



Rollout of Plexus Connect at GSK, a brief history and update

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1. What GSK said we'd do (.....at last years CXN UGM talks)
2. A reminder of the history of forms based SAR tools at GSK and why we need to move to Plexus Connect
3. Status of Plexus Connect rollout at GSK today
4. What next and future challenges?

Previous Presentations. What did we say we'd do?

Find these on the ChemAxon web site



- **Consistent Stereochemical Search at GSK: UK UGM 2015**
 - Delivered a v3000 mol file infrastructure in GSK to allow complex stereo search capabilities
 - Web services, IJC and JChem Cartridge upgraded to handle V3000 format
 - Some issues still being resolved regarding parent/salt data integrity.
- **Integrating Plexus Suite at GSK: US UGM 2015**
 - GSK working with ChemAxon to ensure Plexus Connect could replace IJC
 - Proposed timeline to deliver wave1 in Early 2016 wave 2 in mid 2016

Instant JChem at GSK. A brief history.



- Initial replacement for ISISBase began 2009. Full rollout IJC 5.6 mid 2011.
 - ChemAxon converted H-views to IJC projects like-for-like. 400 H-views approx half converted.
 - Bespoke tools to create test-prod environments
 - Slow US performance necessitated Citrix.
- Cross Pharma prioritisation of requirements. Uplift to 5.7.2.1 in 2012
- Evaluation of JChem Web Browser 2013
 - GSK database architecture made performance slow.
 - Joining across multiple data sources
- 2014 Uplift to version 6.2 using ChemAxon Services to replace test/prod publication mechanism.
 - Still using Citrix for US users (databases mostly in UK)

Why Move to Plexus Connect; the start of a Web-based Chemistry Desktop.



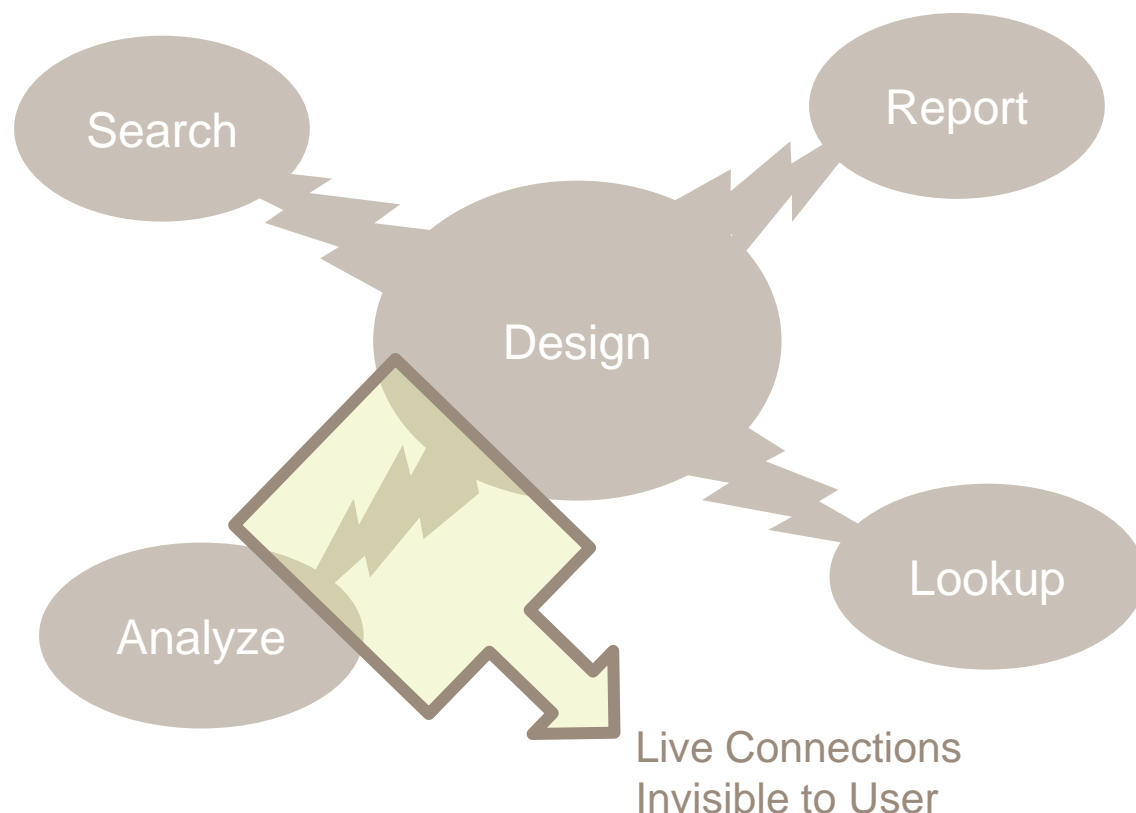
GSK roadmap and vision

- More unified Chemistry Desktop Experience
 - Seamless interactions between other Desktop tools.
 - Ability to share securely with partners
- Performance Enhancements
 - Plexus Connect server co-located with scientific data
 - In contrast to IJC thick clients remotely accessing scientific data
- Fewer application conflicts and dependencies (e.g. Java)
 - Marvin JS instead of Marvin Beans (structure edit and render)
 - Plexus Connect instead of IJC (search, analysis, reporting)
 - Plexus Enumeration instead of bespoke solutions (reaction/scaffold enumeration for virtual libraries)
- Easier to Update Globally
 - No need to script a new client for Citrix Deployment
 - Deploy once via server and patch centrally.

Vision for the Chemistry Desktop in GSK



• Future Chemistry Desktop- Integrated Interfaces



- Web-based editing tool
 - No IJC Thick client
- “Bookmarkable” Plexus Connect Searches.
 - Open Plexus Connect to a saved query
 - Open Plexus Connect to structures/query parameters in the URL
- Speed
 - Server leverages connection pools to improve search performance
- More Web-based tools
 - Allows for more rapid deployment, easier support, fewer desktop conflicts, sharing with external partners and easier migration to touch and mobile interfaces

Plexus on the GSK Chemistry Desktop Today

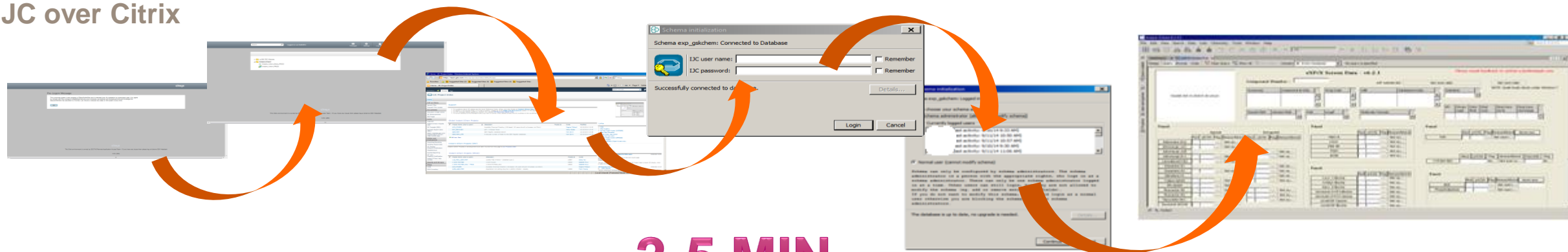


- Working with ChemAxon to align with the Plexus roadmap and vision.
 - Web-based tools allow for more rapid deployment, easier support, fewer desktop conflicts, and easier migration to touch interfaces
 - Web-based tools also address architectural and security problems with desktop data analysis
- GSK/ChemAxon collaboration on IJC Web/Plexus Connect
 - October 2014. IJC to Plexus Connect gap analysis complete and addressing key gaps
 - November 2014. Project form load took **10 MINUTES**.
 - March 2015. Project form load improved to between **10 and 30 SECONDS**.
 - August 2015. “IJC Web,” wave 1, initiated to deliver the 5 most used IJC Projects via Plexus Connect
 - February 2016. “IJC Web,” wave 2, migrate remaining 63 (from 170) IJC Projects to Plexus Connect

User Experience: Opening an IJC project



– IJC over Citrix



– Plexus Connect



Instant JChem (Thick Client)

Form-based Searches and Visualizations



Design Query Browse Code Clear Query Show All Run Query Domain: No query is specified

Cpd Props | Project Assays | Selectivity panel | P450 | In vivo PK | Availability

Details

UCS_ID	
Create Date	
Mod Date	
Registry Del Date	
ACD MDL Number	
CAS Number	
Molecular Formula	
Molecular Weight	

CAS Number
ACD MDL Number
Create Date
Mol Weight
Formula
Molecular Formula
Molecular Weight

GSK LACIR Compound

STRUCTURE_ID	
Status Cd	
Salt Name	
Database Key	
Molname	
Ext Regno	
Parent Mw Low	
Parent Mw High	
Parent Salt Low	
Parent Salt High	
Parent Salt Mf	
Parent Mf	
Hazards	
Store Cond	
Solubility Data	
Sbmaccs Intreg	
CAS Number	
Gw Sop Regno	
Last Updated Date	

Registry Gsk Compound | Compound Number Only

Registry Gsk Compound	Compound Number Only

Proj Code | Comments

Proj Code	Comments

GSK LACIR GSK Lot

Lnb Ref	Date Submitted

Physchem Summary

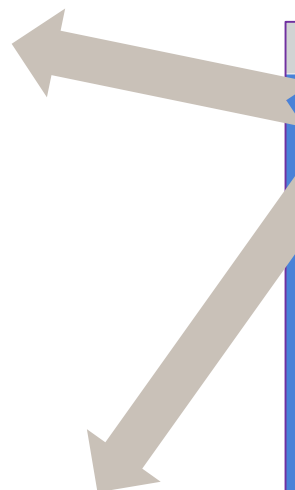
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Chrom Logd Ph74 Range	
Chrom Logd Ph74 N	
Chi Logd Ph74 Mean	
Chi Logd Ph74 Range	
Chi Logd Ph74 N	
Chi Logp Mean	
Chrom Logp	
Acid Or Base	
Pfi	
Pct Chance Low Sol	
Perm Num Mod Ph705	
Perm Num Ph705 Mean	
Perm Num Ph705 Range	
Perm Num Ph705 N	
Hsa Pct Bind Mean	
Hsa Pct Bind Range	
Hsa Pct Bind N	
Link Hsa Mean	

Calculated Properties

Parent Number	
Clogp	
Clogp Comment	
Psa	
Hba Lipinski	
Hbd Lipinski	
Cmr	
Hba	
Hbd	
Pmw	
Flexibility	
Rotbond	
Heavy	
Abe	

Plexus Connect (Web Client)

Form-based Searches and Visualizations via a Web Interface



Export the selected fields of the current recordset

- ChemAxon MRV format (*.mrv)
- MDL SDF file (*.sdf)
- MDL RDF file (*.rdf)
- Tab separated text (*.txt)
- JChem for Excel with structures (*.xlsx)
- Microsoft Excel with structure images (*.xlsx)

Export

Tables Forms Enumeration Help

1 of ?

Cpd Props Project Assays Selectivity panel P450 In vivo PK Availability

Details	
UCS_ID	
Create Date	
Mod Date	
Registry Del Date	

CAS Number	
ACD MDL Number	
Create Date	
Mol Weight	
Formula	

GSK LACIR Compound	
STRUCTURE_ID	
Status Cd	
Salt Name	
Database Key	
Molname	
Ext Regno	
Parent Mw Low	
Parent Mw High	
Parent Salt Low	
Parent Salt High	
Parent Salt Mf	
Parent Mf	
Hazards	

Physchem Summary	
Last Cind Pid	
Cind Conc Mod	
Cind Conc Um M...	
Cind Conc Um Ra...	
Cind Conc Um N	
Comment Flag	
Chrom Logd Ph7...	
Chrom Logd Ph7...	
Chrom Logd Ph7...	
Chi Logd Ph74 M...	
Chi Logd Ph74 R...	
Chi Logd Ph74 N	
Chi Logd Mapp	

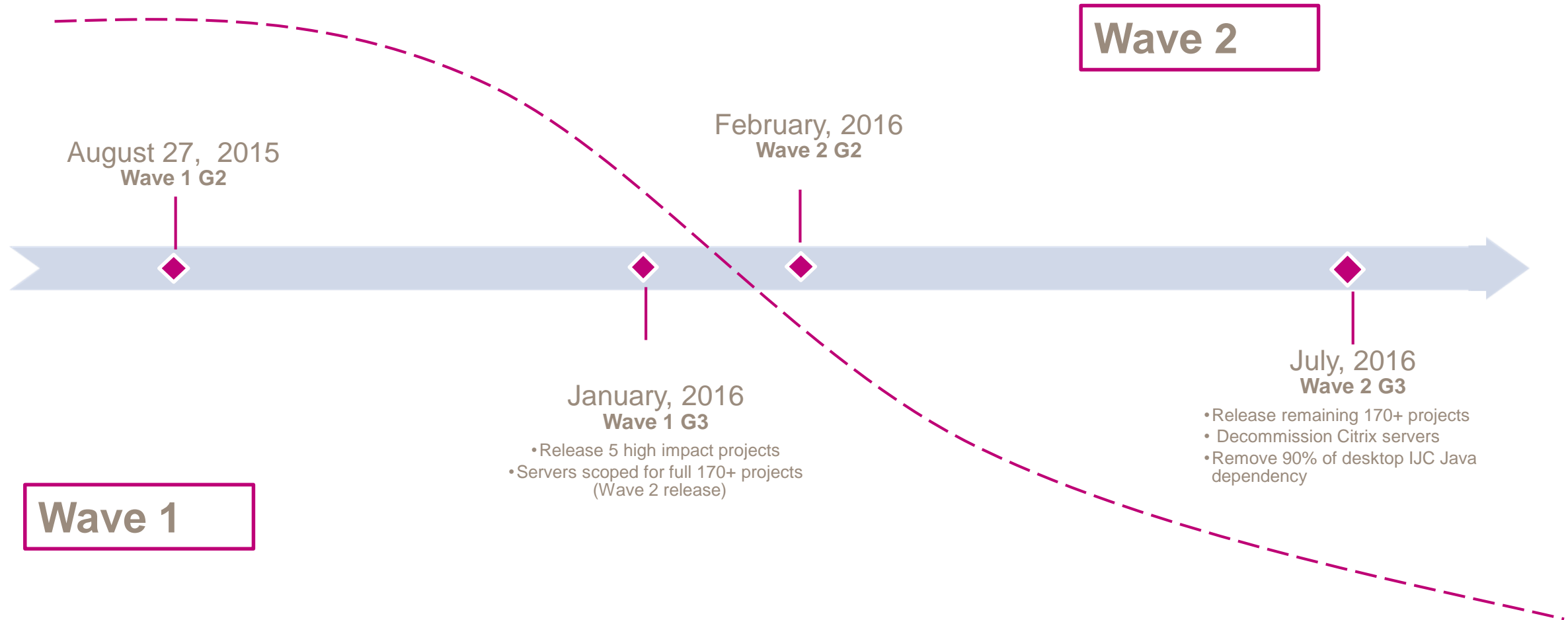
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Cmr	
Hba	
Hbd	
Pmw	
Flexibility	
Rotbond	
Uvw	

Registry Gsk Compound	Compound Number Only

Proj Code	Comments

GSK LACIR GSK Lot	
Lnb Ref	Date Submitted

Instant JChem Web: Waves 2015-2016



Plexus Connect Deployment: Wave 1 Completed Jan 16

- Five projects deployed. US and UK users get benefit. (4 team use, 1 broad use.)
 - Approx 900 unique logins tried it. 250 users stayed with it
 - Feedback from users positive especially performance.
 - Negative feedback around missing features and desire for their project
- Tool to migrate forms developed by ChemAxon (Used in wave2)
- Feedback from application usability session fed into wave 2 for layout, workflow, and functionality optimization

Plexus Connect minimum features delivered for wave 1

Similarity Search	Export List Selection
Keyboard Commands	List Logic
Grid View	Export Child Tables
Cancel Search	Project Form List / Dashboard

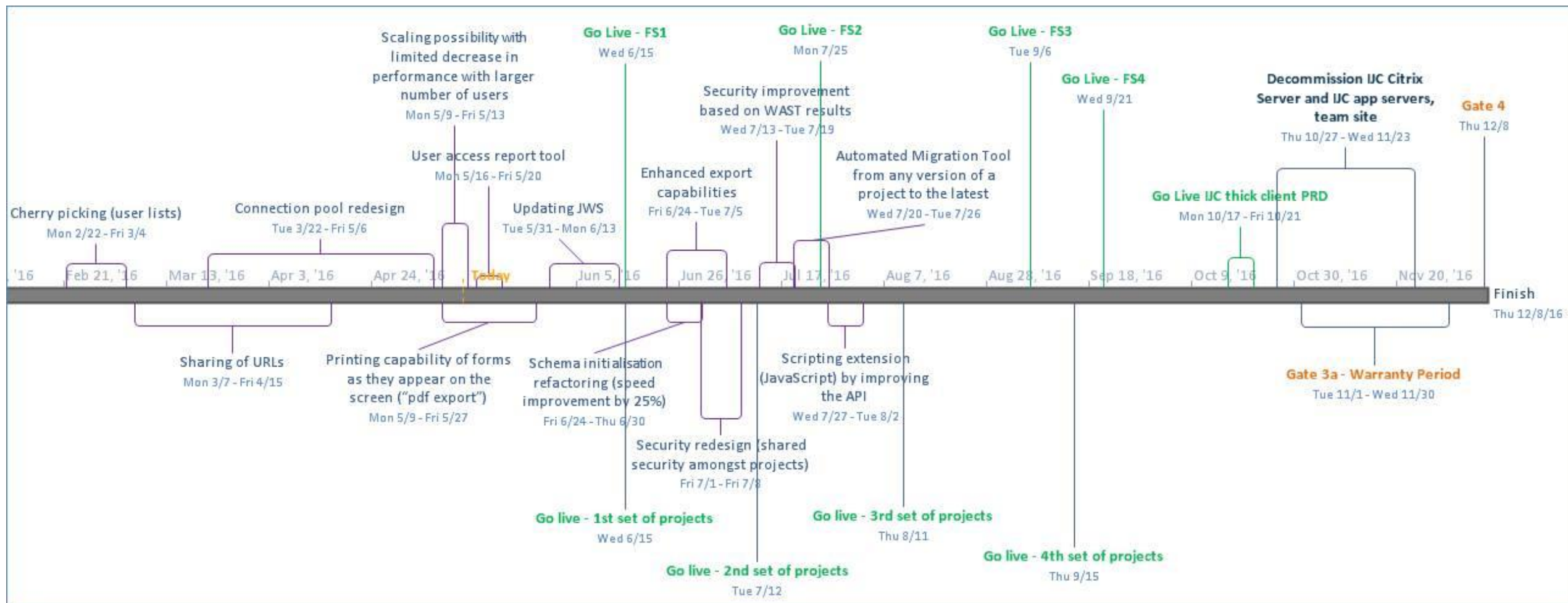
Plexus Connect Deployment: Wave 2 rollout: Mid June



- Cleanup of inactive projects gave total of 63 projects (from 170+) and 124 forms
- Complete May Feature rollout
- Update the IJC Thick Client and Cartridge to latest version to allow Plexus form editing
- Rollout first 15 projects in June. Follow-on batches of 15 approx 3 week intervals
- Retire Citrix interface

Additional Features to be delivered			
Enhanced Export Capabilities (SDF)	May 16	Cherry Picking	May 16
URL Bookmarking	May 16	Connection Pool Redesign	May 16
Performance Scaling	Jun 16	Access Reporting Tool	Jun 16
Form Printing (via pdf)	Jun 16	(List management)	Jun 16
Schema refactoring	July 16	Security Redesign	July 16
Migration Tool Finalised	Aug 16	Scripting Extensions	Aug 16

Plexus Rollout timeline for 2016



What is planned and what are the next challenges?



• Plans

- Continue to rollout as per schedule and complete the feature upgrades with ChemAxon.
- Migrate a reaction database (end July)
- Deliver form editing on web (late 2016)
- Get JChem4XL in line with the rest of the toolset (office 2013 rollout 3Q16)
- Deliver Multi-tabbed form queries (roadmap end 2016 early 2017)
- Deliver form creation on browser (roadmap in 3Q17)

What is planned and what are the next challenges?



• Challenges

- Scalability now all forms loaded. Load time has increased.
- Thick client cannot be retired until end 2017 as it will be needed to create forms and maintain complex databases
- On-premises R&D Information Platform rolls in early 2017. Future direction for project data via HDFS based ecosystem. How will we run structure search over HDFS?
- External partners and security
- Connection of web services to forms

In Conclusion



- We are now ready to deploy Plexus Connect much more broadly as the next step toward delivering our vision of a web-based Chemistry Desktop.
- We have and will continue to work with ChemAxon to deliver and deploy new features of Plexus Connect throughout 2016.
- Despite a very complicated architecture at GSK, we are making progress.
- There are many future challenges as the infrastructure and business model changes.

Thank you for your attention



Questions?