
ChemAxon Informatics Services

*Consultancy, application development
and migration support*

Tim Dudgeon

*ChemAxon US UGM
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Informatics Services Team

- New team to better support customers needs
- Seasoned problem solvers
- Broad expertise in
 - Cheminformatics, Bioinformatics
 - IT, Databases, Software ...
 - Life science sector
- Experienced with ChemAxon products
- Experienced with our competitors products

Locations



- Erin Bolstad

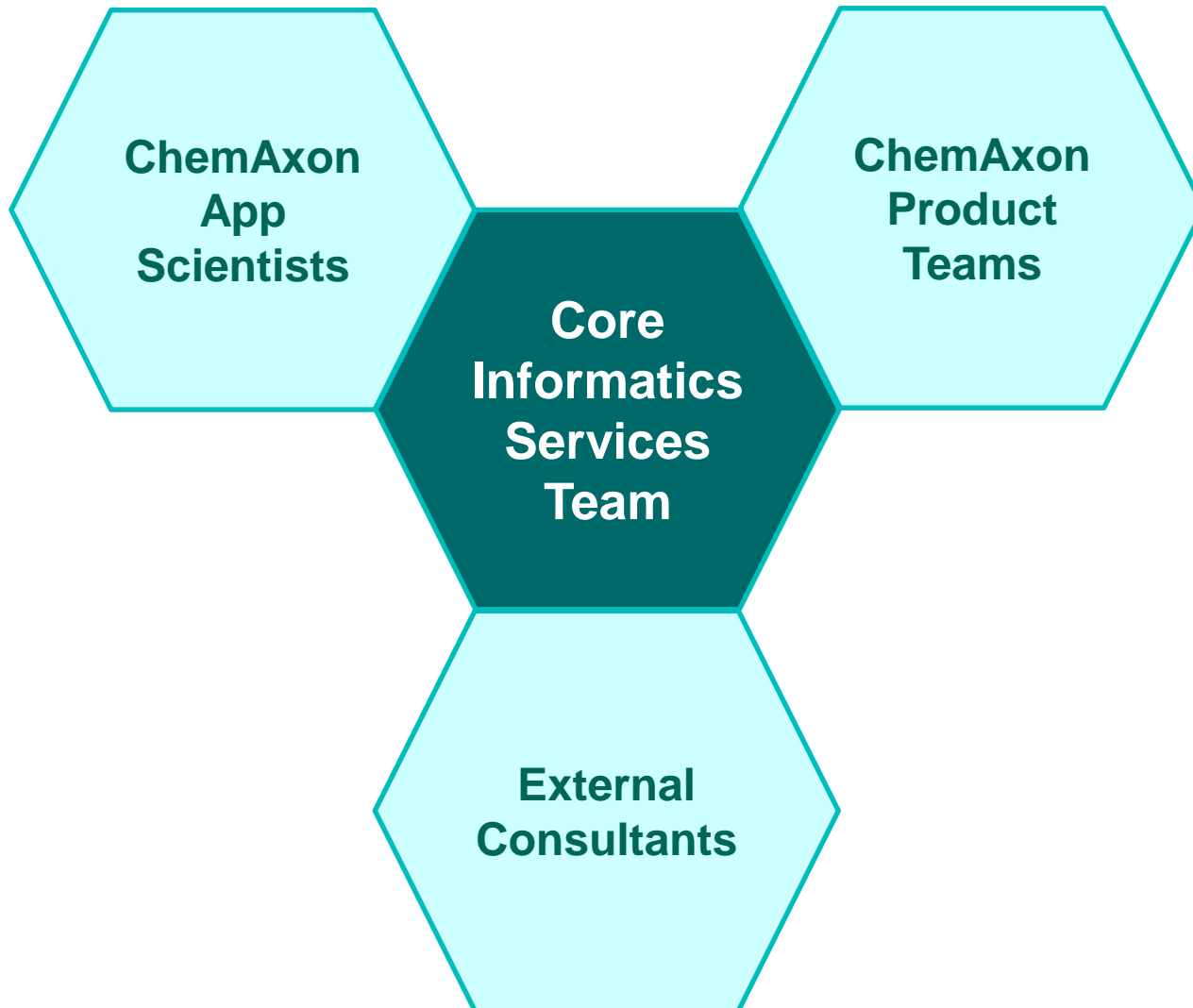
Hiring now



- Tim Dudgeon
- Daniel Butler

Hiring now

Extended team



Key product areas

- Instant JChem
- JChem cartridge
- Markush
- Registration
- Sharepoint

Two main expected areas

Migration support

- Planning
- Commissioning
- Data migration
- Training

App development

- Providing generic apps
 - Registration
 - Inventory
 - Reporting
- Building custom apps
 - Multiple platforms
 - RAD toolkits

Our interest is...

- To understand your needs
- To work out with you how to solve it
- To solve it efficiently
- To transfer the knowledge
- To ensure satisfaction

Tools of the trade

- Creating ‘consultancy toolkits’
 - Tools to assist data migration
 - ETL tools
 - Tools for better integration of products and APIs
 - Domain Specific Languages (DSL)
 - Pipelining
 - Components for building applications
 - Web components
 - ORM tools
 - Composable, embeddable solutions
- Should become products over time



$$1 + 1 = 3$$

Example 1: Migration assistance

GSK

Successful migration of ISIS forms for 100's of projects to IJC

Novartis

Migration of 100's of local ISIS databases to IJC

Pharma 3

Assisting in migrating reporting solution to IJC + cartridge

Example 2: Building SAR database



- Assisting in building and maintaining a compound and assay database
- Instant JChem + MySQL

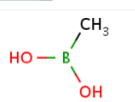
Example 3: NRD

- Reactions data warehouse
 - Import from various legacy databases (ISIS)
 - Live feed from CambridgeSoft ELN
- AJAX-style web application providing query and filtering capabilities
- Web services interface for fitting into SOA

NRD NIBR Reaction Database Gregory Landrum [FEEDBACK](#)

Structure

Search type
SUBSTRUCTURE



Options

Source

Other fields

Chemist

Project

Product yield greater than
80

Search Reset

Reaction

yield 100% with K3PO4:SK-CC01-A in Dioxane by [redacted]

yield 100% with K3PO4:SK-CC01-A in Dioxane by [redacted]

yield 100% with K3PO4:SK-CC01-A in Dioxane by [redacted]

yield 100% with K3PO4:SK-CC02-A in PhMe:H2O b [redacted]

yield 100% with K3PO4:SK-CC02-A in PhMe:H2O b [redacted]

yield 100% with K3PO4:SK-CC02-A in PhMe:H2O b [redacted]

yield 100% with K3PO4:SK-CC01-A in Dioxane by [redacted]

yield 100% with K3PO4:SK-CC02-A in PhMe:H2O b [redacted]

yield 100% with K3PO4:SK-CC02-A in Dioxane by [redacted]

yield 100% with K3PO4:SK-CC02-A in Dioxane by [redacted]

Showing 1 to 3 of 3 << < 1 > >>

Source

Check all | Uncheck all

<input type="checkbox"/> Novartis Backlog	20
<input type="checkbox"/> NovRes	19
<input checked="" type="checkbox"/> SynLab1	16
<input type="checkbox"/> TanPromoted	15
<input type="checkbox"/> SynLab2	8

Reagent

Solvent

Check all | Uncheck all

<input type="checkbox"/> CH2Cl2	17
<input checked="" type="checkbox"/> Dioxane	11
<input type="checkbox"/> H2O	10
<input type="checkbox"/> THF	10
<input type="checkbox"/> PhMe	7
<input type="checkbox"/> nPrOH	6
<input type="checkbox"/> Et2O	4
<input type="checkbox"/> EtOAc	4
<input type="checkbox"/> Hexane	3
<input type="checkbox"/> EtOH	3
<input type="checkbox"/> MeCN	2
<input type="checkbox"/> DME	2
<input type="checkbox"/> AcOH	2
<input type="checkbox"/> MeOH	1
<input type="checkbox"/> Benzene	1

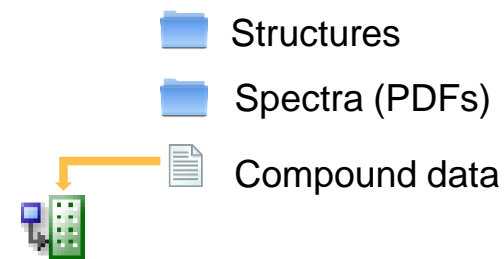
When undefined

Add reactions to final results



Example 4: MSSM

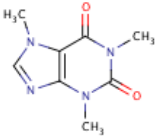
- Customized registration script
- Transition of old library data
- User training and documentation
- (All script based!)



The 'Register Compounds' dialog box is shown with the following options:

- Select compound type:
- Custom Made Compounds (CM)
- Commercial Compounds (MS)
- Spectra PDFs?

Buttons: OK, Cancel

Cdid	Structure	CM Corporate ID	MS Corporate ID	Lots	CAS No	Chemical Name	Catalog I
1		CM0000746	MS0001267	3	58-08-2	1,3,7-trimethyl-1H-purine-2,6-dione 3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione	AP1000

Modes of interaction

- Provide hands-on assistance and specialist knowledge
- Knowledge transfer/training
- Outsourced development
- Joint development
- Product enhancement

Contact us

- Through your sales contact

or contact me directly at

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