

A Web Based Screening Application That Accesses JChem Base via JChem Webservices

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About SkunkWerks

- Vancouver based software company that specializes in building highly interactive, data-driven, enterprise level, web applications.
- Started with Information Management for Biotech and then expanded into an EMR system, iClinic. We have since further expanded our services/products.
- Vertical Markets = SkunkTracks, SkunkVault, iContact
- Biotech/Pharma = iColony, CellLines, iChem, SkunkDNA



Outline

The problem we faced

- Our context
- Why Adobe Flex
- Why JChem and why WebServices
- Our solution

How we did it

- Demo
- Behind the scenes

Q & A



First, a bit of history

- Client was using ChemOffice
- Our preference was to use clients' existing software
- ChemOffice does not integrate well with existing high throughput screening.
- Chose ChemAxon due to excellent technical support and "open" architecture.
- ChemAxon does all the "heavy lifting" for us – we are not chemists.
- Our solution provides the "glue", user interface, and company wide access.



The Problem & Context

- Key feature was to implement sub-structure searching.
- Needed to implement searches over multiple modules.
- Solution required web access. Solution had to be Web based (RIA).



Why Adobe Flex

- Existing Application based in Adobe Flex
- Very powerful RIA framework
- Easy to interface with WebServices

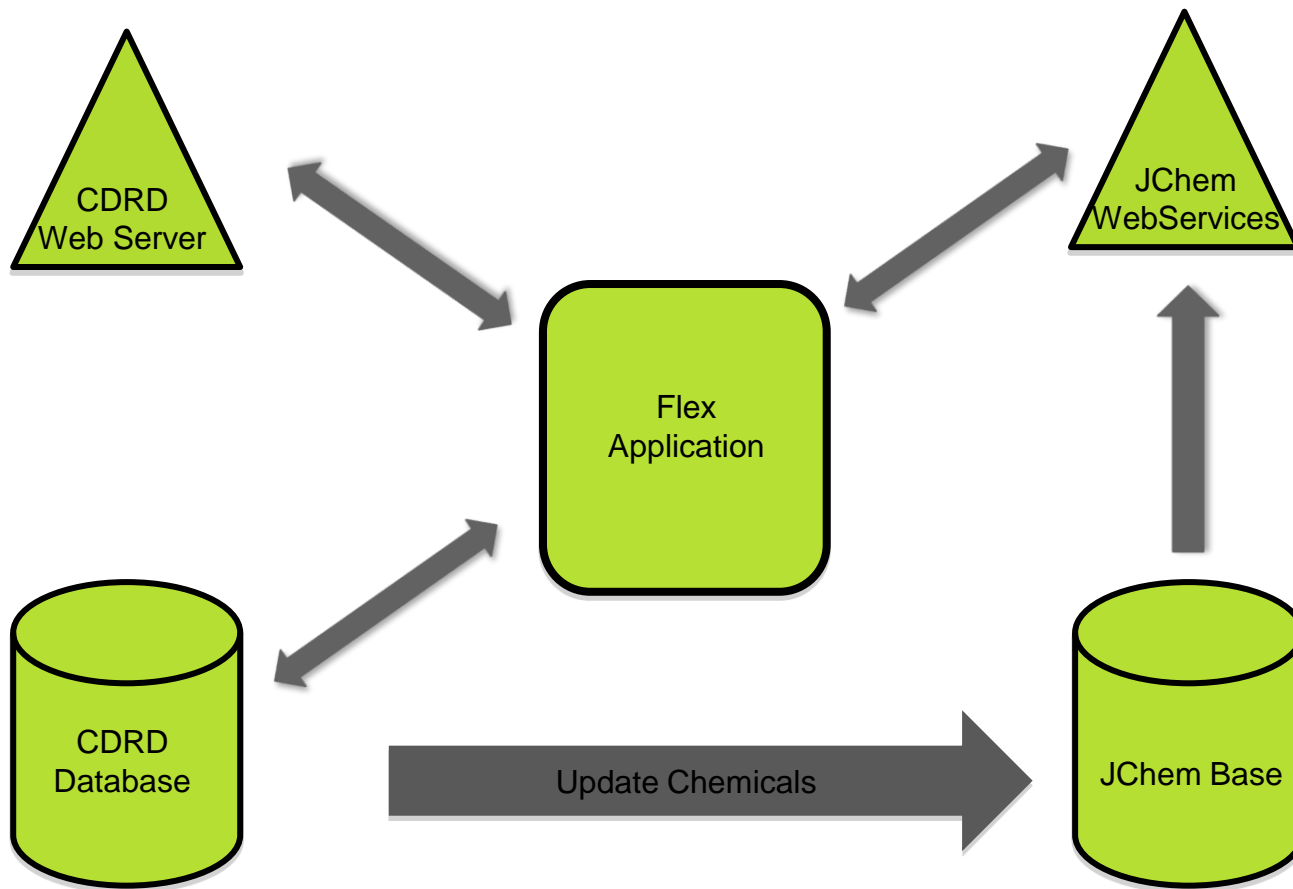


Why JChem Base & Jchem WebServices

- Marvin already used in the application
- Flex interfaces easily with WebServices
- Interlink JChem Base to existing database was fairly easy and straightforward



Our Solution



How we did it

Demo...



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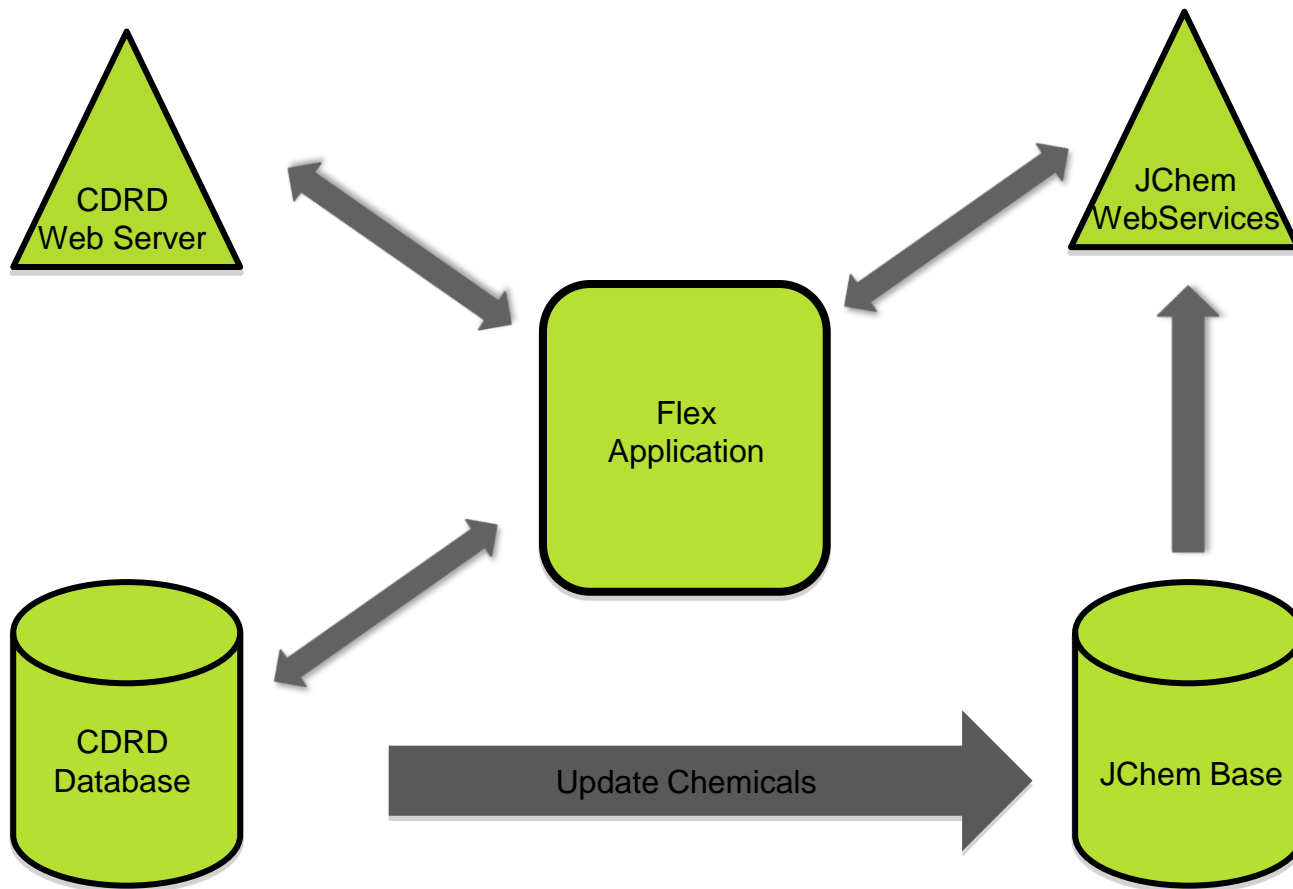
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Behind the Scenes...

- Many Servers In Play...
 - CDRD Database Server
 - CDRD Web Server
 - JChem Server
 - JChem Base
 - JChem Webservices server
 - Tomcat



Behind the Scenes...

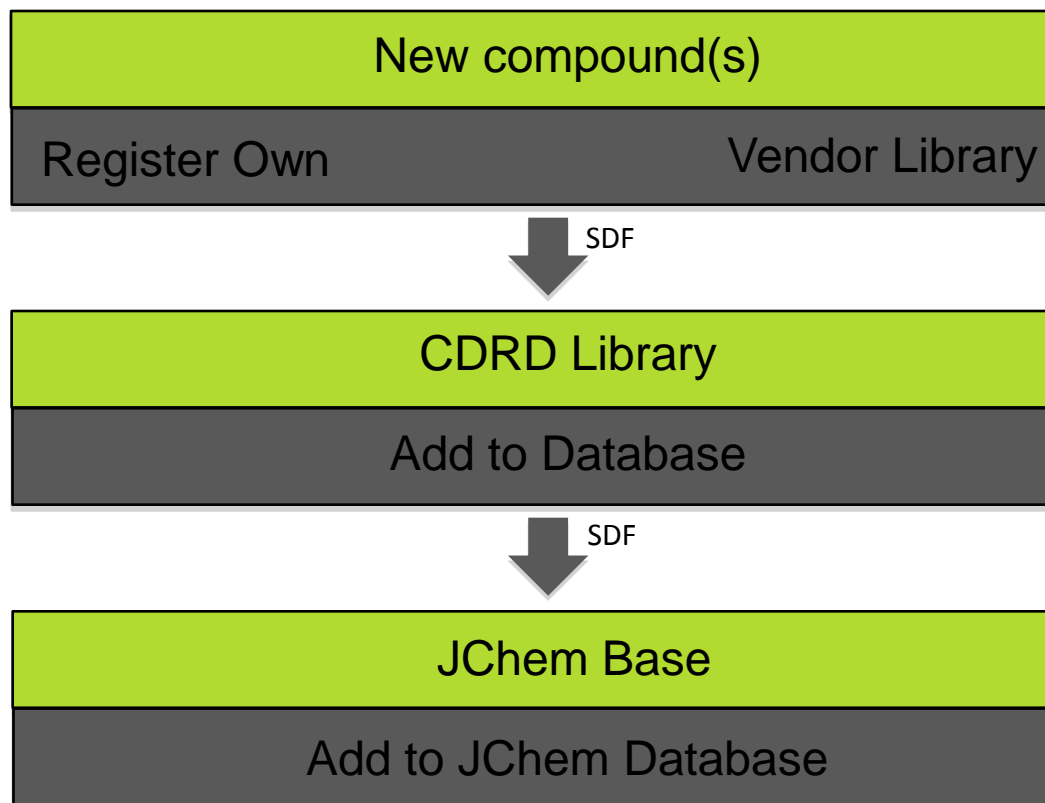


Behind the Scenes...

- JChem Base Integration
 - Databases are kept in sync
 - One way only updates
 - SDF files sent to JChem Base
 - Databases linked by cd_CDARDID extra field

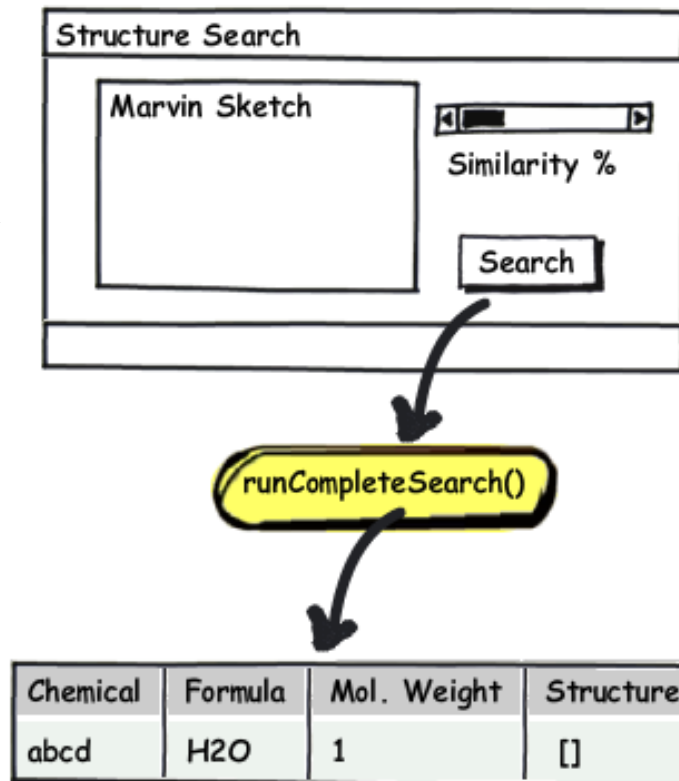


Behind the Scenes



Behind the Scenes...

- Search Dialog in Flex calls `runCompleteSearch()`
 - SDF or SMILES used for search
- Returned fields include `cd_CDRDID`



Behind the Scenes...

- Results presented on a list
 - cd_CDRDID gives the link to the Screening Library records
 - Structure image pulled via JChem Webservices JSP call



Other uses of JChem Webservices

- Adding Chemicals to the Database
 - Calculate various attributes from SDF
 - SMARTS (cxsmarts)
 - Formula
 - Mol. Weight
 - IUPAC name
 - Generate Structure Image



Conclusion

- Client response was exceptionally positive.
- Now in discussions with other clients that require a similar solution to high throughput screening/chemistry problems.
- ChemAxon has provided excellent technical support.



Q & A



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Thank You!



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