

# Integrating with and extending JChem for Excel

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*Solutions for Cheminformatics*

# When?

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- You have an existing in-house Excel integrated application
- Custom corporate data source, web services
- You make an Excel integrated tool for different purposes, but also want structure integration
- You have various custom VBA macros, but need cheminformatics functionality

# Why?

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- You want the cool structure rendering in your application what JChem for Excel has
- You need other cheminformatics capabilities of JChem for Excel
- **But you do not want to worry about these**

# Possibilities

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- Customizable UI
- API
  - VBA
    - Built in macro language of Microsoft Office
  - COM Add-Ins
  - VSTO Add-Ins
  - External Applications interfacing with a running JChem for Excel
- Read – write JChem for Excel specific workbooks without Excel
  - Binary: Apache POI
  - XML

# Customizable UI

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- Change, customize, redefine using XML
  - JChem for Excel, menu and toolbar in Excel 2003
  - JChem for Excel Ribbon in Excel 2007
- We will provide many reusable actions
  - 2D Clean, 3D Clean, Add-Remove Explicit H
  - Put your favorite formulas on the UI
- Combine actions together
  - Convert to Image, Copy, Convert from Image
- Execute action with specific Option
  - Edit structure with xDraw

- AddStructuresToColumn
- GetStructuresFromColumn
- GetStructuresByFormula
- ImportFromFile
  
- *More to come....*

# Demonstration

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- Custom UI
- VBA Sample
- External C# Application