

# JCHEM FOR OFFICE

Ákos Papp  
Budapest Annual Meeting  
2016

# Chemistry in Excel, PowerPoint, Word, Outlook

Excel interface showing the JChem ribbon and spreadsheet data. The formula bar contains the JChem structure function: `=JCSYSStructure("871CA571F995E785BE44901E11FI"`. The spreadsheet displays chemical structures in column A, molecular weight (MW) in column B, and logP in column C.

Outlook interface showing the JChem ribbon and a table of chemical data. The table has columns for CD\_ID, CD\_STRUCTURE, CD\_FORMULA, and CD\_MOLWEIGHT.

CD_ID	CD_STRUCTURE	CD_FORMULA	CD_MOLWEIGHT
		C18H20N2O	280.3642
		C24H32N2O3S	428.587
		C15H15N3	237.2997

	<b>4.18</b>			<b>4.13</b>		
		<b>3.34</b>	<b>5.04</b>	<b>2.71</b>		
				<b>5.04</b>	<b>3.71</b>	<b>3.77</b>
				<b>2.86</b>		<b>5</b>

# Example Use Case: Data analyzis and reporting

The screenshot shows an Outlook window with an email from Akos Papp. The email subject is "FabH measurements ready" and the body contains a list of compound IDs. The list is as follows:

ID
CXN533577024
CXN533577127
CXN533577145
CXN533577158
CXN533577177
CXN533577198
CXN533577205
CXN533577212
CXN533577251
CXN533577266
CXN533577308
CXN533577340
CXN533577350
CXN533577353
CXN533577359
CXN533577407
CXN533577458
CXN533577474
CXN533577647
CXN533577651
CXN533577670
CXN533577706
CXN533577708
CXN533577719
CXN533577780
CXN533577964

The email also includes a header with the sender's name and email address, a subject line, and a body of text that reads: "Hi Akos, The FabH activity of the compounds below have been measured and the results are available in the corresponding view of the central DB: Best regards,". The Outlook interface shows various toolbars and a sidebar with folders like "Inbox", "Drafts", and "Sent".

# Roadmap

- Q2:
  - Windows 10 and Office 2016 support (64-bit)
  - ChemDraw 15 support
- Q3:
  - Document conversion to a journal style
- Q4:
  - Further SAR table improvements

# ACKNOWLEDGEMENT

Attila  
Vasanits

Tamás Pelcz Gergely Kovács



Anna Forró