Delivering Instant JChem to the Masses

A User Perspective

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CRISP & SAR Tools (4Q 2009)

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

- SAR Tools Replacement Project
  - Chemistry Desktop - suite of applications
    - ISIS, Discovery Explorer, Chemically Aware Spreadsheet, Autostructure, ChemRetriever
  - Replace with **Helium in Excel/Spotfire** & **Instant Jchem**
  - High Change Programme
  - IT-Business Partnership critical for success of project

SAR Tools User Representation

- Core User Group
  - Business Lead + 7 Scientists (UK, US & Europe)
    - Cross Site & Function (mostly discovery chemistry)
    - Responsibility for local site
      - e.g. Requirement gathering & communication
    - Weekly meeting with IT Team
      - Decision-Making

- Extended User Group
  - ~ 40 Scientists
    - Additional sites represented
    - Reps from business functions with specialist use cases
  - Generate User Stories
  - Application Testing

SAR Tools – Phase 1

- SAR Tools - 2009-2010
  - Development and Launch of Helium for Excel/Spotfire
    - Removal of DE, CAS, Autostructure, ChemRetriever
    - Enthusiastic uptake by scientists – no tears shed for loss of legacy apps!
  - Switch from Spotfire Decision Site to TIBCO Spotfire (DXP)
    - Professional Client - Enterprise Player Model
    - Many Decision Site users found adjustment to DXP difficult
    - Loss of Decision Site Customisations
- Developing Support Model – New User Roles
  - Business System Owner (BSO)
    - Single point of contact representing the strategic use view
  - Business Expert Users (BEUs)
    - Provide local assistance with application functionality
    - Identify future user requirements

SAR Tools - From ISIS to Instant JChem

- This would be different.....potentially a much harder sell
  - Why change?

- ISIS Desktop
  - ISISDraw
    - Earlier CRISP Project to replace with ChemDraw
    - Goal of ”single drawing package” (ChemDraw also in eLNB & incorporated into Helium)
  - ISISNet & Databases
    - ISISNet - GSK Federation of ISISHost databases
    - GSKChem & ACD Finder – many users view as “gold standard” for structure searching
    - Programme specific, highly customised “Hviews” – structures + biological data
    - Use of Hviews embedded in most medicinal chemistry programmes
    - Many processes evolved around ISIS functionality
    - Hviews tuned for optimal performance over many years
    - Hviews set up and supported by Research Data Management (IT)
    - ISIS Hview Performance in UK better than US – would this change?

Instant JChem – First Impressions

- Initial testing by small number of users in UK – GSKChem & ACD Finder
  - Performance – OK for a non-tuned system but slower than ISIS
    - Structure searching – SSS times could be significantly longer than ISIS
    - A few seconds “pause” when browsing between records – should be “instant”
  - Functionality – similar to ISIS but different – fairly intuitive
    - Positives Query & List Handling, Grid View,
    - Negatives Sorting, Domain Searching, Exporting, Printing.....+ too many error messages
- Testing at US sites
  - Significant drop in performance – GSKChem worse than ACD
    - GSK Structure database located in UK
- ISIS Programme Hviews converted to IJC Projects
  - US performance “unacceptable”
    - GSK Biological database located in UK

General Testing Issues

- Poor performance in US reduced engagement of local testers
  - Similar for extended user group members in Asia
- User Feedback on Performance
  - A slow IJC login time was manageable – it could become a once-a-day activity
  - Slightly slower search speeds also bearable – do something else while it's running!
  - **Scrolling between records was most critical problem**
  - Performance issues resulted in many users attempting to cancel IJC tasks but this is poorly handled by IJC – results in IJC hanging – a significant irritation
- Special Use Cases
  - Most users worked with hit lists of <1000 compounds, but for those that needed to handle large lists (>100K) then performance was a major problem
  - e.g. ISIS/GSKChem – SSS returning >1 million hits ran in less than 60 sec; IJC/GSKChem took >30 minutes

US & Asia Performance Solution

- Access to IJC on CITRIX Servers
  - Separate Citrix installation & access issues for users
  - Citrix/IJC login slower but optimised to avoid unacceptable “spikes”
  - IJC performance acceptable once connected
    - Slower than UK but similar to US ISIS Hview performance
  - Citrix solution also adopted by site in France; Spain also considering approach to improve performance over direct IJC connection

- However.....user frustration at the two-tier Instant JChem experience
  - Global IJC awareness sessions run from UK – excellent performance!
  - Local overall experience is less impressive
  - High Priority User feedback
    - Remove reliance on Citrix
    - Improve overall performance

Migration of Programme Hviews to IJC

- Conversion of programme specific ISIS Hviews to IJC Projects
  - Conversion carried out by IT team
  - Redesign/Customisation in collaboration with programme leads
  - Individual UAT/sign-off required by lead user / IJC Owner
    - Tracking down and engaging with leads – slow process
      - Programmes, scientists had moved on!
      - Hviews with small user bases – was conversion to IJC critical?
      - Opportunity to reduce support burden
  - 387 ISIS Hviews
    - 184 migrated to new IJC Projects
    - 203 not migrated
      - Underlying data available via Helium

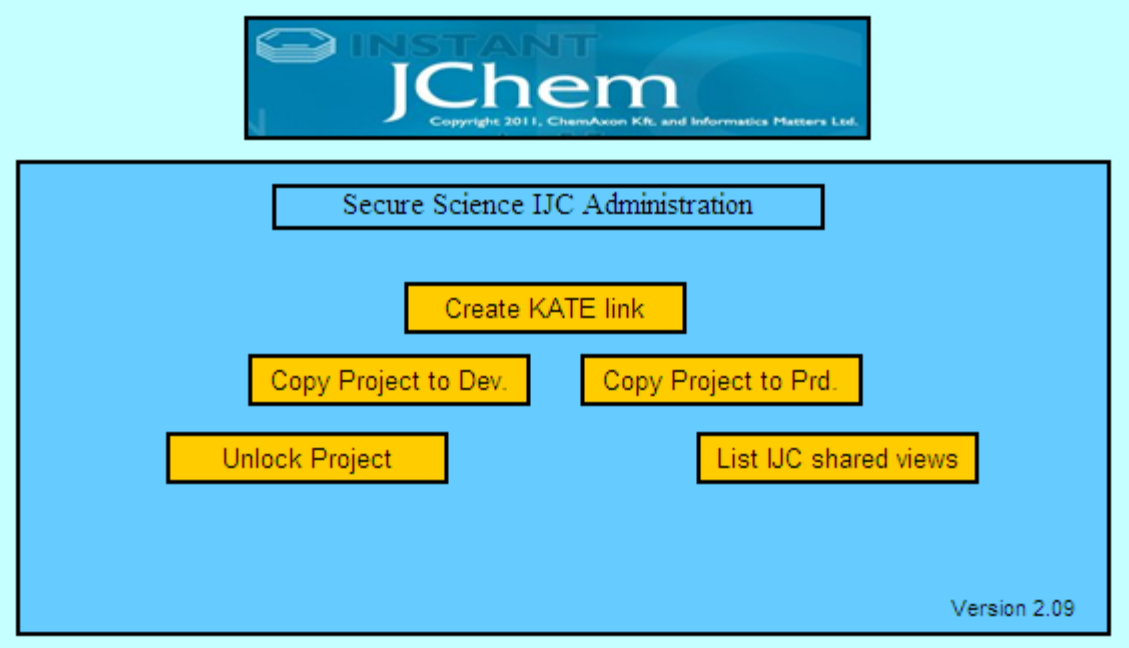
- **Owner - responsibility for future customisation & maintenance of IJC**
  - new data, forms etc

Functionality Gaps & Issues

- SubStructure Searching
  - Still very slow for more complex queries and for large hit list
- Domain Searching
  - Workaround “acceptable” to key users, but still significantly longer than ISIS process
  - Query Builder – non-intuitive
- Exporting SAR Data
  - Additional IJC requirements identified, though Helium provides alternative approach for creating SAR Tables
- Printing
  - Non-chemists in the user group failed to understand why a 21st century scientist might want to view their data in paper format, yet many chemists considered the effective printing of IJC Project forms to be critical functionality – a showstopper for IJC deployment!
- Sorting
  - Does architecture make effective sorting (e.g. on biological activity) unachieveable?

IJC Project Owners

- Greater role for IJC owners (scientists) to develop and maintain programme specific IJC Projects
- Significant push-back from users - owner “pain points” identified
  - Working with Development/Production Environments
  - Creating links to biological data tables
- Creation of IJC Admin Website
  - Project Owners very grateful!



Back at Chemical Structure Drawing.....

- Part of CRISP to consolidate chemical drawing/sketching tools
  - Driven by IT maintenance & support considerations; not by chemists
  - ChemDraw selected as preferred drawing tool to replace ISISDraw
  - Helium in Excel (incorporating JChem) developed with ChemDraw integration
- Instant JChem-ChemDraw integration also enabled
  - Issues identified with Substructure Searches using ChemDraw structures
  - Decision to launch IJC with Marvin as default drawing tool until issues resolved
    - Issues now resolved, but the users continue to use Marvin – they like it for querying
- What prospects for future consolidation?

Conclusions

- Engagement of user community critical to successful deployment
- Non-uniform performance of applications at global sites can be serious issue
- GSK Implementation of IJC - a work in progress
- Improvements in IJC performance required and functionality gaps remain to be addressed