

Chemistry Excel Add-In Game

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Solutions for Cheminformatics

Introduction

- Past, Present and Future of Excel Add-Ins
- Categories and brand names
- Case studies
- Future directions

- Less what's new
- Less fancy pictures and features
- Less demonstration

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?

- 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 – Excel Shape based

- ChemDraw for Excel, Accord for Excel
- Pros:
 - Structures are visible even for those not having the application
 - Copy – Paste to other Office application easier
 - No overhead in printing
- Cons:
 - Slow
 - Resizing of structure images
 - Import
 - Large workbook size
 - Limited number of structures
 - Certain functionality not possible

Add – In Categories – “Window Rendering”

- ISIS – Isentris for Excel, JChem for Excel
- Pros:
 - Fast
 - Import
 - Resizing
 - Unlimited (almost) number of number of structures
 - Smaller workbook size
 - More functionality – structure functions like Reactor
- Cons:
 - Structure are not visible for those not having the add-in
 - Copy – Paste with conversion overhead
 - Printing with conversion overhead

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 - 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

- **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

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

What we did since last year?

- Moved rendering from .NET to C++
- Office 2010 Support
- New functions:
 - MCS, Structure Checker, MarkushMatch,...
- Import – Export Enhancements
- Import from Database
 - Oracle Views, other schemas
 - 3rd party Oracle provider – 5.5
 - Convert IDs to structures – 5.5
- ...
- <https://www.chemaxon.com/jchem4excel/changes.html>

Team

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