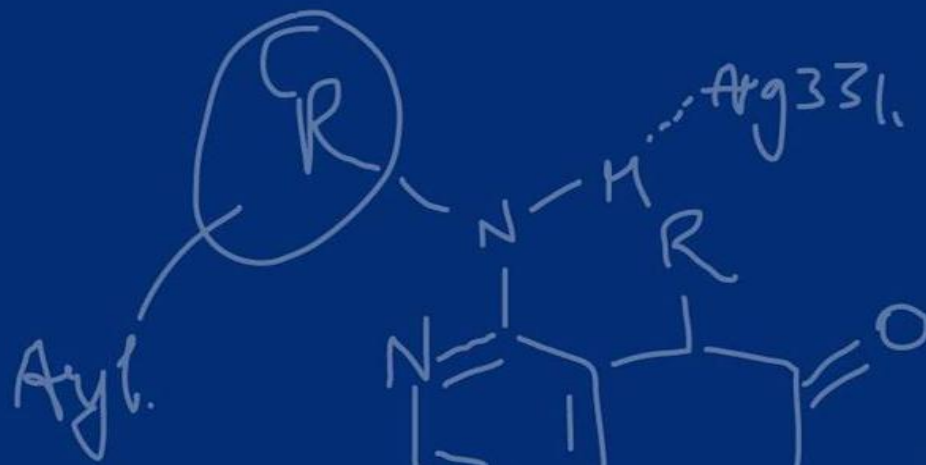


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# Integrating JChem and Marvin with an ELN

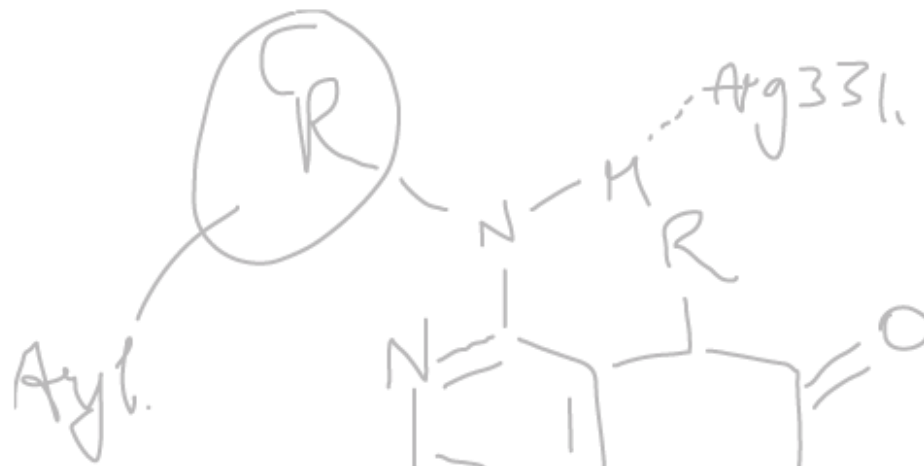
Creating integrated drug discovery  
innovation alliances



# Agenda

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



# Evotec: A proven track record

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## Evotec at a glance

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- 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
<ul style="list-style-type: none"> <li>Assay development</li> <li>(u)HTS</li> <li>High content screening</li> <li>Electro-physiology</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>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>Computational chemistry and structure-based drug design</li> <li><i>in silico</i> ADMET</li> <li>Structural biology</li> <li>ADMET and zebrafish screening</li> <li><i>in vivo</i> pharmacology</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> </ul>	<ul style="list-style-type: none"> <li>Clinical alliances</li> <li>Clinical project management</li> </ul>

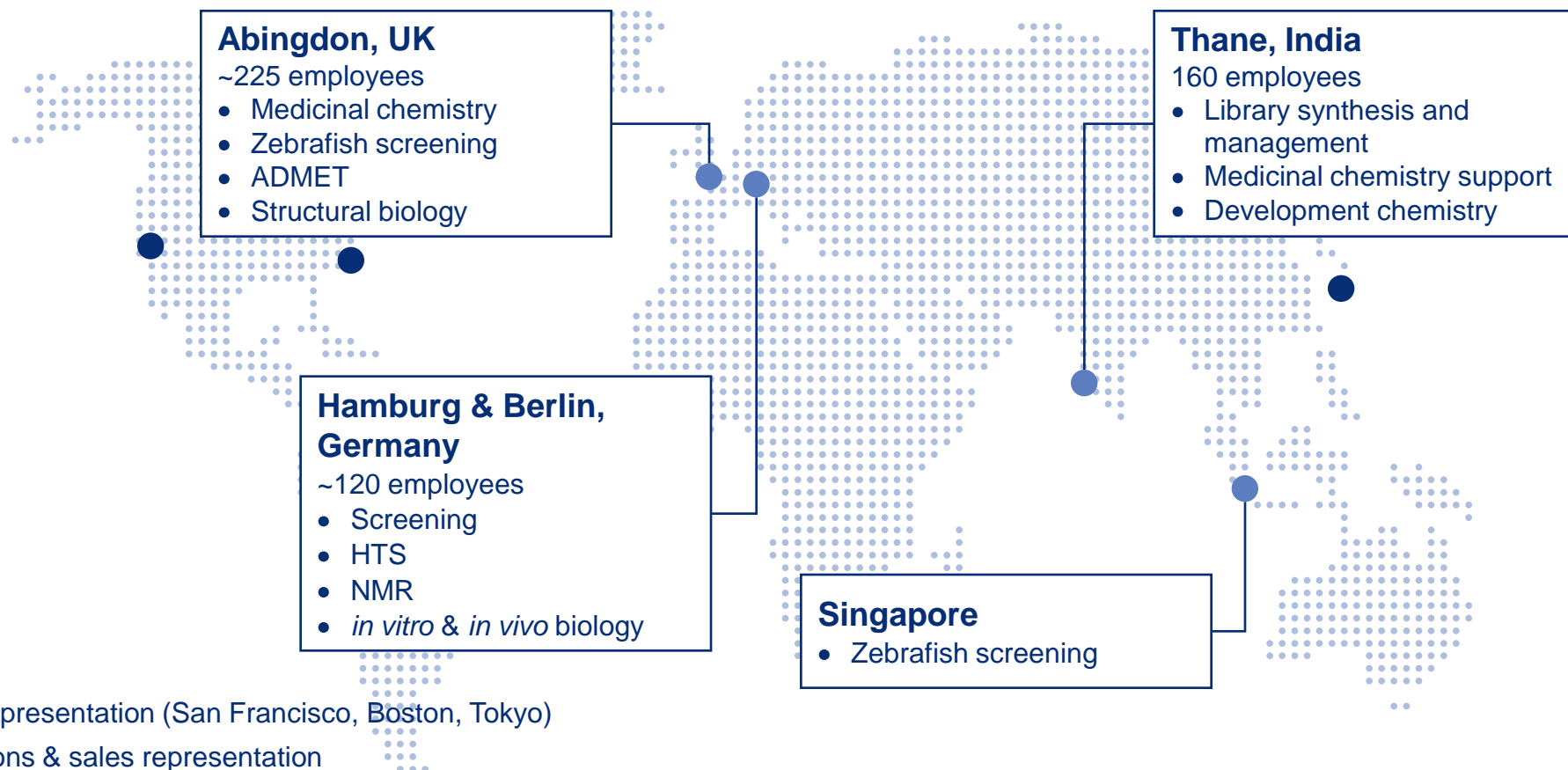


Technology and scientific leadership for numerous target classes and indication franchises

- 1 CNS 
- 2 Oncology 
- 3 Inflammation
- 4 Metabolic disease
- 5 Others, ion channels, GPCR's, kinases,...

# Global reach

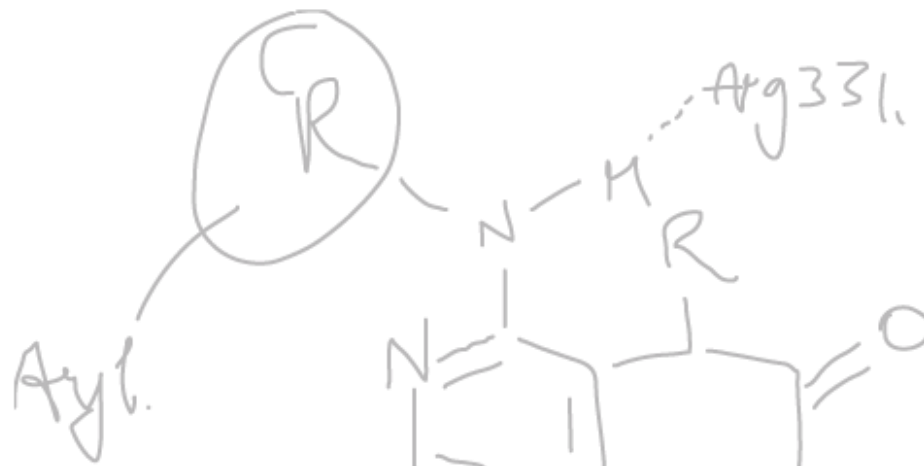
Ca. 500 Evotec employees worldwide



## Agenda

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



# Contur ELN

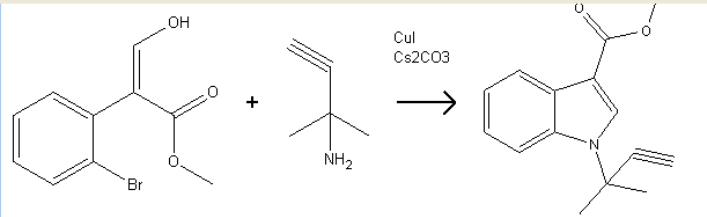
## Chemistry and Parallel Chemistry

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

testuser - EXP-10-AA0894 - (untitled)

File Edit View Insert Format Tools Table Help

Times New Roman 12



Reactants:

Name	Formula	Density	Volume	MolWT	Amount	Mass	Ratio
methyl $\alpha$ -formyl(o-bromophenyl)acetate	C10H9...			257.08	1.945 mmol	0.5 g	1 *
1-Methylbut-3-yn-2-yl-amine	C5H9N	0.79	204.66 $\mu$ l	83.13	1.945 mmol	0.162 g	1

Reagents:

Name	Formula	Batch	MolWT	Amount	Mass	Solvent	Ratio
CuI	CuI		190.45	0.097 mmol	0.019 g		0.05
Cs <sub>2</sub> CO <sub>3</sub>	CCs203		325.82	3.89 mmol	1.267 g		2

Products:

ID	Name	Formula	Density	Yield	Calc. Y...	% Yield	MolWT	Purity
	methyl 1-(2-methylbut-3-yn-2-yl)-1H-in...	C15H1...		0.357 g	0.469 g	76.07%	241.29	100%

Solvents:

Solvent	Quality	Volume	Comment
Methanol		15 ml	
N,N-Dimethylformamide		8 ml	

Method

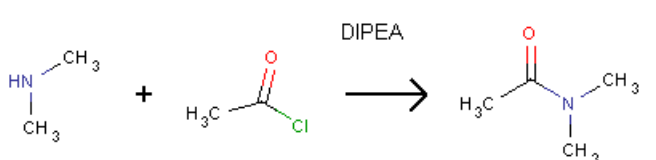
1-Methylbut-3-yn-2-yl-amine (0.161 g, 205  $\mu$ l, 1.95 mmol) was added in one step to a solution of methyl  $\alpha$ -formyl(o-bromophenyl)acetate, 0.5 g, 1.95 mmol) in methanol (15 ml), refluxed for 3 h, and the solvent was removed *in vacuo*. The residue was dissolved in DMF (8 ml) and cesium carbonate (1.271 g, 3.9 mmol) and copper (I) iodide (18.5 g, 0.1 mmol) were added to

Section Type: Chemical reaction EDIT MODE

# Contur ELN

## Chemistry and Parallel Chemistry

**Combi Chem**



DIPEA

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	C2H3Cl	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	MoW...	Amount	Batch	Mass	Molec...	CAS N...	Its Par...	MFCD...
Piperazi...		C4H10N2	86.1356	1.2 m...		103.3...	86.1356	6091...	10622	MFCD...
N,N'-Di...		C4H12N2	88.1515	1.2 m...						


Import SD file with reactants

Acid Chloride

MolNa...	Struct...	Formula	MoW...	Amount	Batch	Mass	Molec...	CAS N...	Its Par...	MFCD...
Acetyl ...		C2H3Cl	78.498	1.26 m...		98.91 ...	78.498	75-36-5	10247	MFCD...

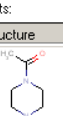

Automatic Page Break

Acid Chloride

MolNa...	Struct...	Formula	MoW...	Amount	Batch	Mass	Molec...	CAS N...	Its Par...	MFCD...
Propen...		C3H3Cl	90.508	1.26 m...		114.0...	90.508	814-6...	11009	MFCD...

Enumerate products

Combinatorial Products:

MolName	Structure	Formula	Mol...	Amount	Batch	Mass	Yield
Product 1		C6H12N2O		128.1723		153.81 mg	84.52%
Product 2		C7H12N2O		140.183		168.22 mg	71.34%



# Contur ELN

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## Out of the box features

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**Integrate with a Chemical Cartridge**



- ChemAxon JChem cartridge

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**Choose a Drawing package**



- Marvin Sketch

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**Authentication via AD**



- Via a Group
-

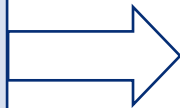
## Contur ELN

---

### Out of the box features

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**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**

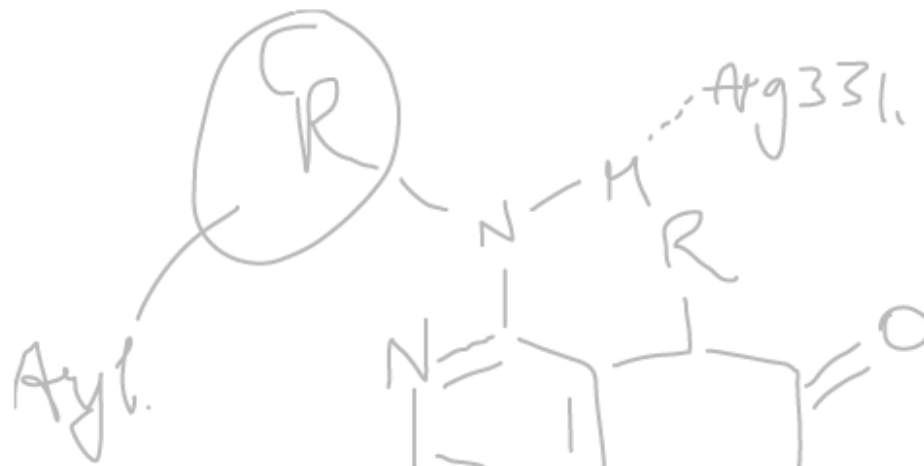


- Integrate with EVOequip and EVOasap
-

## Agenda

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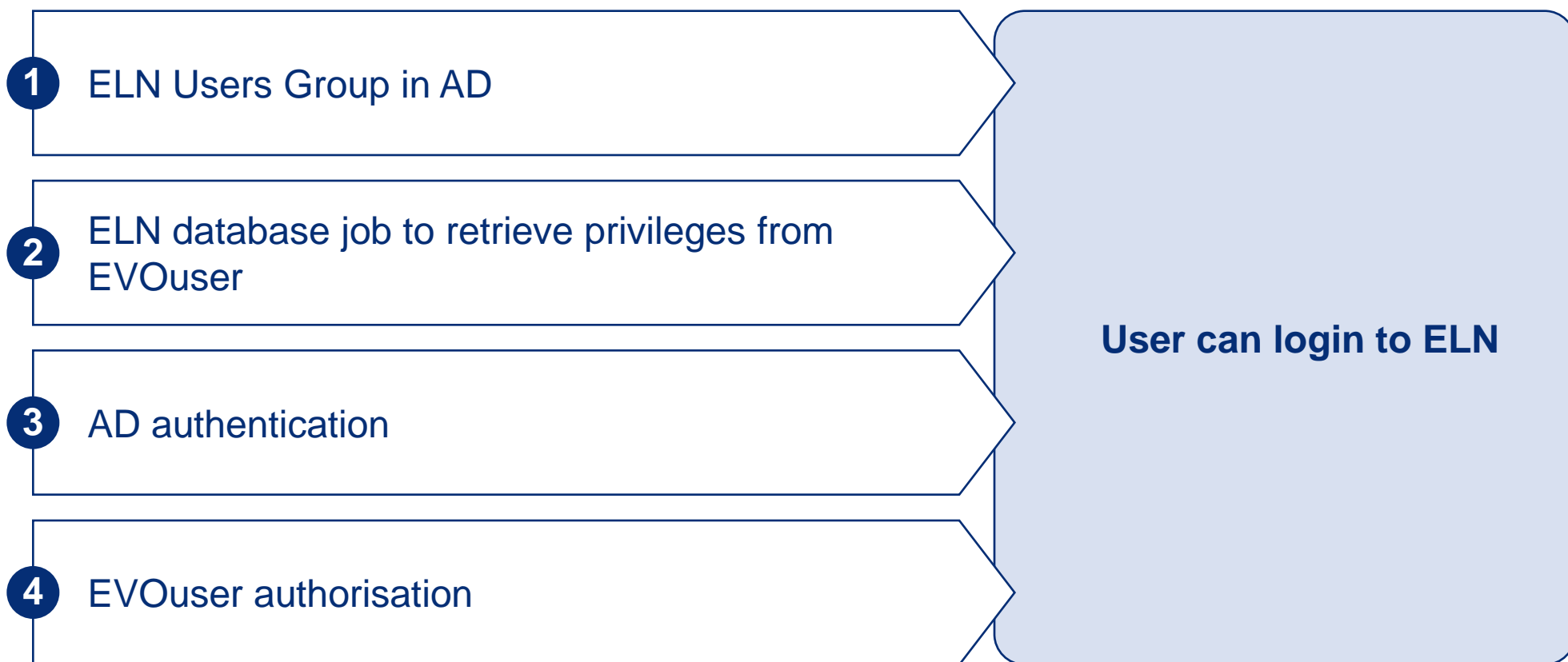
- About Evotec
- Contur ELN
- **Integration with Evotec in-house Applications**
- Conclusion





## EVOuser – ELN Integration

Maintaining users & roles from a centralized Evotec application



## Evotec in-house Applications

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### EVOsource – compound sourcing

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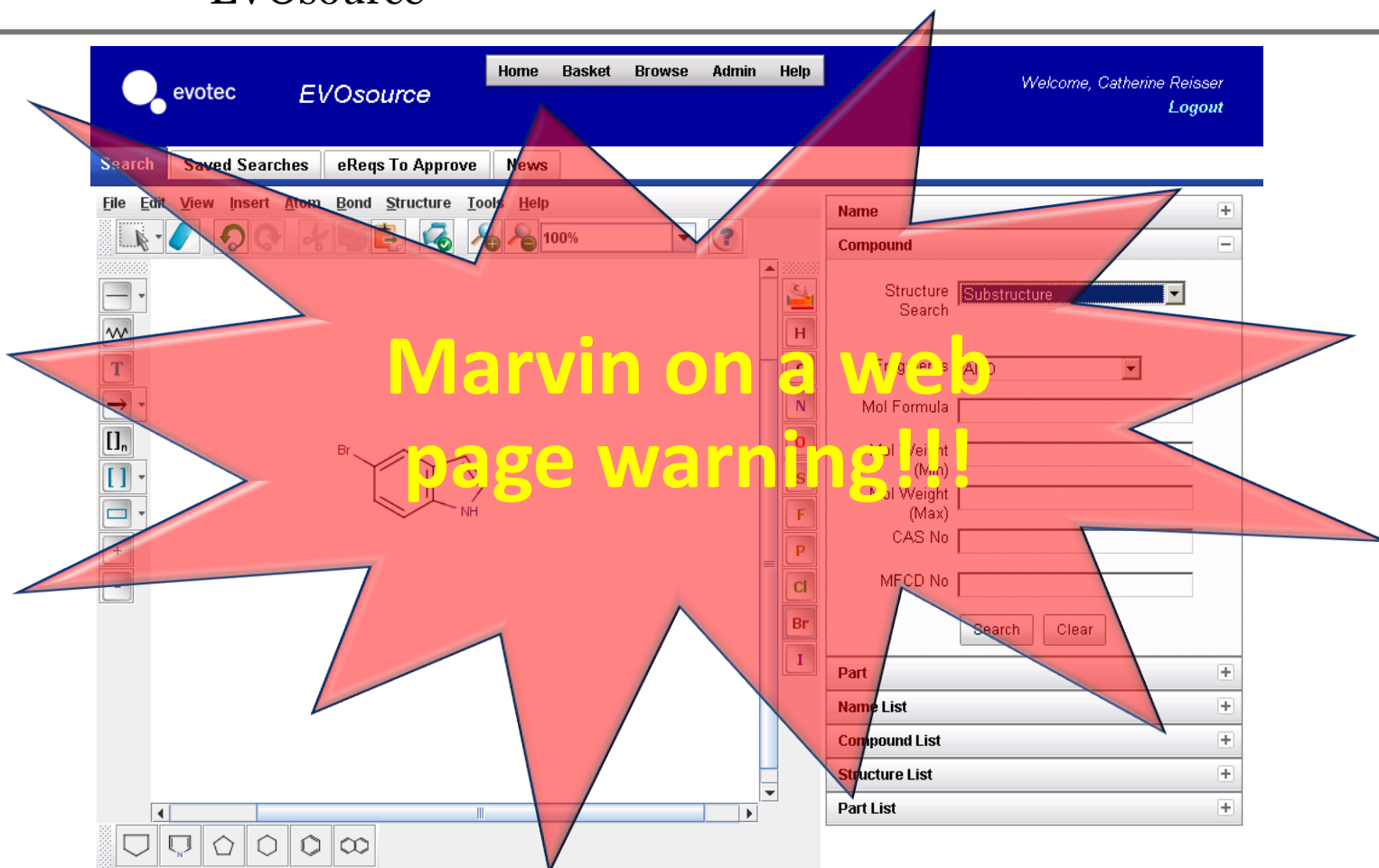
- Evotec's compound sourcing and ordering Application
- Aims to unify and streamline the process of ordering compounds
- Create & request quotes from Suppliers
- Return unused chemicals to Stores & request stock chemicals from Stores
- Directly linked to our ERP System

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

---

# Evotec in-house Applications

## EVOsource



The screenshot displays the EVOsource web application interface. At the top, a blue navigation bar contains the Evotec logo, the text "EVOsource", and links for "Home", "Basket", "Browse", "Admin", and "Help". On the right side of this bar, it says "Welcome, Catherine Reisser" and "Logout". Below the navigation bar, there are tabs for "Search", "Saved Searches", "eReqs To Approve", and "News". A menu bar includes "File", "Edit", "View", "Insert", "Atom", "Bond", "Structure", "Tools", and "Help". The main workspace shows a chemical structure of a benzimidazole derivative with a bromine atom. A large red starburst warning is overlaid on the center of the screen, containing the text "Marvin on a web page warning!!!". To the right of the main workspace is a sidebar with a search form. The search form has a "Name" field, a "Compound" section with a "Structure" dropdown set to "Substructure" and a "Search" input field, and several other input fields for "Mol Formula", "Mol Weight (Min)", "Mol Weight (Max)", "CAS No", and "MFCD No". At the bottom of the sidebar are buttons for "Search" and "Clear". Below the search form are expandable sections for "Part", "Name List", "Compound List", "Structure List", and "Part List".

## 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 !**

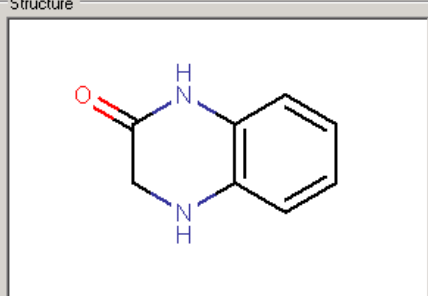


# EVOsource – ELN Integration

## Searching EVOsource directly from the ELN

**Find Reactant** [?] [X]

Structure



[Edit structure...](#) [Clear structure](#)

Structure search method

Substructure  Exact match

CAS Number

Enter CAS Number

Name

Enter Chemistry Name

NameEx

Enter Exact Chemistry Name

IFSPartID

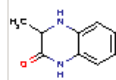
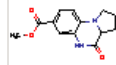
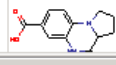
Enter IFS Part No

Find

Use Selected

Close

Help (F1)

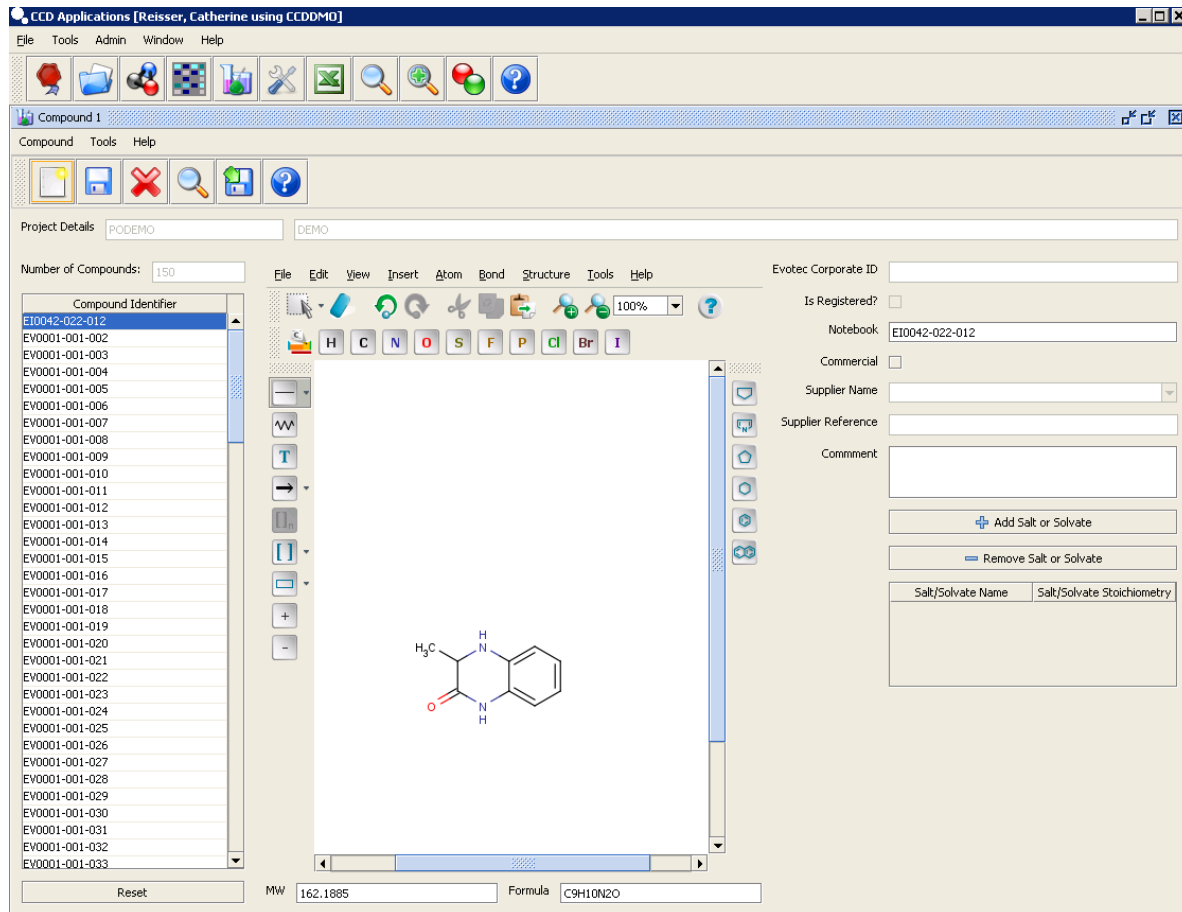
Select	Structure	Name	Source
<input type="checkbox"/>		3-methyl-3,4-dihydroquinoxalin-2(1H)-o...	EVOsource
<input type="checkbox"/>		methyl 4-oxo-1,2,3,3a,4,5-hexahdrop...	EVOsource
<input type="checkbox"/>		4-oxo-1,2,3,3a,4,5-hexahydropyrrolo[1...	EVOsource

20 items (0 selected)      20 items found

# 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



The screenshot displays the CCD Applications software interface. The main window is titled "Compound 1" and contains a "Project Details" section with a "DEMO" project name and a "Number of Compounds" field set to 150. A list of compound identifiers is shown on the left, with "E10042-022-012" selected. The central area features a chemical structure editor with a toolbar and a central canvas displaying the chemical structure of a benzimidazole derivative. The right side of the interface includes a form for "Evotec Corporate ID" and other fields such as "Is Registered?", "Notebook", "Commercial", "Supplier Name", "Supplier Reference", and "Comment". At the bottom, there are buttons for "Add Salt or Solvate" and "Remove Salt or Solvate", along with a table for "Salt/Solvate Name" and "Salt/Solvate Stoichiometry". The status bar at the bottom shows "MW 162.1885" and "Formula C9H10N2O".

# 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**

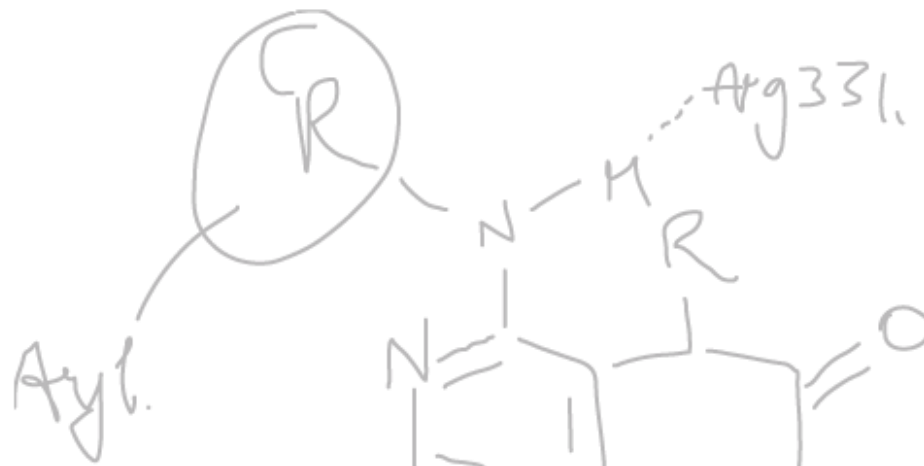
**Open ELN from CCD Application**

**Perform semi-automated pre-registration of compounds**

## Agenda

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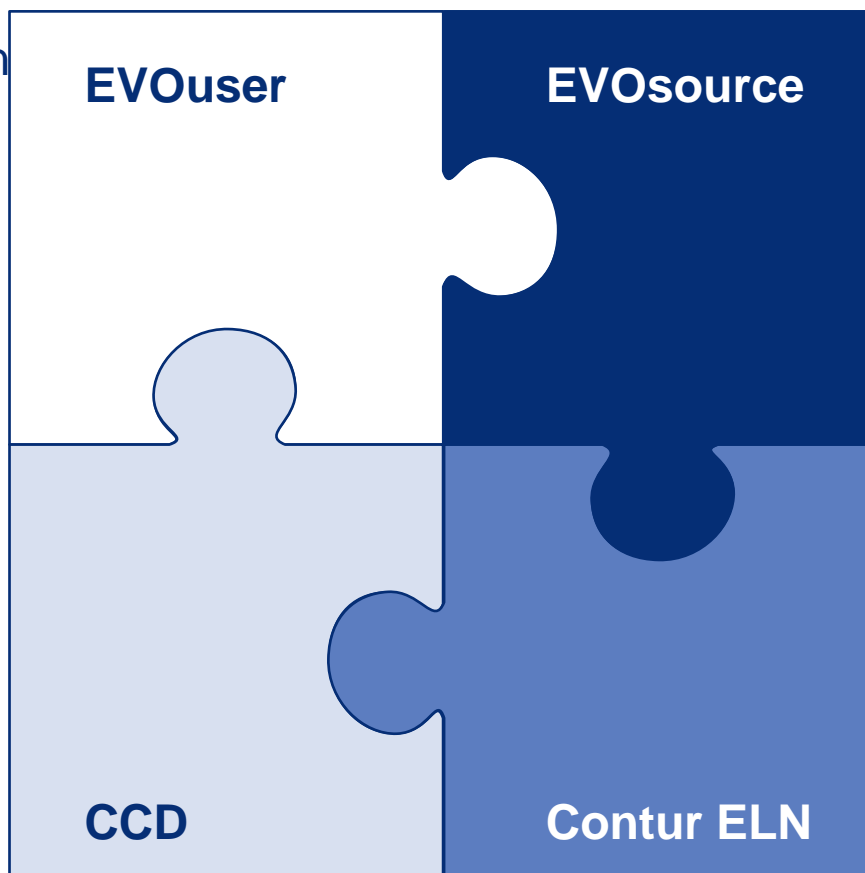
- About Evotec
- Contur ELN
- Integration with Evotec in-house Applications
- **Conclusion**



## Conclusion

4 Applications linked together, 3 relying on ChemAxon technology

- Java Web Application



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

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

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

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