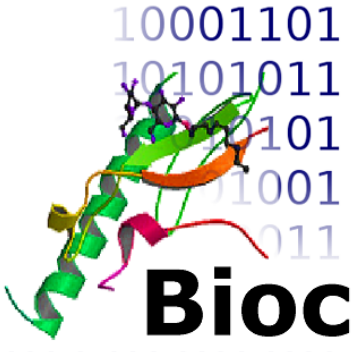
# Macromolecule registration and analysis

*Jan Holst Jensen*
*CEO, Biochemfusion ApS*




Biochemfusion

# Biochemfusion

- Based in Copenhagen, Denmark
- Developing the Proteax software suite since 2007

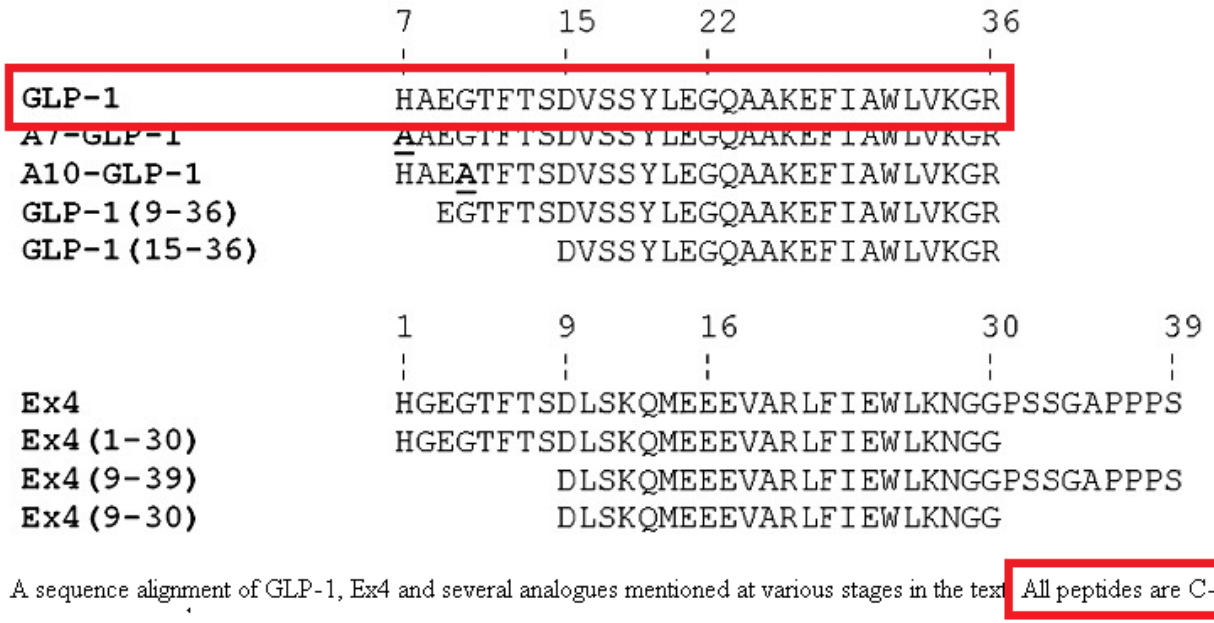
- Let's see what it does...

# Literature – linear peptide

http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3415635/figure/fig01/

**Figure 1**






A sequence alignment of GLP-1, Ex4 and several analogues mentioned at various stages in the text. All peptides are C-terminally amidated.

PLN (Proteax® **P**rotein **L**ine **N**otation) version :

H-HAEGTFTSDVSSYLEGQAAKEFIAWLVKGR-[NH2]

# Literature – cyclic peptide

Cyclosporins are natural undecapeptides derived from cyclosporin A (CsA), cyclo-(-MeBmt[1]-Abu[2]-Sar[3]-MeLeu[4]-Val[5]-MeLeu[6]-Ala[7]-D-Ala[8]-MeLeu[9]-MeLeu[10]-MeVal[11]-), where MeBmt = (4*R*)-4-[(*E*)-2-butenyl]-4,*N*-dimethyl-L-threonine [(2*S*,3*R*,4*R*,6*E*)-3-hydroxy-4-methyl-2-(*N*-methylamino)-6-octenoic acid)] (Fig. 1), by formal substitution of one or two amino acids. Cyclosporin A is nowadays widely used as immunosuppresant for organ transplantations and treatment of autoimmune diseases (*Consupren*®, Galena; *Sandimmun*®, Novartis). Although cyclosporins are structurally almost identical, they strongly differ in their pharmacological activity[1]. Several crystal structures of cyclo-

PLN version :
(cyclo)-[MeBmt]-[Abu]-[Sar]-[MeLeu]-Val-[MeLeu]-Ala-dAla-[MeLeu]-[MeLeu]-[MeVal]-(cyclo)

**CRYSTAL STRUCTURE OF CYCLOSPORIN E**

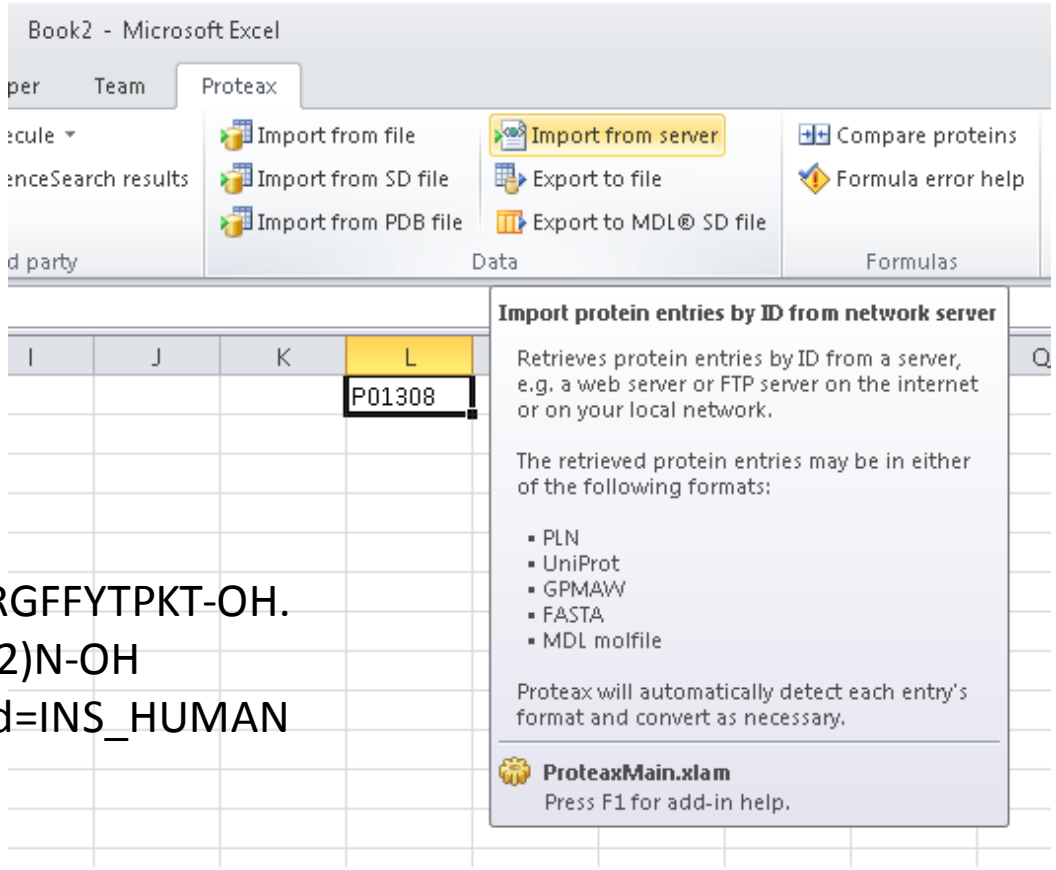
Collect. Czech. Chem. Commun. (Vol. 63) (1998) (pp.115 - 120)

Michal HUSAK[a1], Bohumil KRATOCHVIL[a2], Martin BUCHTA[b], Ladislav CVAK[b] and Alexandr JEGOROV[c,*]

[a] *Department of Solid State Chemistry, Prague Institute of Chemical Technology, 166 28 Prague 6, Czech Republic; e-mail: [1] husakm@vscht.cz, [2] kratochb@vscht.cz*
[b] *Galena Co., R.&D., 747 70 Opava-Komarov, Czech Republic*
[c] *Galena Co., Research Unit, Branisovska 31, 370 05 Ceske Budejovice, Czech Republic; e-mail: husakm@marvin.jcu.cz*

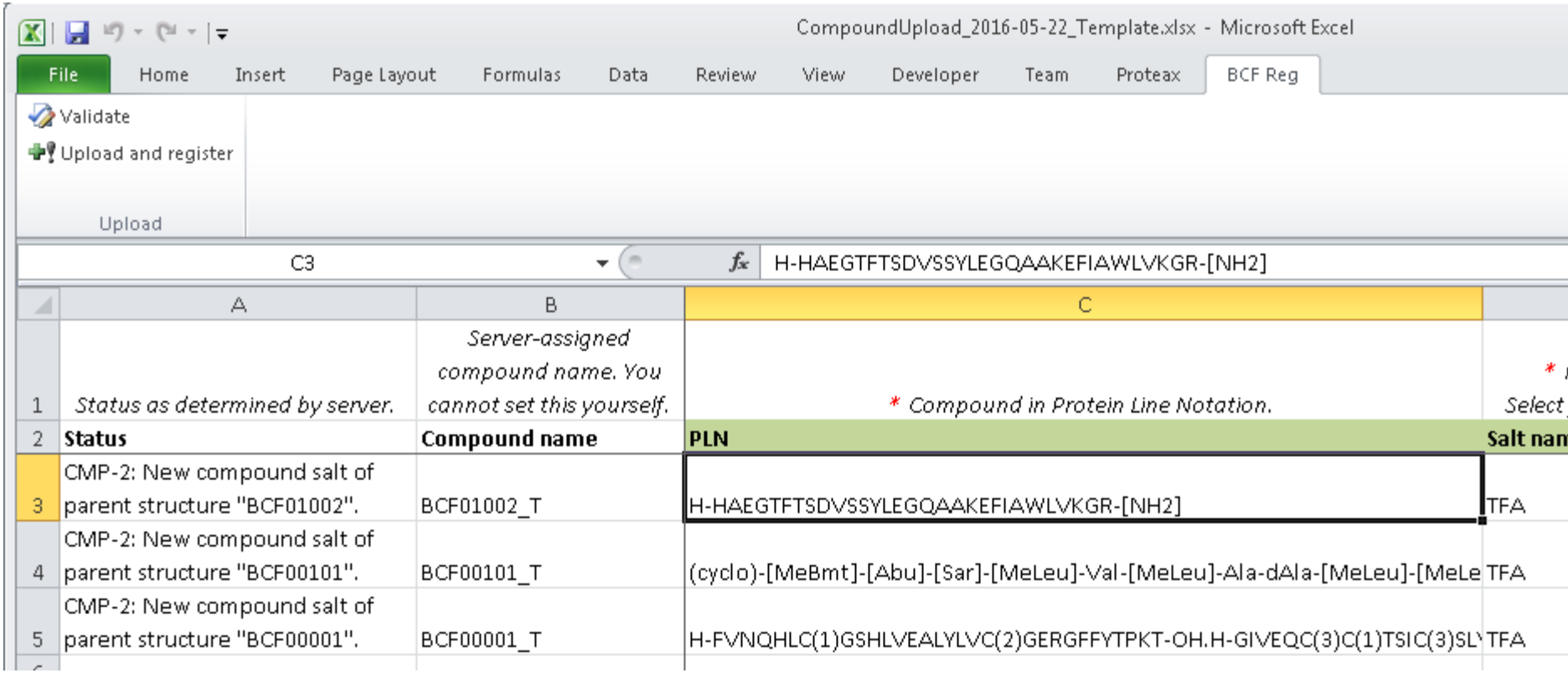
# Multi-chain peptide

- Let's "cheat" – import from UniProt




PLN version :
H-FVNQHLC(1)GSHLVEALYLVC(2)GERGFFYTPKT-OH.
H-GIVEQC(3)C(1)TSIC(3)SLYQLENYC(2)N-OH
name="RecName: Full=Insulin;..." id=INS_HUMAN

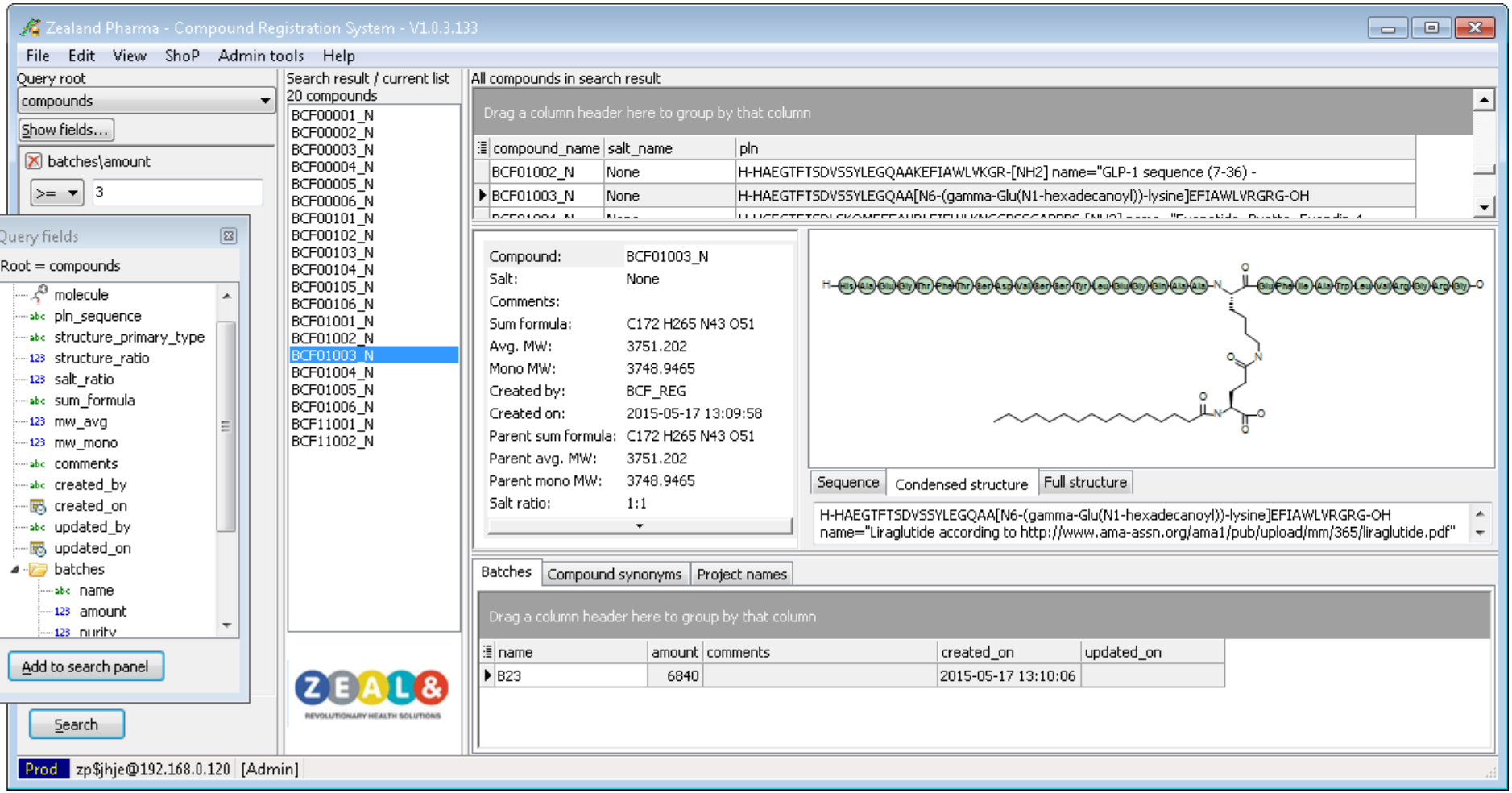
# Registration in Biochemfusion's Proteax-based database BCFReg




| | A | B | C | |
|---|---|---|---|---|
| 1 | *Status as determined by server.* | *Server-assigned compound name. You cannot set this yourself.* | * *Compound in Protein Line Notation.* | * *Select* |
| 2 | **Status** | **Compound name** | **PLN** | **Salt nam** |
| 3 | CMP-2: New compound salt of parent structure "BCF01002". | BCF01002_T | H-HAEGTFTSDVSSYLEGQAAKEFIAWLVKGR-[NH2] | TFA |
| 4 | CMP-2: New compound salt of parent structure "BCF00101". | BCF00101_T | (cyclo)-[MeBmt]-[Abu]-[Sar]-[MeLeu]-Val-[MeLeu]-Ala-dAla-[MeLeu]-[MeLe | TFA |
| 5 | CMP-2: New compound salt of parent structure "BCF00001". | BCF00001_T | H-FVNQHLC(1)GSHLVEALYLVC(2)GERGFFYTPKT-OH.H-GIVEQC(3)C(1)TSIC(3)SL | TFA |

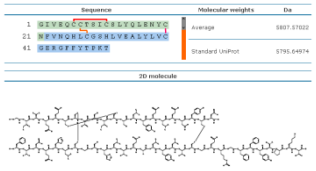
- In production at Danish biotech Zealand Pharma since 2015.

# BCFReg – registration system



# Proteax – broad tooling support

**Proteax for Spreadsheets**
Spreadsheet functions,
macro programming



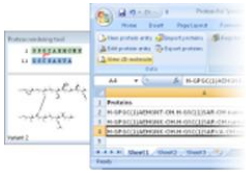
**Proteax for KNIME**
KNIME nodes for graphical processing of protein data

**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

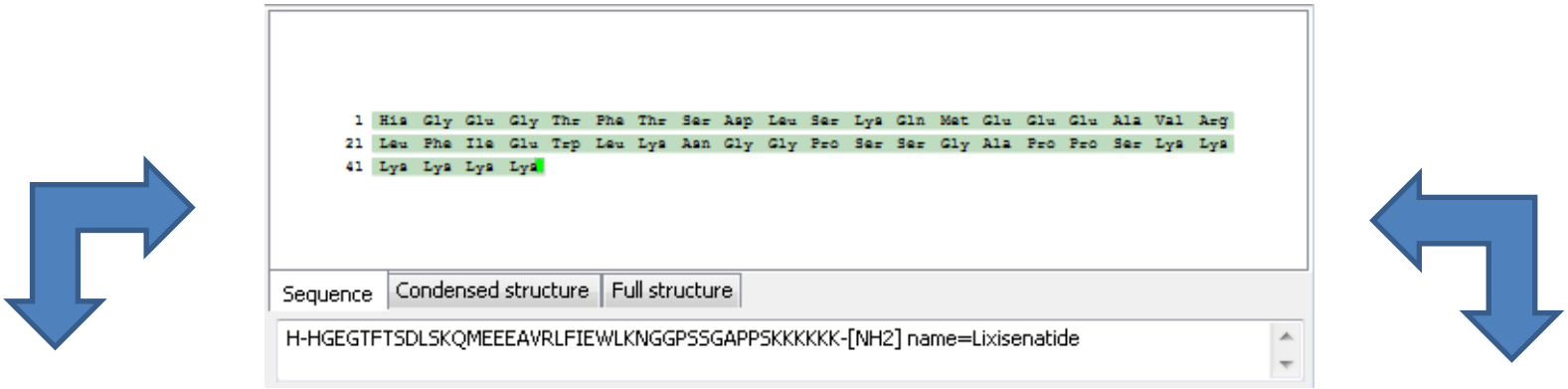
Oracle®

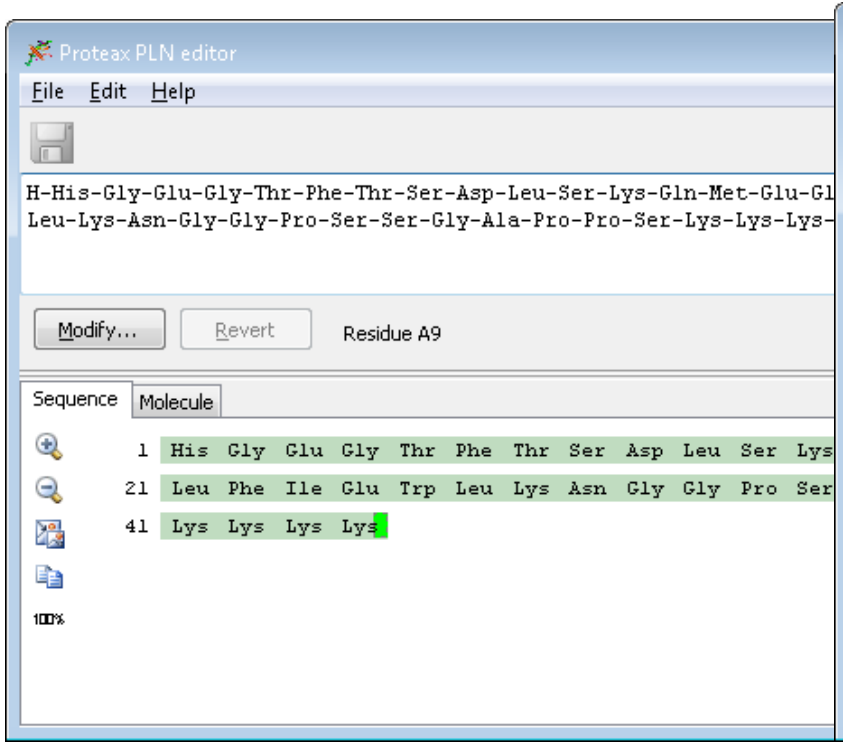
```
select * from compounds
 where proteax.mw_avg(protein_text) > 5000;
```

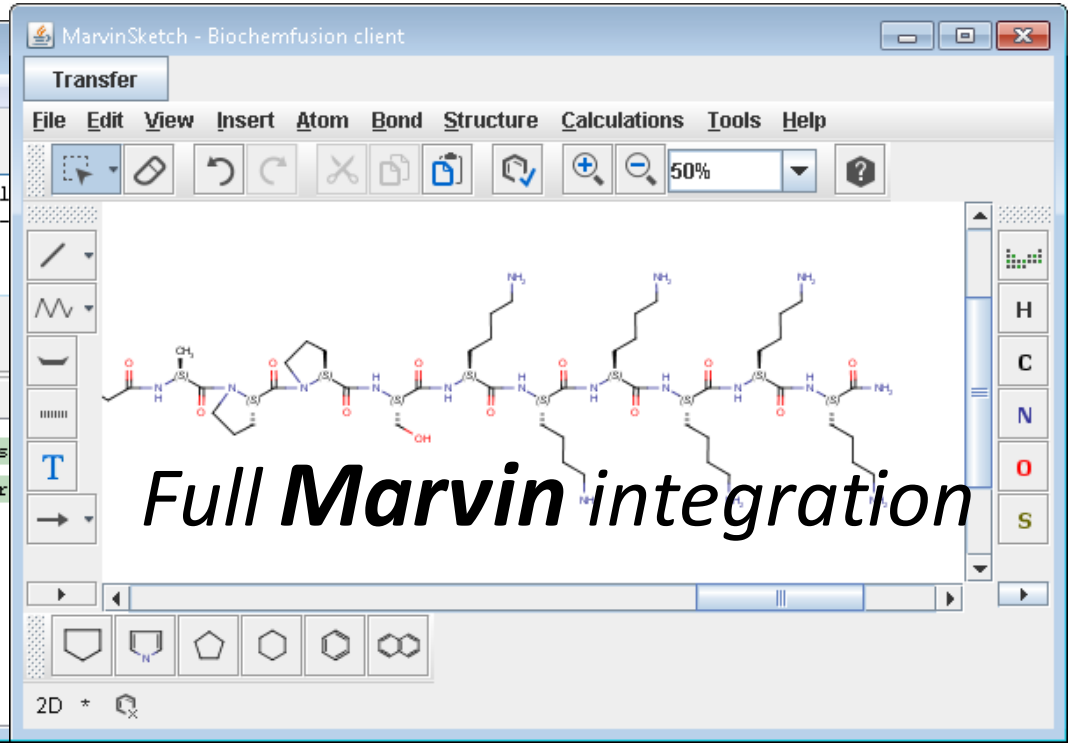
PostgreSQL®

Does not replace yourchemistry cartridge. Works *together* with.e.g. **JChem Cartridge**.

# BCFReg – flexible editing

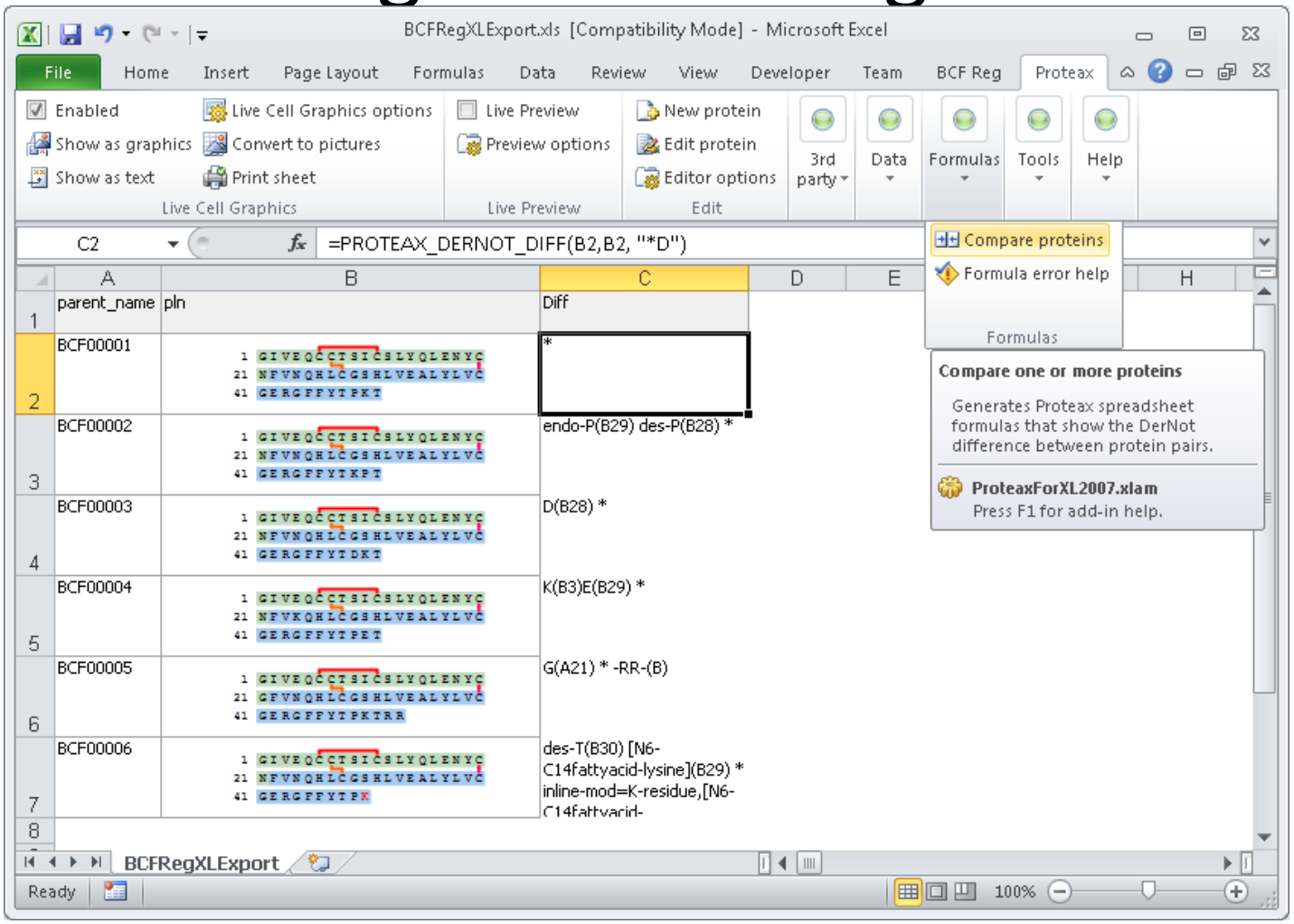



*Full **Marvin** integration*

# BCFReg – Excel integration




- Export to peptide SAR tables.
- **Peptides can be directly converted to JChem for Excel structures**

# Thank you for your attention

- Please check our booth and see BCFReg in action.