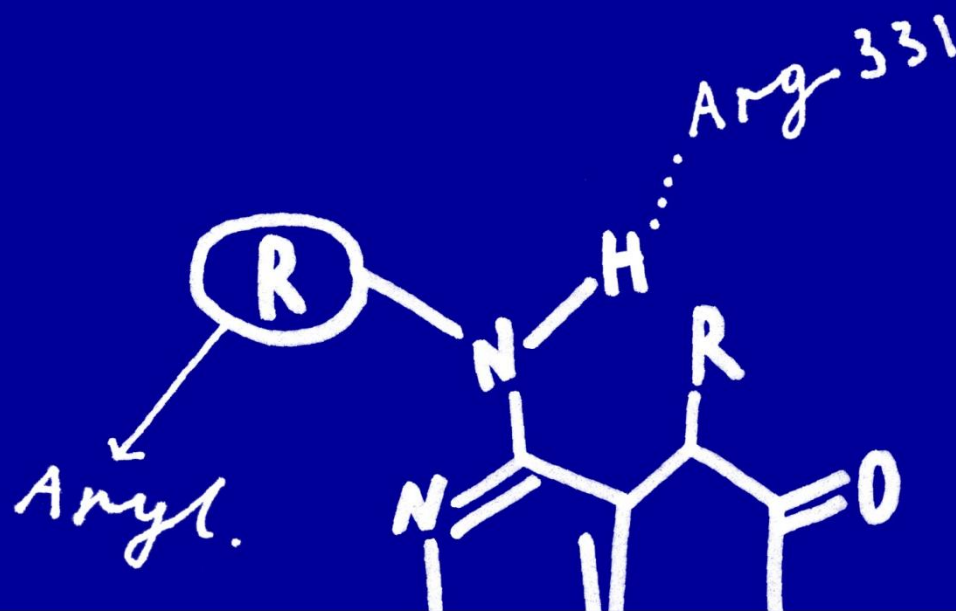


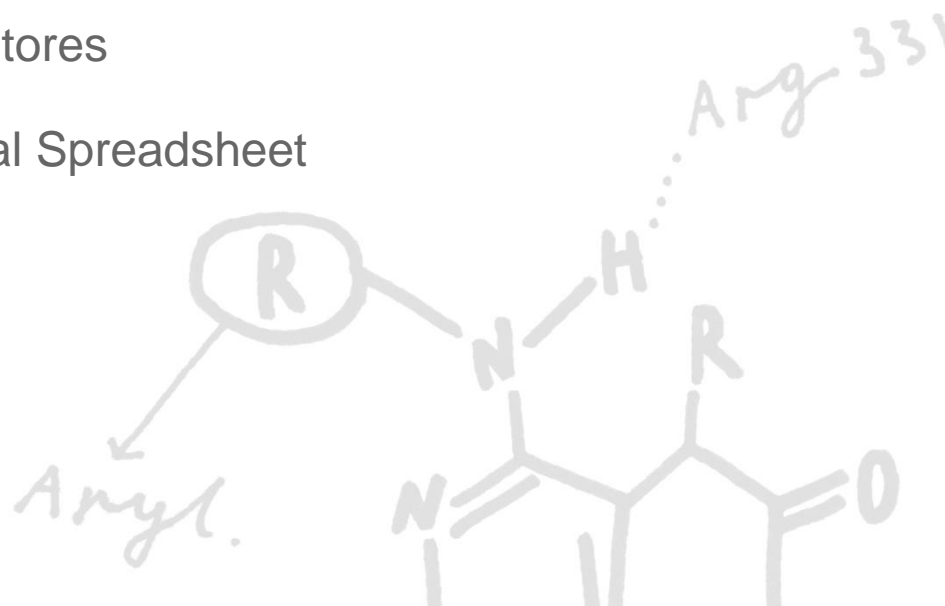
# Migrating to ChemAxon



## Agenda

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- **Evotec**
- Why migrate ?
- Searching for Library Enumeration Replacement
- Migrating a small activity database
- Migrating Chemical Stores
- Using a new Chemical Spreadsheet
- Conclusion



## Evotec's Mission

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Partner of choice for drug discovery alliances

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PEOPLE

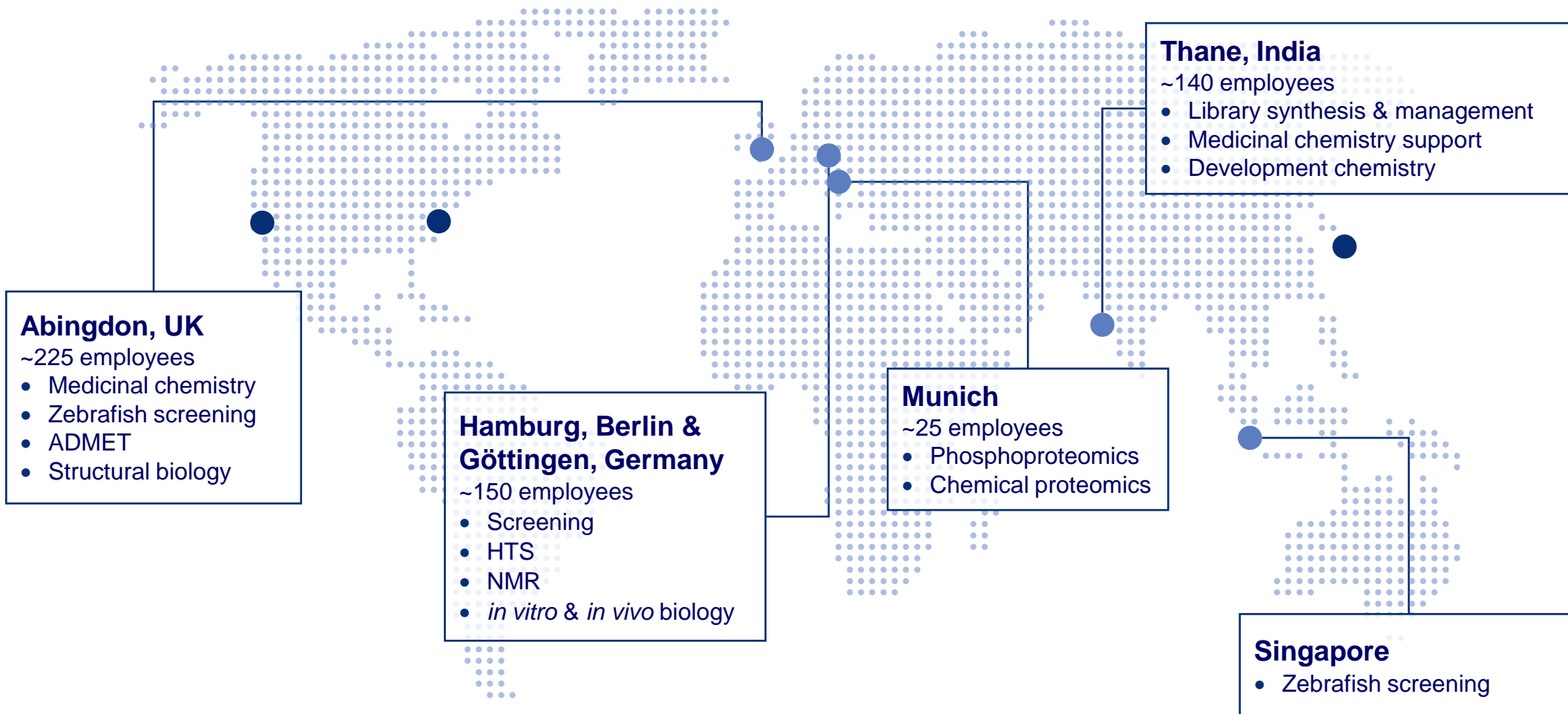
THERAPEUTIC AREA EXPERTISE

**To build innovative and integrated drug discovery alliances to accelerate and maximise the success of our partner's drug discovery efforts by leveraging outstanding scientists, state-of-the-art integrated capabilities and therapeutic area expertise**

INTEGRATED DRUG DISCOVERY PLATFORM

# Global reach for global projects

Ca. 550 Evotec employees worldwide



- Sales representation (San Francisco, San Diego, Boston, Tokyo)
- Operations & sales representation

# Building high value, integrated partnerships

## From target to IND

Target ID & validation	Screening	Hit-to-lead	Lead optimisation	Preclinical development	Clinical development
<ul style="list-style-type: none"> <li>Molecular biology and cloning</li> <li>Bioinformatics</li> <li><i>In vitro</i> target validation</li> <li><i>In vivo</i> target validation</li> </ul>	<ul style="list-style-type: none"> <li>Assay development &amp; screening</li> <li>(u)HTS</li> <li>High content screening</li> <li>Electrophysiology</li> <li><i>In silico</i> screening technologies</li> <li>Fragment-based drug discovery</li> </ul>	<ul style="list-style-type: none"> <li>Medicinal chemistry</li> <li>Hit expansion</li> <li>Library design</li> <li>High throughput chemistry</li> <li>Target deconvolution</li> <li>Protein-ligand crystallography</li> <li><i>In vitro</i> biology</li> <li>Early ADMET</li> </ul>	<ul style="list-style-type: none"> <li>Medicinal chemistry</li> <li><i>In vitro</i> biology</li> <li>Disease biology and target class expertise</li> <li>Cellular selectivity analysis</li> <li>Cellular MoA analysis</li> <li>Computational chemistry and structure-based drug design</li> <li><i>In silico</i> ADMET</li> </ul>	<ul style="list-style-type: none"> <li>Custom synthesis</li> <li>Analytical development</li> <li>Process R&amp;D</li> <li>Large scale synthesis</li> <li><i>In vivo</i> pharmacology</li> <li>Biomarker discovery</li> </ul>	<ul style="list-style-type: none"> <li>Clinical alliances</li> <li>Clinical project management</li> </ul>



**Superior drug candidates in a time and cost efficient manner**

For example:

- 1 CNS 
- 2 Oncology 
- 3 Inflammation
- 4 Pain 
- 5 Metabolic diseases 
- 6 Huntington's disease 

### Disease biology expertise

- CNS
- Inflammation
- Pain
- Oncology
- Metabolic Diseases

### Proven program management

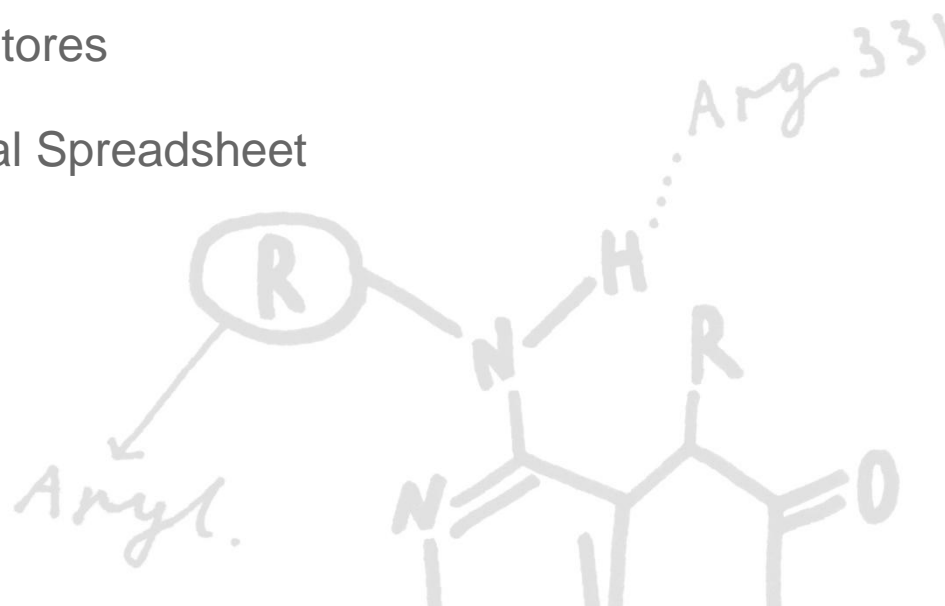
- 320 assays developed
- >110 hit to lead and lead optimisation projects
- 28 PDCs
- 20 compounds approved for clinical trials

### Flexible deal structures

## Agenda

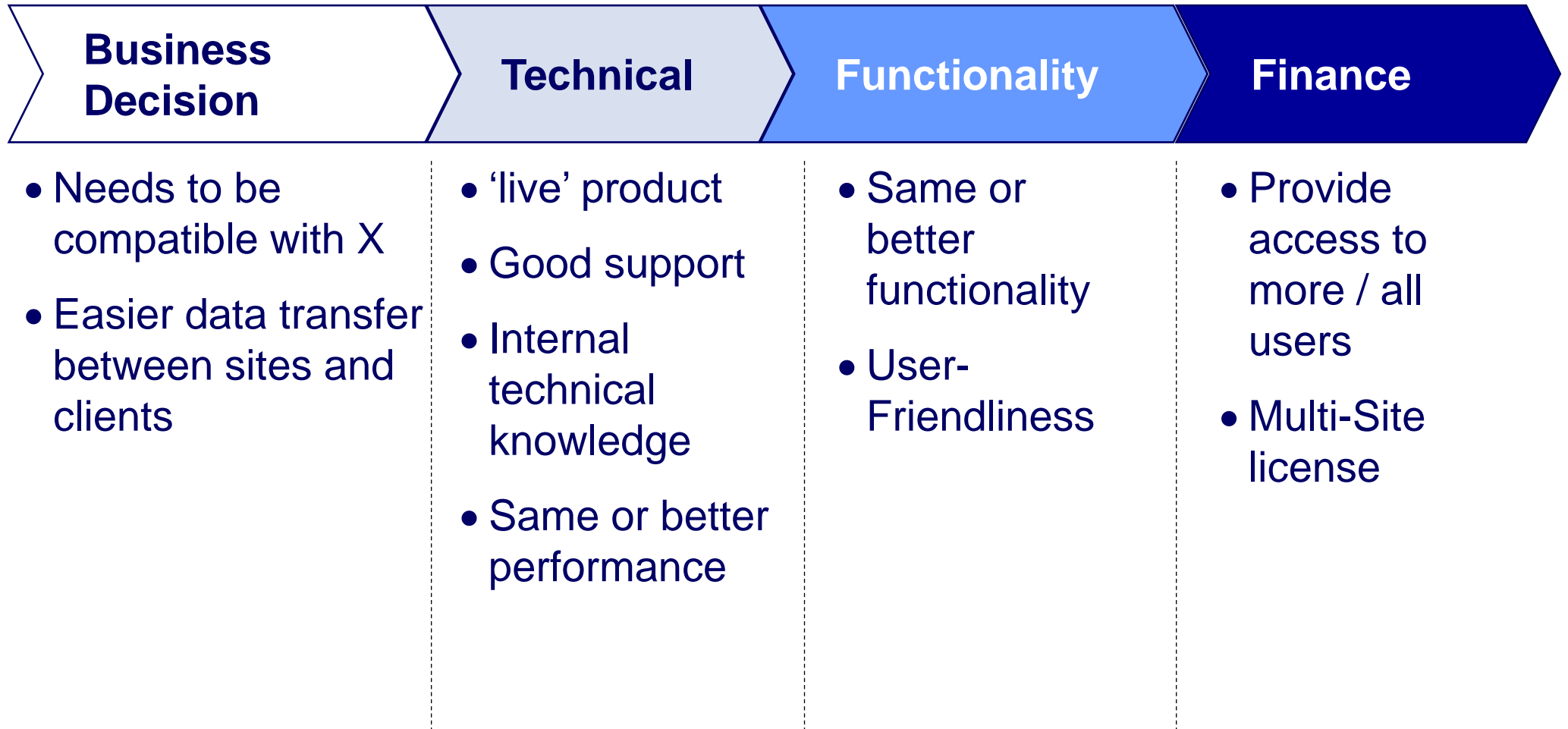
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- Evotec
- **Why migrate ?**
- Searching for Library Enumeration Replacement
- Migrating a small activity database
- Migrating Chemical Stores
- Using a new Chemical Spreadsheet
- Conclusion



## Why migrate ?

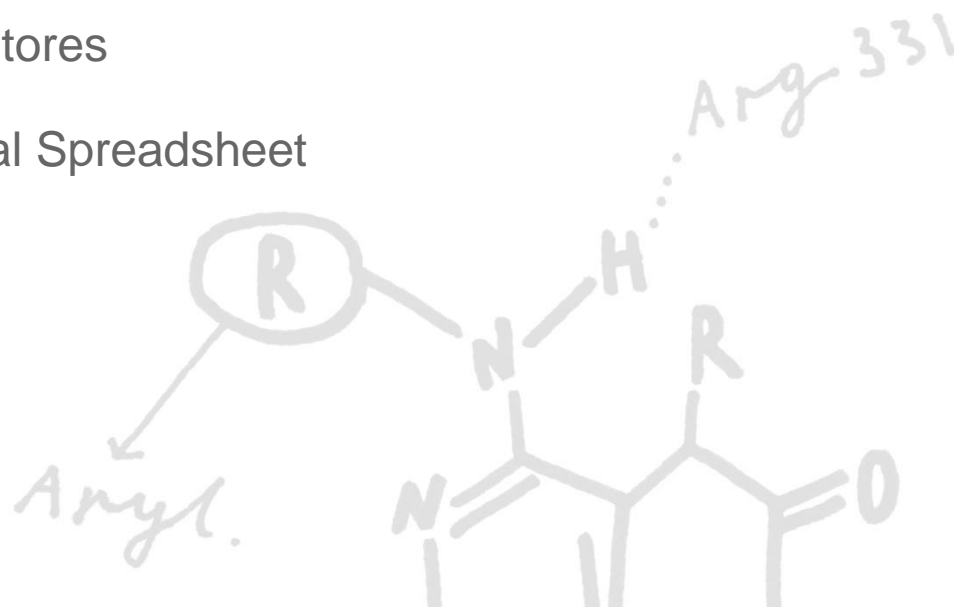
How is the decision made ?



## Agenda

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- Evotec
- Why migrate ?
- **Searching for Library Enumeration Replacement**
- Migrating a small activity database
- Migrating Chemical Stores
- Using a new Chemical Spreadsheet
- Conclusion

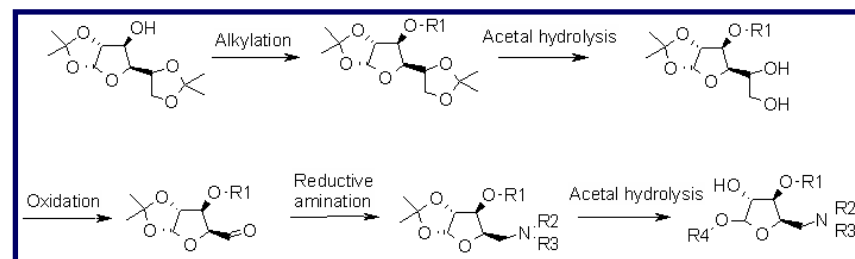
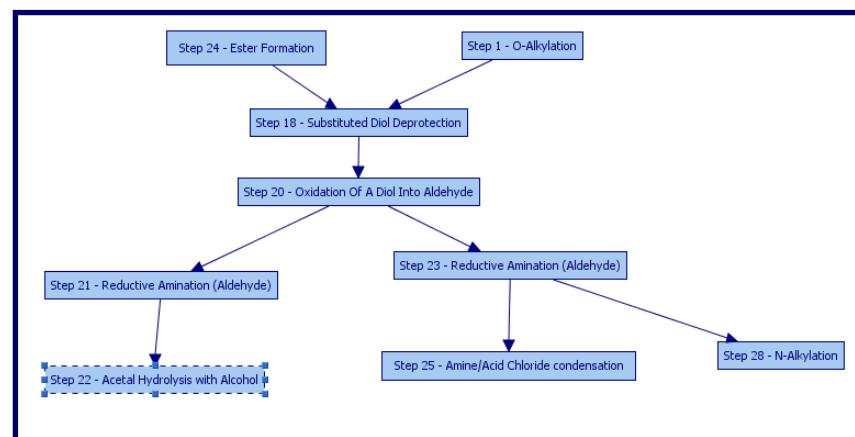




# Searching for a Library Enumeration Replacement?

## Essential Required Features

- User-friendly
- Produces Product Identifier
- Speed
- Multi-Step Libraries
- Enumerate up to 1 million structures
- Chirality support



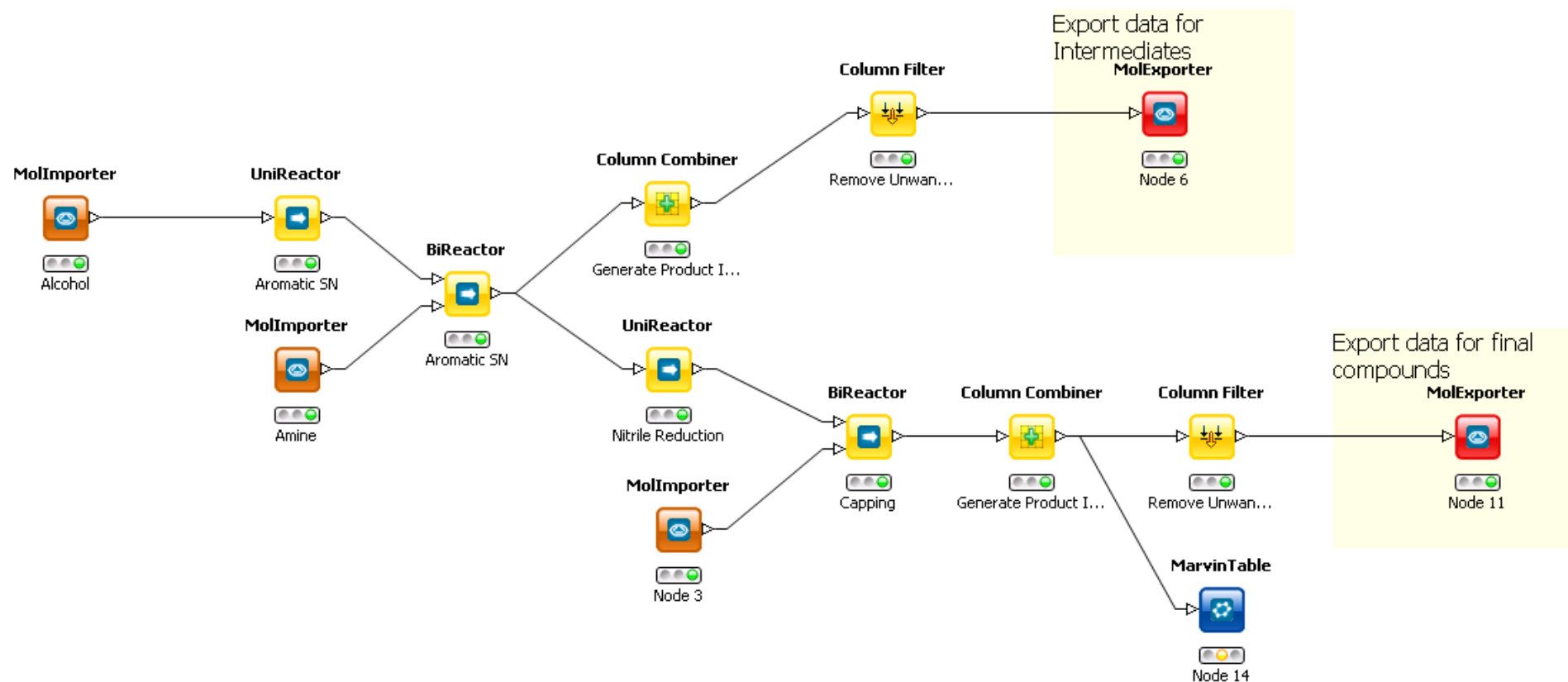
## Searching for a Library Enumeration Replacement ?

What options did we consider ?

Feature	Existing Solution	Evotec CCD	Reactor GUI	Reactor cmd line	IJC	Knime / Infocom
User-Friendly	OK	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	OK	<input checked="" type="checkbox"/>
Speed	<input type="checkbox"/>	OK	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	OK	<input checked="" type="checkbox"/>
Product Identifier	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/> (available in latest version)	<input checked="" type="checkbox"/> (static format)	<input type="checkbox"/> (available in version 5.5)	<input checked="" type="checkbox"/> (flexible format)
Up to 1M	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Not tested	<input checked="" type="checkbox"/>
Multi-Step	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>

# Library Enumeration Tool selected

## Knime and the Infocom ChemAxon nodes



# Library Enumeration Tool selected

## Knime and the Infocom ChemAxon nodes

**Dialog - 0:8 - BiReactor (Capping)**

File


Options | Reactor Options | Advanced | Flow Variables | Memory Policy

Reaction file

S:\eScience\Shared\Training\KNIME\enumeration demo\step4.mrv Brows...

1. Unnamed

Reverse direction



Structure column

The reactant 1 column Product molecule1 (#2)

Keep properties of reactant 1

The reactant 2 column Molecule

Keep properties of reactant 2

OK Apply Cancel

**Dialog - 0:10 - Column Combiner (Generate Product Identifier)**

File

Settings | Flow Variables | Memory Policy

Delimiter -

Quote Character  Quote always

Replace Delimiter by

Name of appended column Product Identifier

**Exclude**

Column(s): Search

Select all search hits

- Product molecule1 (#2)
- Product molecule1 (#1)
- Product molecule1
- Molecule
- Molecule (#1)
- Molecule (#2)
- Product molecule1 (#3)

**Select**

add >>

add all >>

<< remove

<< remove all

**Include**

Column(s): Search

Select all search hits

- BB Code
- BB Code (#1)
- BB Code (#2)

OK Apply Cancel

## Library Enumeration Tool selected

Temporary Storage Solution for the Libraries

---

**1** Structure and Text Searching

**2** Easy to Import and Export Data

**3** Data can be edited easily based on the Product Identifier

**4** Centralised, multi-user access

**Instant JChem  
Shared Project  
Oracle Database**

# Library Enumeration Solution

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## Migration & Implementation

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- Exported data from previous system as SD File (one for each Library)
- Imported data into Instant JChem (a separate table for each Library)
- Process has been streamlined
- One main user of the system (in India)

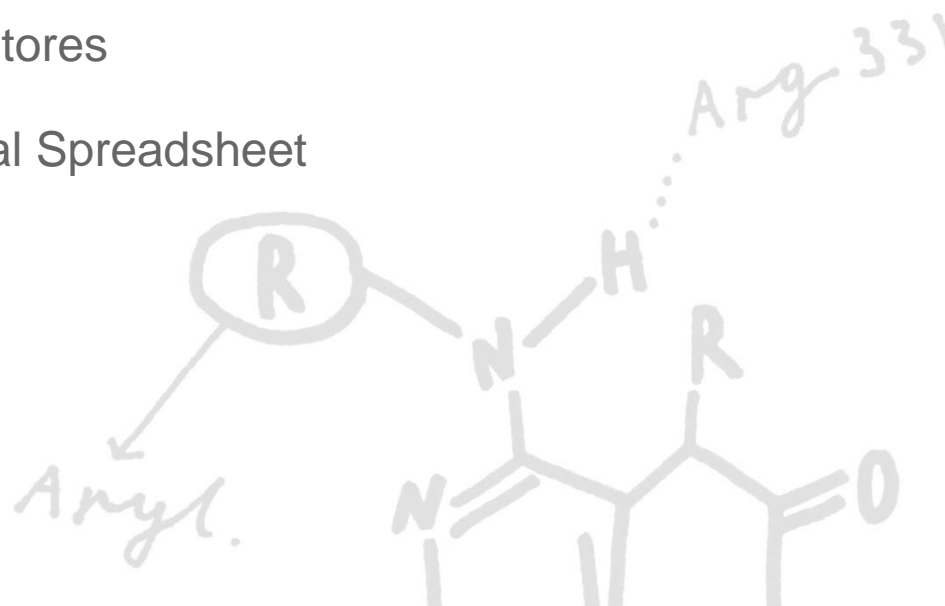
### Summary

- Smooth transition
- Data stored as Smiles (not an encrypted / vendor specific format)
- Easy to trouble-shoot enumeration failures either in Knime or InstantJChem
- Need to remember to map the reactions for enumeration
- Database server is located in Abingdon (a bit too slow for use from India), hopefully will be moved locally soon !

## Agenda

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- Evotec
- Why migrate ?
- Searching for Library Enumeration Replacement
- **Migrating a small activity database**
- Migrating Chemical Stores
- Using a new Chemical Spreadsheet
- Conclusion



# Migrating a small activity database

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From local ISIS Base

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## Pro

- Nice forms
- Options to save Import /Export settings
- Option to query the database using ISIS 4 Excel

## Contra

- Only one user at a time
- Database often became corrupt
- Limited licenses
- Design was not very flexible



# Migrating a small activity database

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## IJC Solution

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- First used in 2008 for an integrated project across several sites
- Shared Instant Jchem project
  - Oracle database
  - JChem cartridge/JChem base tables
- User-friendly
- Most of the features needed are present
- Bonus – access to calculators
- Knime workflows are used for more complicated export and data conversion

## Summary

- Currently the preferred tool for chemistry and biology project databases

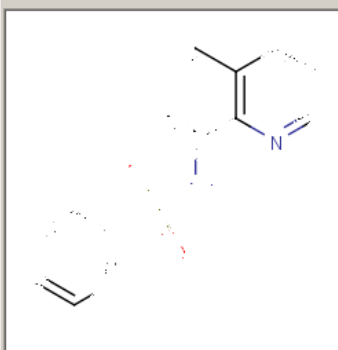
# Migrating a small activity database

## Example IJC Solution

Overview, ADMET Assay details, In Silico, Assay details

Design Query Browse Entity: all\_struct...

Structure



CorpID:

NotebookNo: EV0865-010-006

PlateID: OP-292888

Well: A06

Date: 04-Mar-2010

Mol Weight:

Formula:

FreeMW:

Salt\_Weight:

Salt\_Fomula:

salname:

saltcount:

NMR:

LCMS: y

Purity: 100

Supplier: ChemBridge

Cat\_no:

Comment:

Series: Cluster 9

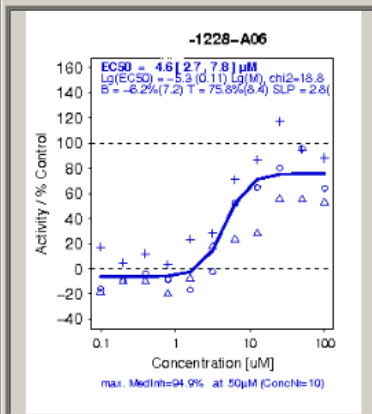
assays\_opera

...	Plate	Well_ID	LNB	FPN date	Test_Date_reported
1	OP-292888	A06	EV0865-010-006		

Ferroportin assay

...	op	IC50 [µM]	comment	op	retest 1	comment	op	retest 2	comment	op	retest 3	comment
1		4.59	efficacy 82%									

Ferroportin assay IC50 test 1



Ferroportin assay IC50 test 1 link to image

...	Fpn R0 Mfluo Pngchart	Link public 2 CRC MFLUO R0
1	Fpn.MembFluo-Batch20-100311_VIT-1228-A06.png	file:///\\ge-ham-ora14\IJC_SHARED\vifor_images\Fp

Ferroportin ligand efficiency -RT ln(IC50)/NHA

...	LE	retest 1 LE	retest 2 LE
1	0.38		

MDCK ATP

...	op	IC50	op	retest
1		123.90		

HEK ATP

...	op	IC50	op	retest
1	>	100.00		

Transferrin counter assay

...	op	IC50 [µM]	op	retest
1				

Ferritin counter assay

...	op	IC50
1		

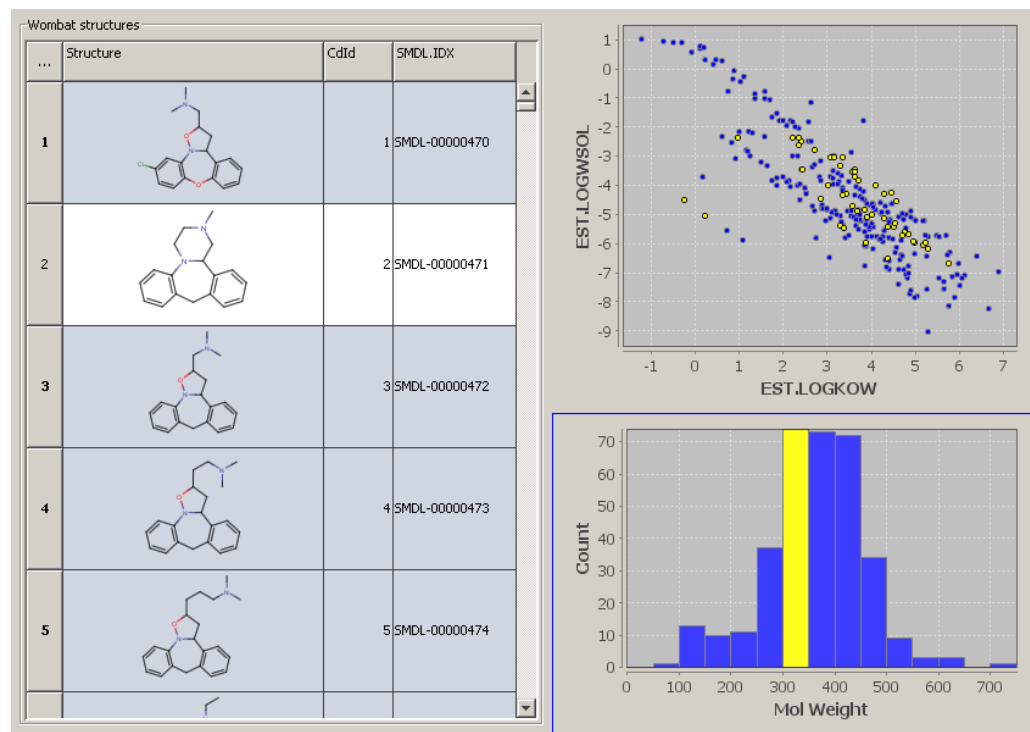
Cytotox HEK cells

...	op	IC50 [µM]	comment
1			

# Migrating small activity database

What is next ?

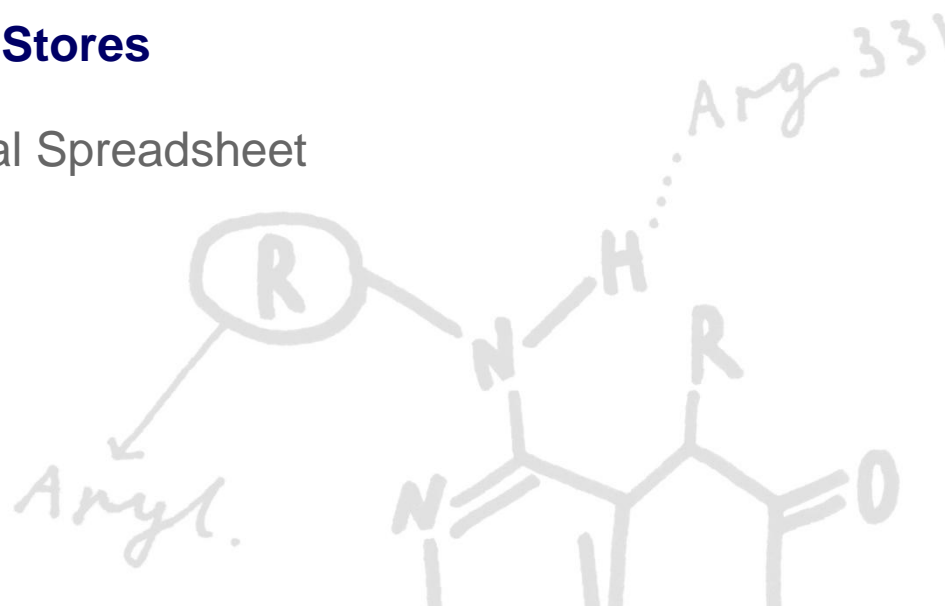
- Planning to migrate the few remaining ISIS databases to IJC in 2011
- Currently running IJC version 5.3.1
- Users are looking forward to all the new features available in 5.5!



## Agenda

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- Evotec
- Why migrate ?
- Searching for Library Enumeration Replacement
- Migrating a small activity database
- **Migrating Chemical Stores**
- Using a new Chemical Spreadsheet
- Conclusion



# Migrating Chemical Stores data

## Comparison of the Options

Feature	Commercial Inventory Software	EVOsource /ERP System
User-Friendly	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Integrated Ordering	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Integrated Quote System	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Supplier Catalogue Data	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Identify each Compound	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Identify Each bottle	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Locate each bottle	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> (only when in stores)

# Migrating Chemical Stores data

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What was the process ?

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- How much data needs to be migrated?
  - Ca. 10k bottles, 4k structures
- Exporting data from the current Chemical Stores Application
  - Did not work
  - Could not export shelf location
  - Could export quantity, but not unit
- Exporting data directly from the database
  - Structures encrypted, finally found cartridge functions to convert!
  - Understanding the data model was not too bad
  - Exported selected data from selected tables
  - Created scripts (PL/SQL) to migrate stores stock data into Finance system
  - Discovered about 3k bottles with Lab location – Really ??? Massive stores return requested !!!



# Migrating Chemical Stores data

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## Potential Issues

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- Compound Identifiers will replace bottle identifiers
- Scientists attached to Numbers e.g. '10125' = benzoyl chloride
- Some functionality loss
  - EVOsource will need to be extended to allow tracking of Compounds in the Lab
- Some functionality gained
  - Access to more catalogue data
  - Integrated ordering and quote system

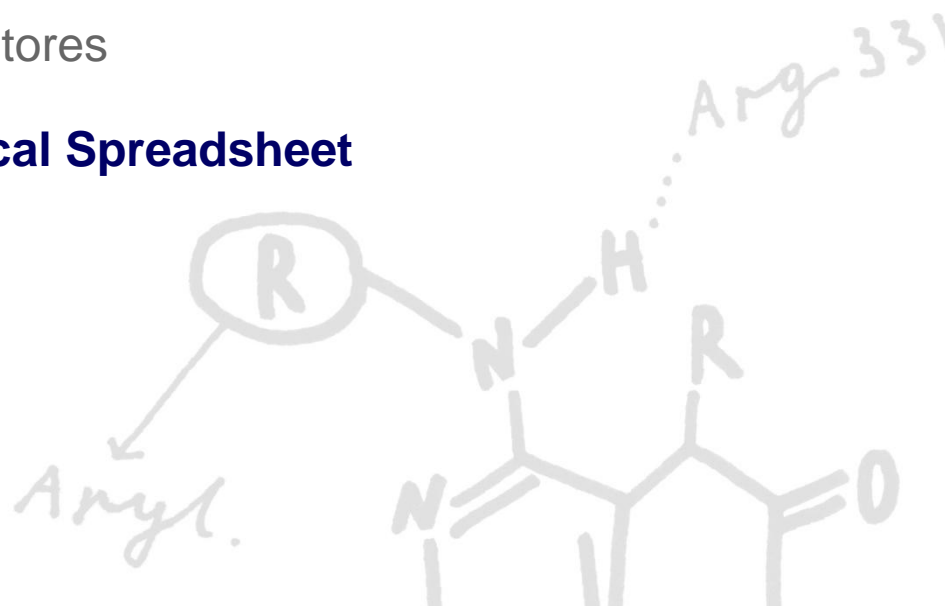
## Summary

- Will the benefits outweigh the functionality loss ?

## Agenda

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- Evotec
- Why migrate ?
- Searching for Library Enumeration Replacement
- Migrating a small activity database
- Migrating Chemical Stores
- **Using a new Chemical Spreadsheet**
- Conclusion





## Using a new Chemical Spreadsheet

### Comparison of Tools

Feature	Software A (UK)	Software B (India)	JChem4XL
Licensed to all	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Plug-Ins	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> (limited by number per day)	<input checked="" type="checkbox"/>
Import/Export SD File	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
SMILES Support	OK (problems with chirality)	??	<input checked="" type="checkbox"/>
Conversion to Images	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Copy to Report	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> (Not always nice)

## Migrating to JChem4XI

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### What the users like

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- Be able to send the spreadsheet to another site and they can see and copy/paste active structures
- Be able to send structures as 'Images' to Clients who do not have chemical spreadsheet tools
- Be able to calculate all the properties using the JChem4XL functions
- Be able to use R Group decomposition, and do simple enumerations

## Migrating to JChem4XI

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What are the users moaning about ?

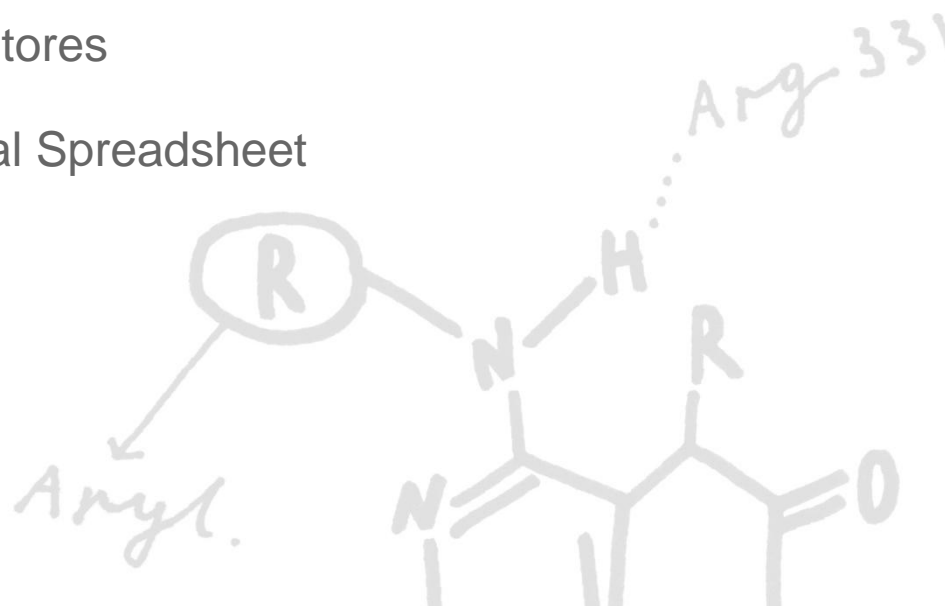
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- I have been using Software A for 20 years...
- I Don't know how to use Marvin
- It does not look pretty when I copy/paste to my report or PowerPoint slide
- It is an extra click to do this.....
- My structures are disappearing
- Difficulty in installing/ upgrading
  - Application tested in the department with sometimes extra spreadsheet tools installed
  - Test Installation and upgrades on 6 PCs
  - Why does it all go wrong on a scientist 's desktop ?
- Thanks for all the support we have received from ChemAxon !

## Agenda

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- Evotec
- Why migrate ?
- Searching for Library Enumeration Replacement
- Migrating from ISIS Local database to IJC
- Migrating Chemical Stores
- Using a new Chemical Spreadsheet
- **Conclusion**



# What makes migration easier ?

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How to convince users ?

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- Small team of friendly scientists
- Computer Literate
- Equivalent or better functionality
- Always keen if the new software is going to facilitate their daily tasks
- Process changes are limited
- Selective 'Memory Loss' from users

**Your contact:**

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*Senior Application Developer 1*

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catherine.reisser@evotec.com

