Challenges in Updating an Enterprise Environment: Progress toward updating the ChemAxon tools at GSK

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Abstract

- ChemAxon has been a strategic partner with GSK for many years now and has allowed for GSK to envision a comprehensive Chemistry Desktop that works seamlessly from molecule design to all the related lead optimization tools and given us the infrastructure and tools to afford advanced, consistent search capabilities. Efforts to keep the systems consistent and up-to-date have been challenging in recent years due to inconsistent upgrade strategies at GSK and ChemAxon and diverse use cases at GSK but a concerted effort has allowed GSK to work toward that goal. This topic will cover what progress and challenges still await us as we move toward consistency and stability on our chemistry desktop.

Agenda

1. What is GSK trying to accomplish?
2. Why are updates so hard?
3. Delivering the Solutions
4. Preparing for the future

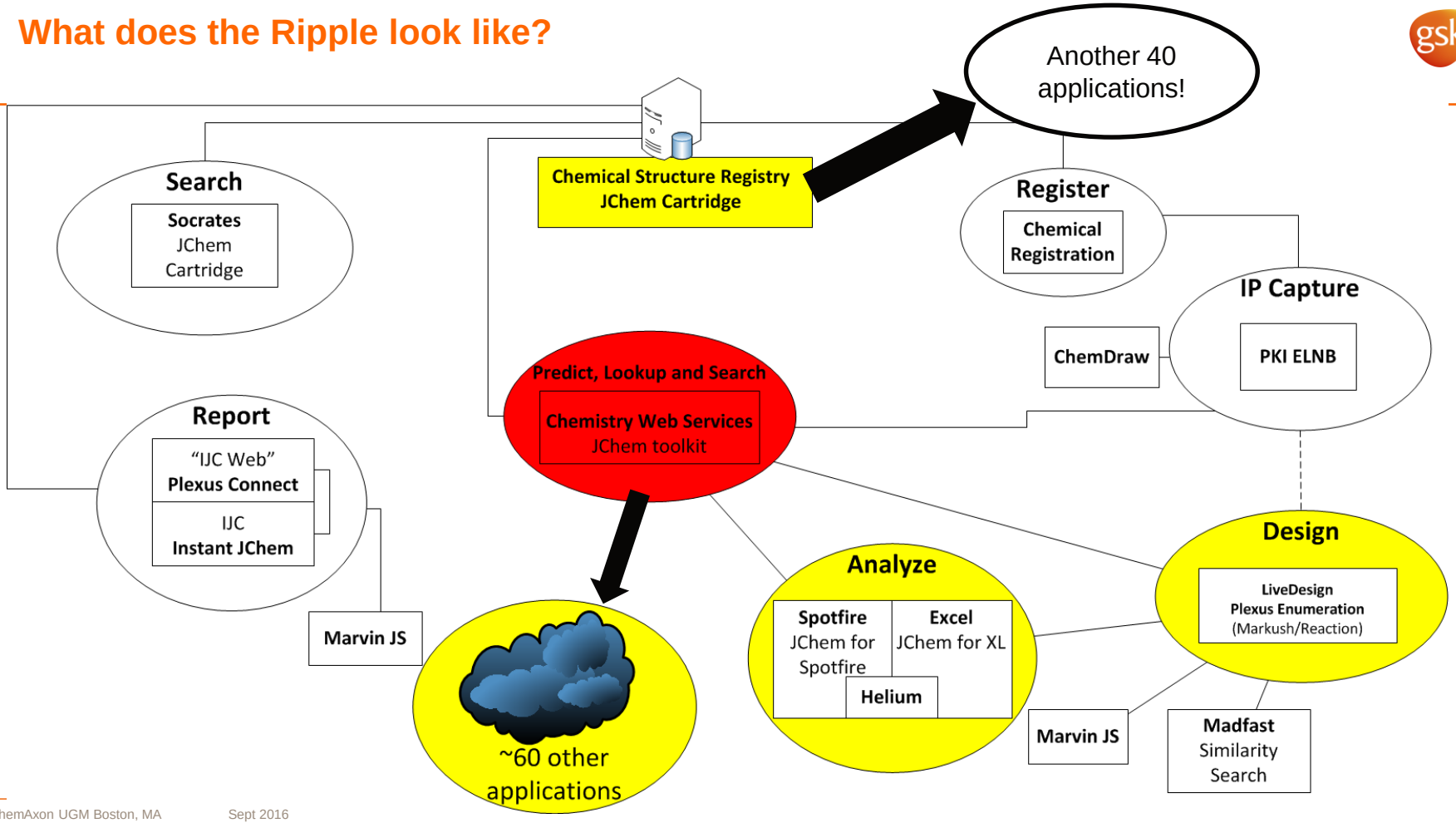
What is GSK trying to accomplish?

- Move to more limited and supportable set of Chemistry-related tools and architecture- e.g., Simplify!
- Move to the V3000 molfile standard from SMILES and V2000
- Gain search consistency across our Chemistry tools
- Take advantage of developing technology more quickly

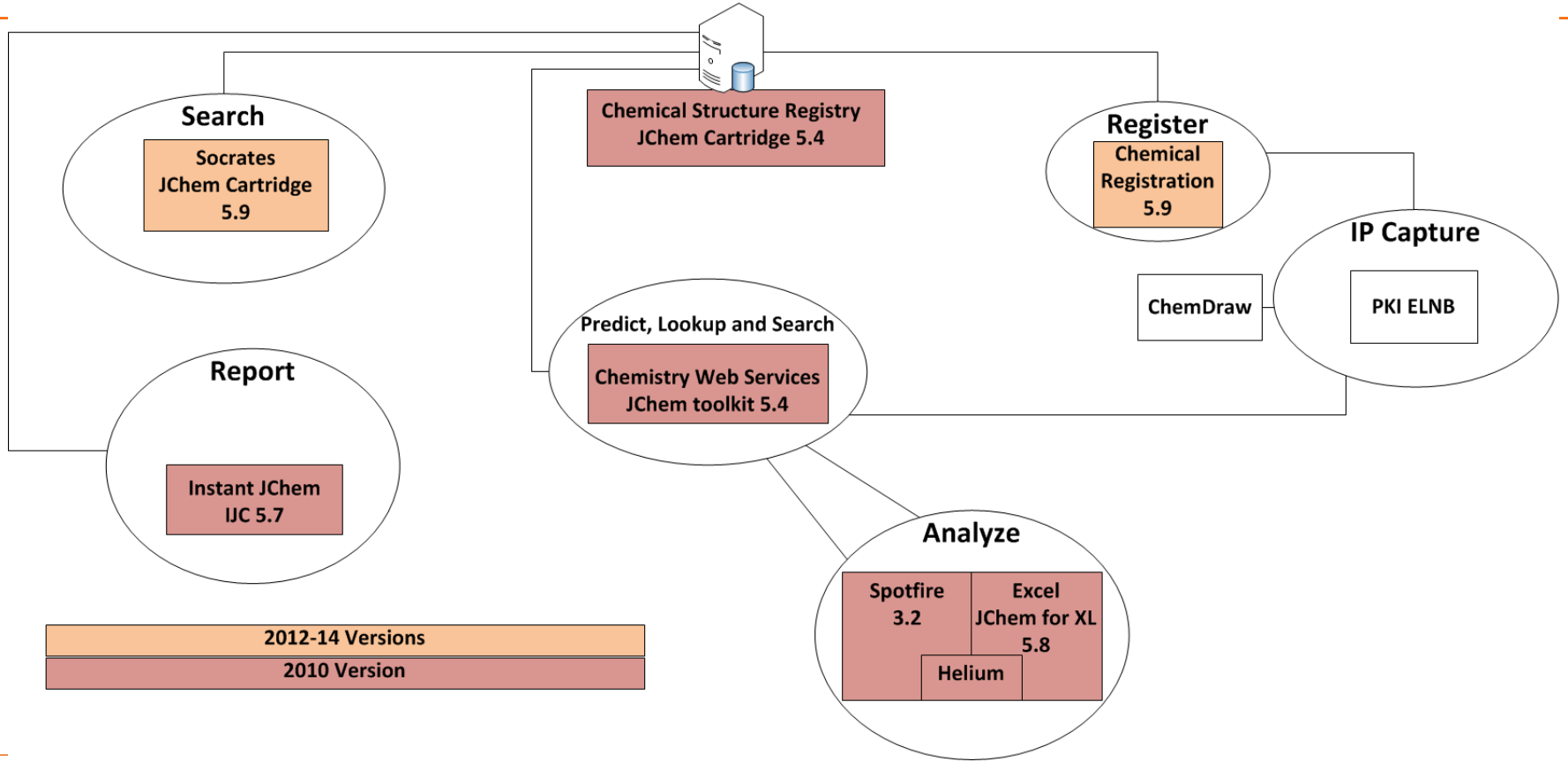
Why are ChemAxon updates so hard?

- ChemAxon tools are interconnected to multiple applications and processes at GSK- some of which include other ChemAxon tools/Apps
- Changes to one system make ripples across the whole pond as all updated applications and tools need to be tested
- We aren't the only ones on the pond
- IT Budgets get squeezed. The upgrade costs often outweigh the benefits of simply "keeping the trains running"

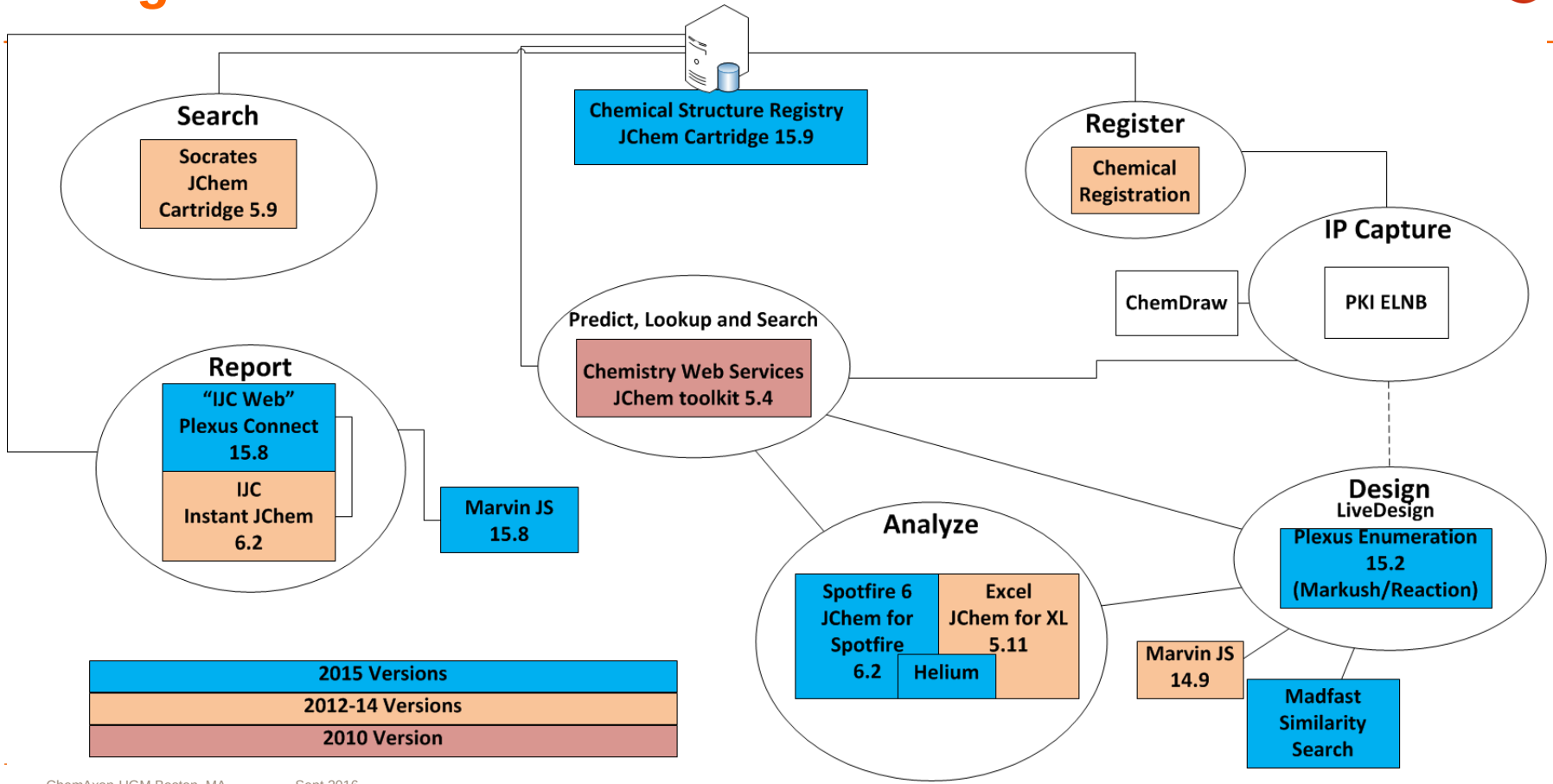
What does the Ripple look like?



A look back at our systems in 2014



Progress in 2015



Successes and Challenges

- Successes
  - Upgraded JChem Cartridge
  - Upgraded JChem for Spotfire
  - Deployed Plexus Connect
  - Plexus Enumeration in LiveDesign
- Challenges
  - IJC 6.2 and JChem Cartridge incompatibility– bespoke cartidge
  - JChem Cartridge and Toolkit incompatibility
  - V3000 molfiles not handled in all systems
  - Copy and paste of chemical structures

What were we trying to accomplish?

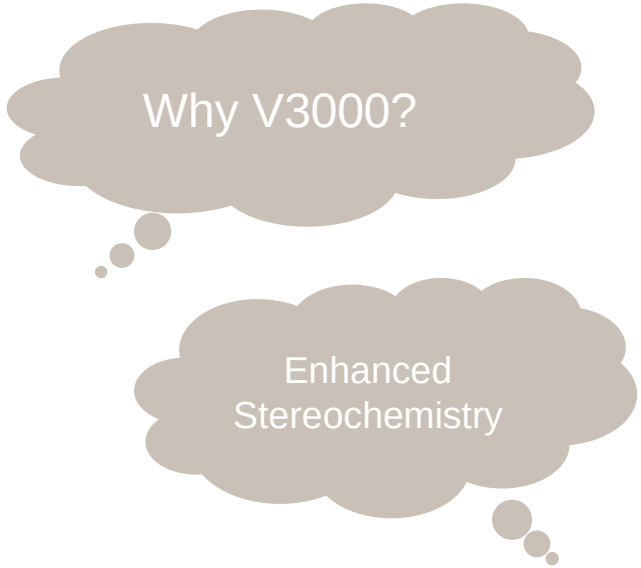
- Move to Web-Based tools.. Getting there
- Enhance the infrastructure and tools to handle V3000 molfiles (or an equivalent there of)… still have some challenges to overcome.
- Expose structure search inconsistencies and move to eliminate them where we can… need to dig deeper

2016-17 Goals: Move to Web-based tools

- **Design**
  - LiveDesign
    - Ongoing expansion
  - Plexus Enumeration
    - Available as an embedded component in LiveDesign
    - Plans to deploy a stand alone instance outside of LiveDesign to test additional capabilities
- **Report**
  - Plexus Connect (IJC Web)

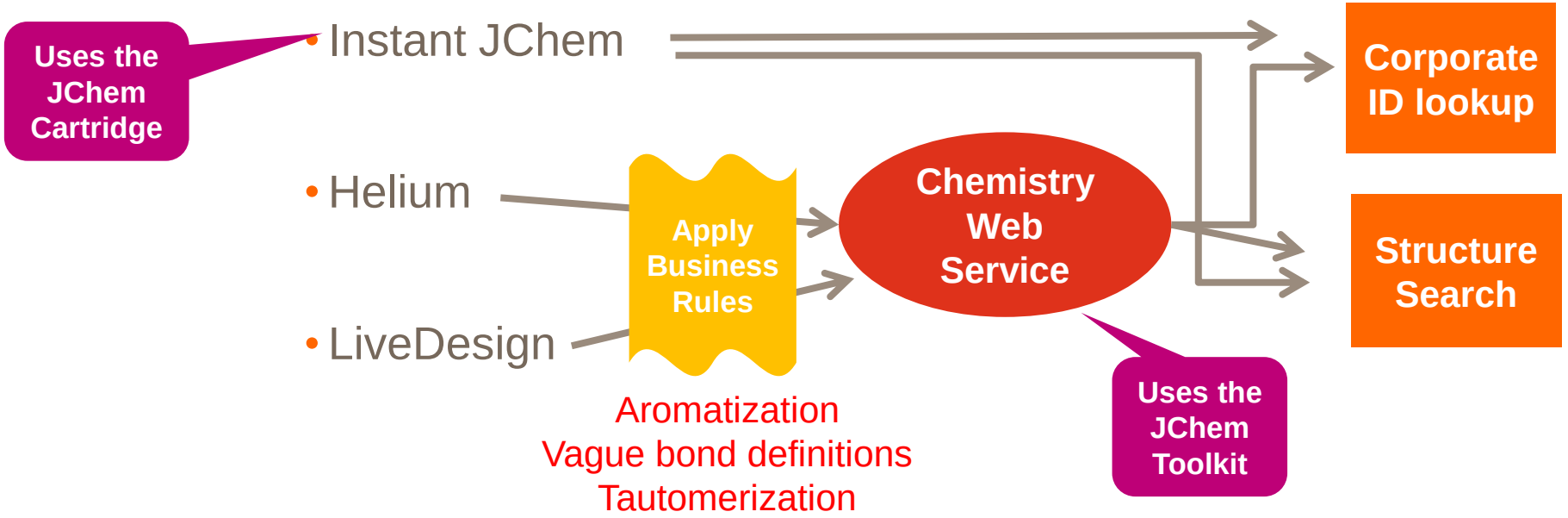
2016-17 Goals: Enhance V3000

- **Predict, Lookup, Search**
  - –Chemistry Web Services
    - JChem Toolkit and JChem Cartridge to handle and search V3000 inputs and outputs
- **Analyse**
  - –Helium
    - Uses the V3000 methods provided by the Chemistry Web Services
- **Report**
  - –Tweak Instant JChem project forms to view and search V3000 structures

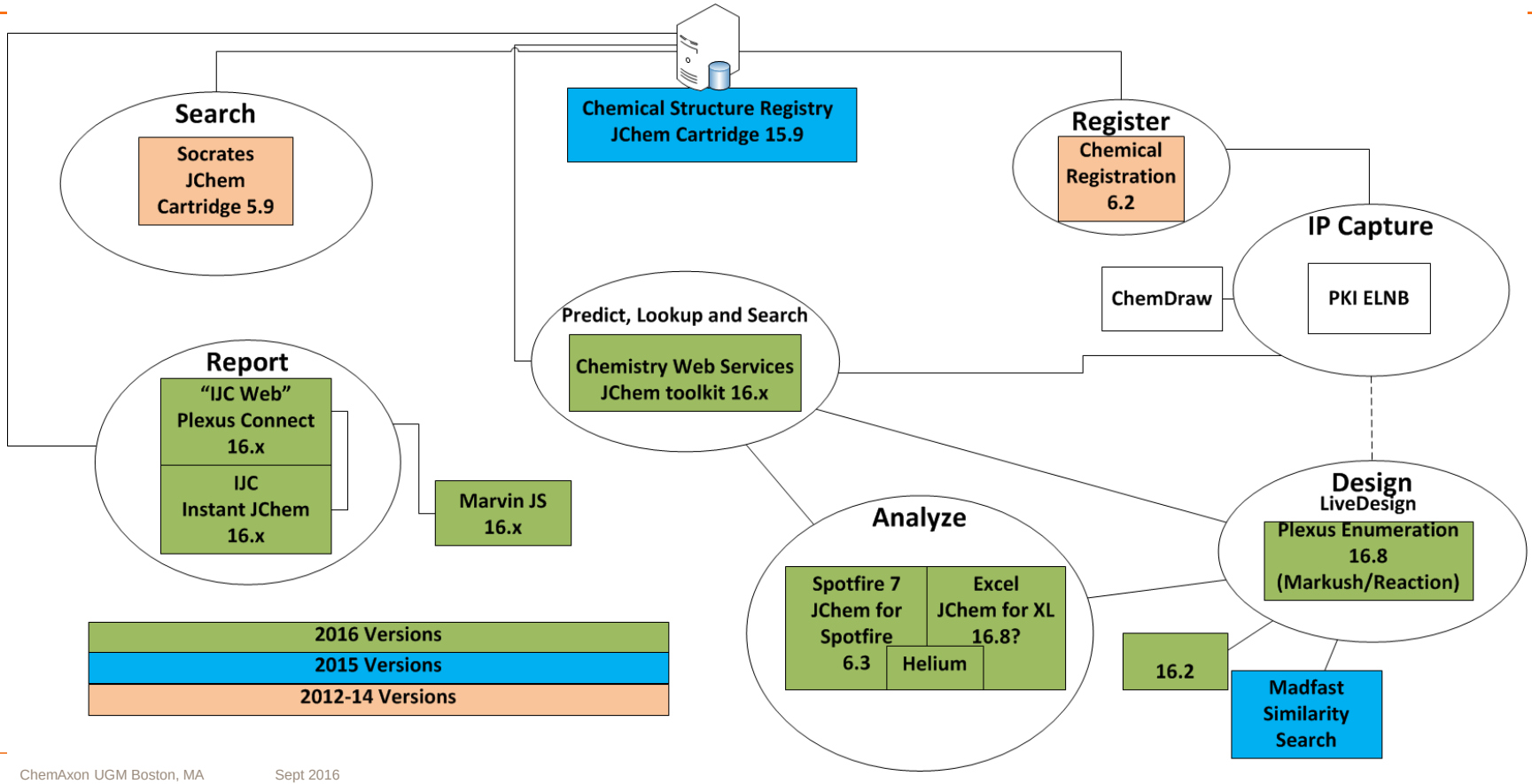


2016-17 Goals: Consistency Across Structure Queries

Structure Search and Lookup



How is going so far in 2016?



Successes and Challenges

- Successes
  - Upgraded JChem Toolkit on most of the Web Services
  - Upgraded JChem for Spotfire
  - In the process of Deploying Plexus Connect
  - In the process of upgrading JChem for XL (because we have to)
- Challenges
  - IJC still needed to make changes to Plexus Connect
  - Still on a bespoke version of JChem Cartridge
  - Struggled with Flag settings on JChem Toolkit
  - V3000 molfiles still not handled in all systems
  - Licenses are handled inconsistently across applications
  - Copy and paste of chemical structures

Preparing for the Future: Supportability

- Help us help you help us.
- Everyone wins with regular updates, but upgrades are hard.
- We need:
  - Stable, tested, and documented enterprise releases
  - Backward Compatibility testing across multiple products (Cartridge and IJC and…)
  - Establish diverse testing framework
  - Simplified consistent license management

Preparing for the future: structure search

- Expose more search options across ChemAxon tools (help with consistency)
- Searching chemical structures on unstructured databases
- Madfast for substructure search?
- Biological structure editor based on HELM

- Oh and... copy paste between applications not based on SMILES

Thank you for your attention

Questions?