

Chemistry Excel Add-In Game

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Solutions for Cheminformatics

Introduction

- Things to consider when evaluating an Excel Add-In
 - Past, Present and Future of Excel Add-Ins
 - Categories and brand names
- Evaluation and Migration
 - Case studies
- What is new?
- Future directions

Why in Excel?

- Is it better than custom applications?
 - Probably not.
- Is it the best choice for chemistry applications?
 - Not really.
- Is it easy to develop this under Excel?
 - Are you joking?

Why shall you use an Excel Add-In?

- Possible answers:
 - It is there on every desktop.
 - Almost everybody knows how to use it.
 - Familiar user interface.
 - Standard for spreadsheet applications
 - Used in other areas of research

Add – In Categories

Feature	Excel Shape based	Window Rendering
Examples	Accord for Excel ChemDraw for Excel	ISIS and Isentris for Excel JChem for Excel
Structures visible without Add-In	Yes	No
Print sheet as it is	Yes	No (insertion-removal required)
Structure resize with cells	No	Yes
Max # of structures	~3000	No limit
Import Speed	Slow	Fast
Workbook Size	Large (contains images)	Small
Advanced Functionality (like structure functions)	No	Yes

Evaluation - Migration

- Open to new feature requests
 - Work closely with the customer
- Release every ~two months
 - Access to development releases
- Work on features or issues providing the highest value
 - Sometimes it is not worth fixing an issue which are not used by many
- Migration
 - ISIS for Excel workbooks

Case Study - GSK

- Integrated with own add-in, Helium for Excel
- **Users:** ~1200
- **Communication:** Monthly meetings during evaluation
- **Issues:**
 - Deployment
 - OLE Conversions not working
- Requests from integration side
 - Load CLR in background because of VSTO
 - To be able to use the .NET API

Case Study – GSK - Continued

- **Requested user features:**
 - ChemDraw Integration
 - OLE and ActiveX based
 - OLE Copy Improvement
 - Copy structures and data in a single step to the clipboard
 - Copy filtered structures to new sheet
 - Import from File - Rename worksheet to file name

Case Study – GSK - Continued

- **Demonstration of requested features:**
 - ChemDraw Integration
 - OLE and ActiveX based
 - OLE Copy Improvement
 - Copy structures and data in a single step to the clipboard
 - Copy filtered structures to new sheet
 - Import from File - Rename worksheet to file name

Case Study - Evotec

- **Migrating from: ISIS for Excel**
- **Issues:**
 - Deployment: Ribbon going gray, add-in not present (disabled)
 - ISIS for Excel coexistence
 - Custom macros causing problems on structure sheet
 - Apply structure display options to calculated structures
 - JCImage referring to special Excel address functions
 - Convert from CXSMILES lost coordinates

Case Study – Evotec - Continued

- **Demonstration of requested features:**
 - Import from File
 - Start at current cell
 - Export to File
 - Selection only
 - Matrix of structures
 - No structure – to be able to create SDF
 - Default export format
 - Convert to Image
 - Option to remove formula

Case Study - GNF

- **Migrating from:** Accord for Excel
- **Issues:**
 - Structure sheet
 - Structure drawing using Terminal Services
 - Printing issues
- **Requested features:**
 - Turn on and off drawing in API
 - R-Group decomposition on same page
- **Partial Success**
 - Some chemists use printing and copy-paste to PowerPoint frequently

What we did since last year?

- Moved rendering from .NET to C++
- Office 2010 Support
- Import from Database
 - 3rd party commercial provider
 - Oracle Views, other user's schema
- Simple structure transformation actions
- JCHitColorSimilarityStructure
- Many fixes and small improvements

What will be new in 5.6?

- Advanced copy-paste to Office applications
- R-Group Decomposition Functions
- Structure Editor in Task Pane
- Import from File by key
- Import from Database
 - Import by key
 - Relational import
 - Use IJC connection definitions

What will be new in 5.6?

- Samples for reading from / and writing JC4XL specific workbooks in OpenXML
 - .NET Example: JChem for SharePoint
 - Java
- KNIME Nodes

Future – Technical

- Deployment
 - Installation validation checker – self diagnostics
 - Necessary dlls, registry,
 - OLE
- Performance
 - Load time
 - IKVM Class loading – at the moment it loads everything
 - JChem.dll size: 5.3: 18MB, 5.4: 23MB, 5.5 28MB
 - Necessary IKVM Dlls
 - Caching of function results
 - Asynch structure and normal functions
- “Hybrid” Add-In
 - Support for both Excel shapes and rendering
- Structure Storage
 - Database, file
- 64 bit
- WPF UI

Future – Functional

- Features
 - Import from Database improvements
 - Import from Web Services
- Task Pane
 - Structure Editor
 - Dialogs – Import, Export, Filter
- Instant JChem
 - Import – Export OpenXML
 - Handling IJC Datatree?
- SharePoint Integration

Team

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