

Marvin and JChem + Proteax

- Benefits of integration

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CEO, Biochemfusion

biochemfusion
- *Enabling biochemformatics*

Bridging the gap

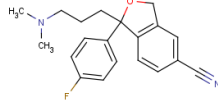
Cheminformatics

Bioinformatics

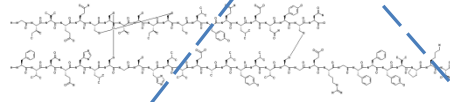
neither-nor

Molecule graphs

Sequences



```
1  GIVEQCCTSICSLYQLENYC  
21 NFVNQHLCGSHLVEALYLVC  
41 GERGFFYTPKT
```



```
1  MVSQALRLLCLLLCLGQCCLAAGGVAKASGCETRDMPWRPG  
41  PHRVFVTQEEAHCVLHRRRRANAFLEELRPGSLERECREE  
81  QCSFEFARIFKDAERTKLFMISYSDGDQCASSPCQNGGS  
121 CRDQLQSYICFCLPAFEGRNCETHRDDQLICVNENGCCRQ  
161 YCSDHTCTKRSCRCHEGYSLLADCVSCTPTVEYPCGKIPI  
201 LEKRNASKPQCRIVGCKVCFKGCPWVLLLVNCAQLCGG  
241 LLINTIWVVSAAHCFDKIKNWRNLIAVLGEHDLSEHDCDE  
281 QSRRVAQVIIPSTYVPGTINHDIALLRLHQPVVLDHVV  
321 LCLPERTFSERTLAFVFSLVSGWCQLLDRCATALELMVE  
361 NVPRLHTQDCLQQSRKWCDSPNITETHFCACYSDGSKDSC  
401 KGDSGGPHATHRGTWYLTGIVSWGQCCATVGHFGVYTRV  
441 SQYIEWLQKLMRSEPRPCVLLRAPFF
```

100

10k

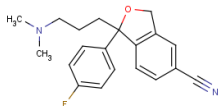
1M

MW
Da

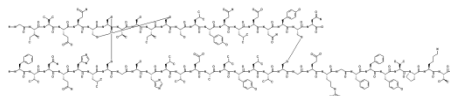
JChem for Excel
 JChem Extensions for KNIME
 Structures4MorphIt
 JChem Cartridge
 ...

Proteax for Spreadsheets
 Proteax for KNIME
 Proteax4MorphIt
 Proteax Cartridge
 ...

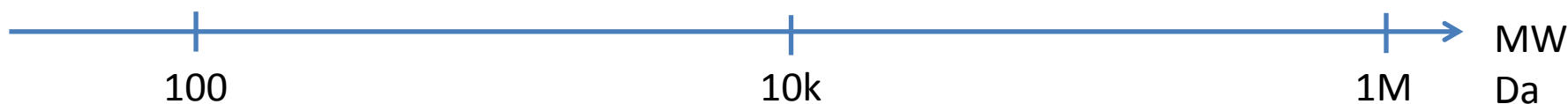
product integration



1 GIVEQCCTSLYQLENYC
 21 NFNQHLGSHLVEALYLVC
 41 GERGFFYTPKT



1 MVSQALRLLCLLLGLGCLAAAGVAKASGCETRDMPWRPG
 41 PRRVFTQEEAHCVLHRRRANAFLLELRPGSLERCKRE
 81 QCSFSEARRIFKDAERTKLFWISYSDGDCASSPCQNGCS
 121 CRDQLQSYICFCLPAFEGRCNCETHRDDQLICVNEGGCEQ
 161 YCSDHITGTRRSRCRCEGYSLLADCVSCTPTVEYPCCKIPF
 201 LEKRNASKPQGRIVGCKVCFKGECPWQVLLLVNGAQLCGG
 241 LLIMTIWVVSAAHCFDKIRNWRMLIAVLGEHDLSEHDGDE
 281 QSRVAQVLIIPSTYVPGTIMHDIALLRLHQPVVLTDRHVV
 321 LCLPERTFSERTLAFVVFSLVSGWQLLDRCATALELHVE
 361 MVRRLHTQDCLQQSRKWCDSPNITZYHFCACYSDGSKDSC
 401 KDGSGGPHATHYRGTWYLTGIVSWGQCCATVGHFQVYTRV
 441 SQYIEWLQKLMRSEPRFCVLLRAPFF

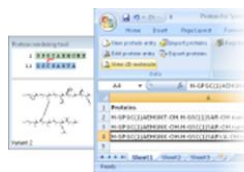


Proteax[®] – easily integrated

Proteax for Spreadsheets

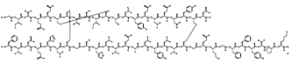
Spreadsheet functions,
macro programming

MS Excel[®]
OpenOffice.org[®]



Sequence	Molecular weights	Da
1 NEVQDQVETGK	Average	5887.51922
21 NEVQDQVETGK	Standard Unifrac	5795.64874
41 NEVQDQVETGK		

3D molecular



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

Structure and
sequence visualization

Proteax for KNIME

KNIME nodes for graphical
processing of protein data

KNIME[™]
graphical workflows



Proteax Desktop

.NET, Java[®], Python,
C/C++, Pascal

Scripting,
programming

Proteax toolkit

Proteax Cartridge
Database integration
registration and querying

Oracle[®]

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

PostgreSQL[®]

Vendor example – Sysment, Hungary

- Using ChemAxon's JChem and Biochemfusion's Proteax toolkits together
- Using Proteax's .NET API and JavaScript renderers

Available Section Types

- [New Html Section](#)
- [New Text Section](#)
- [New Reaction Section](#)

Existing Sections

- [Synthesis of ε-NB29-dehydrocholyl insulin](#)

Synthesis of ε-NB29-dehydrocholyl insulin

Include in Extract

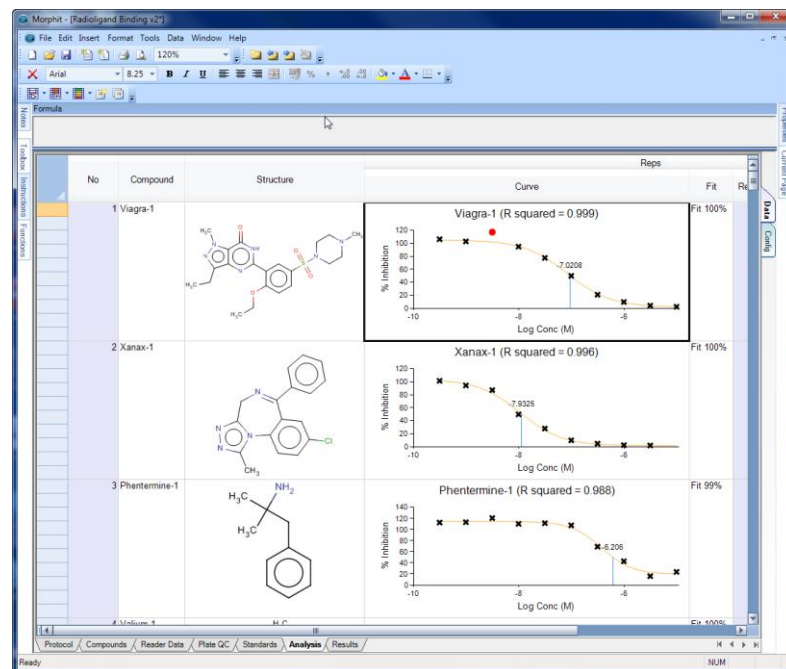
1 G I V E Q C C T S I C S L Y Q L E N Y C
21 N F V N Q H L C G S H L V E A L Y L V C +
41 G E R G F F Y T P K T

1 G I V E Q C C T S I C S L Y Q L E N Y C
21 N F V N Q H L C G S H L V E A L Y L V C
41 G E R G F F Y T P ~~K~~ T

- Resulting in the web-based *Sysment Notebook* ELN with full chemistry *and* biologics support

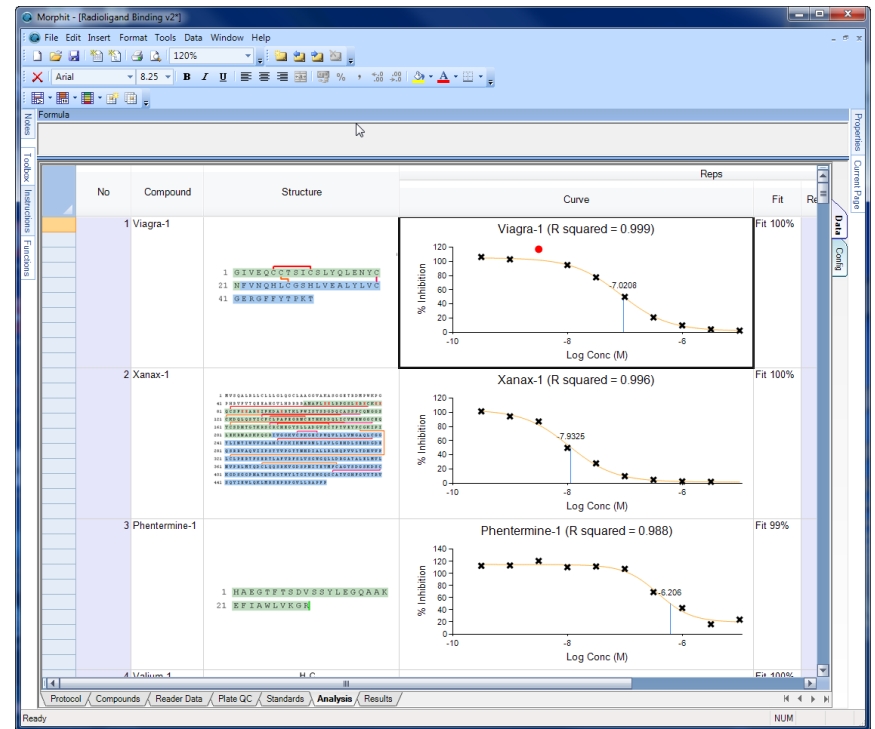
Vendor example – The Edge, UK

- The Edge's *MorphIt* is a relational spreadsheet – specifically designed to handle research data
- *Structures4MorphIt*
 - a MorphIt plugin that uses ChemAxon renderers for chemical structure visualization



The Edge - Proteax4MorphIt

- Proteax plug-in
 - Adding protein sequence and structure visualization capabilities to MorphIt
 - Using Proteax's .NET API and .NET renderers
- Full access to Proteax API
 - Protein manipulation and analysis via spreadsheet formulas



Mock-up – check the booth for a live demo

Links...

- Proteax for Spreadsheets
 - <http://www.biochemfusion.com/downloads/#ProteaxForSpreadsheets>
 - <http://www.chemaxon.com/download/jchem-for-excel/>
 - Direct data link from Proteax for Spreadsheets to JChem for Excel
- Sysment ELN
 - <http://www.sysment.hu/>
- The Edge
 - http://www.edge-ka.com/products/morphit/morphit_plugins
 - *Structures4Morphit* - structure visualizer plug-in using ChemAxon renderers
 - *Proteax4Morphit* - protein plug-in using Biochemfusion's Proteax toolkit and renderers - available later this year