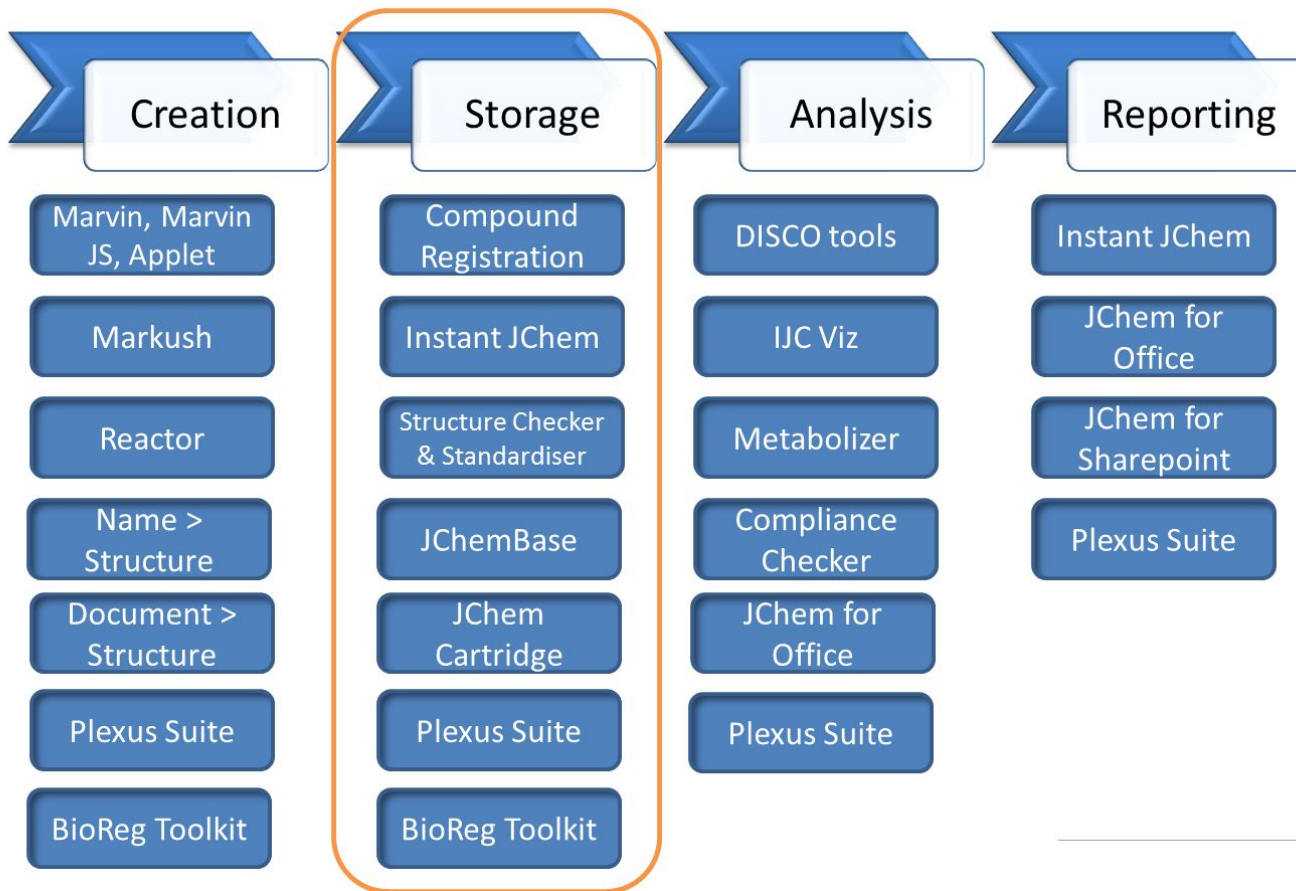


Storage & Correction

Petr Hamernik

How ChemAxon manages Scientific Data

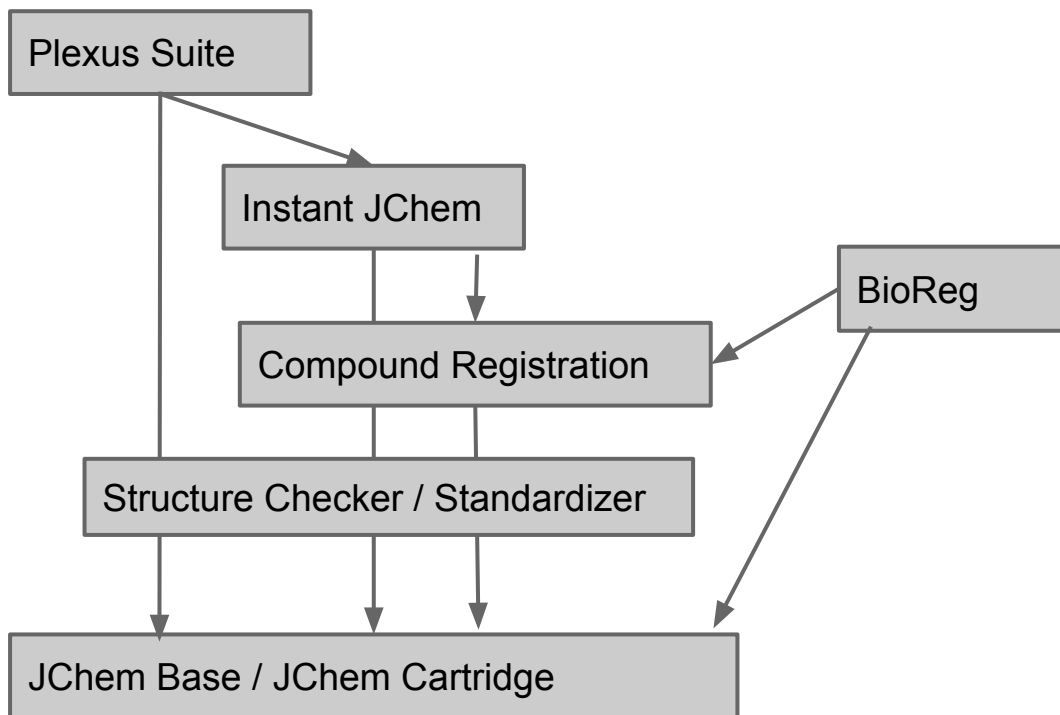


Storage & Correction

How to store data?

- One of the oldest cheminformatics topic
- Fundamental needs solved (storage, molecule representation, chemical search)
- Various use cases/applications:
 - Registration systems
 - Reporting tools
 - ELN

ChemAxon technologies for storage



Platforms?

- Java APIs, .NET APIs
 - Relational databases - Oracle, MySQL, MS SQL Server, Java DB, PostgreSQL
 - Operating systems
 - Microsoft Sharepoint
 - Microsoft Office
- => The same (for example) search results everywhere

JChemBase and JChem Cartridge

- Core technology behind other products
 - Integrated in
- Mature product (ver 1 in 2000!)
- Belongs among top technology in the market
- Great support
- Accessible through its own APIs or through other products
- New: improvements for Compliance Checker

JChemBase and JChem Cartridge

- Industry changes / new challenges:
 - big data
 - cloud
 - distributed systems
- Tell us your ideas
 - => Andras Volford (avolford@chemaxon.com)

Structure Checking & Correction

- Part of storage story
- ChemAxon coverage:
 - Structure checker
 - Standardizer
 - Compliance checker -> Tim's presentation

Structure checker

- Integrated with other ChemAxon tools (Compound Registration)
- Major trends:
 - Migration from Accelrys Cheshire (Lilly, BI -> Edith's presentation)
 - Custom structure checkers & fixers -> Consultancy team (Erin's presentation?)

Compound registration

- DEMO - 2min video
- Trends:
 - Easy deployment
 - User interface
- Integration options:
 - Web services (with ELNs for example)
 - Instant JChem
- Aptuit presentation link!
- BioReg -> Roland's presentation

Instant JChem

End user desktop application... but not only

- Application platform
- Base for Plexus Suite
 - Instant JChem Web client became part of Plexus Suite
-

Instant JChem - Chemistry application platform

- Extensible through plugins, scripts or possible to integrate in other products
 - APIs, connecting to Web Services, etc.
- Mini-apps (consultancy -> Erin's presentation)
 - Mini - registration
 -



Instant JChem

- MS SQL Server
- Pick list

Future:

- UX, backend integration (PS), better support for developers

Plexus Suite

Acknowledgement

JCB: Volfi

Structure

Checker/Standard:

Zsolt

RegSys: Csaba

Attila