A User Experience of ChemAxon Software @ GSK

Past, Present & Future

Stephen Swanson
R&D Tech, GSK

do more
feel better
live longer

GW/GSK Chemistry Life B.C. (Before ChemAxon)

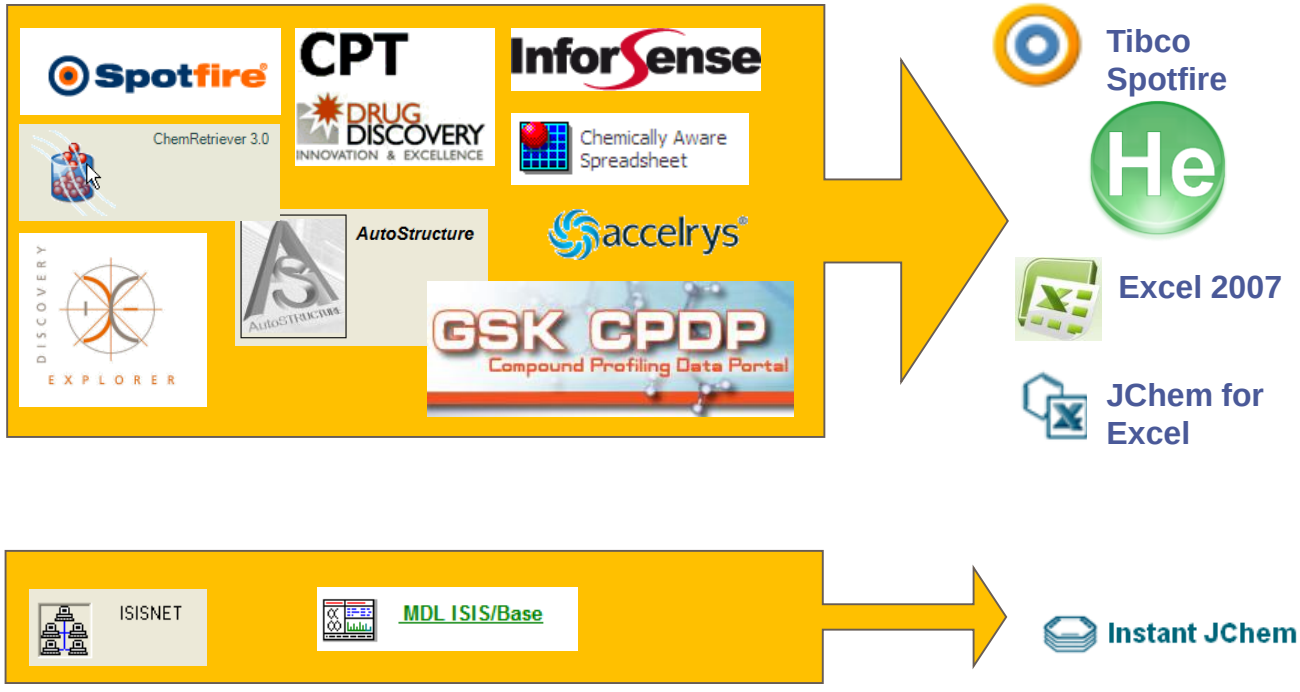
- 1998
  - GlaxoWellcome
    - MDL ISIS, Daylight + In-house developed SAR Applications
- 2000
  - GlaxoWellcome – SmithKline Beecham Merger
    - All the above plus legacy applications developed across both organisations
    - “Best-of-Both” approach for selecting data systems and applications
- 2009
  - Simplification & Cost Reduction of IT Systems

CRISP & SAR Tools (2009)

- CRISP (Chemistry Research IT Simplification Programme)
  - Highly complex Discovery Chemistry portfolio:
    - Large number of application components (520+)
    - Complex and fragile inter-application dependencies
    - Overlapping functionality, some obsolete and end of life tools

- SAR Tools Replacement Project (SS – Business Lead)
  - Chemistry Desktop – Too many applications – though some “loved” by the community
    - ISIS, Discovery Explorer, Chemically Aware Spreadsheet, Autostructure, ChemRetriever
    - Replace with Helium in Excel/Spotfire & **Instant JChem**
    - Structure Rendering for Helium in Excel using **JChem for Excel**

SAR Tools Objectives



SAR Tools Project Outcomes

2009 - 2010

- Development and Launch of Helium for Excel/Spotfire + **JChem for Excel**
  - Removal of DE, CAS, Autostructure, ChemRetriever.....++
  - Enthusiastic uptake by scientists – no tears shed for loss of legacy apps!

- Switch from Daylight to **ChemAxon Cartridge & Toolkit**

- But what about moving away from ISIS?
  - From….ISIS Draw, ISIS Base, ISIS for Excel
  - To……..**Marvin Sketch, Instant JChem, JChem for Excel**

Moving from ISISBase to Instant JChem

- Early testing indicated a significant drop in performance outside of UK
  - GSK Structure & Assay Databases located in UK
- US and Asia “solution” to access IJC on CITRIX Servers
  - US Performance improved but still slower than UK
  - European sites also impacted

- 2011-2016 - A Two-Tier IJC User Experience
  - High Uptake of IJC amongst UK chemistry groups
    - IJC becomes integral to many UK discovery programmes
  - Poor performance of IJC outside of UK, particularly at US sites, plus a frustrating CITRIX “barrier” results in lower uptake

2016 – The (almost) arrival of Plexus Connect

- Moving to a web solution presents a number of potential advantages, including..
  - A significant performance improvement in the US should increase uptake and usage
  - Removal of Java compatibility issues

But…..

- Several key members of the Chemistry Domain IT Group impacted by site closure
- A rush to get Plexus Connect launched before the IT group was broken up
- More limited engagement of business users during testing
- UK chemists raised major concerns around Plexus Connect project forms, particularly moving between records – so to switch from using IJC to Plexus Connect would be “unacceptable” to business
- Wave 1 launch put on hold

2017 – Plexus Connect - Wave 2 Project

- Greater business engagement (!)
  - UK & US Business Leads on IT Project Team
  - Key IJC Project Owners involved in testing

- Original Proposal
  - Instant JChem for form design and admin functions
  - Plexus Connect to be main tool for querying by programme scientists

- Top Priorities - Performance & Functionality Gaps (Plexus Connect vs IJC)
  - Fix original migration issues, repair project forms, implement new widgets and improve form design (Plexus Connect less “fault tolerant” – testing of individual project forms by owners)
  - Re-launch of Plexus Connect in August 2017

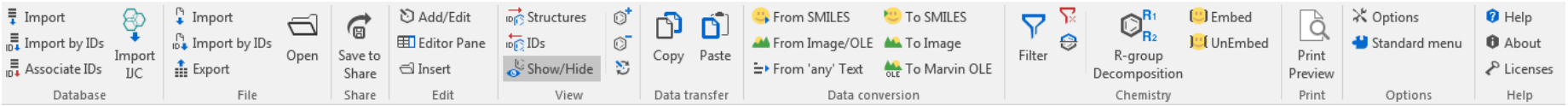
Plexus Connect in 2018

- Plexus Connect and IJC Performance now regarded as very similar by key UK users
- US Plexus Connect Performance (structure & data querying) comparable to UK
- US uptake and usage of Plexus Connect has increased – scientists there are happier!
  - IJC in US for form design and editing etc is OK – but no longer used for querying by scientists

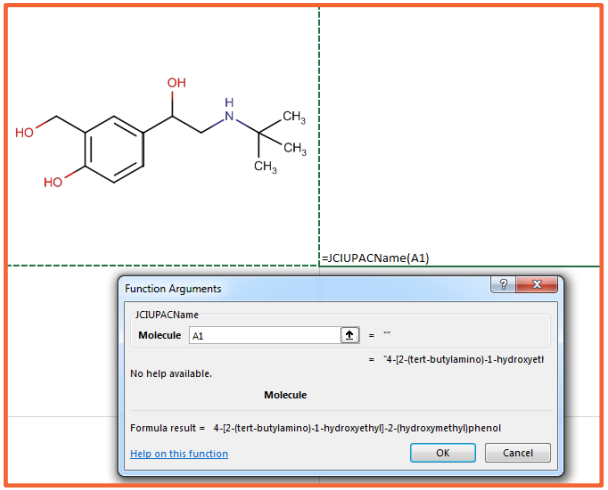
- UK usage now split between Plexus Connect and IJC
- Some established projects continue to use IJC
- New projects use Plexus Connect and existing project templates during set-up

- Functionality gaps between Plexus Connect and IJC still highlighted by some IJC users – e.g. list handling, structure search query options

JChem for Excel (or Office)



- An essential add-in for structure handling – part of the Helium installation
- We didn't promote the JChem for Excel functionality when launched so users end up discovering it for themselves – IUPAC naming a particular favourite
- One of the few tools available to chemists for creating and sharing SD files
- The add-in contributes to slow opening of Excel, particularly following our migration to Office 2016. Plan to move to JChem for Office in 2018.



2018 and Beyond

- Short Term
  - Consolidation of JChem Suite of apps to LTS Versions – Argon or Barium?
    - Plexus Connect v16 “Snapshot”
    - Instant JChem v17.21
    - JChem for Excel v16.12
    - JChem Cartridge v15.8
  - Will this help us deal with the Microsoft Office “Elevator”?
- Medium Term
  - Connection to “Big Data”
    - Hadoop Platform
    - Better Spotfire Integration
    - Containerisation of Plexus

2018 and Beyond

- Slightly longer term…..

- The Compound CV & Even Bigger Data
  - Chemists look at their Plexus Connect project form as an overarching view of a compound's properties, but the form has to be manually created and pre-linked to data sources, so has limited flexibility. A "Smart" form would create itself and make the necessary connections. Otherwise how to keep up with the ever increasing sources of data that need to be processed and analysed?

- Who are to be the future users of ChemAxon Software?
  - Through advances in AI, algorithms, machine learning etc, for enabling data molecular design, there is a real probability that the age of the medicinal chemist may be fast drawing to a close, so how will current, or future, ChemAxon applications fit into the new model?

Acknowledgements

- Plexus Connect & IJC Performance Testing
  - Debbie Needham (UK Lead)
  - Christie Schulte (US Lead)
  - Carl Brooks