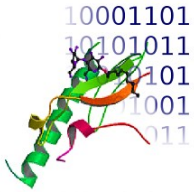
Hall of mirrors

- Reflections on protein registration

Jan Holst Jensen
CEO, Biochemfusion ApS



biochemfusion
- Enabling biochemformatics

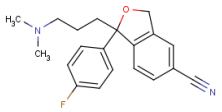
Perceiving molecules

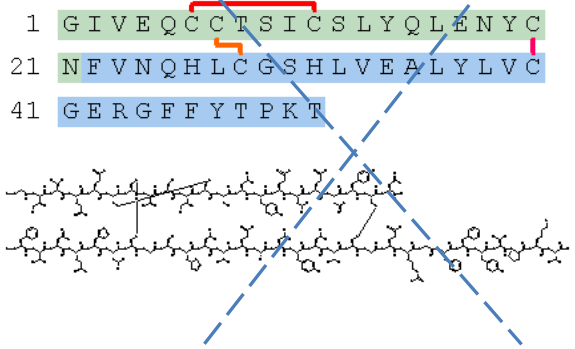
Cheminformatics

Bioinformatics

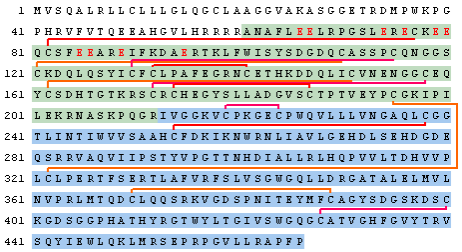
neither-nor / both-and

Molecule graphs





Sequences



100 10k 1M MW Da

Biologics registration

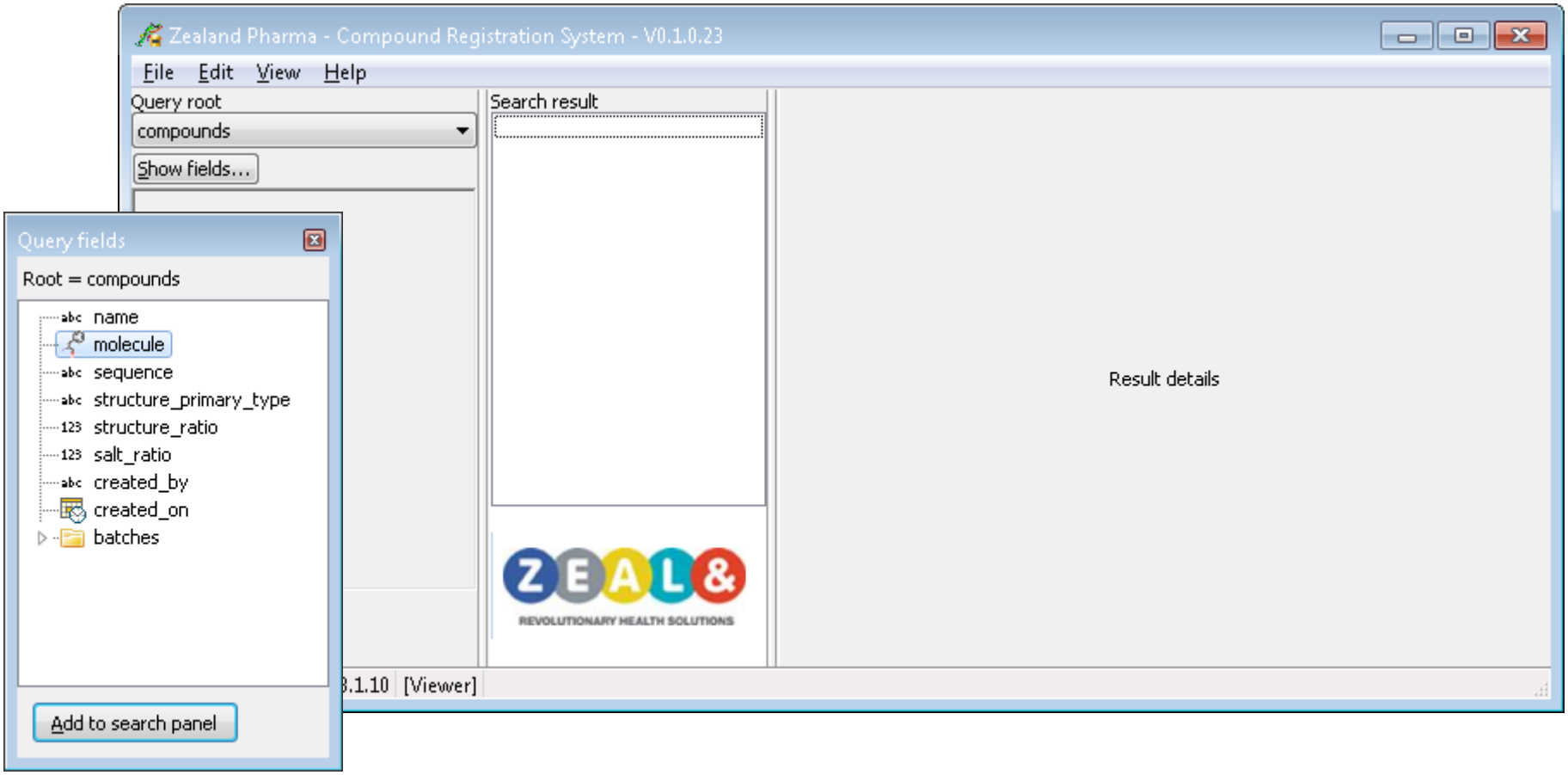
- Zealand Pharma, Denmark
  - Novel peptide drugs for e.g. diabetes and obesity
  - e.g. lixisenatide, marketed by Sanofi as Lyxumia®
- Joint collaboration with Biochemfusion on a new biologics registration system
  - Project started Feb 1st, going live June 30th
  - Using Biochemfusion's Proteax toolkit on both server and client side

Why a joint collaboration ?

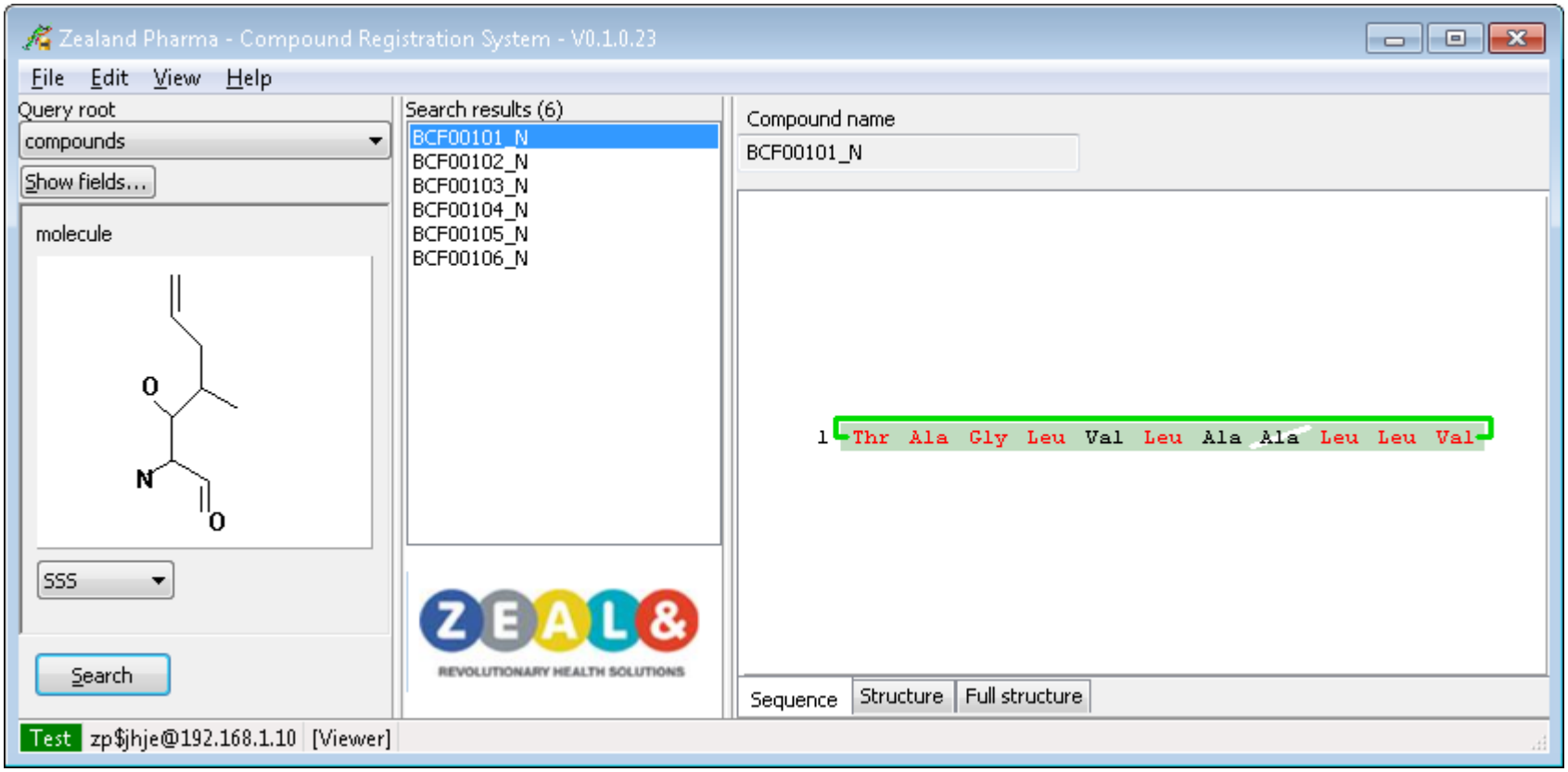
Traditional approach		BCF + Zealand Approach
Off-the-shelf	Bespoke	Bespoke app on standard components
• Many product features irrelevant • 80% of needs covered • 20% must be custom-coded and added in • (and what about that protein chemistry ?)	Everything is possible • (Eventually and with a bit of luck ☺)	• 80% of needs covered from • 100% relevant features available from client selected standard components Remaining 20% done by • Joint development collaboration • Maintained in the future from off-the-shelf BCF product

• Premium price for irrelevant features
• Those last 20% may be very hard to do
	• Huge potential risk
	• Expect and accept prolonged projects
		Build on
		• Proteax protein chemistry cartridge
		• Standard chemistry database cartridge
		• Max. integration with existing tools
		  • Standard chemistry sketchers
		  • Excel (!)

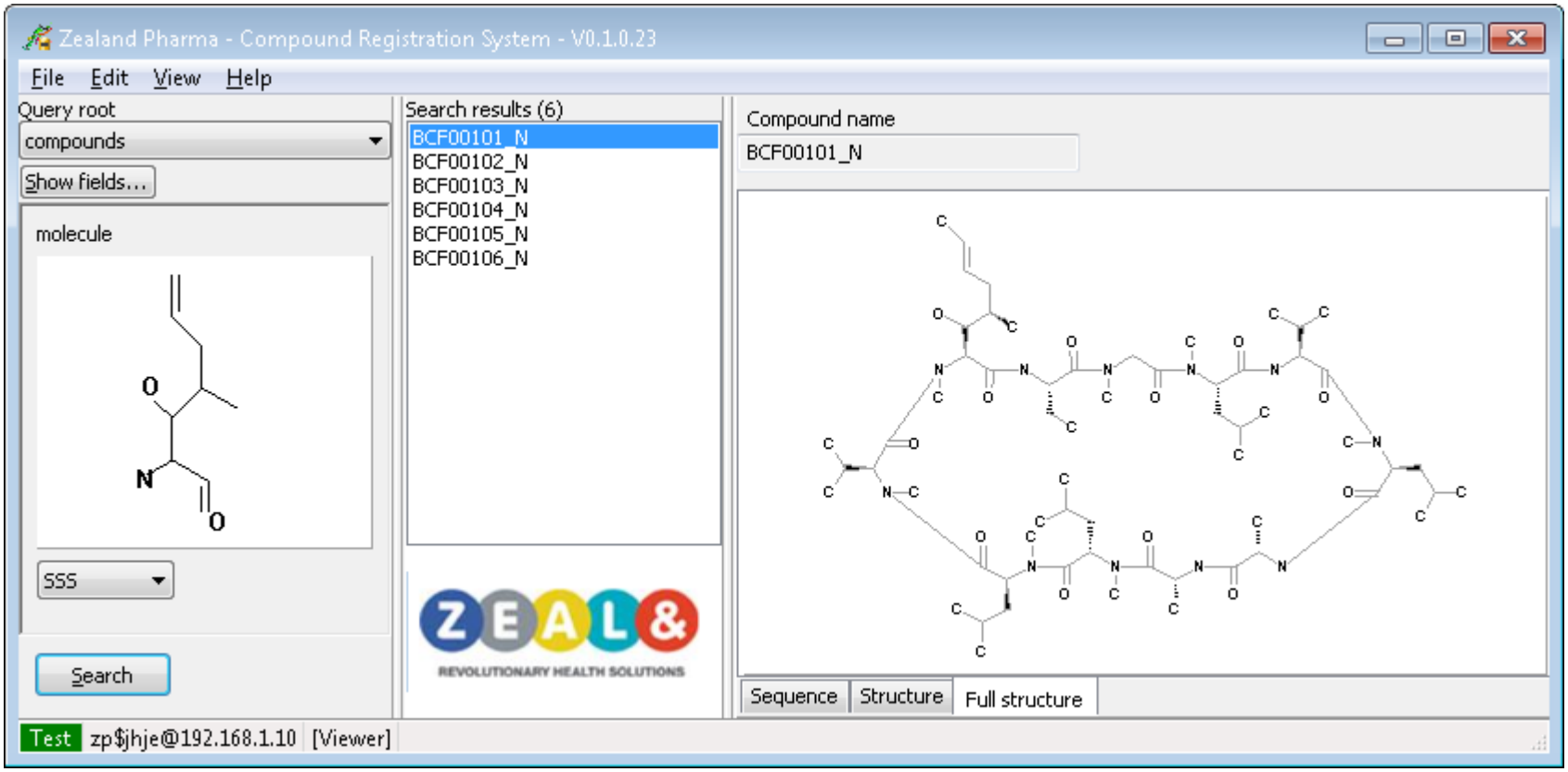
Registration in action



Registration in action

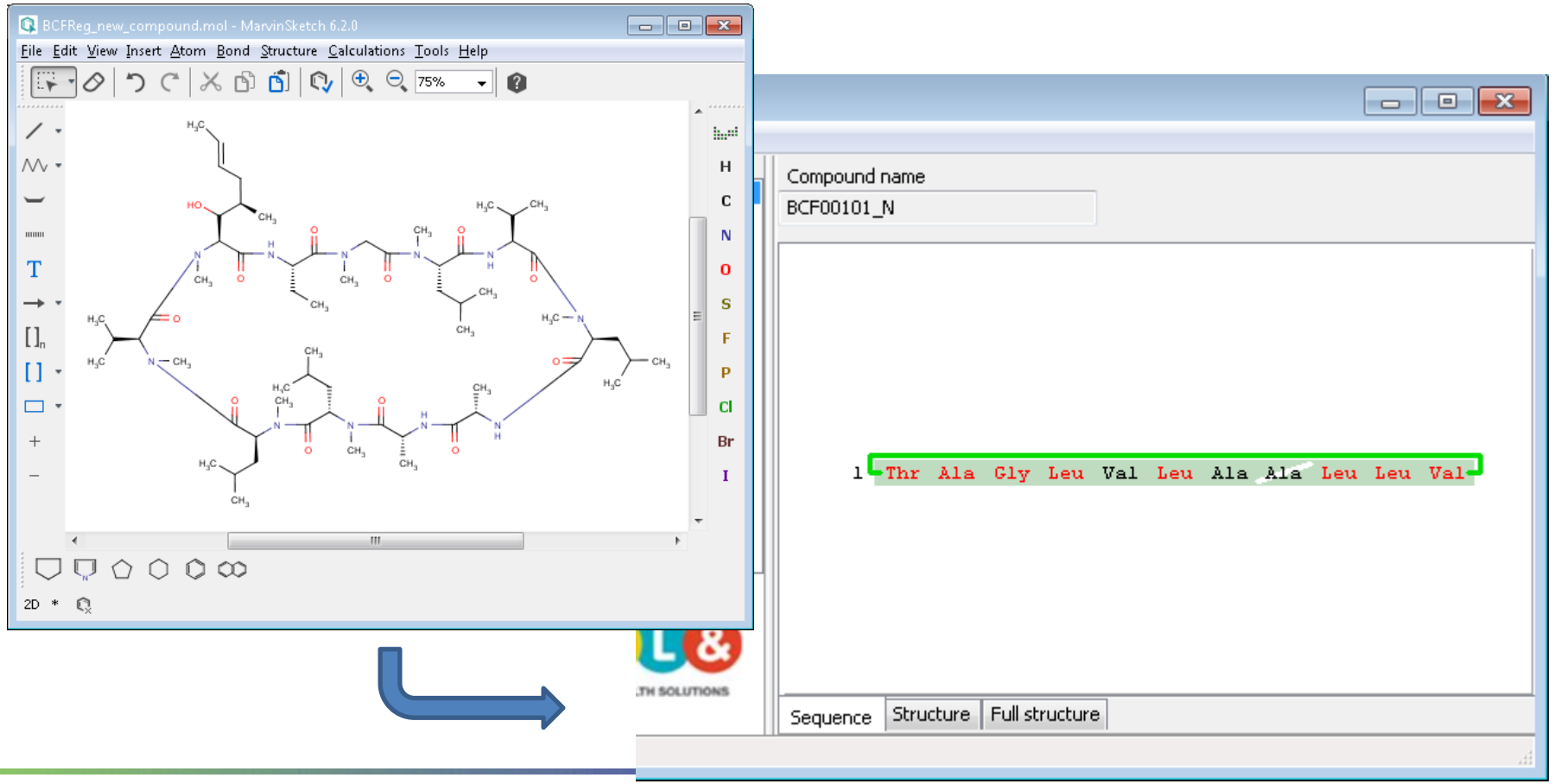


Registration in action



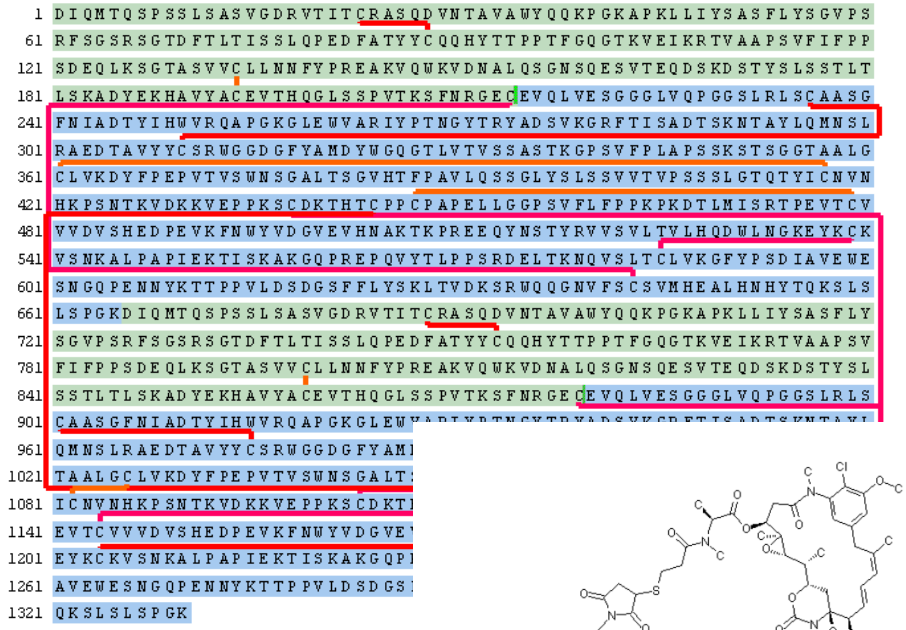
And of course...

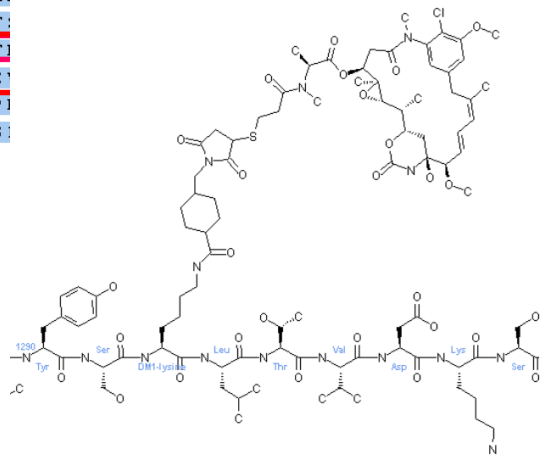
- *Just Works* with MarvinSketch



“What about the big guys ?”

- Proteax composite structure key
- Provides a unique identifier for proteins from 0 – 1 MDa
- Calculated in milliseconds for antibody-drug conjugates

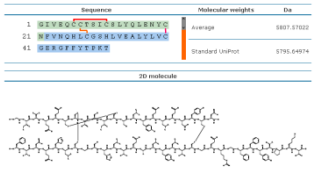




- ICCS 2014, Noordwijkerhout: Presenting the poster “A computationally efficient structure key for large proteins” in collaboration with Gerd Blanke, StructurePendium Technologies, Germany

Proteax® – easily integrated

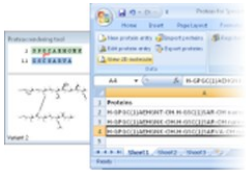
Proteax for Spreadsheets
Spreadsheet functions,
macro programming



Proteax for KNIME
KNIME nodes for graphical processing of protein data

Proteax Desktop
.NET, Java®, Python,
C/C++, Pascal

MS Excel®
OpenOffice.org®



Java® applet, Flash®-based,
JavaScript™, .NET, and Pascal
visualizers

KNIME™
graphical workflows

Scripting,
programming

Structure and
sequence visualization

Proteax toolkit

Proteax Cartridge
Database integration
registration and querying

Oracle®

```
select * from compounds
 where proteax.mw_avg(protein_text) > 5000;
```

PostgreSQL®

Integration partners

- iScienceSearch, by AKos GmbH
  - http://isciencesearch.com/iss/default.aspx
  - Proteax enables sequence searching across multiple chemical structure databases on the web.

- Sysment Notebook and Reaction Tool
  - http://www.sysment.hu/
  - Sysment is using Proteax Desktop so their product line can support both small and large molecules

- Proteax4Morphit, The Edge
  - http://www.edge-ka.com/products/morphit/morphit_plugins
  - Proteax plugin for Morphit provides sequence and structure visualization plus protein comparison and analysis

Thanks

- Zealand Pharma
  - Jakob Anker Hansen
  - Jakob Lind Tolborg
  - Lars Bo Hansen
- StructurePendium
  - Gerd Blanke
- RDKit
  - Greg Landrum

... and of course!

ChemAxon