

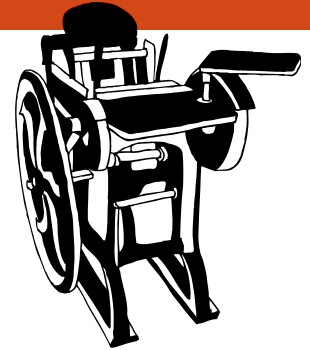


ENTERPRISE DEPLOYMENT OF
JCHEM FOR EXCEL (JC4XL)

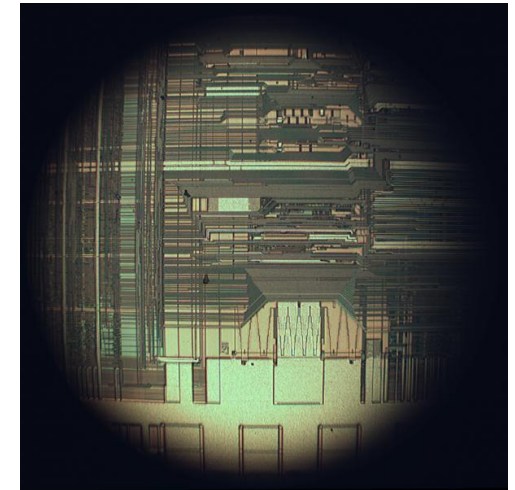
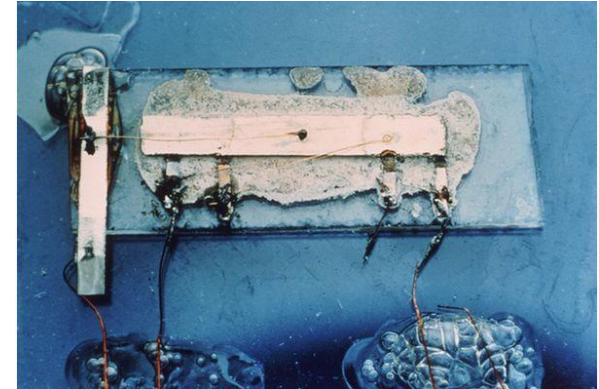
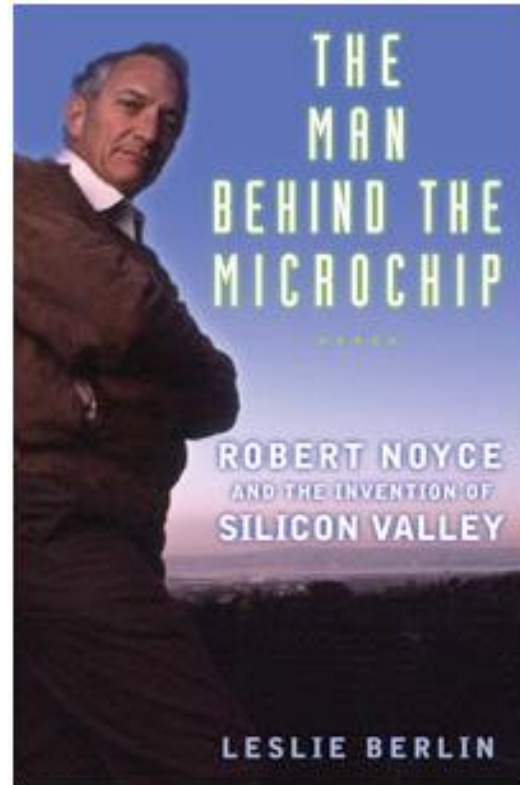
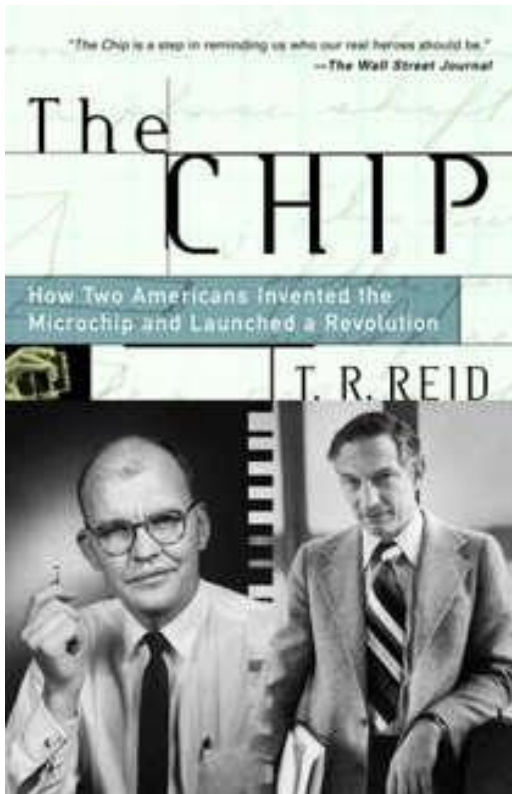
ChemAxon US UGM 2011 – San Diego CA

Name the Inventor

- Who invented the printing press?
 - ▣ Johannes Gutenberg
- Who invented the light bulb?
 - ▣ Thomas Edison & Joseph Swan
- Who invented the telephone?
 - ▣ Alexander Graham Bell
- Who invented the integrated circuit (microchip)?
 - ▣ Jack Kilby & Robert Noyce



The Microchip

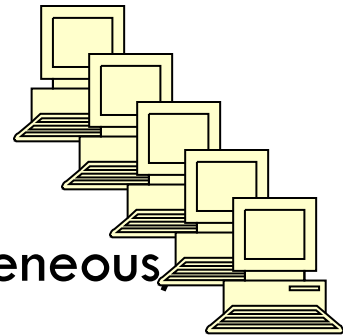


“Tyranny of Numbers”



Installing vs. Deploying Software

- “Installing” Software (Task-centric)
 - ▣ End user, installer, and administrator are same individual (single level permissions).
 - ▣ One or two computers are targeted in a homogeneous, static environment, in one location (house)
 - ▣ Typical of consumer applications (iTunes, Picasa, etc).
- “Deploying” Software (Support-centric)
 - ▣ End user, installer, and administrator are different individuals (multilevel permissions).
 - ▣ Hundreds of computers are targeted in a heterogeneous, dynamic environment in multiple locations
 - ▣ Typical of enterprise applications (ERP, ELN, JC4XL, etc).



“Tyranny of Computers”

Solution Delivery Strategy

- MS Office Suite (Excel):
 - ▣ Familiar and ubiquitous desktop tools targeting all corporate strata.
 - ▣ Usually requires active updating.
- Data query & visualization (IJC, Knime, Spotfire):
 - ▣ Advanced query and visualization targeted to scientists
 - ▣ Historically active updating but more recently passive.
- Web (Sharepoint, proprietary):
 - ▣ Focused operational tools targeting multiple corporate groups.
 - ▣ Passive updating (centrally updated).



Container Frameworks

- TCAL Addin
- R for Excel
- JChem4XL



- Spotfire
- IJC
- Knime



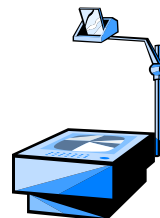
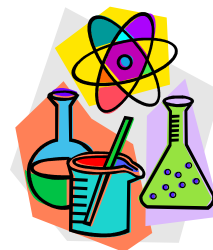
- Sharepoint
- Proprietary
- Portal/Integration
- Browser plugin

**Pick the best
framework for the
solution delivery
need**

Why Microsoft Excel?

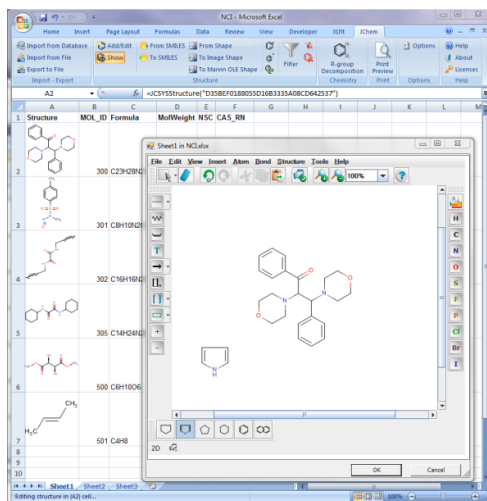


- Well suited for data visualization (tables, charts)
- Familiar and ubiquitous (ELN, SAR, Templates)
- Proven ChemInformatics “addins” Isentris, Accord, Chemdraw
- JC4XL maturation and integration
- Extendable (Templates, Macros, Addins)
- Facilitate communications
 - Printing
 - Presentations
 - E-mail



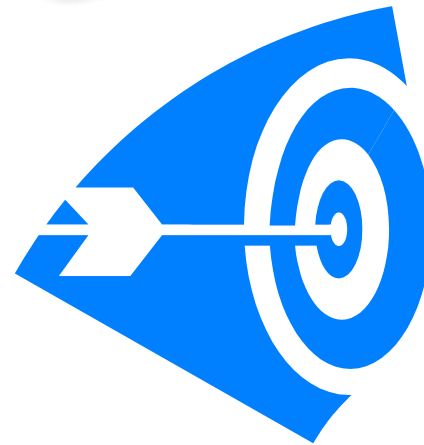
Business Case for JC4XL

- Aligned with our solution delivery strategy (Excel)
- Value proposition (immediate & long term)
- Missing Cheminformatics extension (Takeda Addin)
- Low overhead for Excel “Excel Hijacking”
- Ease of deployment and maintenance



Dynamic IT Infrastructure

- Operating Systems
 - **Windows 7 (32 bit)**
 - Windows XP
 - Windows 2000
 - Linux
- MS Office
 - 2000
 - 2003
 - **2007**
 - 2010



“hit the target”

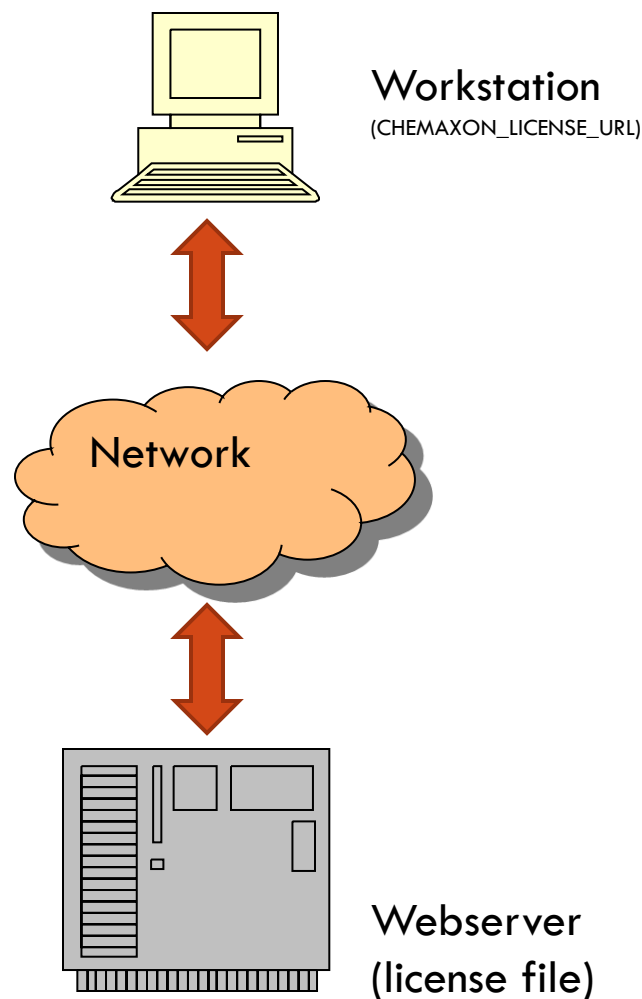
Vendor License File Strategies

- No license file/key
 - ▣ Relies on honesty policy.
 - “Time bomb”
 - ▣ Subscription-based license files that limit execution of software to a time window.
 - Installation or registry key
 - ▣ Key that unlocks or allows installation of the software.
 - Traditional license file
 - ▣ File that is imported or placed in a specific directory to activate the software after installation.
- Central license file/server
 - ▣ License file is deployed to a central server.




JC4XL Deployment Steps

- Deployed license file to apache web server.
- Set CHEMAXON_LICENSE_URL environment variable (logon batch script) to license file on web server.
- Silent install of JC4XL
 - ▣ Force reboot of computers (Windows 7 & Office 2007).
 - ▣ Logon script installs JC4XL .msi for Chemistry profile users.
 - ▣ Users notified of install and asked to perform one-time activation in Excel (not optimal).
- ChemAxon on-site training and distribution of JC4XL user documentation.

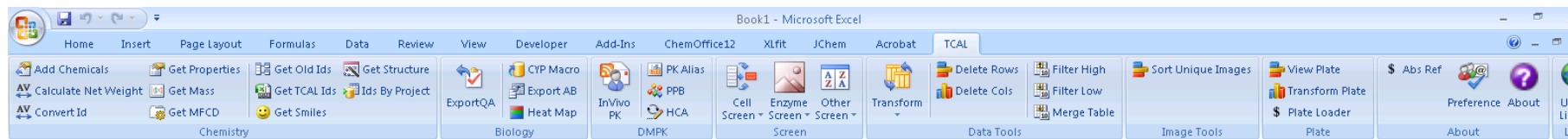


Post-Deployment

- Very few support issues.
 - ▣ Most issues reported related to one-time activation of addin.
- ~30% adoption in Chemistry (used >3 times since training).
 - ▣ Calculate chemical descriptors
 - ▣ View and manipulate SD files
- Non-Users
 - ▣ Get all the information / functionality through other tools.
 - ▣ Not integrated into infrastructure. 

Future Integration & Customization

- ❑ Identifier Services – converting identifiers into live structures (e.g. MFCD ID, T Number, CIS, SMILES, trade names, TAK IDs).
- ❑ Chemical descriptor calculator / profiler
- ❑ Workflow training and demonstrations
- ❑ Refactoring of Takeda Excel “Addin”:
 - ❑ Core
 - ❑ Chemistry – ChemAxon JC4XL
 - ❑ Biology – IDBS XLfit
 - ❑ Pharmacology



Summary

- ❑ Central push deployment of JC4XL successful to >80 workstations (thru login script)
- ❑ License file managed thru web server (CHEMAXON_LICENSE_URL environment variable)
- ❑ Moderate user adoption after 1 training session (~30%) potential improvement thru further integration
- ❑ Successfully patch pushed out to users
- ❑ Switch to live structures for naming/id service in TCAL Excel Addin
- ❑ Minimal support



Acknowledgements

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Thank you!