Round-tripping in sequence and structure space

- Searching across abstractions

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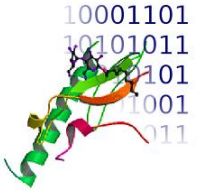
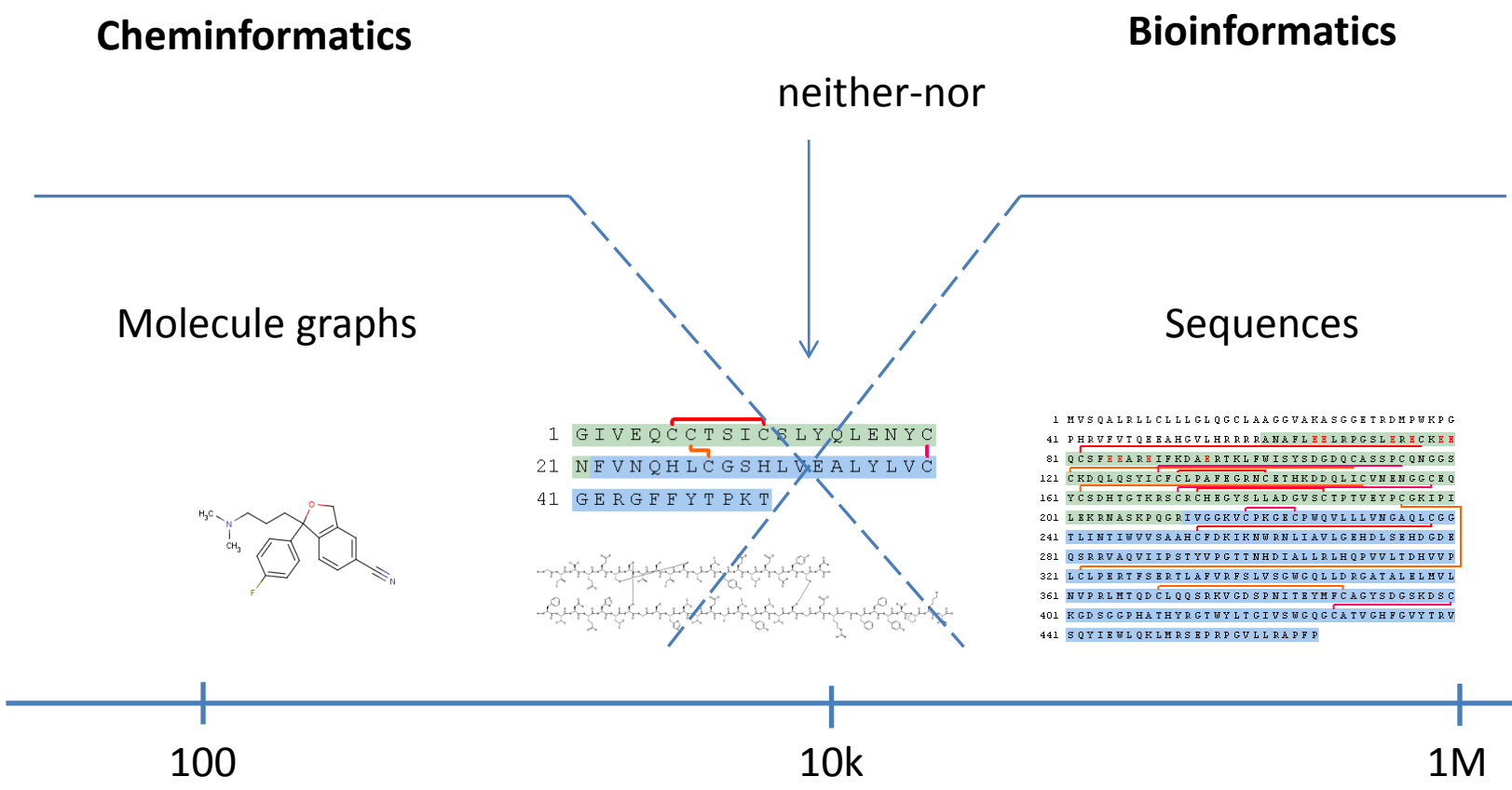


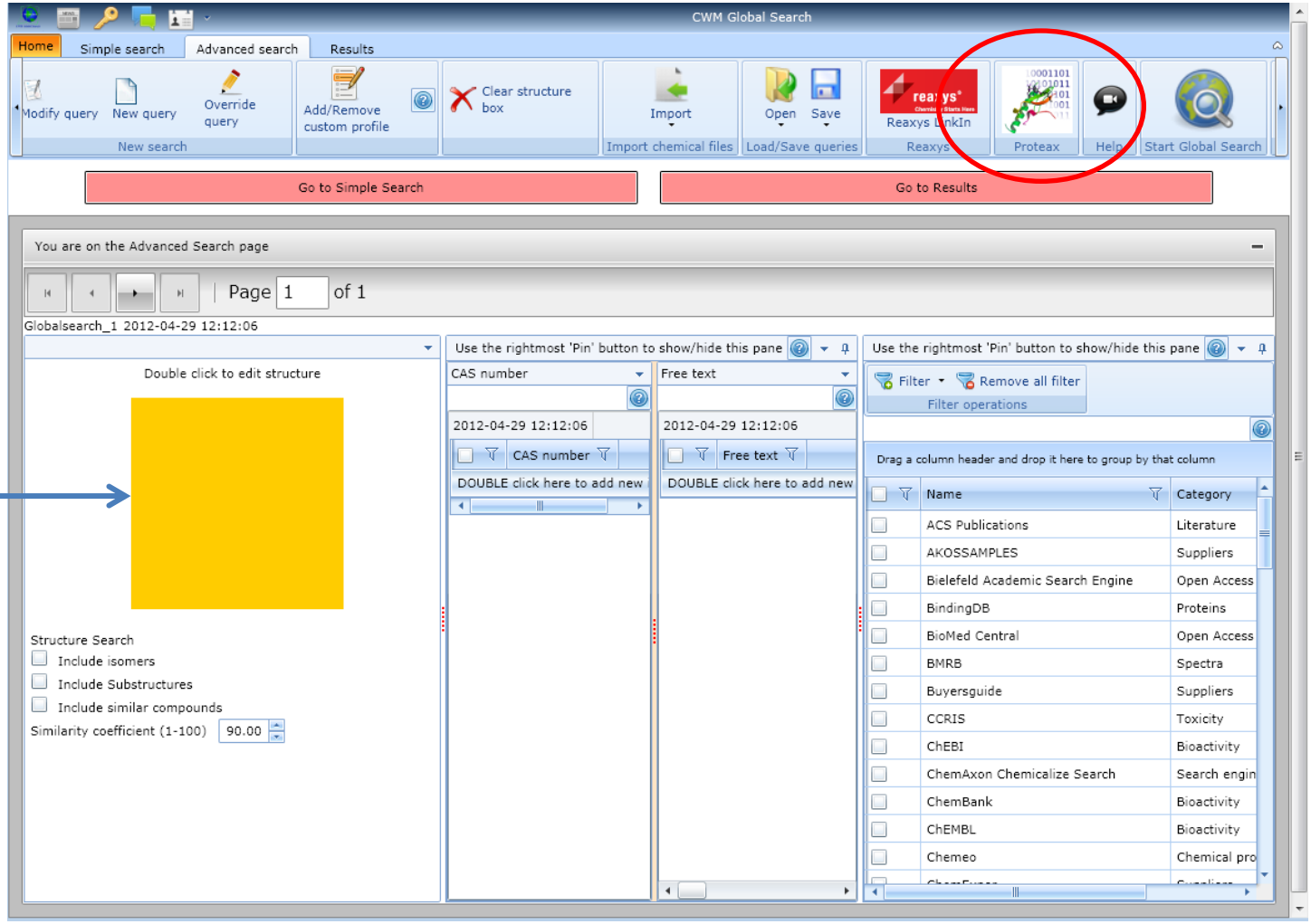
in collaboration with

AKos
Consulting & Solutions GmbH

Bridging the gap



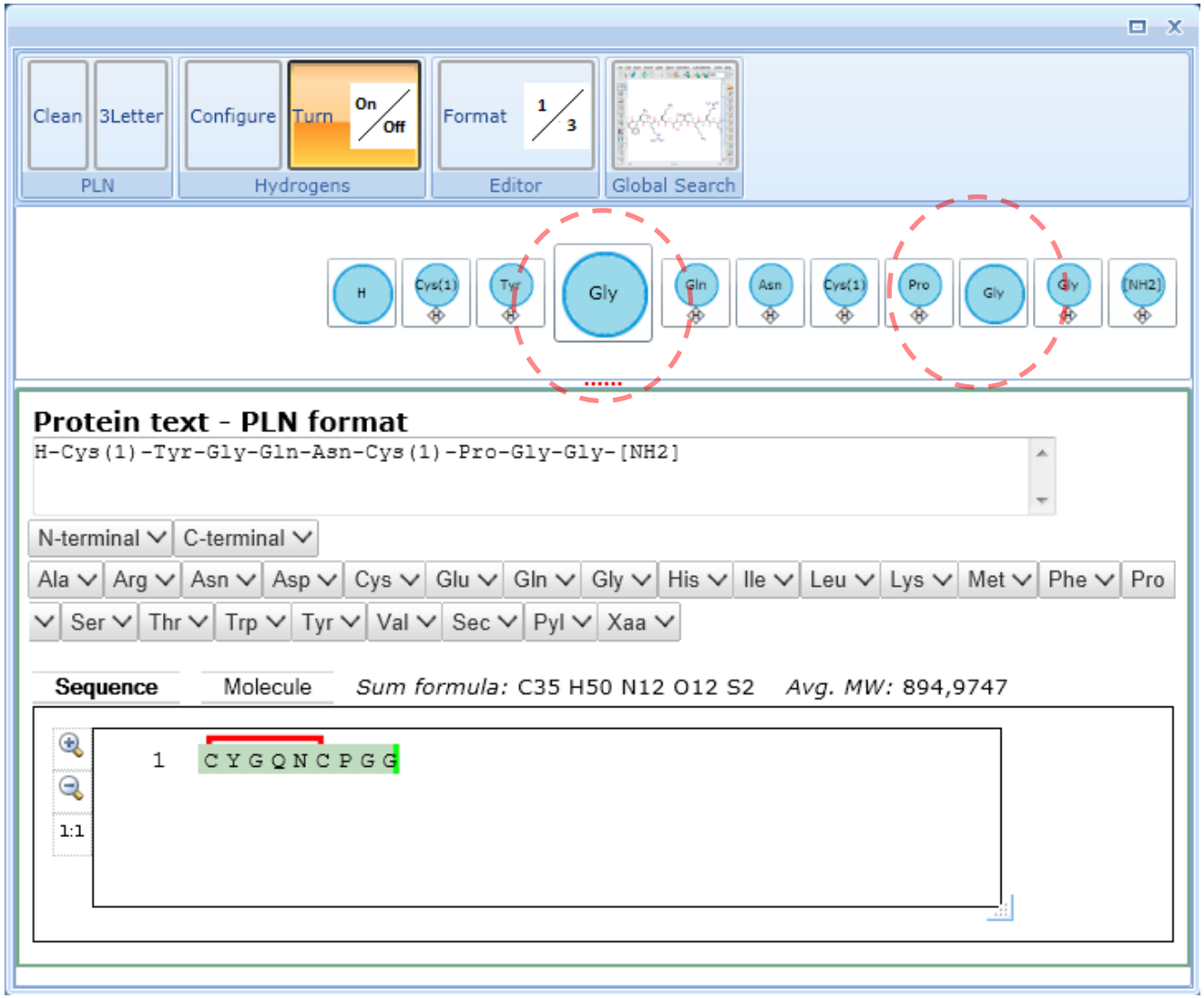
CWM Global Search – now with a “Proteax” button!



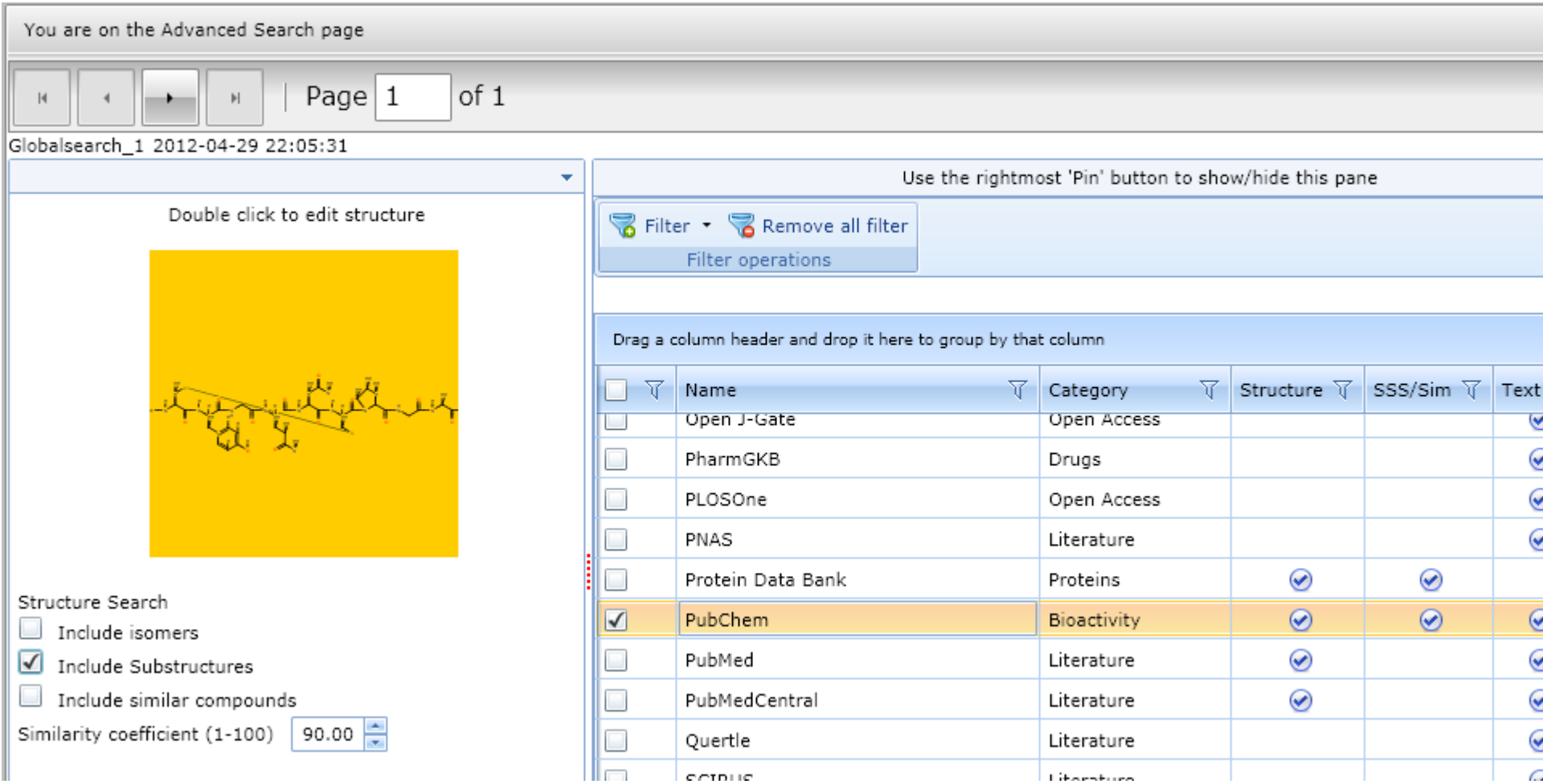
Marvin

Let’s check for Oxytocin look-a-likes

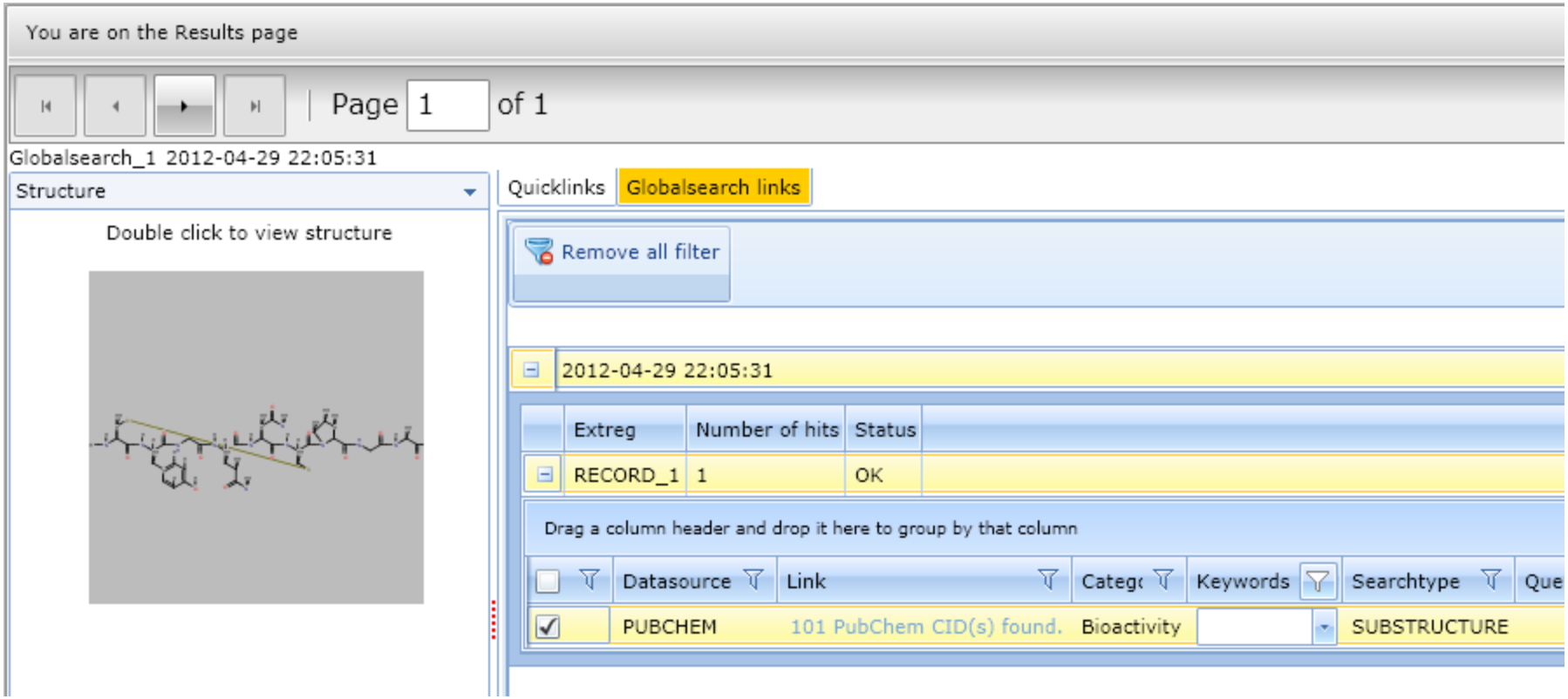
Pos 3 (Ile) and 8 (Leu) are substituted with Glysines and left without explicit hydrogens so any sidechain will be allowed in a substructure mapping.



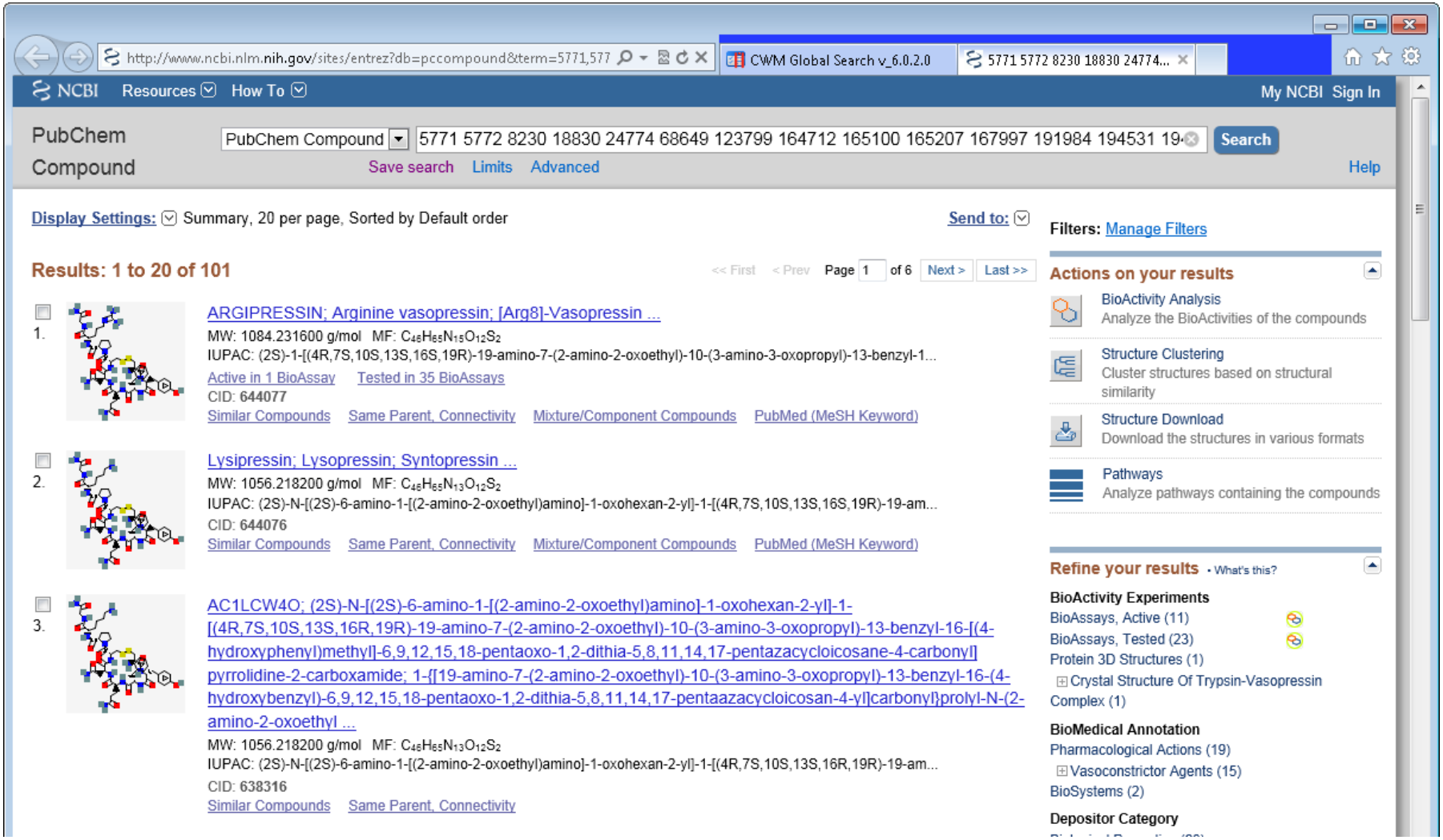
Query structure is generated for you by Proteax; let's start the search



We find 101 hits in PubChem

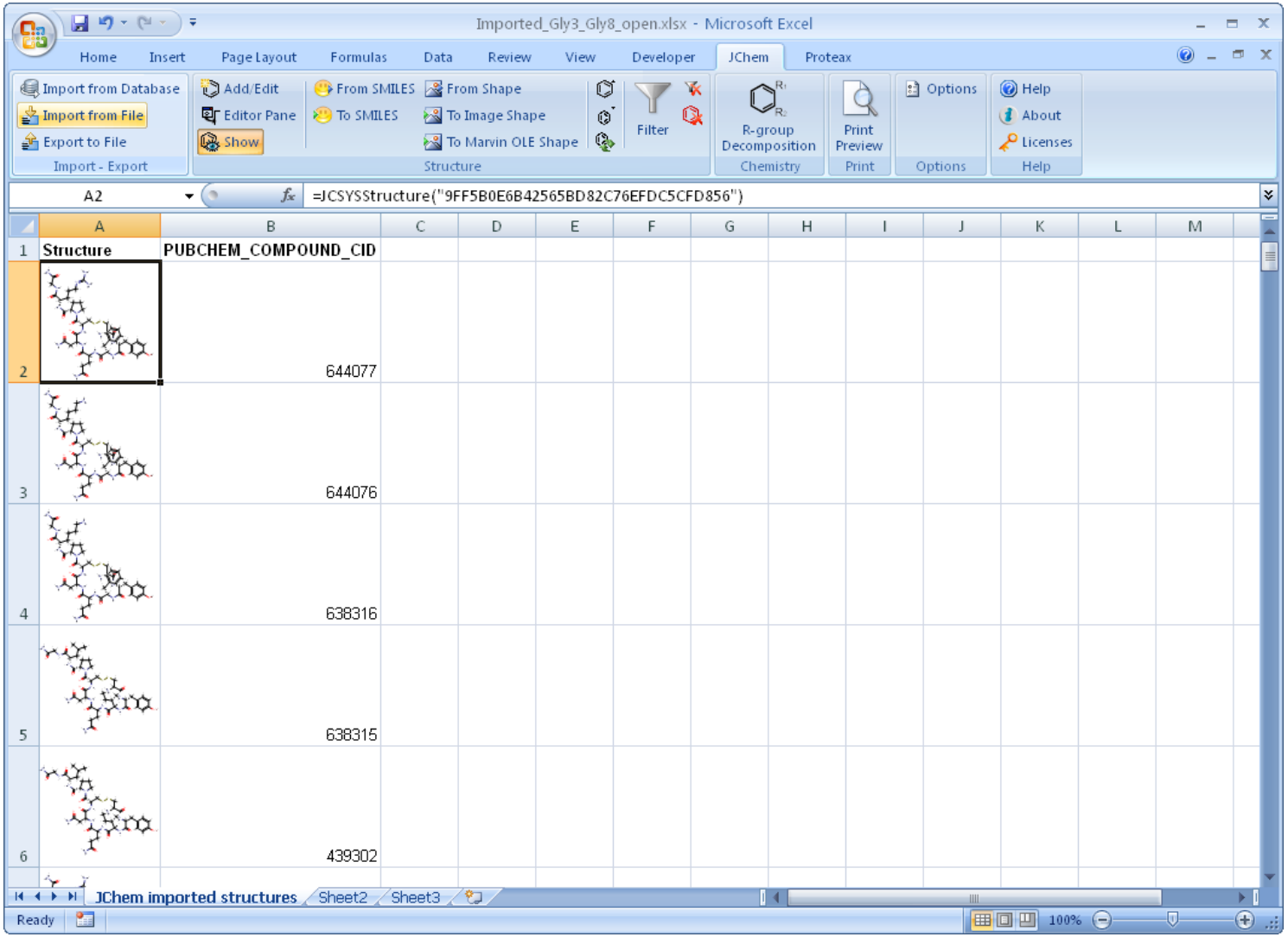


PubChem hit list

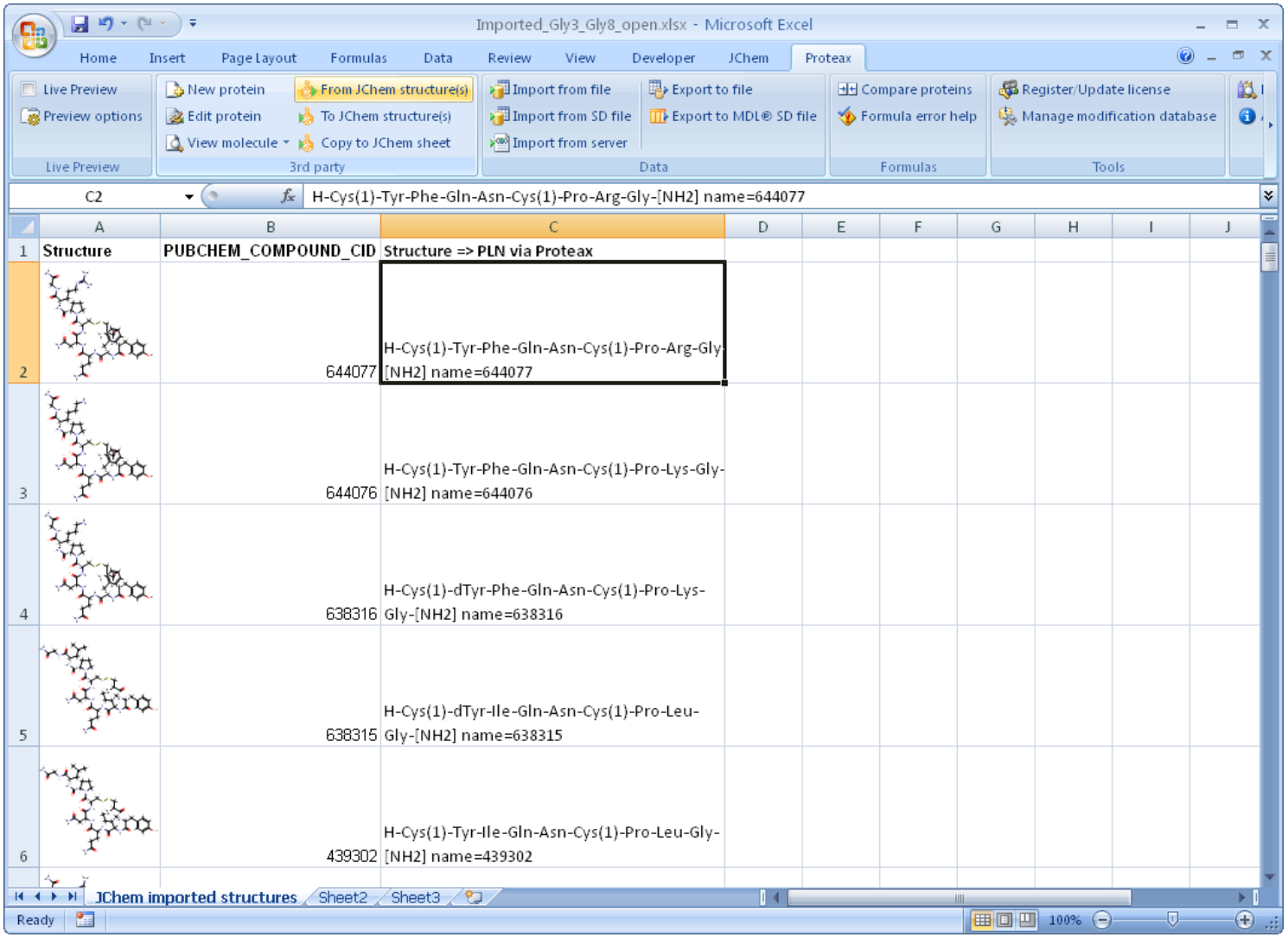


Now, analyze this...

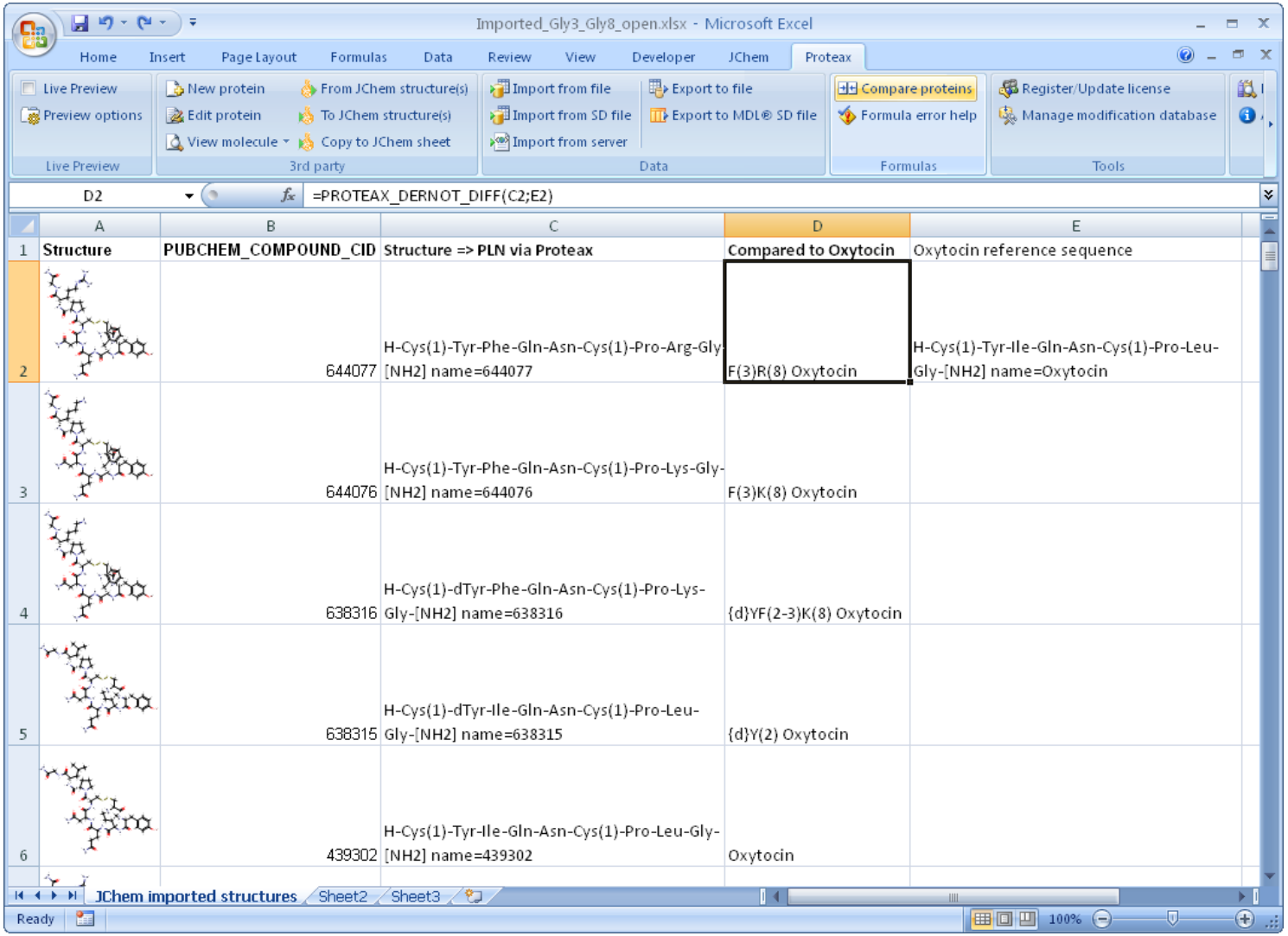
Import PubChem results from SD file with JChem for Excel



Convert structures to Protein Line Notation (PLN) with Proteax



Show variations as Biochemfusion DerNot expressions (“peptide naming”)



Links...

- Proteax for Spreadsheets, by Biochemfusion ApS
  - http://www.biochemfusion.com/downloads/
  - Direct data link to JChem for Excel, by ChemAxon http://www.chemaxon.com/download/jchem-for-excel/
  - Structure => PLN conversion will become available with release 2.0 later this year
- CWM Global Search, by AKos GmbH
  - http://cwmglobalsearch.com/gsweb/