

# Consultancy

Reaching the parts other  
products can't reach

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## Who are we?

- US and EU based
- Background in science + IT
- Wide range of skills
- Good communicators

## Why might you need us?

- Your needs are varied
- Your environments are varied
- One size does not fit all
- You want to explore new ideas
- You need specialist skills
- You need knowledge transfer
- You need extra resource

# What types of things do we do?

UGM

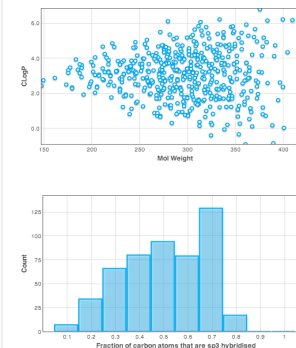
- Build new applications
- Add/extend functionality of existing systems
- Migration/integration support
- Customized end-user and developer training

# Examples: custom app development

**DuPont: Document structure search**  
See Mark Andrews' talk at this UGM

**Novartis Reactions Database**  
See [Greg Landrum's talk](#) at 2012 EU UGM

**D2DB demo site**  
<https://d2db.chemaxon.com>



**European Lead Factory WP9/10 portal**  
Going live Jan 2014

# Custom dev approach

- **Emphasis on PRODUCTIVITY**
  - best of breed technology stack
  - experienced developers
- **Emphasis on REUSABILITY**
  - common toolkit of reusable components
- **Emphasis on FLEXIBILITY**
  - neutral technology stack allows parts/technologies to be interchanged
  - allow your branding
  - fit into your security infrastructure
  - accommodate change

# Custom development/ enhancement within products

UGM

- Compound Registration (GSK)
- Plexus (Eli Lilly)
- IJC (GSK, BMS)
- Structure checkers (BI)
- Marvin (Elsevier, Pearson)

# Examples - extending existing software



...	Structure (Original)	Structure (To)	Status	Errors	LNB	Supplier	Origin	Salt ID	Salt	
1			REGISTERED		D554-51	in-house	in-house	0	0.00	<= Complete Standard Import (GREEN IS mandato...
2			REGISTERED		D554-52	in-house	in-house	0	0.00	Reset STAGE Reset STAGE for new load
3			REGISTERED		D554-53	in-house	in-house	0	0.00	Salt strip 1. Reduce to parent (strip single salt ion)
4			REGISTERED		D554-54	in-house	in-house	0	0.00	Register 2. Register parent
5			REGISTERED		D554-55	in-house	in-house	0	0.00	

## Compound and assay registration and reporting in Instant JChem.

6 projects completed  
2 underway

## Custom structure DBs in Instant JChem

Database design  
Migrate data  
Build forms etc.  
Provide training

Patent Selection

Retrieve the lead patent using our best guess to the location:

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Or, select the patent from the invention to view, and the web location  
Some sites only work with patents from certain countries.

Select patent

Select patent repository

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Some patent sites block external programs, or are not used often.  
Jump to the country specific patent websites using the menu below.

## Patent Markush and structure search

Thomson-Reuters Markush DARC  
+ DWPI data

## KNIME Workflows

Requirements gathering  
Workflow generation  
Rollout  
Training



# Migration and Integration Support

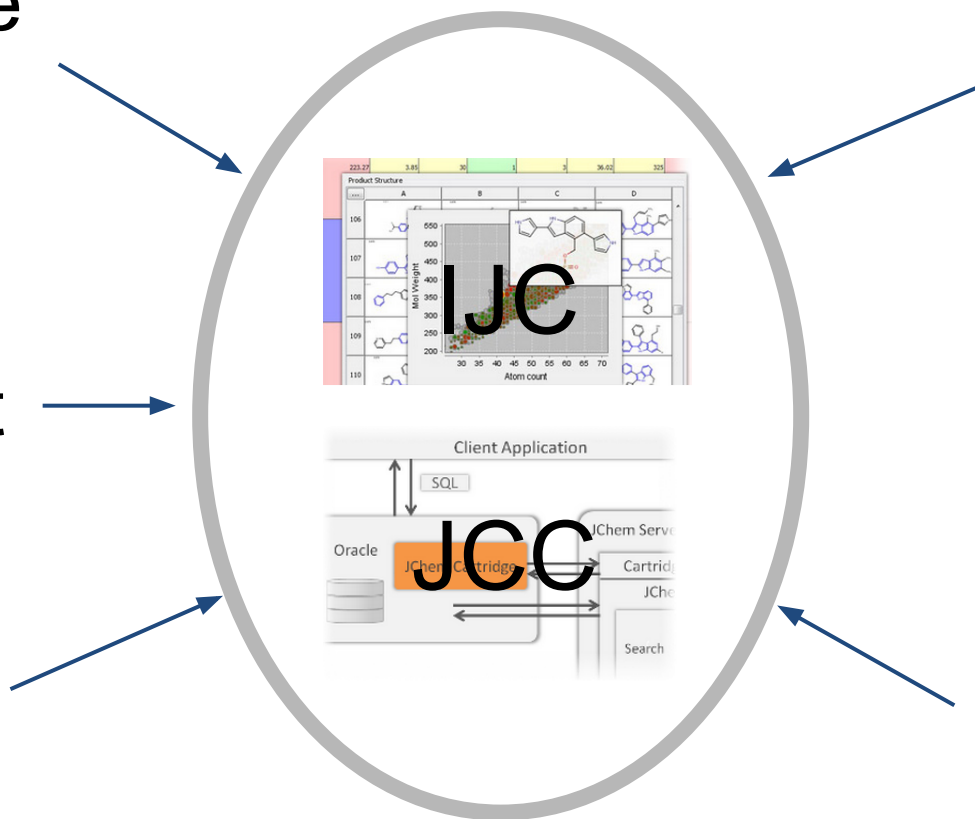
UGM

ISIS/Base

In house apps

ISIS/Host

Accelrys  
Direct



Daycart

# Migration and Integration Support

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- Database redesign
- Data cleaning
- Data migration
- System design
- Chemical business rules
- Workflow review
- Integration with other softwares
- Training

## For more info get in touch

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