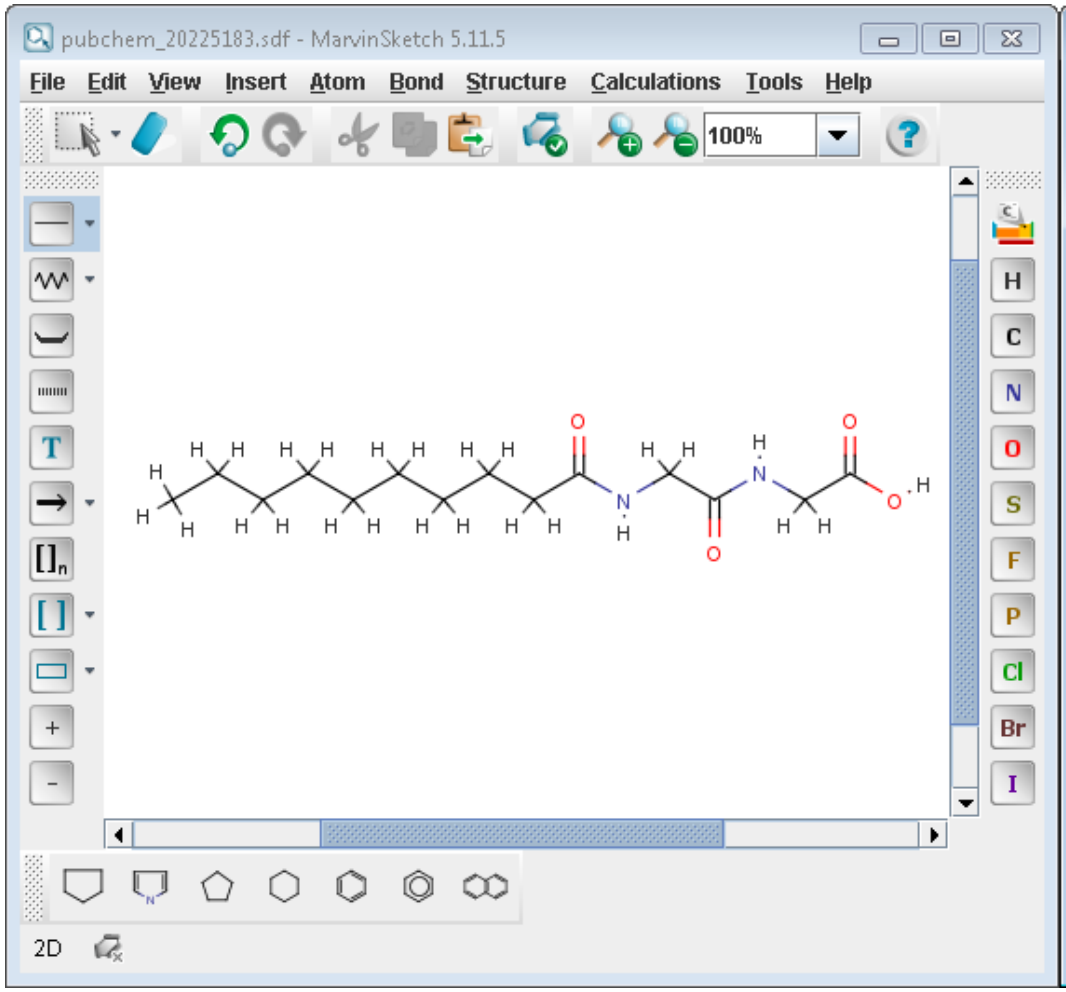


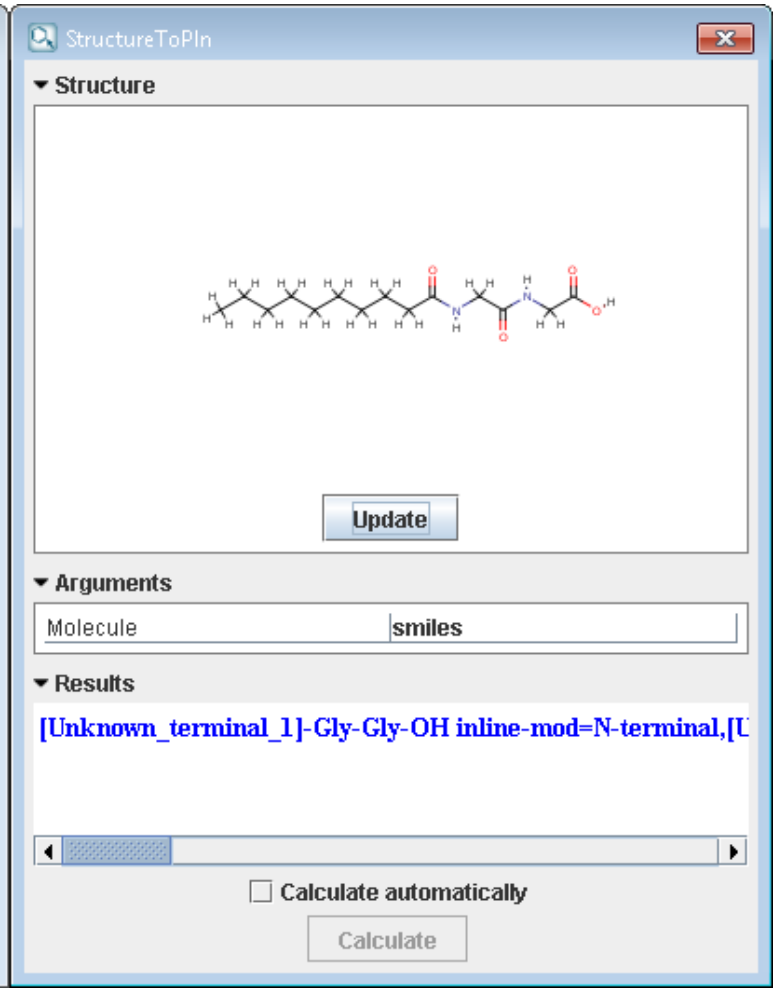
Proteax calculator service example for MarvinSketch

- Just add protein chemistry intelligence

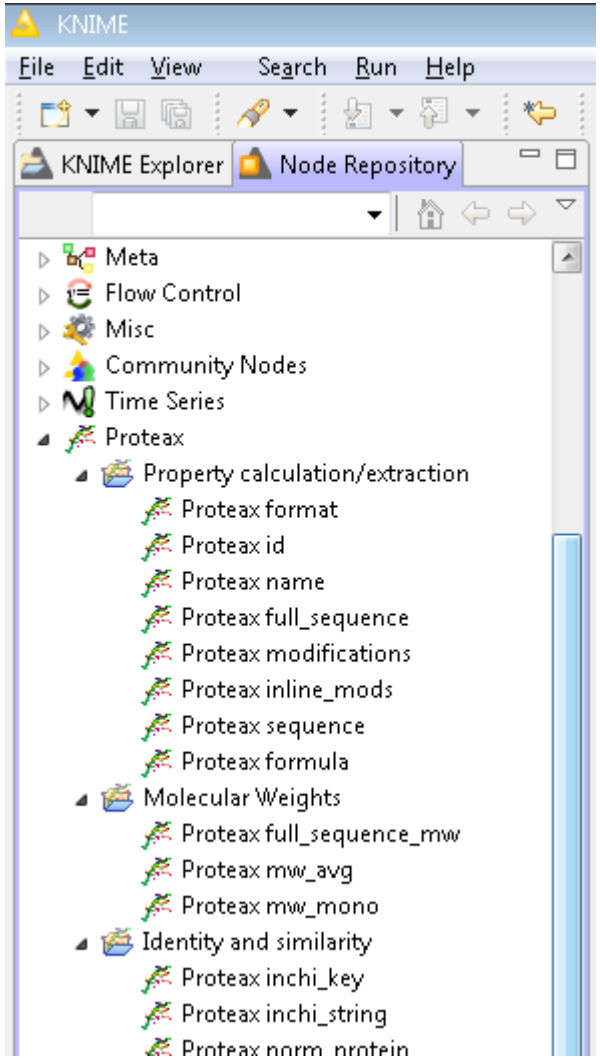


Proteax calculator service in action





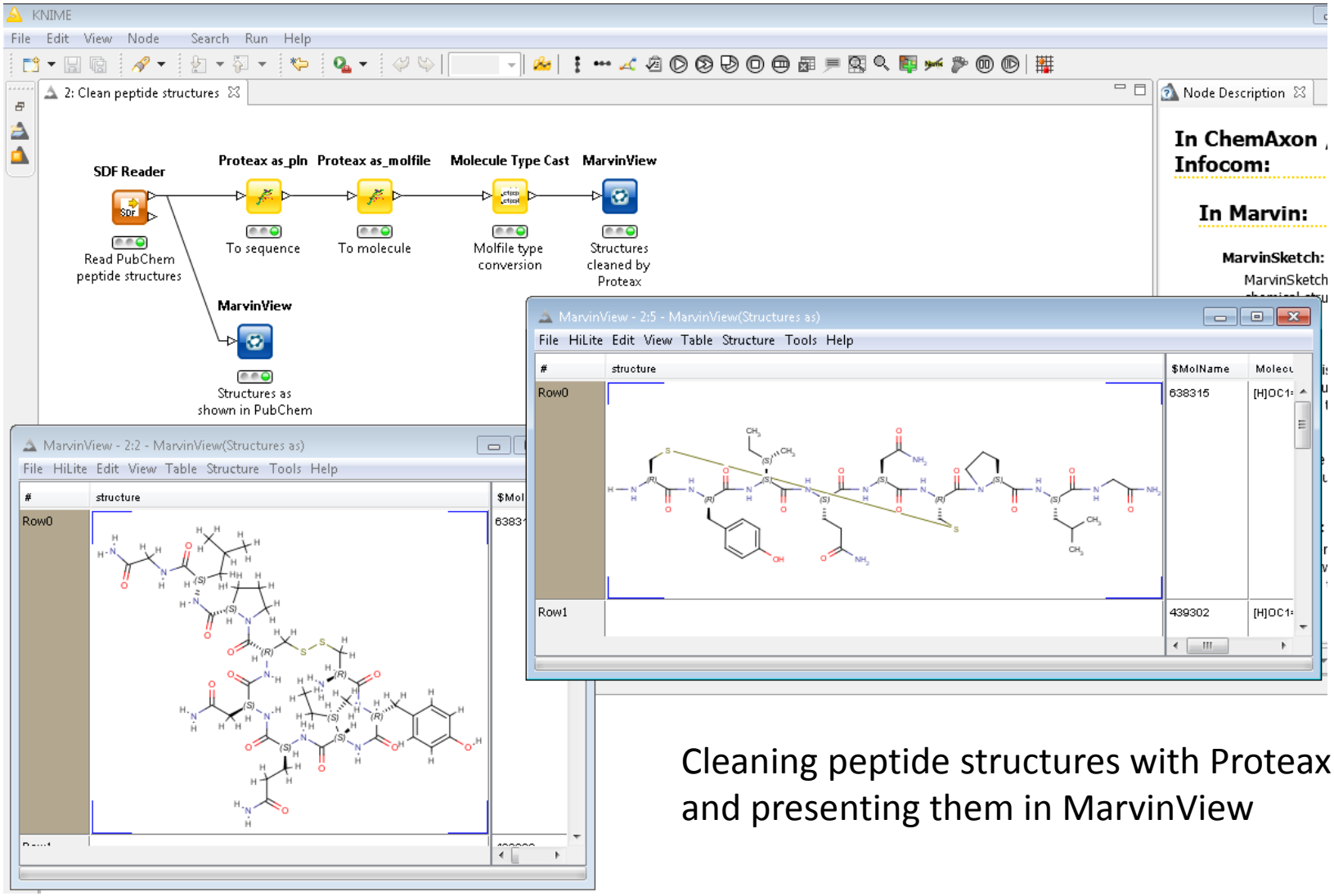
Proteax in KNIME



- Proteax KNIME nodes
  - Released with Proteax Desktop 2.0
- Free download for Proteax users

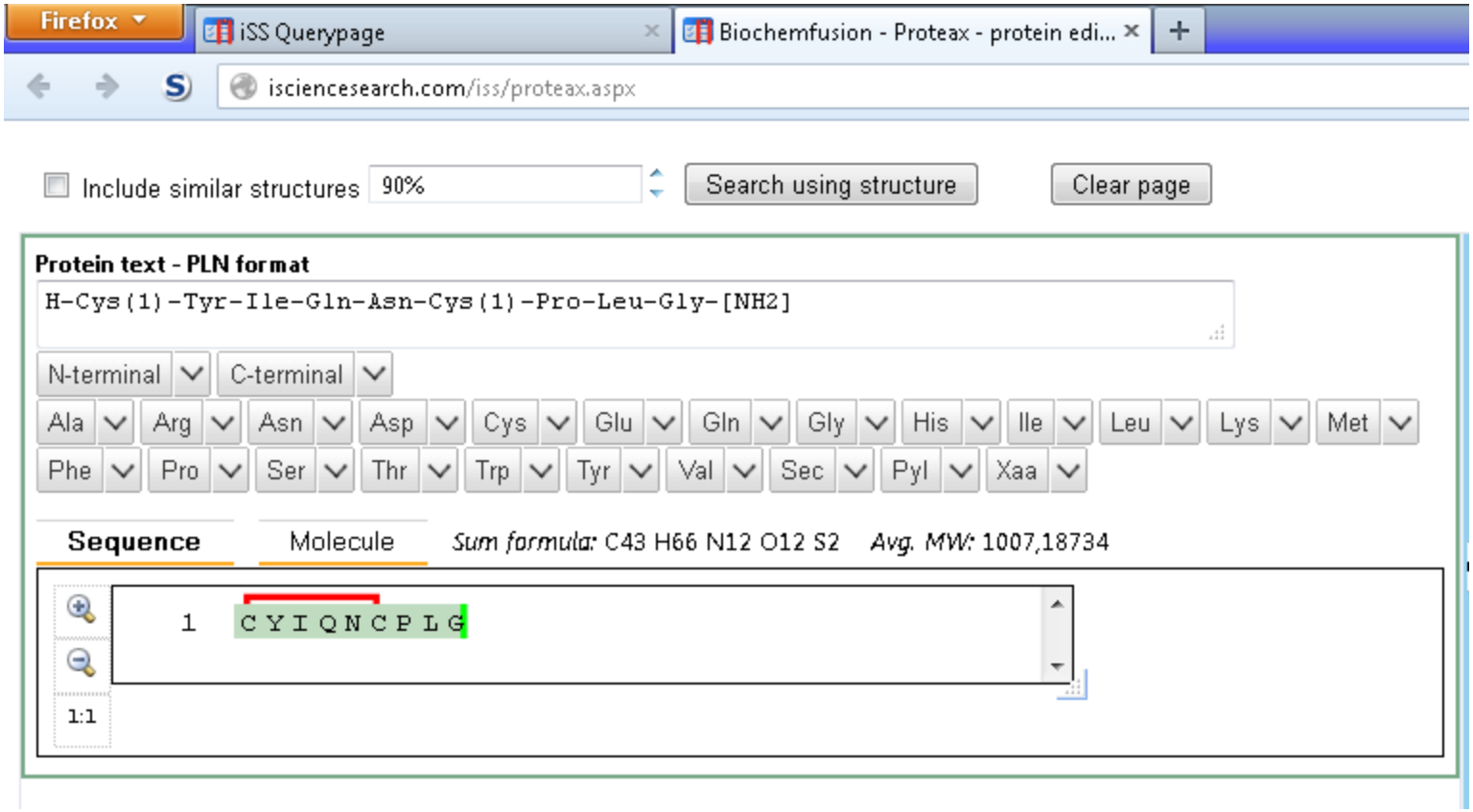
  http://biochemfusion.com/downloads/proteax_knime_nodes/

Easily combined with Marvin nodes



Cleaning peptide structures with Proteax and presenting them in MarvinView

iScienceSearch – by AKos GmbH



- Searches structure databases by queries created from sequence by Proteax
- See also the Biochemfusion Partner Presentation 2012
  - iScienceSearch was formerly known as GlobalSearch

Links...

- Proteax for Spreadsheets, Proteax Desktop, Proteax KNIME nodes
  - http://biochemfusion.com/downloads/
- iScienceSearch, by AKos GmbH
  - http://isciencesearch.com/iss/default.aspx
- Sysment Notebook and Reaction Planner
  - http://www.sysment.hu/
  - Sysment is using Proteax Desktop so their product line can support both small and large molecules