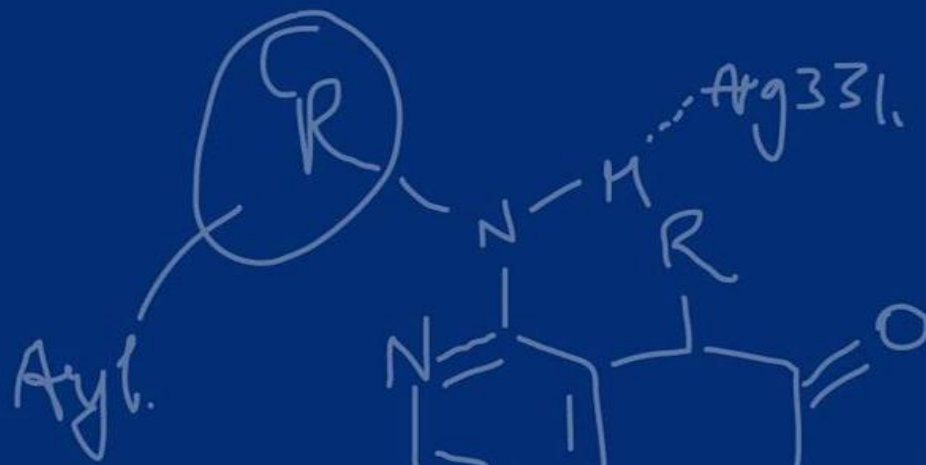
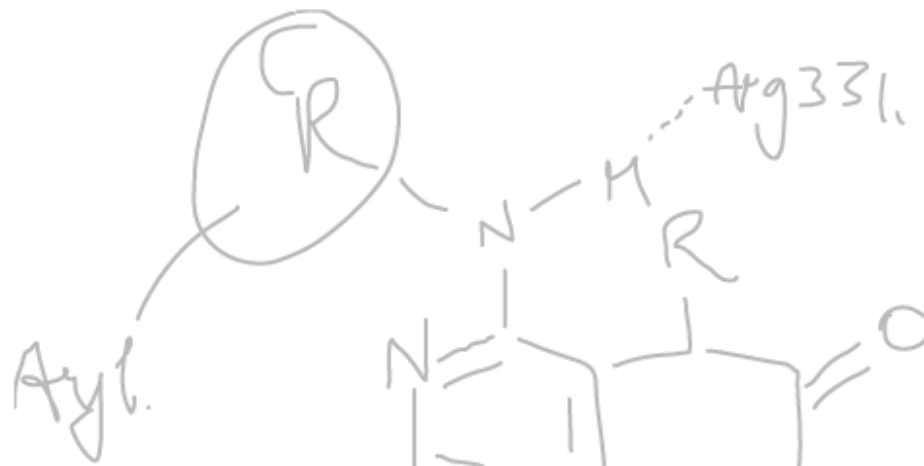

Integrating JChem and Marvin with an ELN

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
<ul style="list-style-type: none"> Assay development (u)HTS High content screening Electro-physiology <i>in silico</i> screening technologies Fragment-based drug discovery 	<ul style="list-style-type: none"> Medicinal chemistry Hit expansion Library design High throughput chemistry Protein-ligand crystallography <i>in vitro</i> biology Early ADMET 	<ul style="list-style-type: none"> Medicinal chemistry <i>in vitro</i> biology Disease biology and target class expertise Computational chemistry and structure-based drug design <i>in silico</i> ADMET Structural biology ADMET and zebrafish screening <i>in vivo</i> pharmacology 	<ul style="list-style-type: none"> Custom synthesis Analytical development Process R&D Large scale synthesis <i>in vivo</i> pharmacology 	<ul style="list-style-type: none"> Clinical alliances Clinical project management

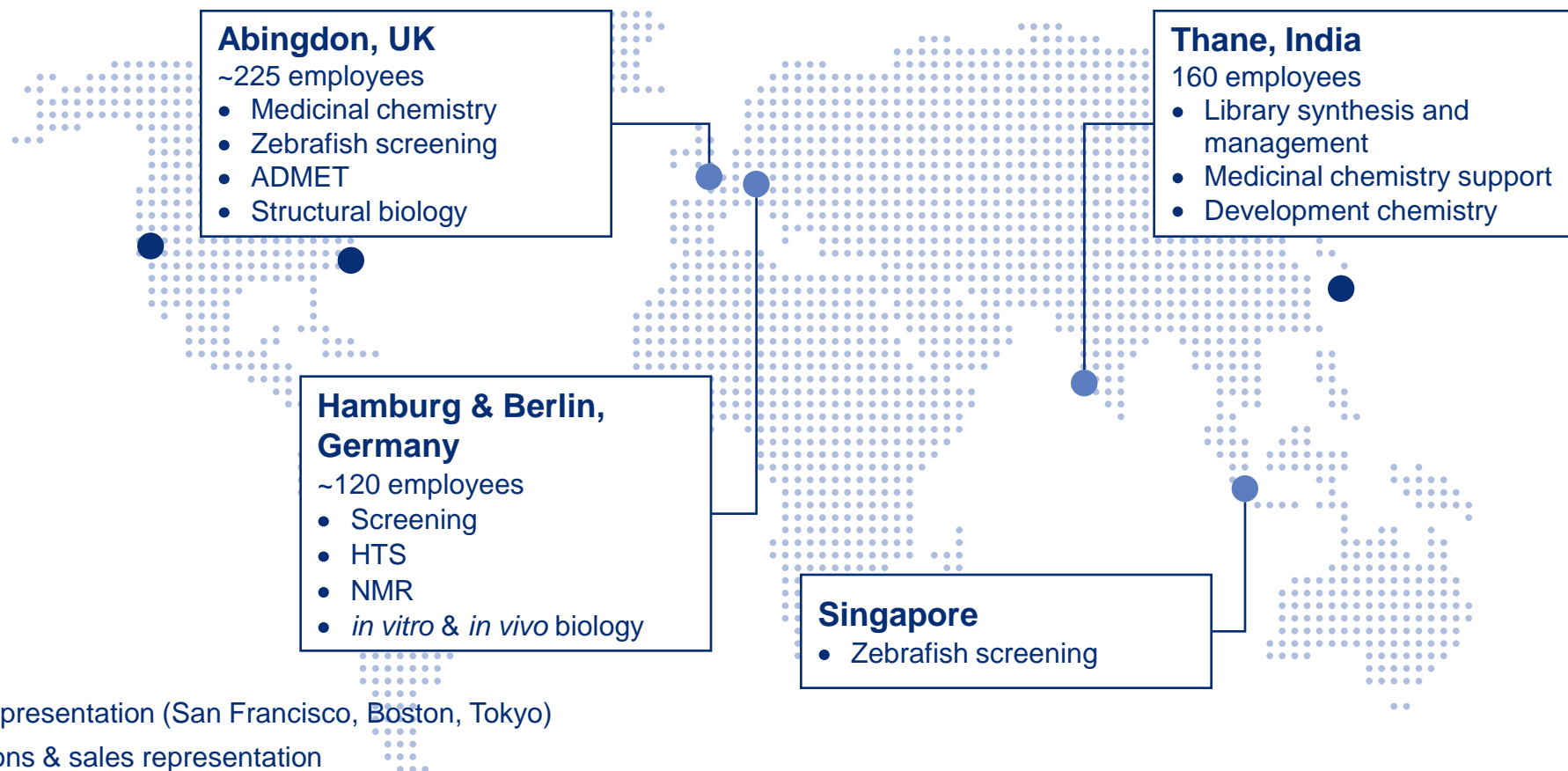


Technology and scientific leadership for numerous target classes and indication franchises

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

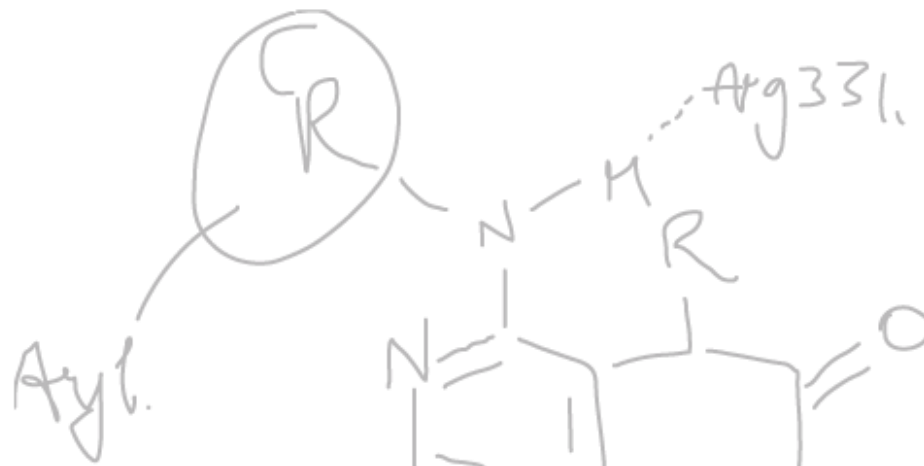
Global reach

Ca. 500 Evotec employees worldwide



Agenda

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



Contur ELN

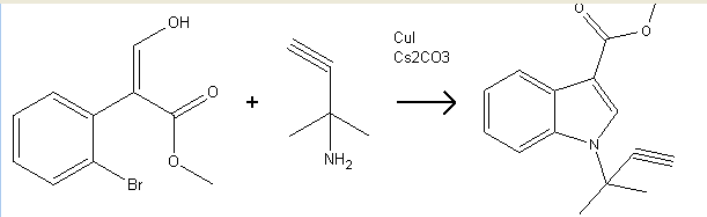
Chemistry and Parallel Chemistry

- 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 α -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 μ 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 ₂ CO ₃	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

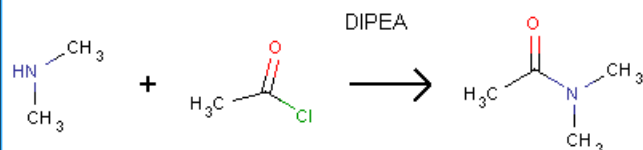
1-Methylbut-3-yn-2-yl-amine (0.161 g, 205 μ l, 1.95 mmol) was added in one step to a solution of methyl α -formyl(o-bromophenyl)acetate, 0.5 g, 1.95 mmol) in methanol (15 ml), refluxed for 3 h, and the solvent was removed *in vacuo*. The residue was dissolved in DMF (8 ml) and cesium carbonate (1.271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



Set up generic reaction

Reactants:

ID	Name	Formula	Mol.WT	Amount	Solvent	Purity	Ratio
	Amine	C ₂ H ₇ N	45.08	1.2 mmol	Dichloromethane	100%	1 *
	Acid Chloride	C ₂ H ₃ Cl	78.5	1.26 mmol		100%	1.05

Reagents:

ID	Name	Formula	Density	Volume	Mol.WT	Amount	Solvent	Ratio
	DIPEA	C ₈ H ₁₉ N	0.742	0.211 ml	129.24	1.212 mmol		1.01



Products:

ID	Name	Formula	Batch
	Amide	C ₄ H ₉ NO	

Solvents:


Solvent	Quality	Volume	Comment
Dichloromethane		10 ml	

Amine

MolNa...	Struct...	Formula	MoW...	Amount	Batch	Mass	Molec...	CAS N...	Its Par...	MFCD...
Piperazi...		C ₄ H ₁₀ N ₂	86.1356	1.2 m...		103.3...	86.1356	6091...	10622	MFCD...
N,N'-Di...		C ₄ H ₉ NO	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 ...		C ₂ H ₃ Cl	78.498	1.26 m...		98.91 ...	78.498	75-36-5	10247	MFCD...

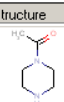

Automatic Page Break

Acid Chloride

MolNa...	Struct...	Formula	MoW...	Amount	Batch	Mass	Molec...	CAS N...	Its Par...	MFCD...
Propen...		C ₃ H ₅ Cl	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		C ₆ H ₁₂ N ₂ O		128.1723		153.81 mg	84.52%
Product 2		C ₇ H ₁₂ N ₂ O		140.183		168.22 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

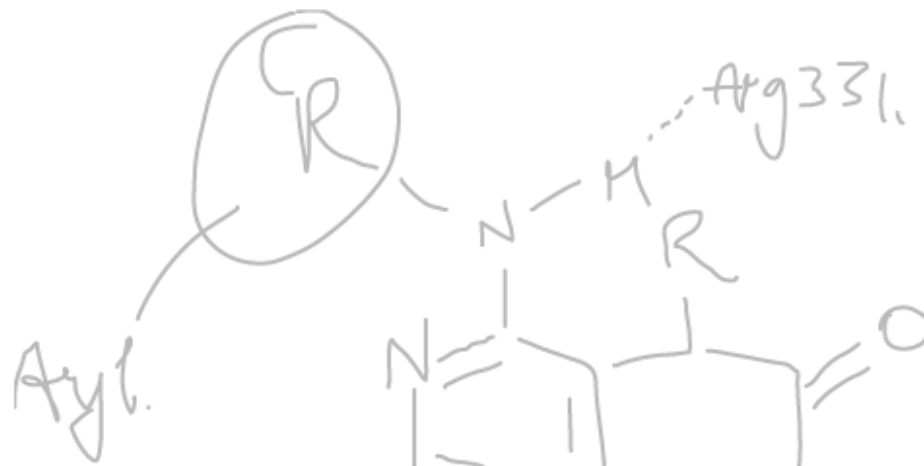
Set up Look Up List for Assays, Species, Equipment



- Integrate with EVOequip and EVOasap
-

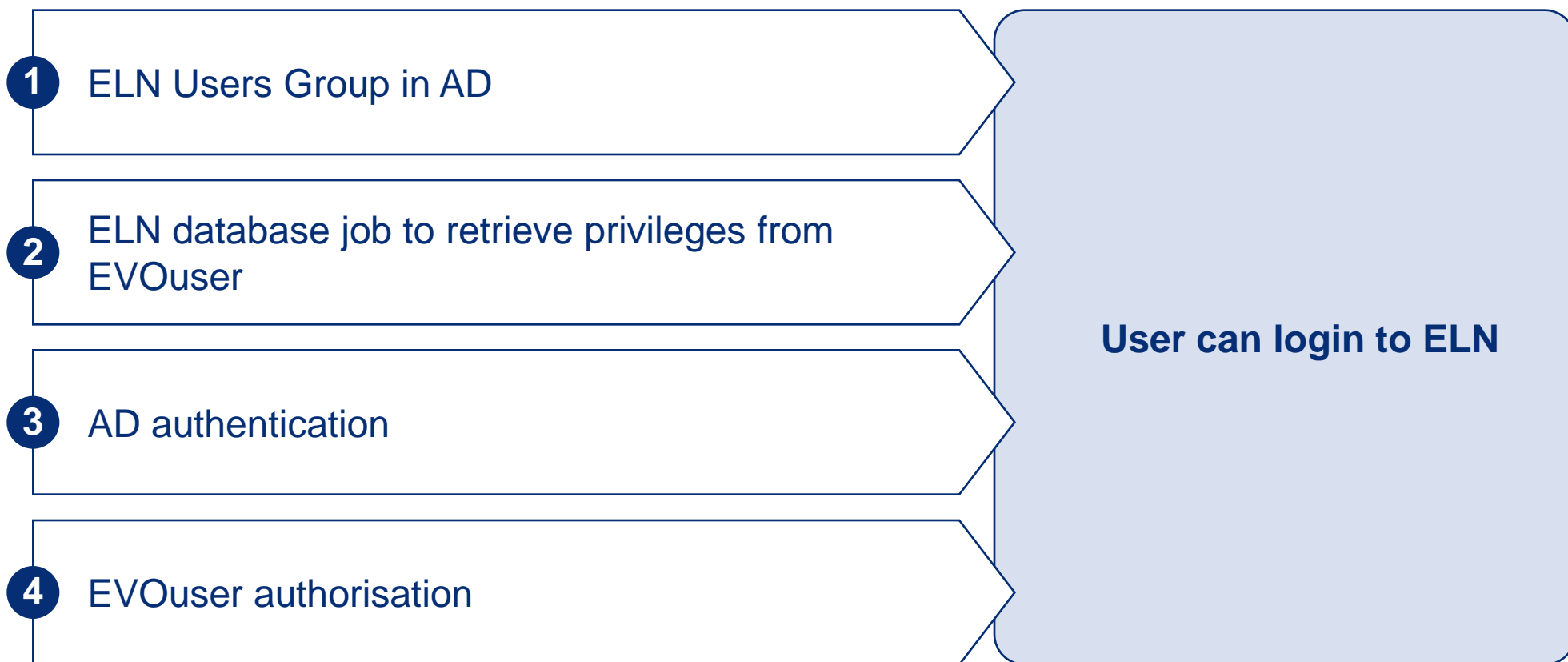
Agenda

- 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

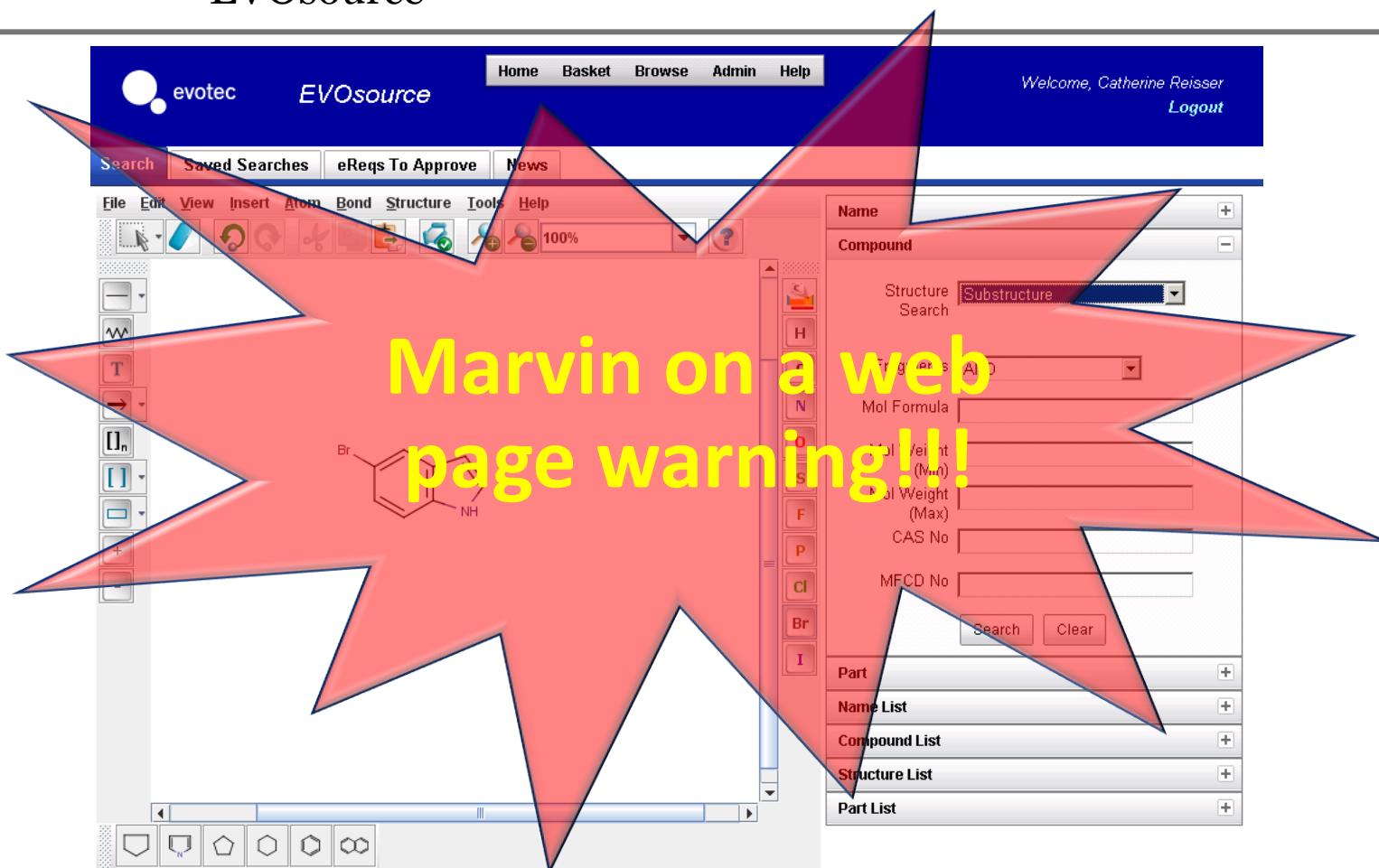
EVOsource – compound sourcing

- 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



The screenshot displays the EVOsource web application interface. At the top, a blue navigation bar contains the Evotec logo, the text "EVOsource", and menu items: 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 benzamide derivative with a bromine atom. A large red starburst graphic 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 menu set to "Substructure", and a "Search" button. Below the search form are several expandable sections: "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

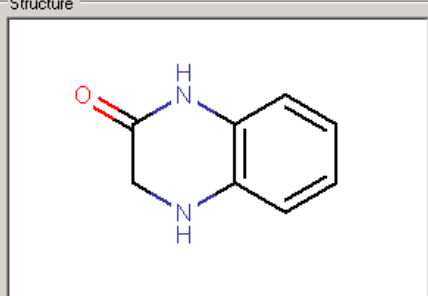
Exact Searching takes 1 second !

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

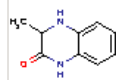
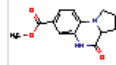
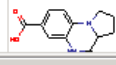
Enter IFS Part No

Find

Use Selected

Close

Help (F1)

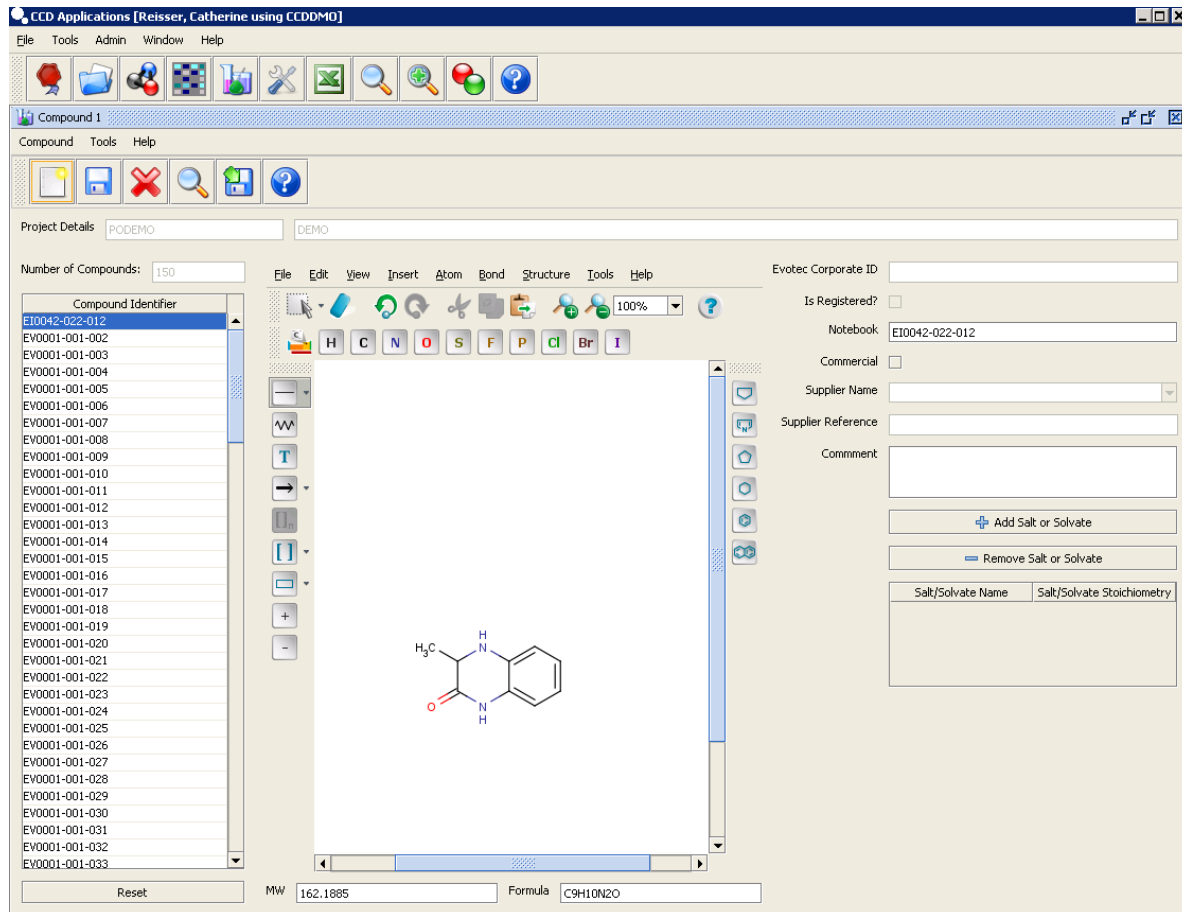
Select	Structure	Name	Source
<input type="checkbox"/>		3-methyl-3,4-dihydroquinoxalin-2(1H)-o...	EVOsource
<input type="checkbox"/>		methyl 4-oxo-1,2,3,3a,4,5-hexahydrop...	EVOsource
<input type="checkbox"/>		4-oxo-1,2,3,3a,4,5-hexahydropyrrolo[1...	EVOsource

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 Identifier" entries is visible, ranging from EI0042-022-012 to EV0001-001-033. The central area shows a chemical structure of a benzimidazole derivative with a methyl group (H₃C) and a carbonyl group (C=O). The structure is displayed in a 2D representation. The right side of the interface includes a form for "Evotec Corporate ID" and other fields: "Is Registered?" (checkbox), "Notebook" (text field with value EI0042-022-012), "Commercial" (checkbox), "Supplier Name" (dropdown), "Supplier Reference" (text field), and "Comment" (text area). Below these fields are buttons for "Add Salt or Solvate" and "Remove Salt or Solvate", and a table for "Salt/Solvate Name" and "Salt/Solvate Stoichiometry". At the bottom, there are fields for "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?

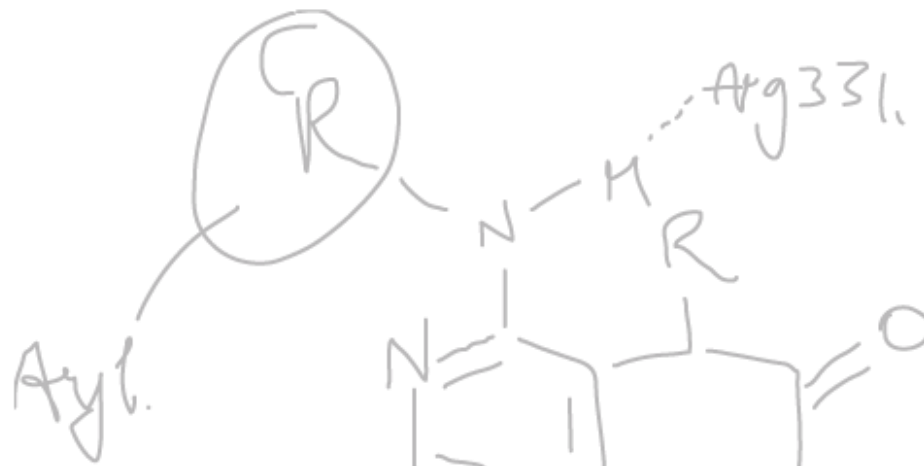
CCD batch numbers can be used for ADMET and Analytical Experiments

Open ELN from CCD Application

Perform semi-automated pre-registration of compounds

Agenda

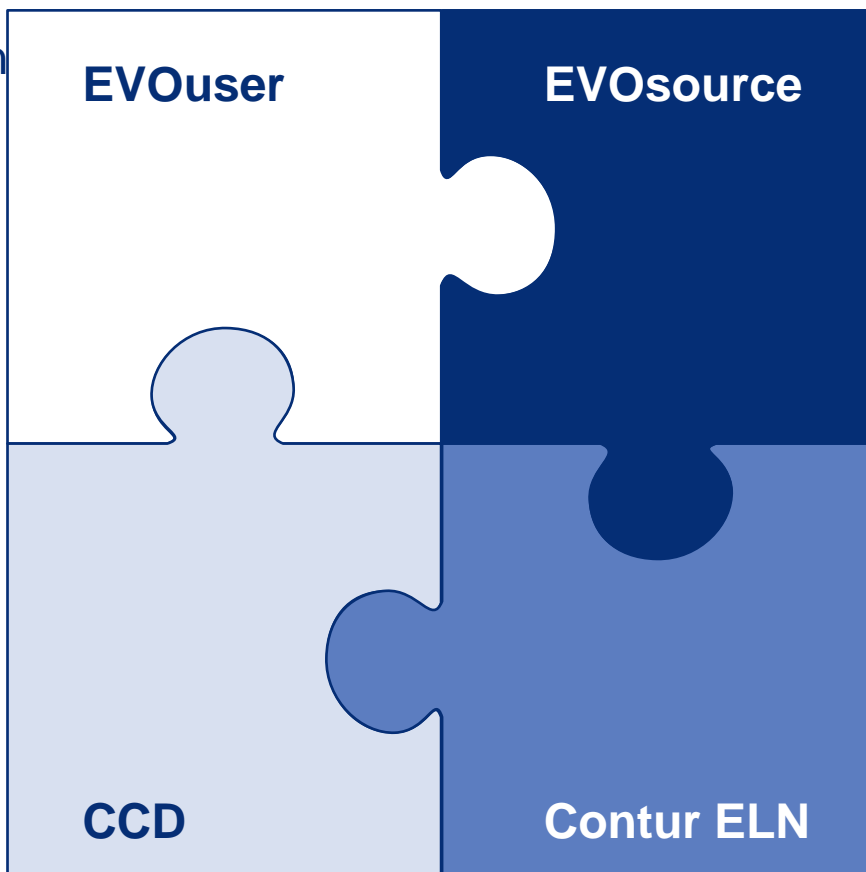
- About Evotec
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- **Conclusion**



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

Your contact:

Dr Ian Berry

Principal Scientific Software Developer

+44.(0).1235.441451

+44.(0).1235.863139 Fax

lan.Berry@evotec.com

