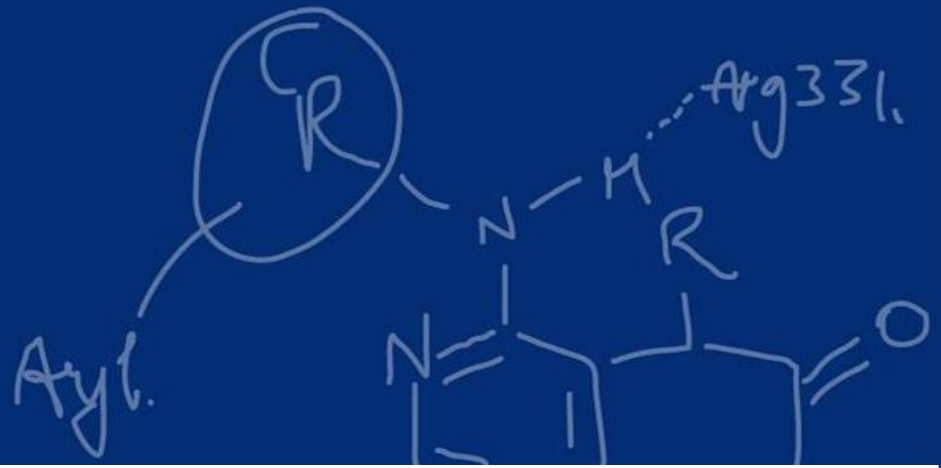
evotec

'RESEARCH NEVER STOPS'

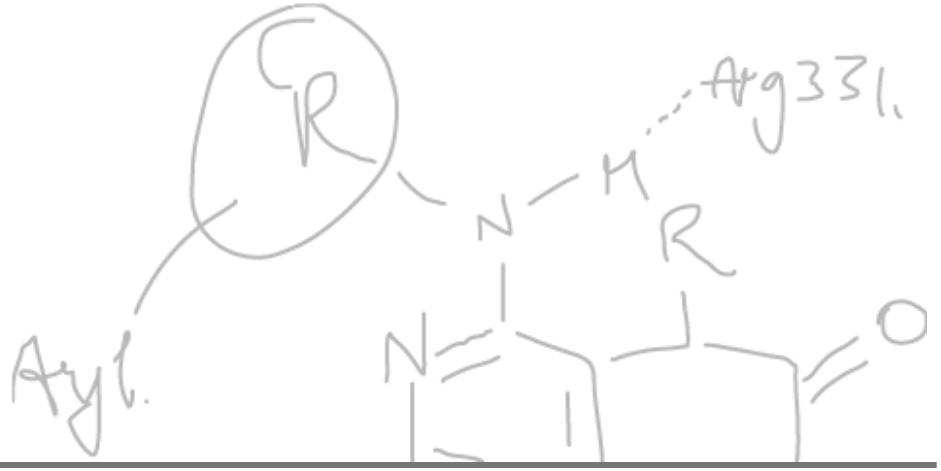
Integrating JChem and Marvin with an ELN

Creating integrated drug discovery innovation alliances



Agenda

- **About Evotec**
- Contur ELN
- Integration with Evotec in-house Applications
- Conclusion



Evotec: A proven track record

Evotec at a glance

- Founded in 1992
- Proven track record with over 150 partners worldwide
- A comprehensive platform that:
  - Focuses on small molecule drug discovery and development
  - Drives a range of discovery alliances in various therapeutic areas
- Global Operations
  - UK, Germany, India and Singapore
- Critical mass
  - 500+ employees
- Flexible deal structures
- TecDax

A drug discovery and development company that delivers innovation to its partners

Fully integrated R&D platform from target to clinic

Technology overview

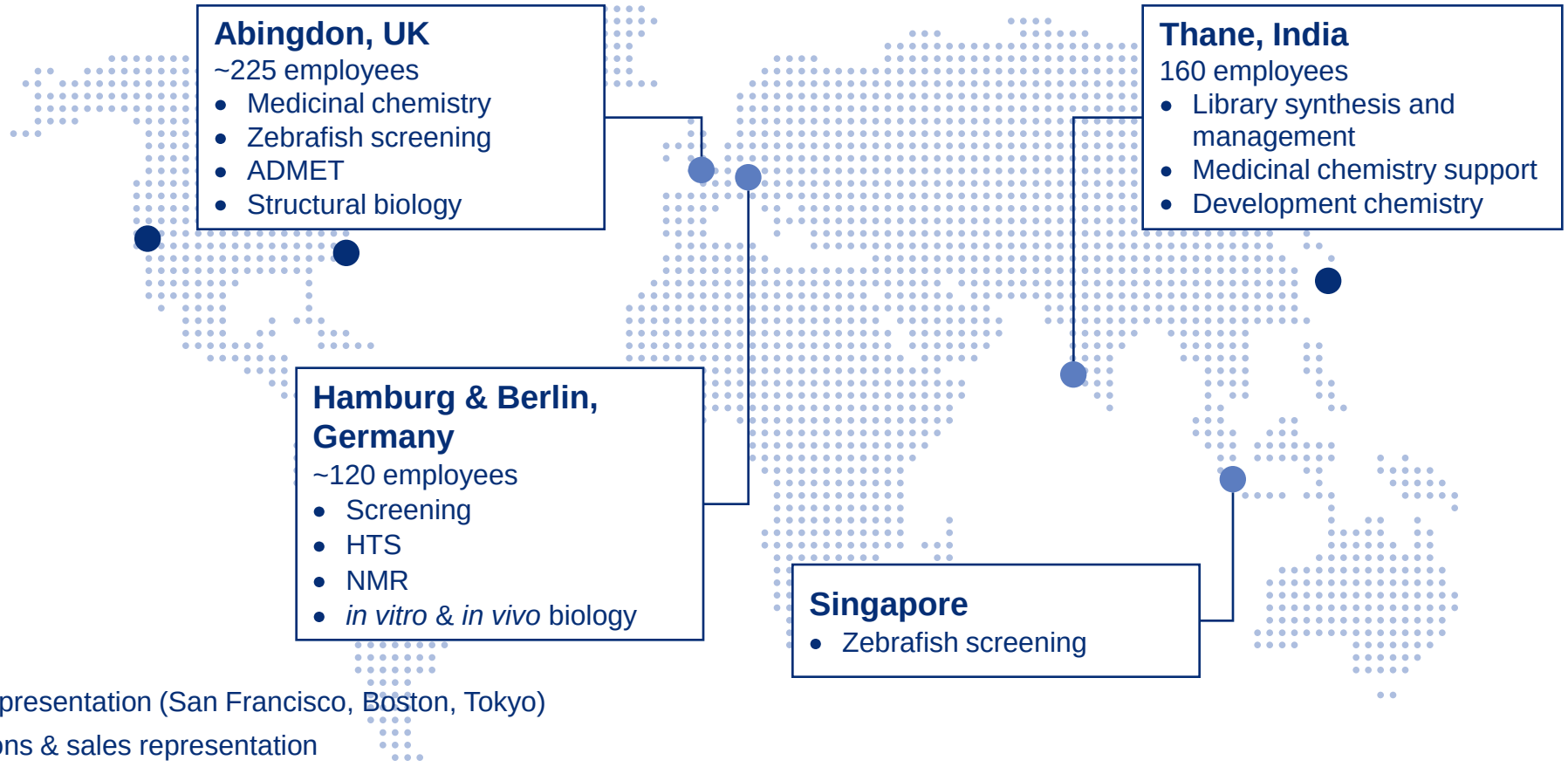
Screening	Hit-to-lead	Lead optimisation	Preclinical development	Clinical development
• Assay development • (u)HTS • High content screening • Electro-physiology • *in silico* screening technologies • Fragment-based drug discovery	• Medicinal chemistry • Hit expansion • Library design • High throughput chemistry • Protein-ligand crystallography • *in vitro* biology • Early ADMET	• Medicinal chemistry • *in vitro* biology • Disease bio-logy and target class expertise • Computational chemistry and structure-based drug design • *in silico* ADMET • Structural biology • ADMET and zebrafish screening • *in vivo* pharmacology	• Custom synthesis • Analytical development • Process R&D • Large scale synthesis • *in vivo* pharmacology	• Clinical alliances • Clinical project management

Technology and scientific leadership for numerous target classes and indication franchises

1. **CNS** (Roche)
2. **Oncology** (Boehringer Ingelheim)
3. **Inflammation**
4. **Metabolic disease**
5. **Others, ion channels, GPCR's, kinases,…**

Global reach

Ca. 500 Evotec employees worldwide



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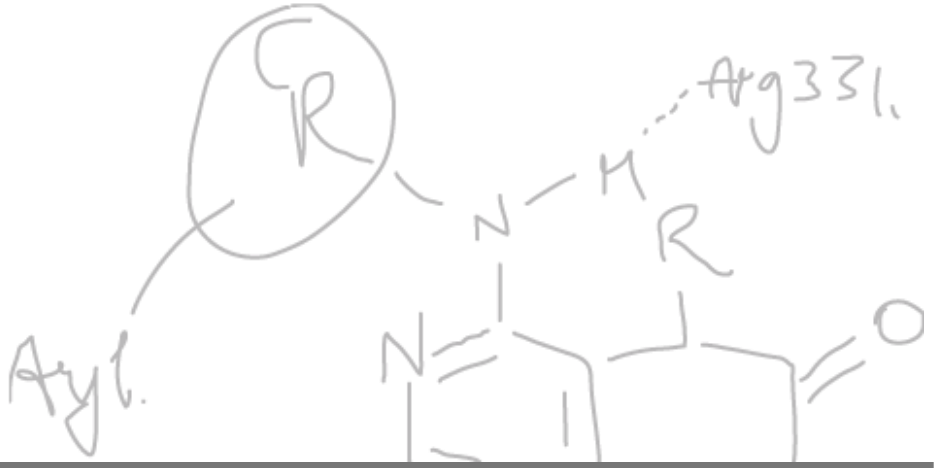
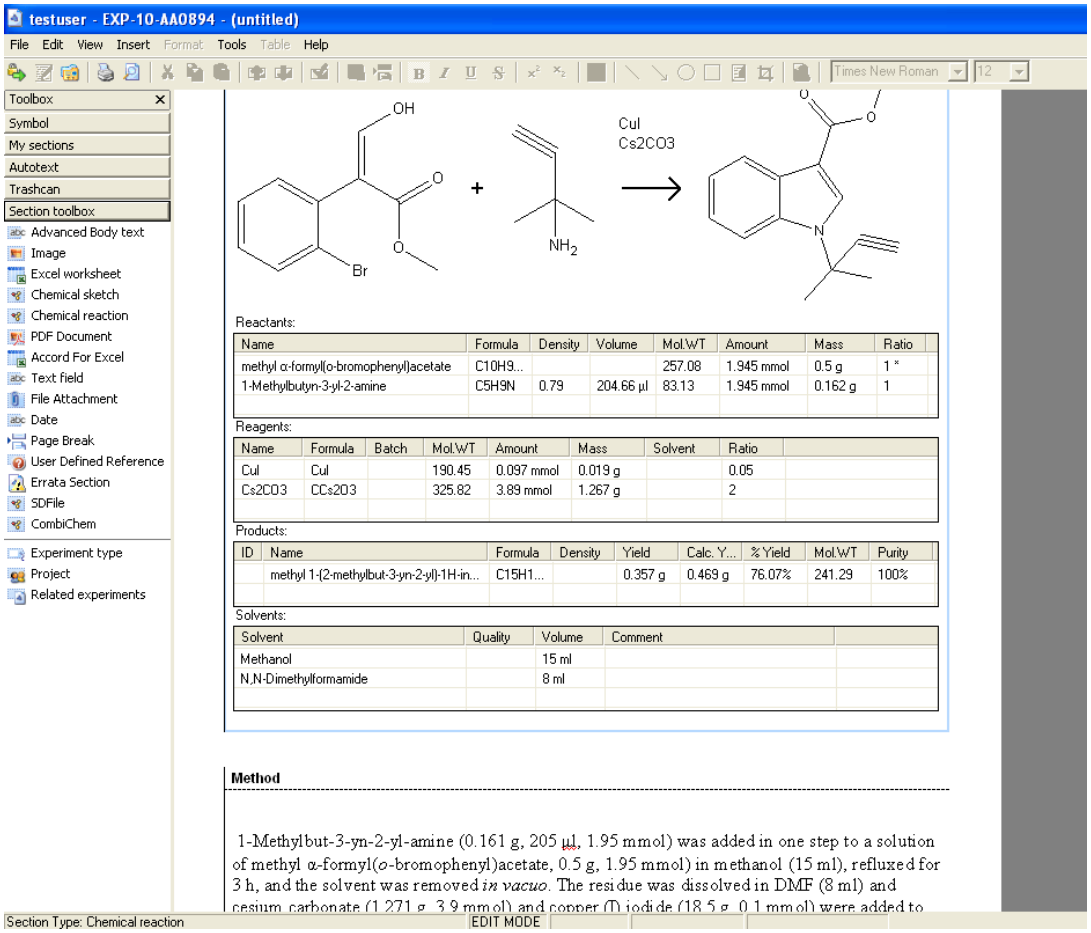


Contur ELN

Chemistry and Parallel Chemistry

- Simple, intuitive, flexible user interface for Chemists and Biologists
- Integrated with ChemAxon Marvin, Reactor, etc.

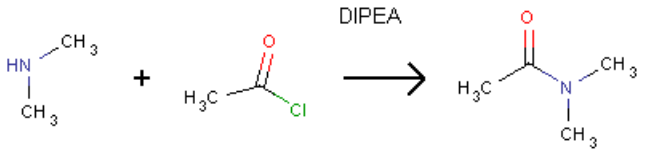


Contur ELN

Chemistry and Parallel Chemistry

Combi Chem

Set up generic reaction



Reactants:

ID	Name	Formula	Mol.WT	Amount	Solvent	Purity	Ratio
	Amine	C2H7N	45.08	1.2 mmol	Dichloromethane	100%	1 *
	Acid Chloride	C2H3C...	78.5	1.26 mmol		100%	1.05

Reagents:

ID	Name	Formula	Density	Volume	Mol.WT	Amount	Solvent	Ratio
	DIPEA	C8H19N	0.742	0.211 ml	129.24	1.212 mmol		1.01

Products:

ID	Name	Formula	Batch
	Amide	C4H9NO	

Solvents:

Solvent	Quality	Volume	Comment
Dichloromethane		10 ml	

Amine

MolNa...	Struct...	Formula	MolW...	Amount	Batch	Mass	Molec...	CAS N...	Ifs Par...	MFCD...
Piperazi...		C4H1...	86.1356	1.2 m...		103.3...	86.1356	6091-...	10622	MFCD...
N,N'-Di...		C4H1...	88.1515	1.2 m...						

Import SD file with reactants

Acid Chloride

MolNa...	Struct...	Formula	MolW...	Amount	Batch	Mass	Molec...	CAS N...	Ifs Par...	MFCD...
Acetyl ...		C2H3...	78.498	1.26 m...		98.91 ...	78.498	75-36-5	10247	MFCD...

Automatic Page Break

Acid Chloride

MolNa...	Struct...	Formula	MolW...	Amount	Batch	Mass	Molec...	CAS N...	Ifs Par...	MFCD...
Propen...		C3H3...	90.508	1.26 m...		114.0...	90.508	814-6...	11009	MFCD...

Enumerate products

Combinatorial Products:

MolName	Structure	Formula	MolW	Mass	Amount	Yield
Product 1		C6H12N2O	128.1723	153.81 mg	130 mg	84.52%
Product 2		C7H12N2O	140.183	168.22 mg	120 mg	71.34%

Contur ELN

Out of the box features

Integrate with a Chemical Cartridge → • ChemAxon JChem cartridge

Choose a Drawing package → • Marvin Sketch

Authentication via AD → • Via a Group

Contur ELN

Out of the box features

Admin console to set up Projects, Users and Roles

- Integrate with EVOuser instead

Use Contur Reactant, Reagent and Solvent List

- Integrate with EVOsource instead

Set up Look Up List for Assays, Species, Equipment

- Integrate with EVOequip and EVOasap

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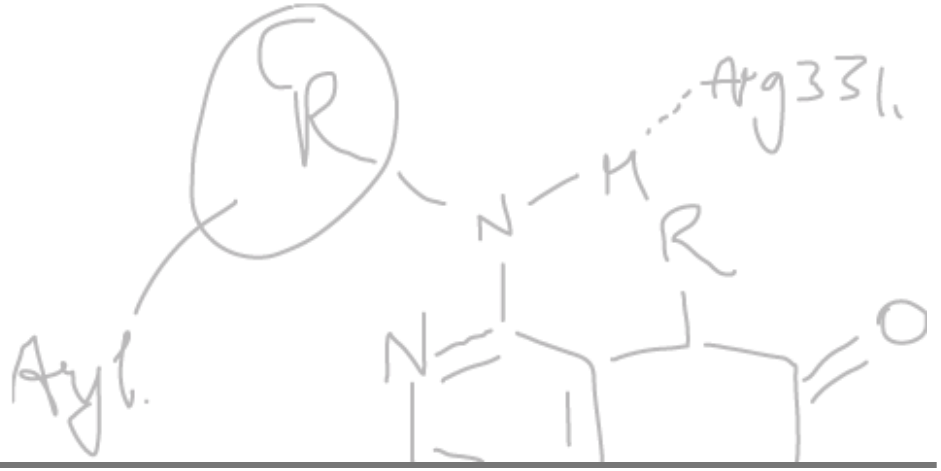
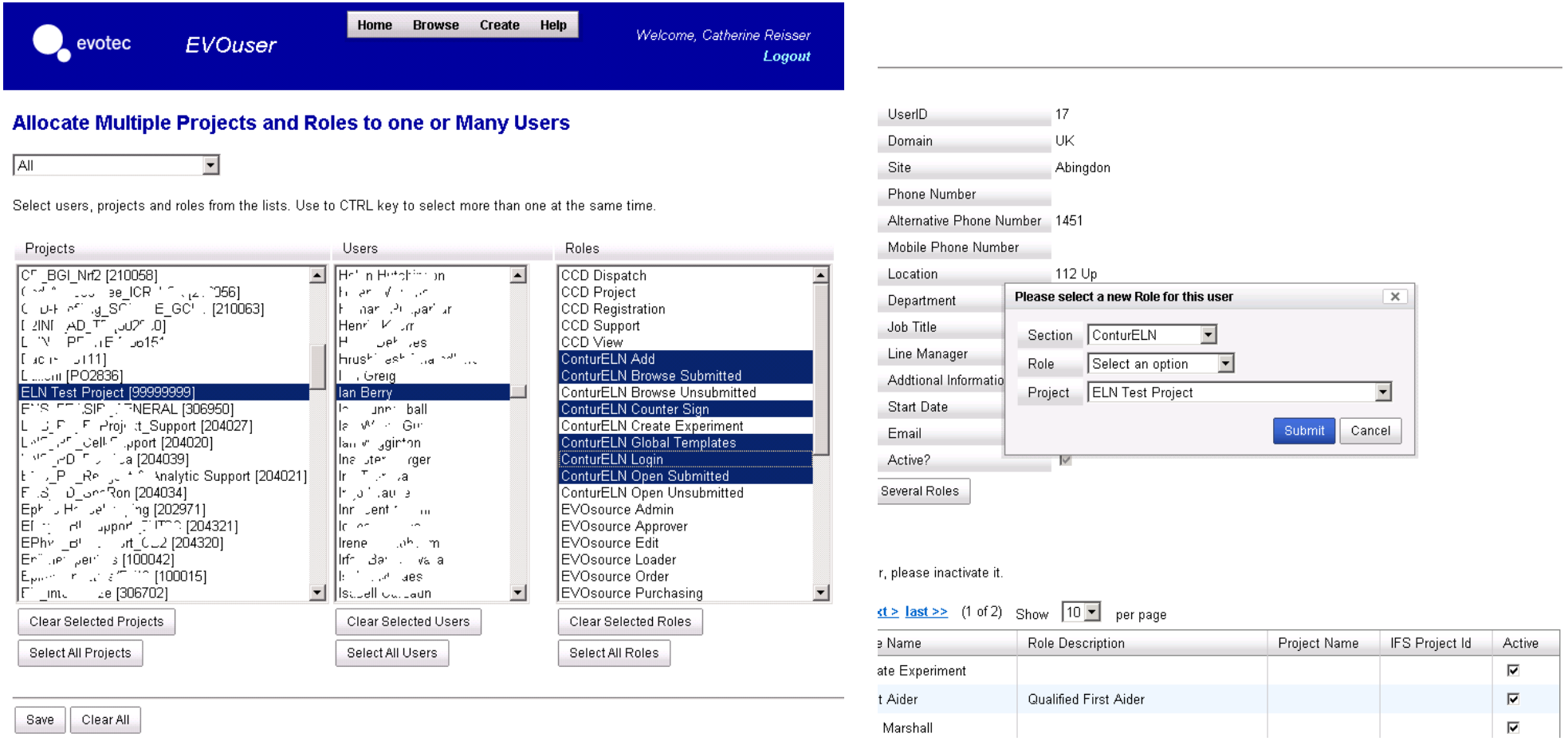


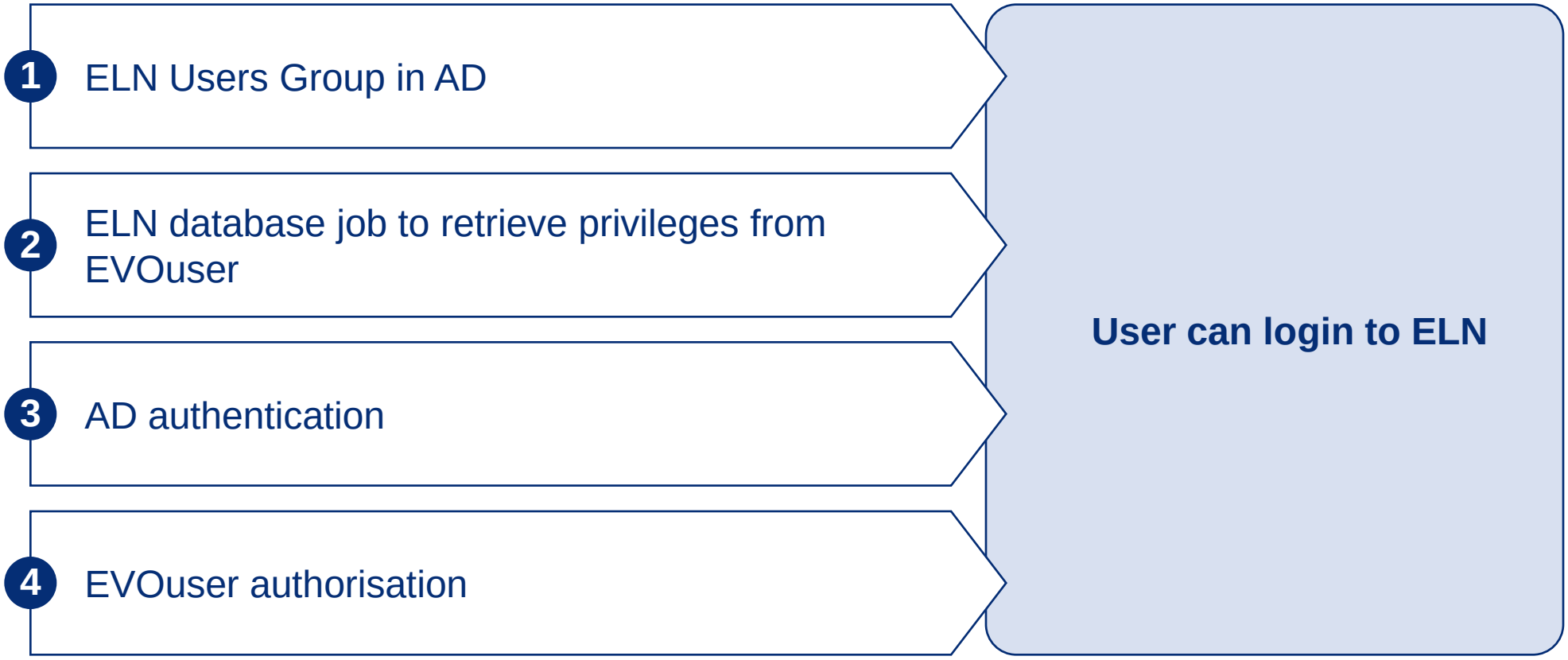
Evotec in-house Applications

EVOuser - User Management Application



EVOuser – ELN Integration

Maintaining users & roles from a centralized Evotec application



Evotec in-house Applications

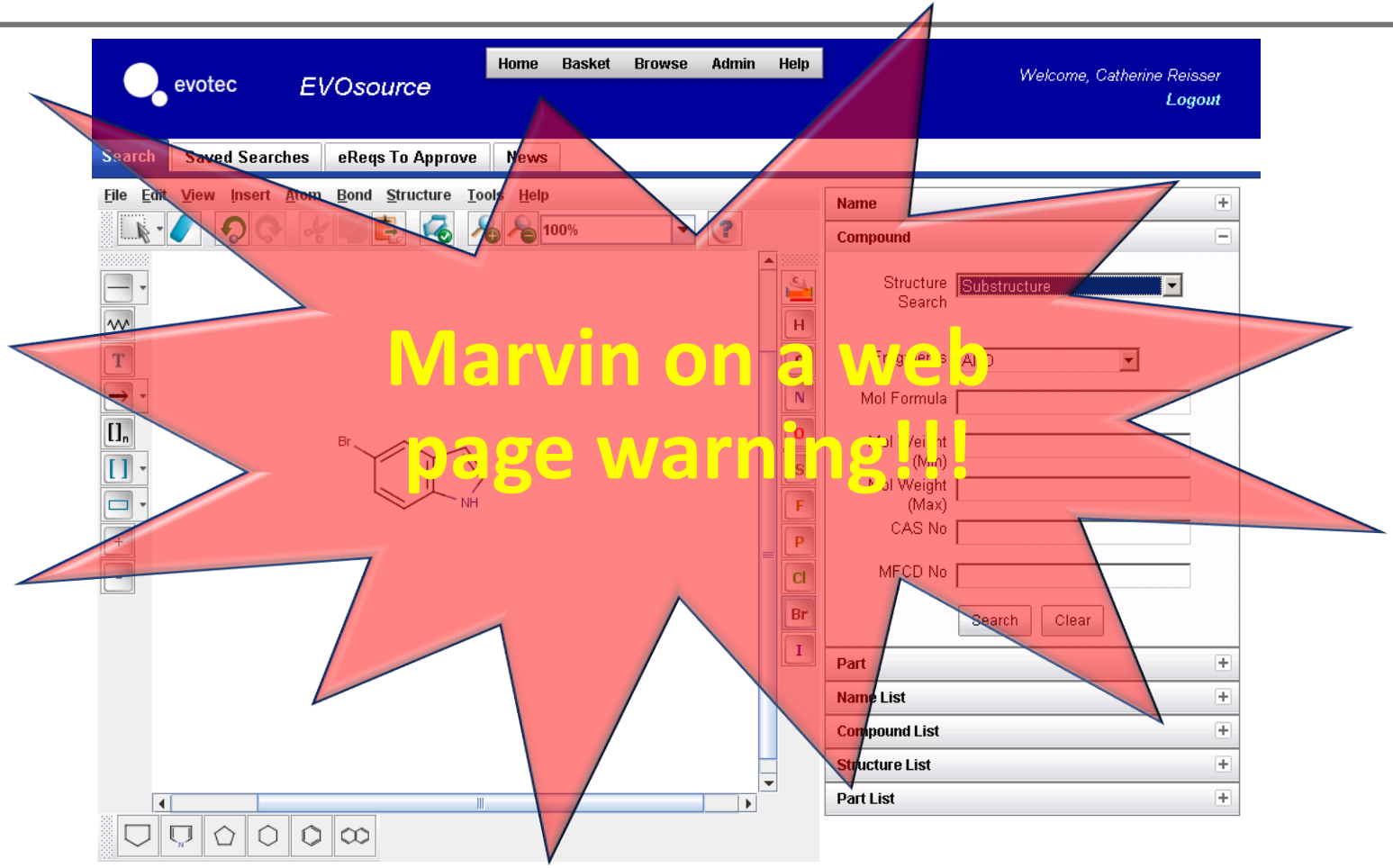
EVOsource – compound sourcing

- Evotec's compound sourcing and ordering Application
- Aims to unify and streamline the process of ordering compounds
- Create & request quotes from Suppliers
- Return unused chemicals to Stores & request stock chemicals from Stores
- Directly linked to our ERP System

Category	Count
• Suppliers	71
• Catalogues	206
• Unique Compounds	9,618,473
• Parts	24,676,106

Evotec in-house Applications

EVOsource



EVOsource – ELN Integration

Searching EVOsource directly from the ELN

1. EVOsource trigger to automatically create Mol File when Loading data
2. EVOsource function to retrieve density for each compound
3. Contur ELN Compound Searcher queries EVOsource directly using a Temporary Table in EVOsource
4. XML files to configure the Contur ELN screen and field names according to Evotec specification

Contur ELN can search EVOsource

Results obtained in less than 5 seconds

Exact Searching takes 1 second !

EVOsource – ELN Integration

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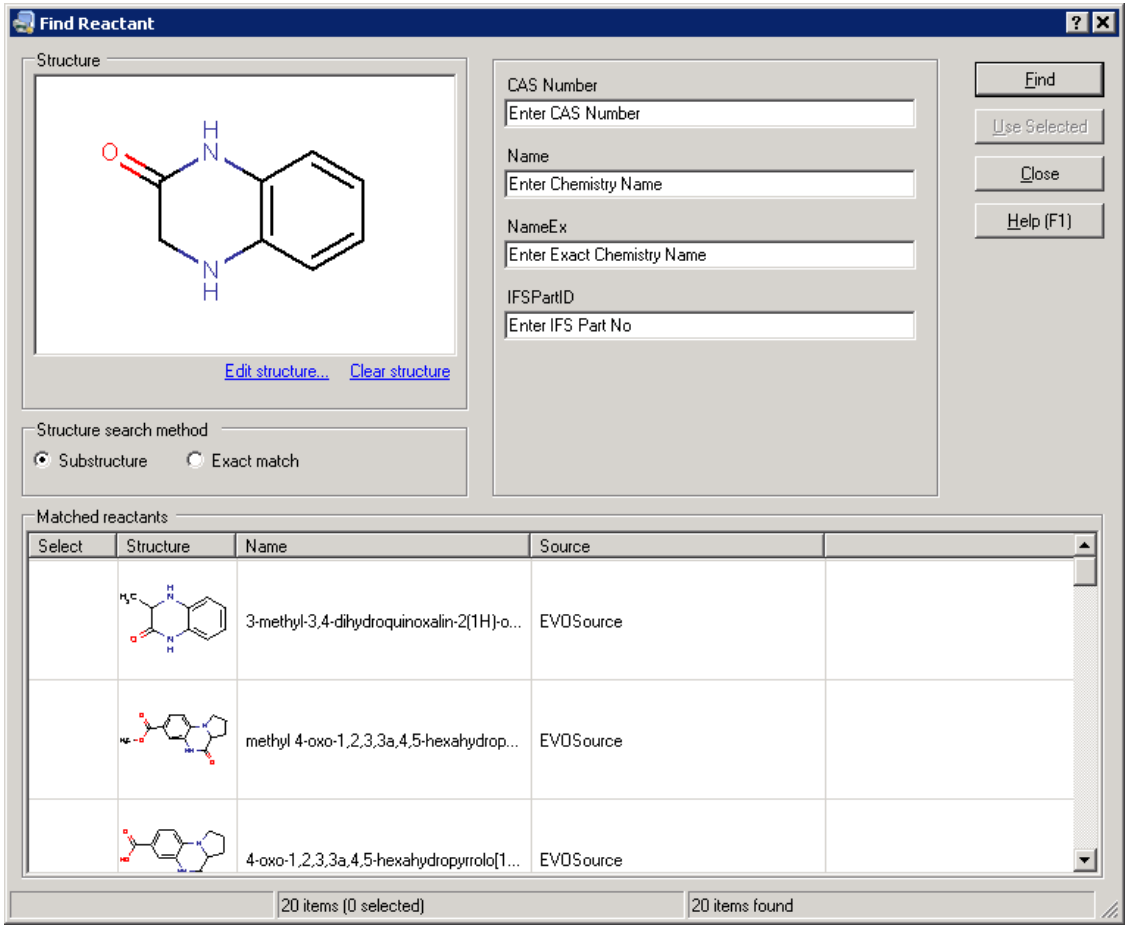
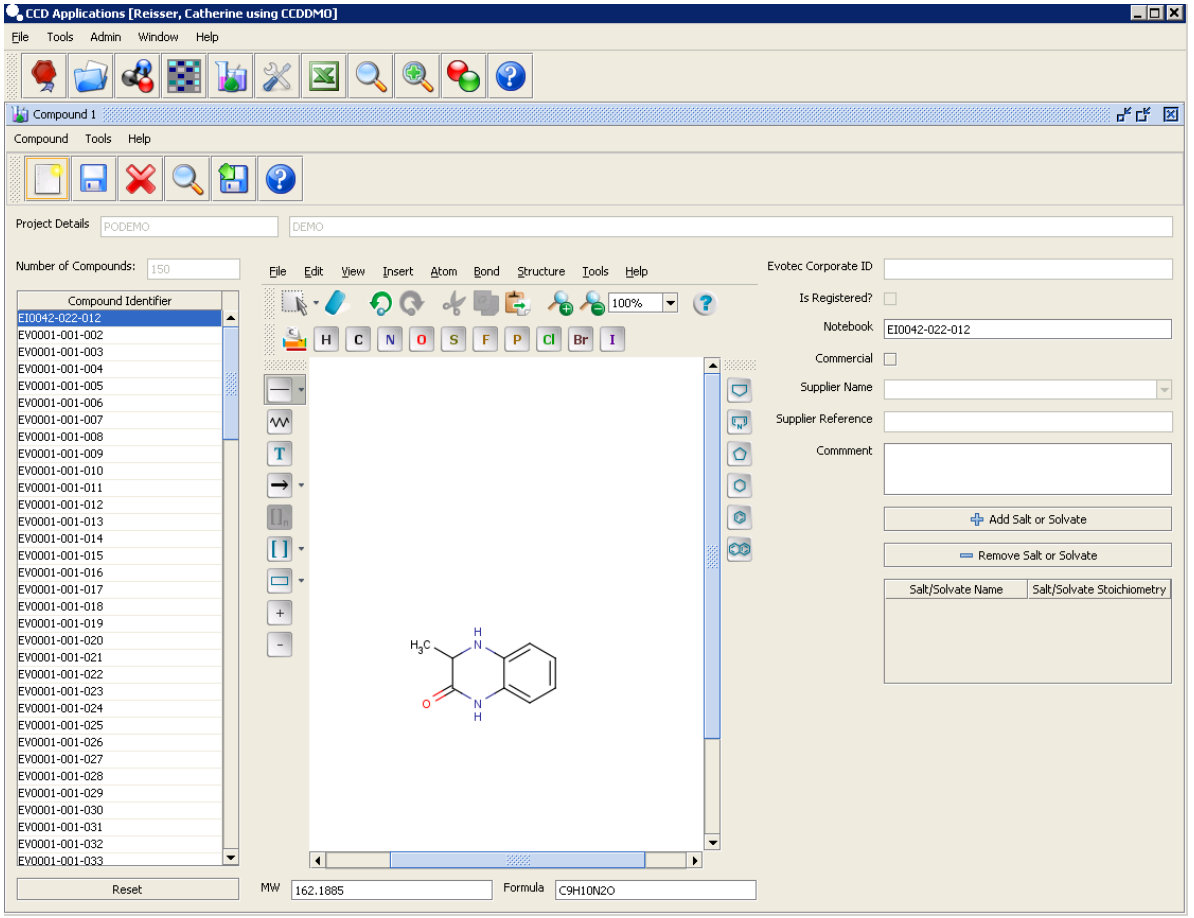


Evotec in-house Applications

CCD (Corporate Chemical Database)

- Evotec's Compound Registration Application
- Keeps a record of all the compounds ever synthesized for an Internal Project or for an External Customer
- Keeps track of all compounds ever dispatched to a Customer
- Allows eScience to enforce exclusivity for each compound



CCD - ELN - CCD Integration

Work in progress!

1. CCD View with all Registered Compounds Batches
2. Open the experiment and ELN from CCD by using the experiment link, e.g.
   http://elntest/ElnStarterWeb/OpenExperiment.aspx?experimentnumber=EXP-10-AA0103
3. ELN View display all Reaction products + CCD Link to Query ELN and bring back compound on Request
4. Chemist discipline to populate the ELN product table with agreed identifier?

CCD batch numbers can be used for ADMET and Analytical Experiments

Open ELN from CCD Application

Perform semi-automated pre-registration of compounds

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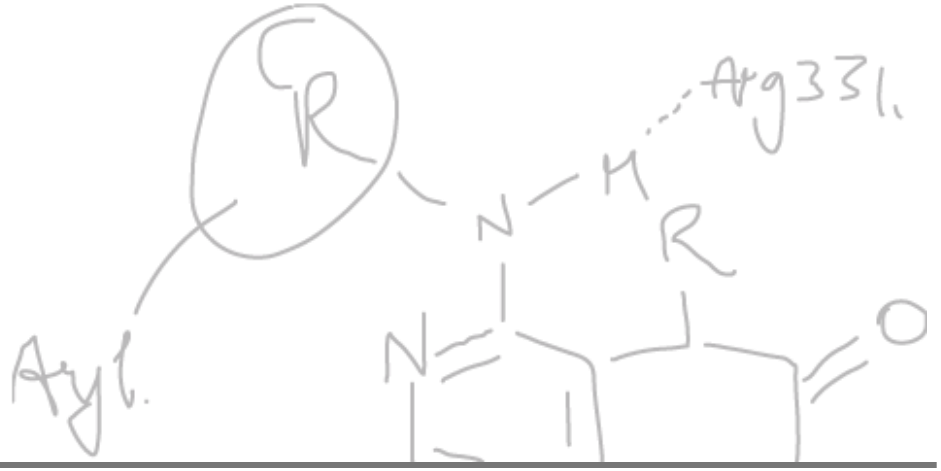
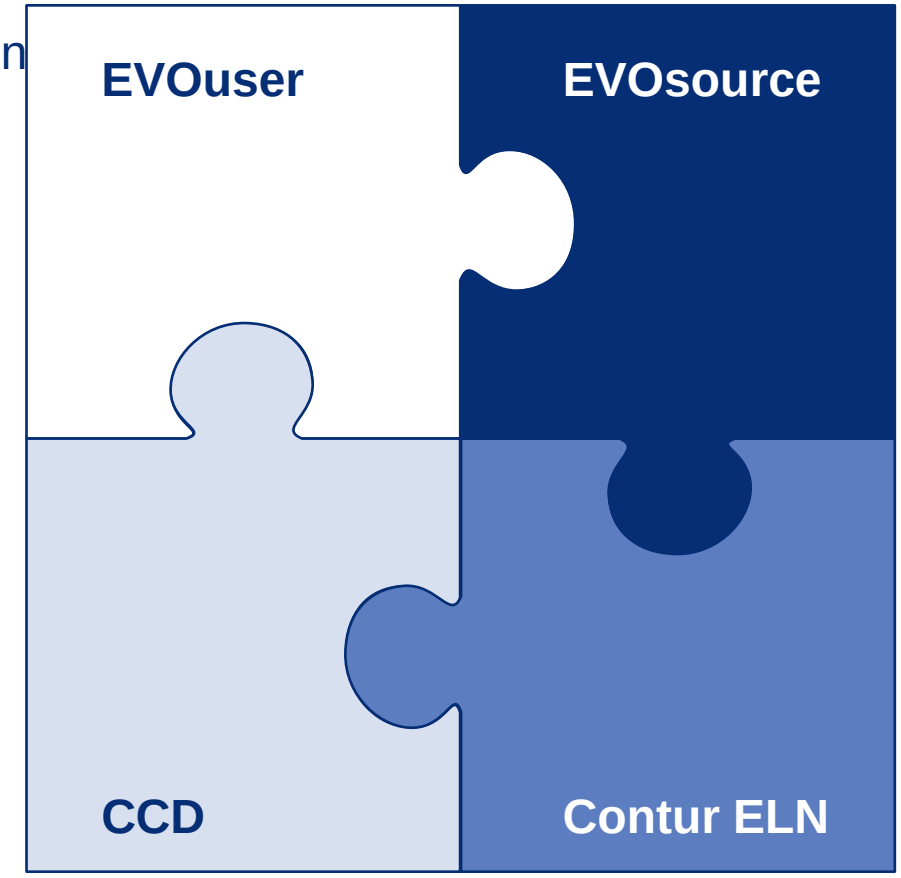


Conclusion

4 Applications linked together, 3 relying on ChemAxon technology

- Java Web Application



- Java Web Application
  - JChem cartridge
  - JChem API
  - Marvin Applet

- Java Client App
  - JChem cartridge
  - JChem API
  - Marvin Sketch

- Rich Client App
  - JChem cartridge
  - Marvin Sketch
  - Reactor
  - JChem tools

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