



ELSEVIER

ChemAxon's technology in Reaxys

ChemAxon's technology supporting Reaxys and Reaxys Medicinal Chemistry (RMC) production, searching and visualization workflows

Derrick Umali at ChemAxon UGM 2019 San Diego

supported by Ralph Hössel Elena Herzog, Stefan Roller, Olivier Barberan, Rosalind Sankey, Jürgen Swienty-Busch, Christian Böhm, and Pieder Caduff

March 2019

My role at Elsevier



Derrick Umali

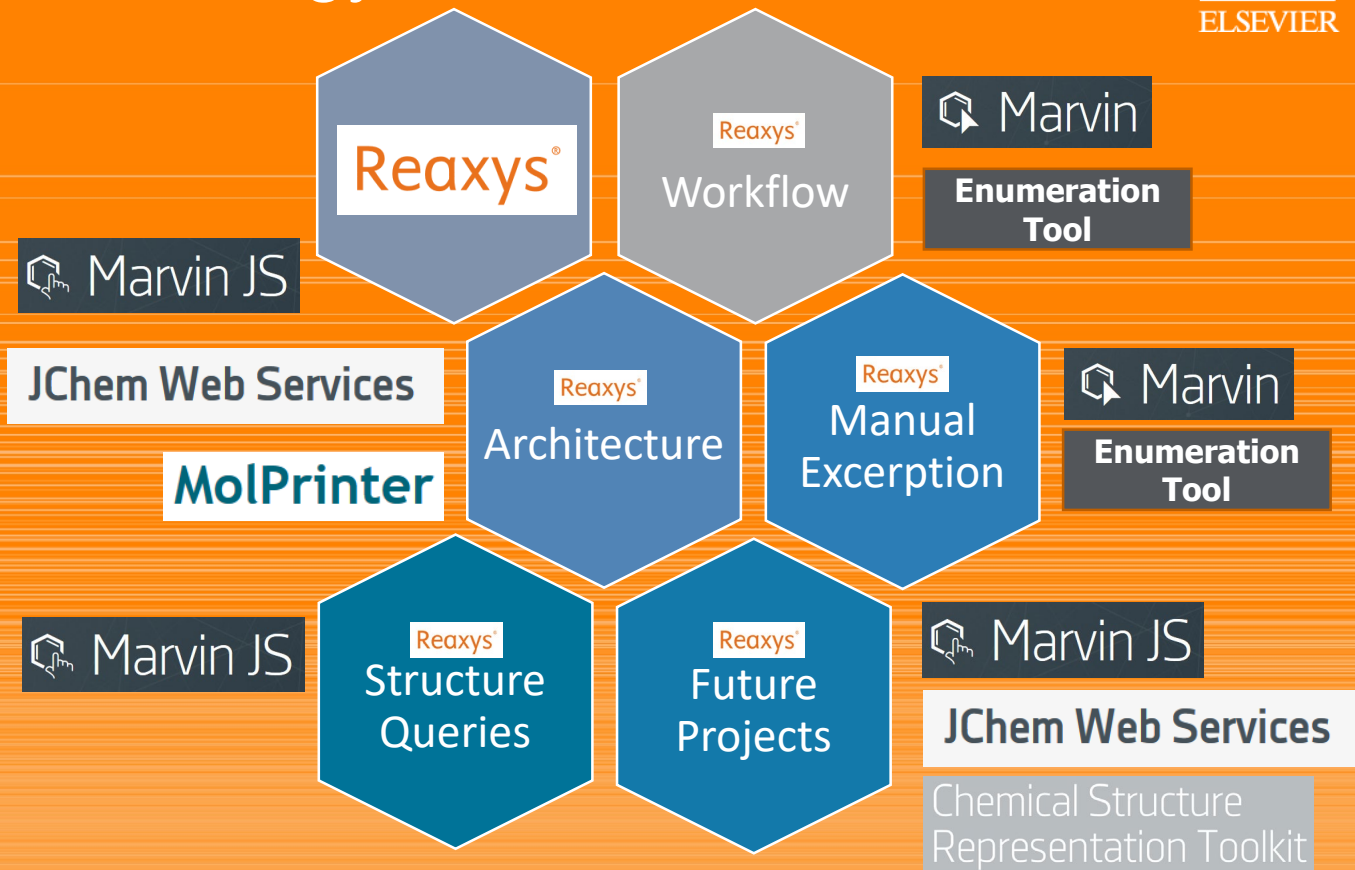
Solution Sales Manager at Elsevier - Life Science Solutions

San Francisco, California Area

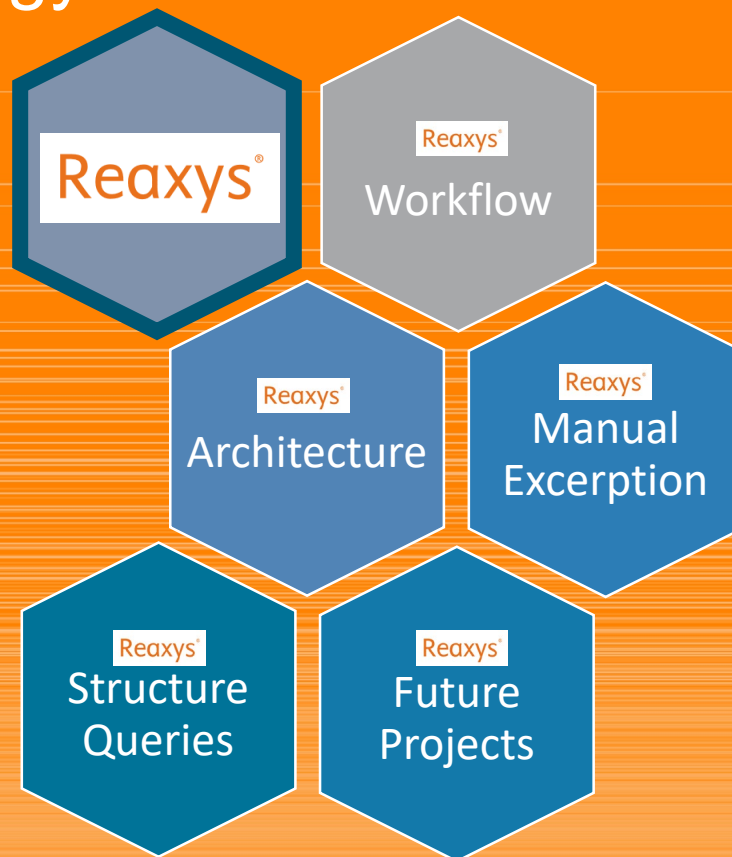
Life Science Solutions

- ~ 20 years at Elsevier
 - MDL Elsevier answering phone calls on ISIS Draw / ISIS Base
 - Cheminformatics / Bioinformatics Consultant
 - Life Science Trainer
 - Life Science Sales
- Worked with Crossfire Beilstein, migration to Reaxys , Reaxys 2.0

ChemAxon's technology in Reaxys

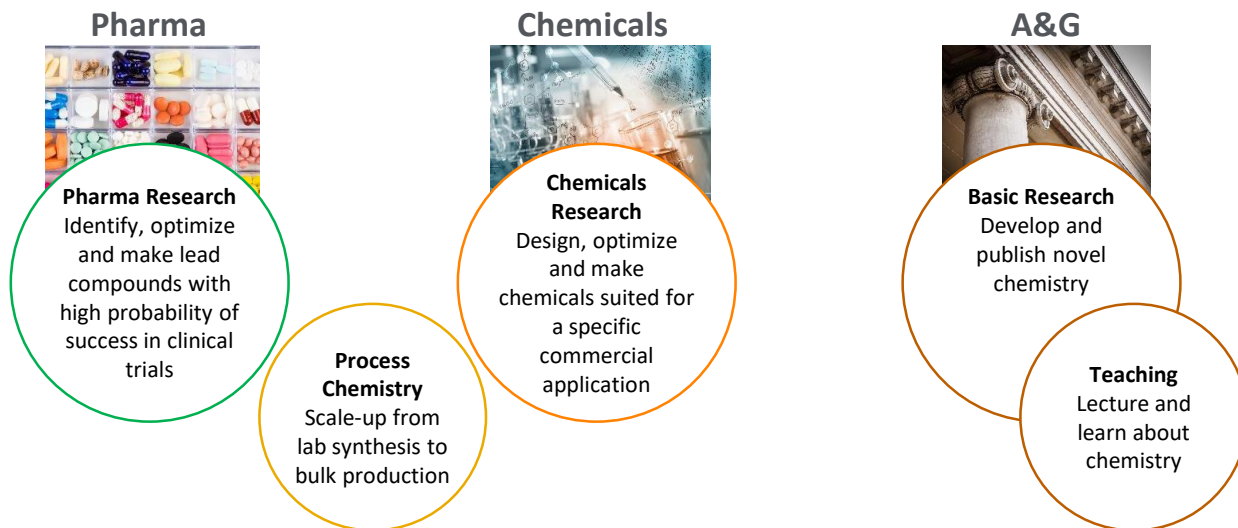


ChemAxon's technology in Reaxys



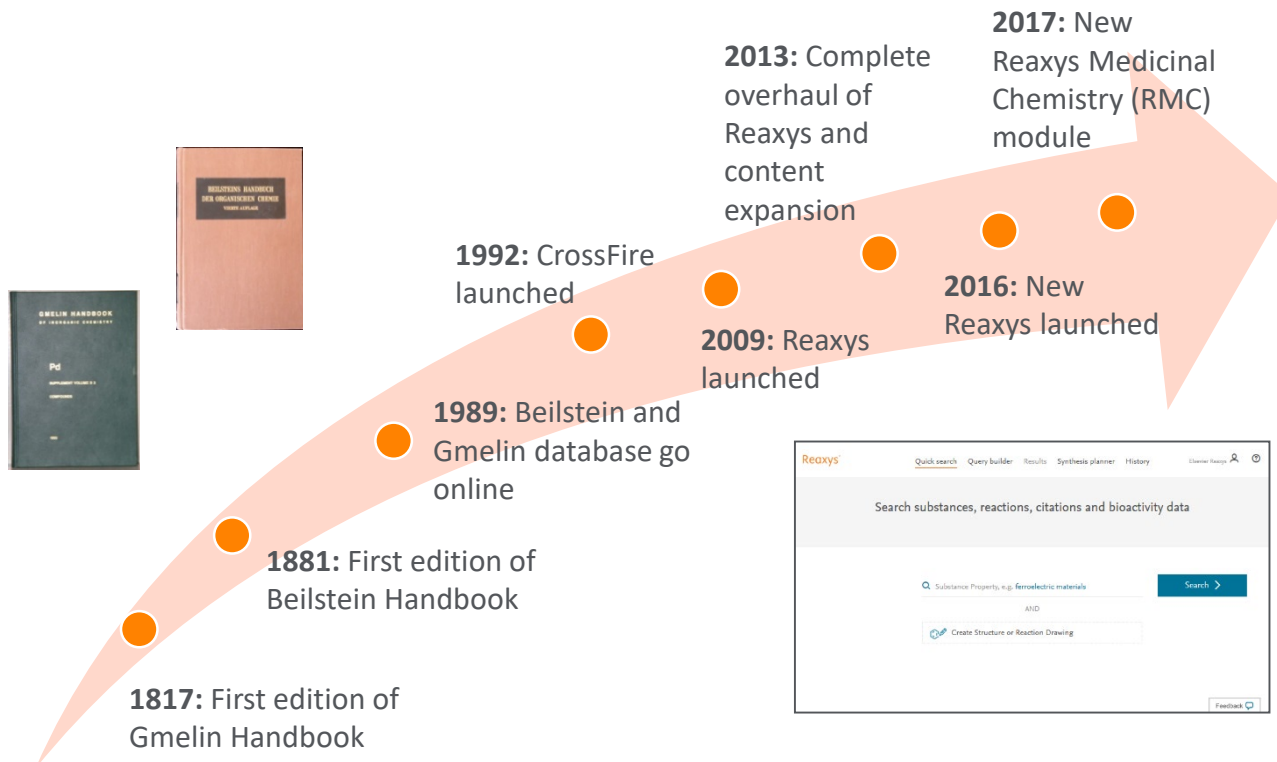
In essence chemistry deals with two core questions across the three segments

1. "Which compound will have the desired property?" **Properties**
2. "How can a compound be made?" **Synthesis – Production**



Due to their common foundation – segments share similar chemistry information needs and challenges

We have a long history in providing chemistry information and driving new developments



The core of our philosophy: Reaxys aims to deliver immediate access to information

The diagram illustrates the Reaxys philosophy. On the left, a magnifying glass icon is connected by an orange line to a bar chart with four bars of increasing height, each topped with a question mark. To the right, a screenshot of the Reaxys interface shows a chemical reaction between acetic acid and aspirin, followed by a 'Physical Data - 532' window displaying a table of dissociation exponents and a list of relevant references.

Chemical Reaction:

CC(=O)O + CC(=O)Oc1ccc(O)cc1 >> CC(=O)Oc1ccc(O)cc1CC(=O)O

Physical Data - 532

Dissociation Exponent (pK _a)	Dissociation Group	Temp (°C)	Log P
3.48	RCOOH	25	
3.47		25	
3.55	COOH	25	
3.6	COOH	25	

References:

- Lyophilized aspirin with trehalose may decrease the incidence of gastric injuries in healthy dogs Cited 1 times
Lin, Lee-Shuan; Kayasuga, Yuko; Shimohata, Nobuyuki; +6 others - Journal of Veterinary Medical Science, 2012, vol. 74, # 11, p. 1511 - 1516
Abstract Index Terms Full Text
- Incidence of aspirin resistance in the patient group of a university hospital in Korea Cited 6 times
Lee, Young Kyung; Kim, Han-Sung; Park, Ji-Young; +1 other - Korean Journal of Laboratory Medicine, 2008, vol. 28, # 4, p. 251 - 257
Abstract Index Terms Full Text
- Increased platelet expression of glycoprotein IIIa following aspirin treatment in aspirin-resistant but not aspirin-sensitive subjects Cited 3 times
Floyd, Christopher N.; Goodman, Timothy; Becker, Silke; +7 others - British Journal of Clinical Pharmacology, 2014, vol. 78, # 2, p. 320 - 328
Abstract Index Terms Full Text

Instead of **delivering lists of references** that may be relevant to a query...

... Reaxys strives to **deliver relevant answers on the spot:**

- References ranked by relevance
- Reactions with experimental details
- Substances with extensive properties

Focus on **using** information, not searching for information

Using a clean and streamlined user interface

The screenshot displays the Reaxys web application interface. At the top left is the Reaxys logo. The navigation bar includes links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History', along with user profile, notification, and help icons. Below the navigation is a search bar with the text 'Search substances, reactions, documents and bioactivity data' and a sub-line 'in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, LabNetwork and SigmaAldrich'. An 'Import' button is on the left. The search input field contains 'Reactions, e.g. phosphorylation'. Below the search bar is an 'AND' operator and a button labeled 'Create Structure or Reaction Drawing'. The footer contains the Elsevier logo, copyright information for RELX Intellectual Properties SA, links for 'Terms and Conditions', 'Privacy policy', and 'Performance Page', the RELX Group logo, and a 'Feedback' button. A thick orange arrow points from the search bar area towards the right side of the slide.

Applying user centered design, extensive user testing and Agile development methodologies helped to create a new user interface:

New Reaxys places powerful text and structure searches front and center on a single, easy-to-use interface.

Everyone can leverage the full capabilities of Reaxys,
from first-year students to expert users

Alternatively, use Query Builder to create your own targeted queries without being an expert

The screenshot shows the Reaxys Query Builder interface. The main workspace contains two query boxes: 'Structure' and 'Melting Point'. The 'Structure' box has a 'Create Structure / Reaction Drawing' button. The 'Melting Point' box has a 'Find any' checkbox and a 'Show fields' dropdown. An 'AND' operator is positioned between the two boxes. On the right, a 'Search Querylets' panel is open, showing a search bar and a list of querylets including 'Basic Indexes', 'Identification', 'Physical Properties', 'Melting Point', 'Boiling Point', and 'Sublimation'. A 'Feedback' button is at the bottom of the panel. The interface includes a top navigation bar with 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. A user profile 'medchem0...' is visible in the top right. The interface also features icons for 'Import', 'Save', 'Reset form', and 'Delete all', as well as 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index' filters.

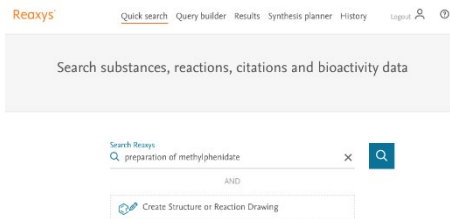
4 Enter search terms and click Search.

1 Search Querylets

3 Combine them with operators

2 Click or Drag and drop them into a query

Retrieving relevant answers and anticipating needs – providing options



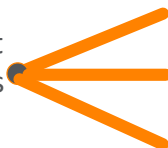
1 Reaxys interprets either natural language, or truncation and operators



2 Recognizes search intention (reactions)



3 Delivers a ranked list of alternative results suggestions



Reaxys Quick search Query builder Results Synthesis planner History Logout

← Back to Quick Search

Choose a result for preparation of methylphenidate

146	Reactions	Product: methylphenidate (exact search)	Preview Results	View Results
1146	Documents	Document Basic Index : formation; formations; make; making; manufacture; prep; preparation; preparations; prepare; prepared; preparing; preps; synthesis; synthesise AND Document Basic Index : methylphenidate	Preview Results	View Results
15842	Documents	Document Basic Index : methylphenidate	Preview Results	View Results
7004798	Documents	Document Basic Index : formation; formations; make; making; manufacture; prep; preparation; preparations; prepare; prepared; preparing; preps; synthesis; synthesise	Preview Results	View Results

Get intended answers directly, plus relevant results you may not have considered

Presenting standardized, normalized and collated data in one record for quick and easy access

The screenshot displays the Reaxys interface for the compound 'cetane'. The main record includes a chemical structure, a list of tabs (Identification, Physical Data - 2307, Other Data - 292, Spectra - 103, Bioactivity - 127), and a detailed data table. Callout boxes provide expanded views of the Physical Data, Other Data, Spectra, and Bioactivity sections.

Physical Data - 2307

- Liquid/Solid Systems (MCS) - 72
- Further Information - 111
- Self-diffusion - 8
- Solubility (MCS) - 23
- Molecular Deformation - 1
- Transport Phenomena (MCS) - 195
- Thermal Expansion - 1
- Compressibility - 9
- Boundary Surface Phenomena (MCS) - 146
- Association (MCS) - 366
- Transition Point(s) of Liquid Modification(s) - 2
- Mechanical & Physical Properties (MCS) - 170
- Ionization Potential - 1
- Azeotropes (MCS) - 3
- Energy Data (MCS) - 250

Other Data - 292

- Biodegradation - 99
- Exposure Assessment - 19
- Concentration in the Environment - 118
- Use - 12
- Stability in Soil - 7
- Abiotic Degradation, Hydrolysis - 1
- Abiotic Degradation, Photolysis - 1
- Transport and Distribution - 8
- Isolation from Natural Product - 25
- Oxygen Demand - 1
- Bioaccumulation, Biomagnification and Biomonitoring - 1

Spectra - 103

- Raman Spectroscopy - 12
- IR Spectroscopy - 26
- Fluorescence Spectroscopy - 1
- ESR Spectroscopy - 3
- NMR Spectroscopy - 35
- UV/VIS Spectroscopy - 4
- Mass Spectrometry - 18
- Rotational Spectroscopy - 1
- Luminescence Spectroscopy - 2
- NQR Spectroscopy - 1

Bioactivity - 127

- Ecotoxicology - 16
- Pharmacological Data - 111

Table Data:

cetane			
Reaxys ID:	1736592		
Chemical Names:	cetane, Hexadecane, Hexadecan		
CAS Registry Number(s):	Substance type:		
Molecular Formula:	C16H34	Linear Structure Formula:	C12H26C4H8
Molecular Weight:	226.446	No of references:	1627
InChIKey:	DCAYPVUWAIBOU-UHFFFAOYSA-N		

All relevant data are accessible for a common point and tabulated for direct use.

Allowing further refinement of results - Filters and Analysis are interactive for fast filtering and evaluation of results

The image displays two side-by-side screenshots of the 'Filters and Analysis' interface, illustrating how selected index terms interact with other filters.

Left Screenshot: Shows the 'Index Terms (List)' section with the following filters and counts:

Filter	Count
stereoselectivity	44
enantioselectivity	24
total synthesis	18
oxidation reaction	18
enantiomer excess	11
catalysed reaction	11
catalyst	10

The 'total synthesis' filter is selected, highlighted with an orange square. Below it, the 'Publication Year' section shows counts for various years:

Year	Count
1998	3
2006	2
2009	2
1994	1
2008	1
2015	0
2007	0

Right Screenshot: Shows the 'Index Terms (ReaxysTree)' section with the following filters and counts:

Filter	Count
stereoselectivity	44
enantioselectivity	24
total synthesis	18
oxidation reaction	18
enantiomer excess	11
catalysed reaction	11
catalyst	10

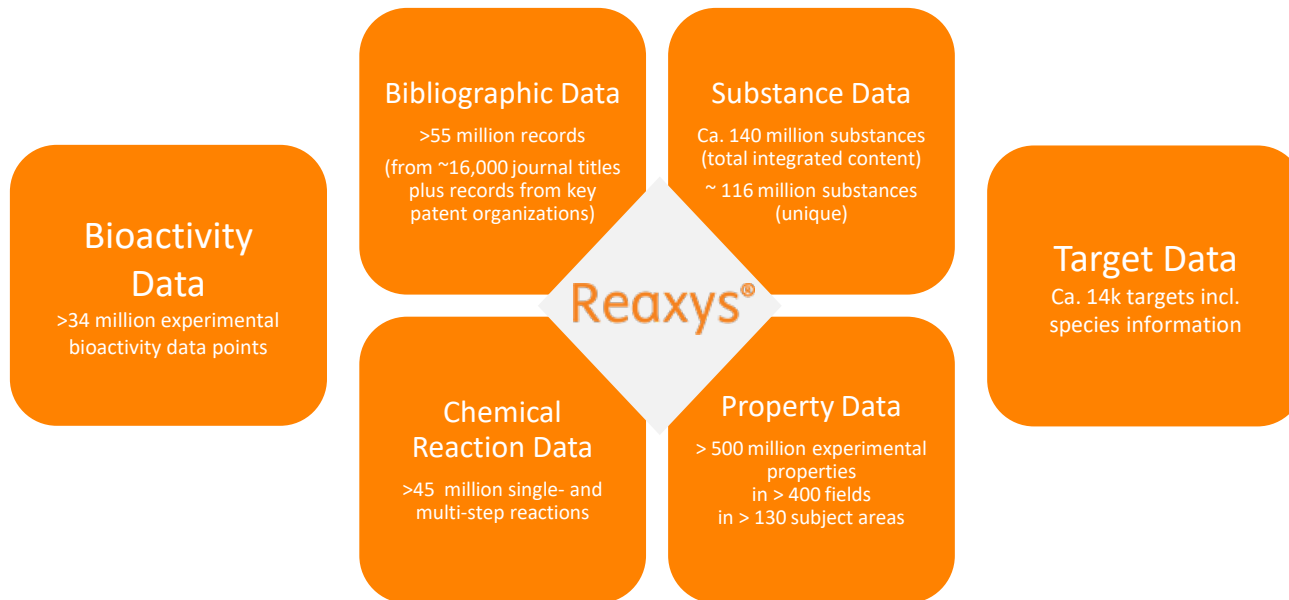
The 'total synthesis' filter is selected, highlighted with an orange square. Below it, the 'Authors' section shows counts for various authors:

Author	Count
weinreb, steven m	2
nakata, tadashi	1
kroutil, wolfgang	0
cha, jin soon	0
oishi, takeshi	0
nakamura, kaoru	0

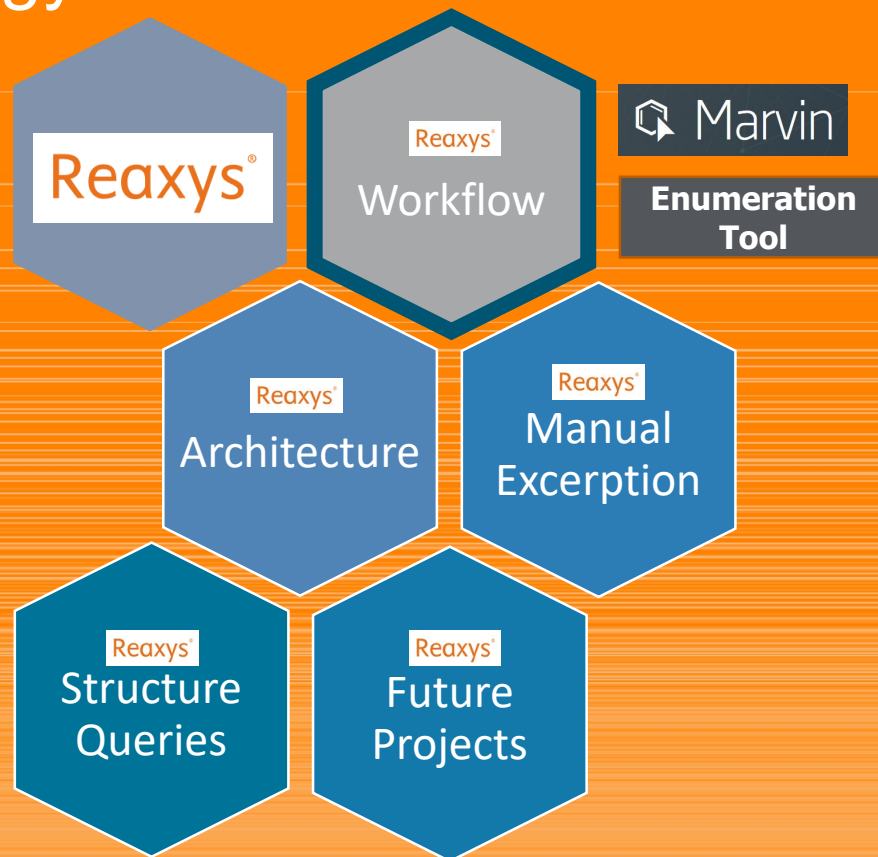
An orange arrow points from the selected 'total synthesis' term in the right screenshot to the 'total synthesis' term in the left screenshot, indicating that the selected index term highlights corresponding records in other filters.

What does Reaxys offer to support chemistry researchers?

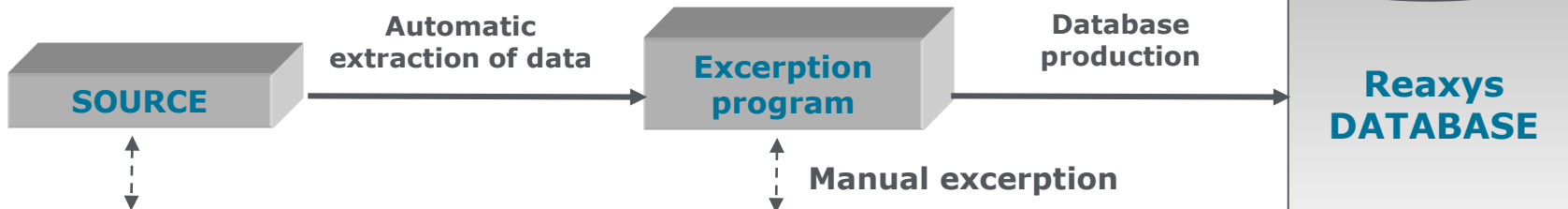
Reaxys and Reaxys Medicinal Chemistry provide access to 6 key chemistry subject areas



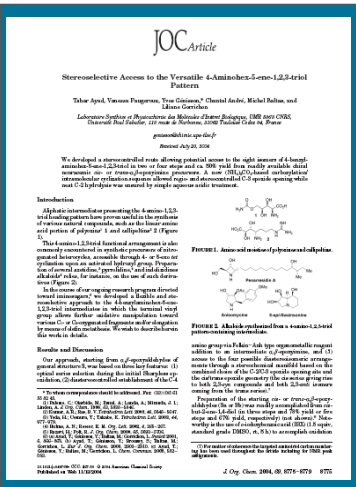
ChemAxon's technology in Reaxys



Reaxys Workflow (simplified)



Paper or electronic file

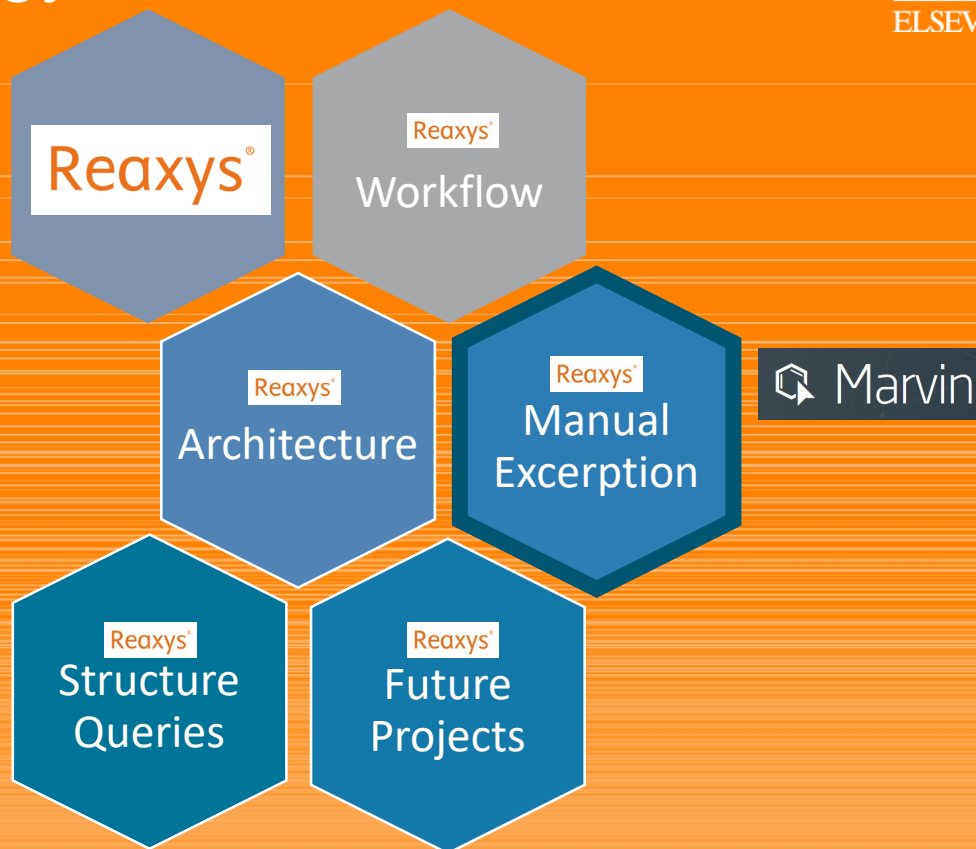


Structures, Markush, chemical names, NMR, IR, MP, USE, ...
Reactions, temp., solvent, ...
Targets, MedChem data

iEI (intuitive Excerption Interface)



ChemAxon's technology in Reaxys



ChemAxon Marvin Sketch in Reaxys excerption



iE1 - version 3.71.21.0. © Elsevier, 2011-2018

File Edit View Exception Checks Extras Window Help

Start Page **ap_002101693_2018...**

Target Pane
inorg. chim. acta, 2018, 473, 121-132, tetranuclear cubane cu4o4 complexes as prospective anticancer agents: design, synthesis, structural ...

Compounds **12.3** **12.3** **LABE** **NW** **QPO**

IDE #1: 2-amino-2-(hydroxymethyl)
IDE #2: 2-hydroxy-3-methoxybenza
IDE #3: H4L
IDE #4: 1
IDE #5: 2
IDE #6: copper acetate monohydrat
IDE #7: triethylamine
IDE #8: piperazine
IDE #9: calf thymus DNA
IDE #11: naloxone

Sign In

121 (1 of 12) ... ?

Inorganica Chimica Acta

Tetranuclear cubane Cu₄O₄ complexes as prospective anticancer agents: Design, synthesis, structural elucidation, magnetism, computational and cytotoxicity studies

Abstract

Introduction

Conclusions

Chemical structure of naloxone

Structure:

abs

Molecular formula:
C19H21NO4

Main name:
naloxone

Synonym(s):
(-)-17-allyl-4,5 α -epoxy-3,14-dihydroxy-6-morphinan-6-one
(5 α)-4,5-epoxy-3,14-dihydroxy-17-(2-propenyl)morphinan-6-one

Modification:

Macroscopic type:

Comments

C. R., F., A., T., B., M., P., M.

ChemAxon Marvin Sketch in Reaxys excerption



The image shows a screenshot of the Reaxys software interface with MarvinSketch.NET 17.10.0 open. The MarvinSketch window displays a 2D chemical structure of a complex polycyclic molecule, likely a natural product or a complex synthetic intermediate. The structure features several stereocenters labeled with (S) and (R) configurations. Key functional groups include a hydroxyl group (HO), a carbonyl group (C=O), and a vinyl group (CH₂=CH₂). The text "abs" is circled in green on the right side of the structure, possibly indicating a specific atom or property. The background shows the Reaxys interface with a search bar, navigation tabs, and a document viewer displaying a research paper snippet from Inorganica Chimica Acta.

MarvinSketch.NET 17.10.0

File Edit View Insert Atom Bond Structure Calculations Services Help

212%

HO

O

H

C

N

O

S

F

P

Cl

Br

I

OH

(S)

(R)

(S)

(R)

N

CH₂

abs

Expand Ungroup

2D *

Comments

ChemAxon Marvin Sketch in Reaxys excerption



iEL - version 3.71.21.0. © Elsevier, 2011-2018

File Edit View Exception Checks Extras Window Help

Start Page x ap_00201693_2018.. x

Sign In

121 (1 of 12) ... ?

inorg. chim. acta, 2018, 473, 121-132, tetranuclear cubane cu4o4 complexes as prospective anticancer agents: design, synthesis, structural ...

Compounds 123

Compound Identification (IDE) #11

IDE #1: 2-amino-2-(hydroxymethyl)

MarvinSketch.NET 17.10.0

File Edit View Insert Atom Bond Structure Calculations Services Help

212%

Attach Data

Field Placement

Context: Fragment Absolute

Name: MORG_FRAGMENT_STEREO Relative

Value: abs Next to objects

racemate

stereic

rel

R(a)

S(a)

Units

Query: none

Units:

Tag:

OK Cancel

abs

CH₂

2D

Expand Ungroup

Comments

C. R., F., A., T., B., M., P., M.

The screenshot displays the MarvinSketch.NET 17.10.0 interface within the Reaxys environment. The 'Attach Data' dialog box is open, showing the configuration for the 'abs' (absolute) stereochemistry field. The 'Context' is set to 'Fragment', and the 'Name' is 'MORG_FRAGMENT_STEREO'. The 'Value' is 'abs', which is circled in green. The 'Placement' options include 'Absolute' (selected), 'Relative', and 'Next to objects'. The 'Display' options include 'racemate', 'stereic', 'rel', 'R(a)', and 'S(a)'. The 'Units' checkbox is checked. The 'Query' is set to 'none'. The 'Tag' field is empty. The 'OK' and 'Cancel' buttons are visible at the bottom of the dialog. In the background, the Reaxys interface shows a search result for 'tetranuclear cubane Cu₄O₄ complexes as prospective anticancer agents: design, synthesis, structural ...' with a chemical structure of a cubane complex highlighted in green. The 'abs' label is also circled in green, and a 'CH₂' group is highlighted in green in the bottom right corner.

ChemAxon Marvin Sketch in Reaxys excerption - Markush structures

iE! - version 3.71.21.0. © Elsevier, 2011-2018

File Edit View Excerpton Checks Extras Window Help

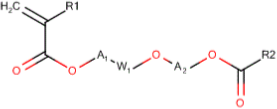
ASSAY TARGET BIOM MEAS PH META... IDE RX NMR MS COL MP IR UV +

Markush Details of IDE #1: I


Patent Number: 20160130210
 Excerptor: K16
 Status:

Comment:

Created: ; last modified: 19.02.2018 03:41:35



Note:

Label	Type	Value	Size	Substitution	Frequency	Attributes
R2	Homology	perfluoroalkyl	1-6C			
	Homology	-CHR1R2				
A2	Homology	alkanediyl	1-6C			
W1	Homology	alicyclic hydrocarbon group	5-18C			divalent
R1	Nomenclature	hydrogen				
	Homology	halogen				
	Homology	alkyl	1-6C	\$halogen	0-1	
A1	Homology	single bond				
	Homology	alkanediyl	1-6C			
	Formula	-A3-X1-(A4-X2)a-(A5)b-				
	Homology					
						
	Homology					

Print Close

ChemAxon Marvin Sketch in iEI - Markush structures



Markush Editor (v.3.71.21.0/3.71.21.0)

File Edit Label Tools Help

Labels

MarvinSketch.NET 17.10.0

File Edit View Insert Atom Bond Structure Calculations Services Help

100%

R-AP

H₂C R1

O A₁ W₁ O A₂ O

2D *

Check Validity

Ready

Periodic Table of Chemical Elements

Periodic Table Advanced

Description

Generic query atoms

A	Q	M	X
AH	QH	MH	XH

Atom query properties

.H+	.v+	.X+	.R+	.r+	.rb+	.s+	.h+	.D+	.u
.H-	.v-	.X-	.R-	.r-	.rb-	.s-	.h-	.D-	.al/A

Periodic Table Groups

G1	G2	G3	G4	G5	G6	G7	G8	G9
G10	G11	G12	G13	G14	G15	G16	G17	G18

Special nodes

Pol	*
-----	---

R-groups

R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16
R17	R18	R19	R20	R21	R22	R23	R24	R25	R26	R27	R28	R29	R30	R31	R32

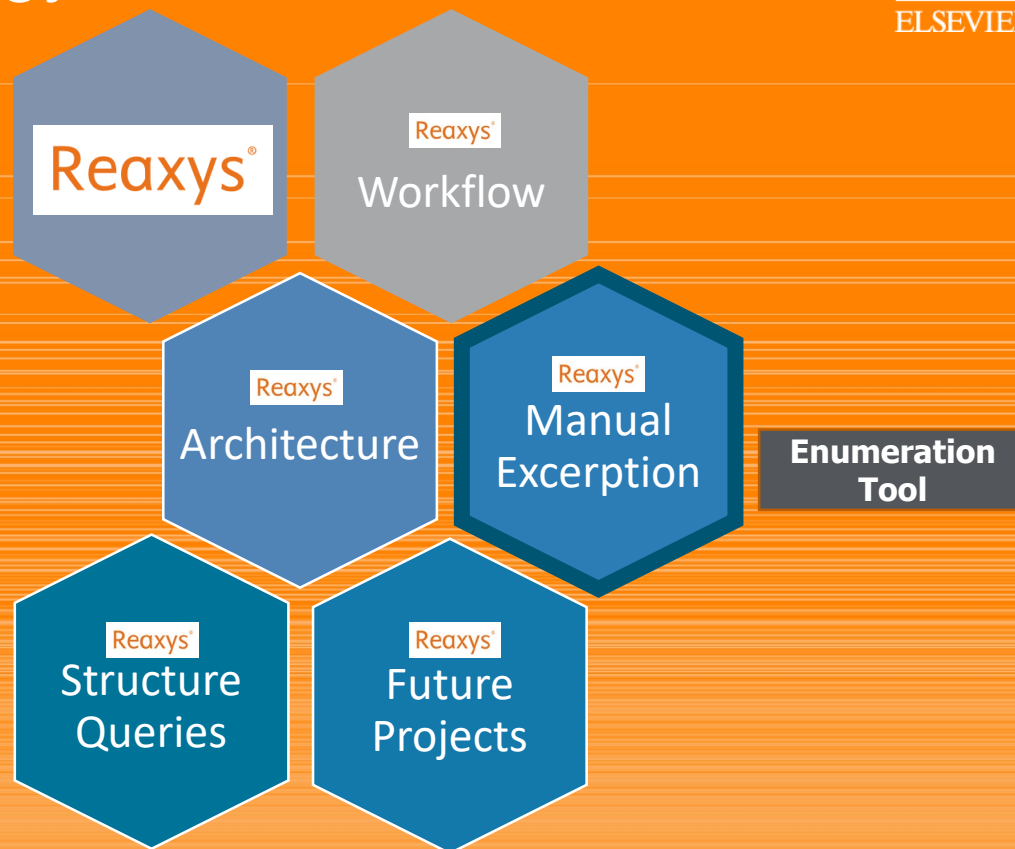
Custom Property

Type: R-group Alias Pseudo SMARTS Value

Value: A1

Close

ChemAxon's technology in Reaxys



ChemAxon Enumeration Tool in iEI

Enumeration
Tool

Marin

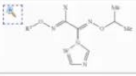
iEI (Intuitive Exception Interface) - version 3.61.955.9200. © Elsevier, 2011-2016

File Edit View Exception Checks Extras Window Help

Start Page **us_2013_20130102..**

TABLE-US-00001

TABLE 1



Compound No.	R ¹	X	W
I-1	Me	Cl	N
I-2	Et	Cl	N
I-3	Pr-n	Cl	N
I-4	Pr-i	Cl	N
I-5	Bu-n	Cl	N
I-6	Bu-i	Cl	N
I-7	Bu-s	Cl	N
I-8	Bu-t	Cl	N
I-9	Pen-n	Cl	N
I-10	Pen-i	Cl	N
I-11	Pen- <i>neo</i>	Cl	N
I-12	Pen-2	Cl	N
I-13	Pen-3	Cl	N
I-14	Hex-n	Cl	N
I-15	CH ₂ CH ₂ C(Me) ₃	Cl	N
I-16	Pen-c	Cl	N
I-17	Hex-c	Cl	N
I-18	CH ₂ Pr-c	Cl	N
I-19	CH ₂ Bu-c	Cl	N
I-20	CH ₂ Pen-c	Cl	N
I-21	CH ₂ CH=CH ₂	Cl	N
I-22	CH ₂ C=CH	Cl	N
I-23	CH ₂ C=CCH ₃	Cl	N
I-24	Me	H	N
I-25	Et	H	N
I-26	Pr-n	H	N

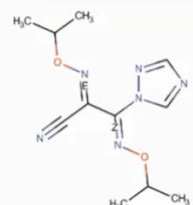
Target Name: us_2013_20130102568_a1, alkoxyimino derivative and pest control agent

Compounds: **IDE #4: 1-(2-cyano-1,2-diisopropoxyiminoethyl)-1H-1,2,4-triazole**

Compound Identification (IDE) #4

Working name: _____ Label: _____

A - Compound B - Compound C1 - Compound C2 - Compound Markush

Structure: 

Prophetic compound

Location: _____

Part of Markush: _____

Molecular formula: C₁₁H₁₆N₆O₂

Main name: 1-(2-cyano-1,2-diisopropoxyiminoethyl)-1H-1,2,4-triazole

Synonym(s): _____

Modification: _____

Macroscopic type: _____

Comments: _____

References

Referred in following compounds:

Referred in following facts:

Referred as product in:

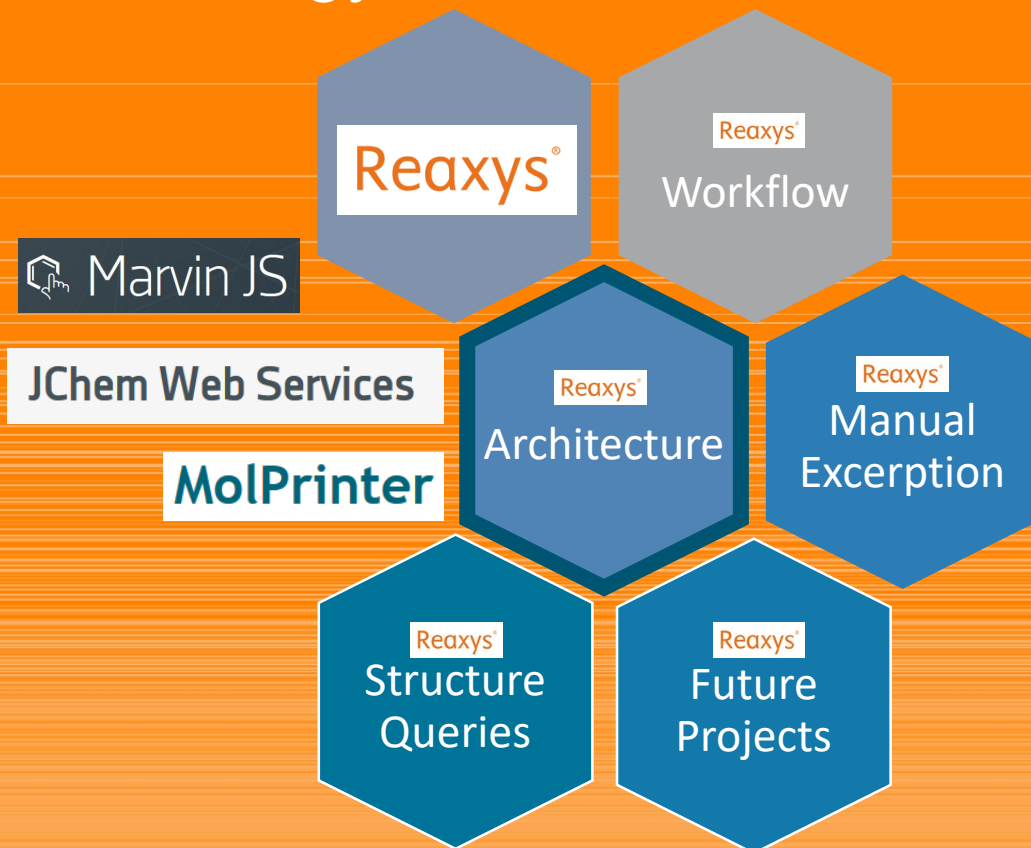
Referred as starting material in:

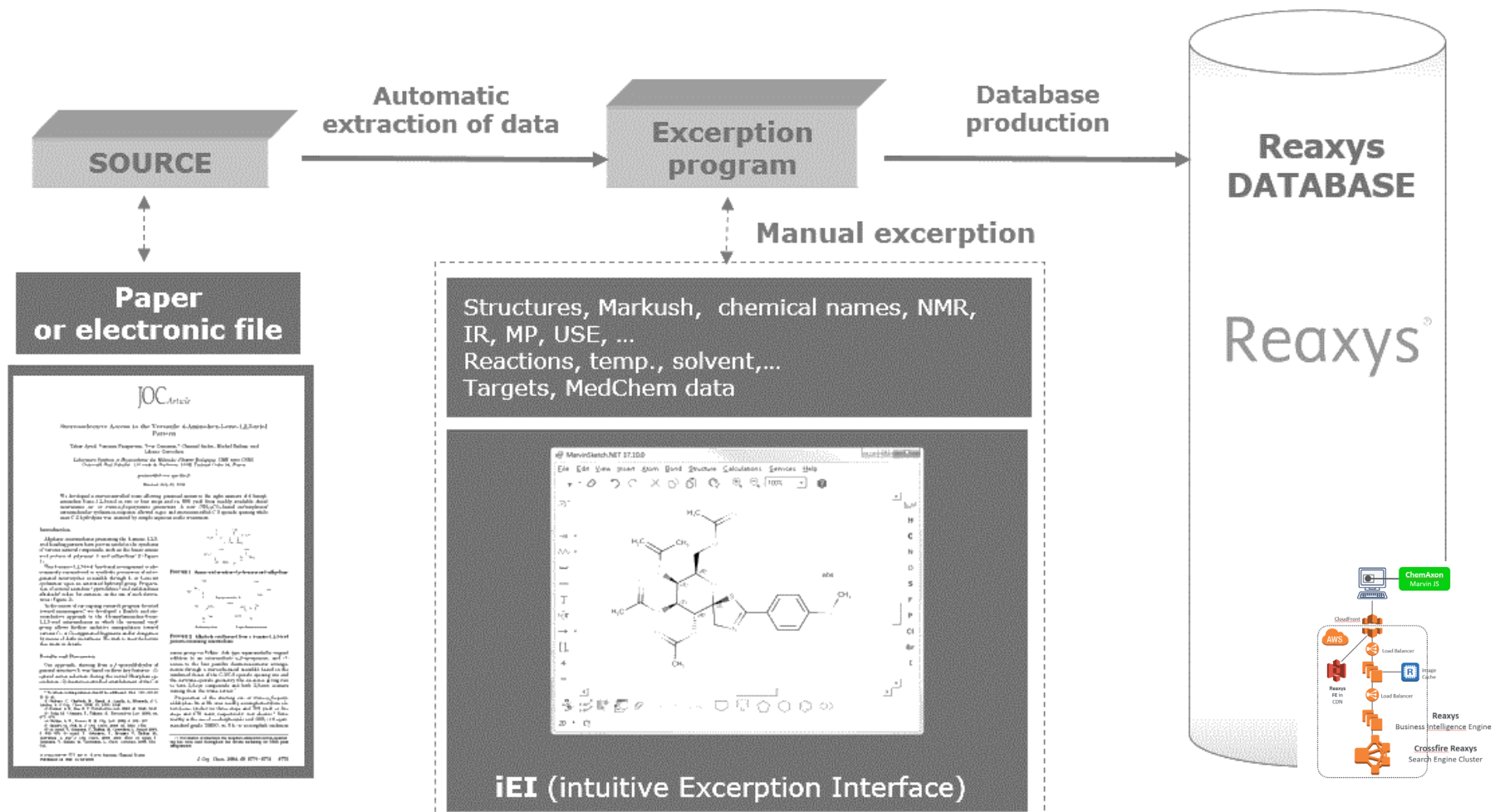
[RX #17: Example 2](#) [RX #23: Example 3](#)

Referred as reagent/catalyst in:

C R F A T B M P M

ChemAxon's technology in Reaxys





SOURCE

Automatic extraction of data

Excerpt program

Database production

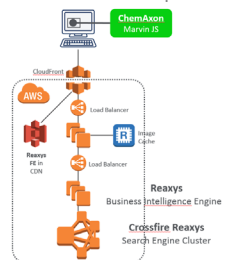
Reaxys DATABASE

Paper or electronic file



Structures, Markush, chemical names, NMR, IR, MP, USE, ...
Reactions, temp., solvent, ...
Targets, MedChem data

iEI (intuitive Excerption Interface)

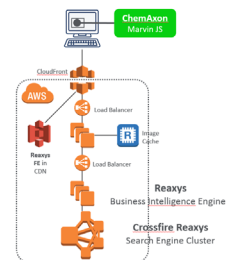
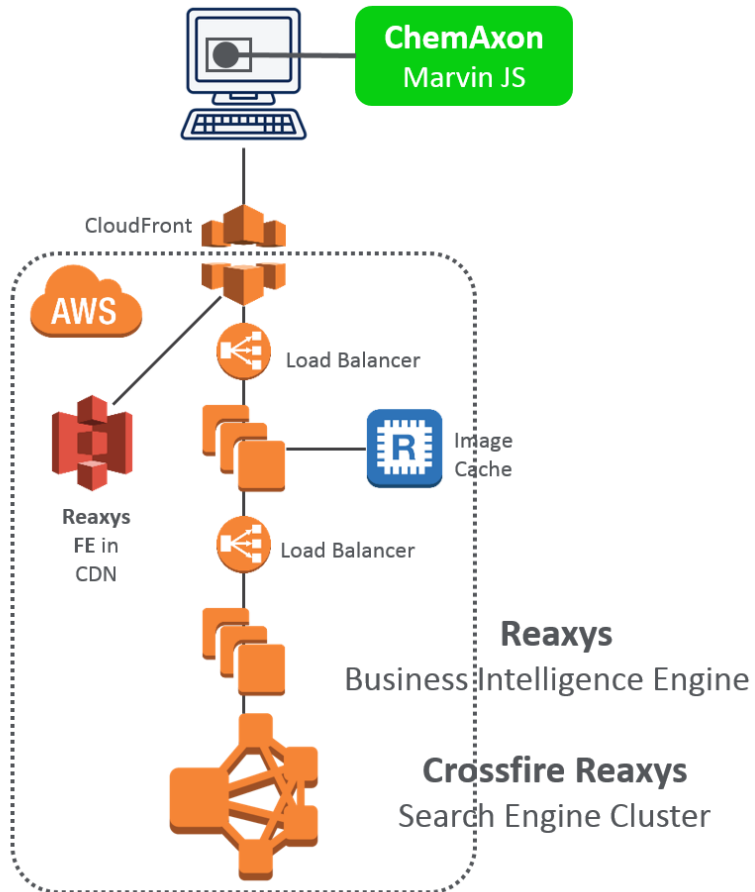


ChemAxon Marvin JS

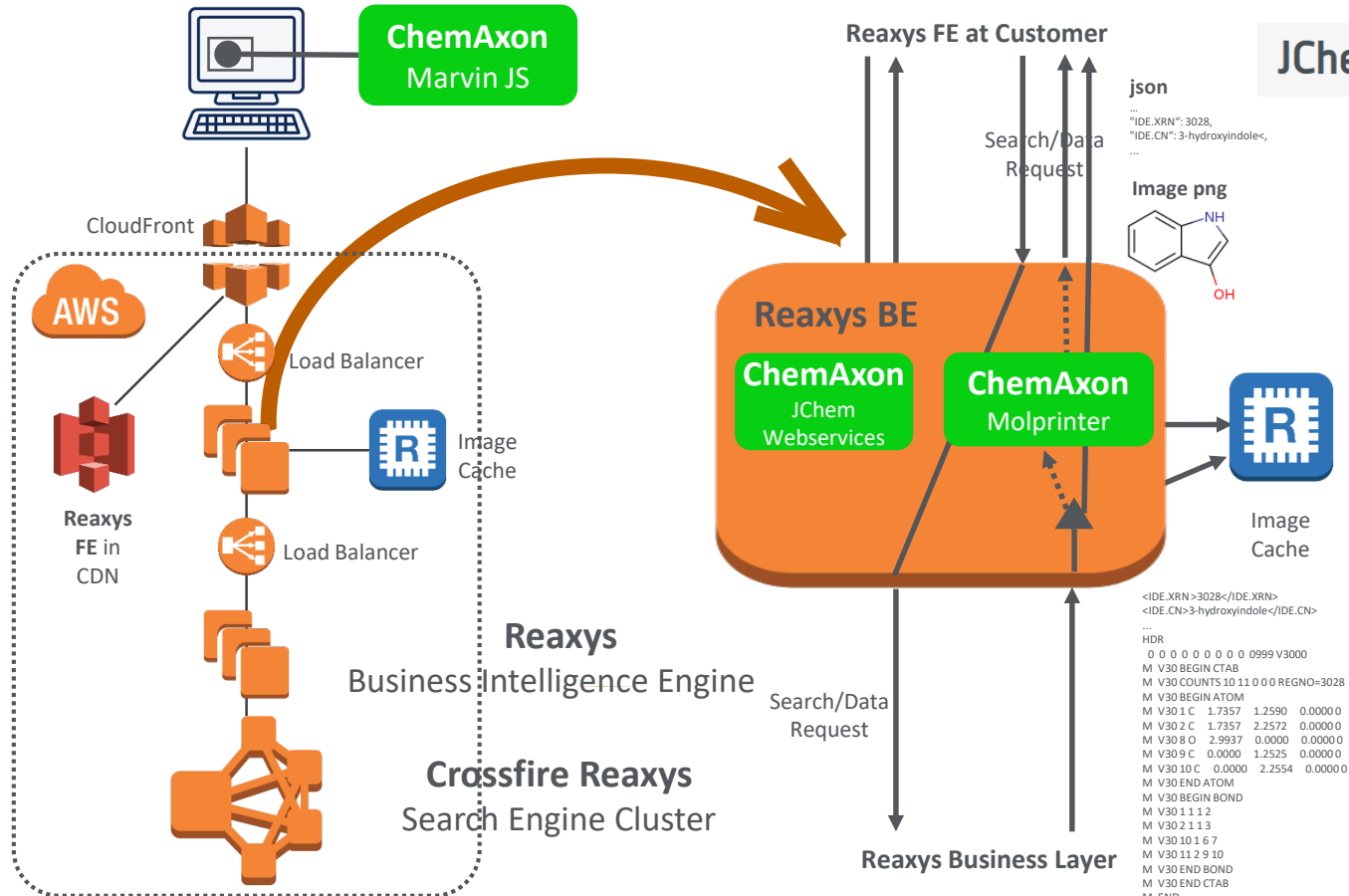
Reaxys Business Intelligence Engine

Crossfire Reaxys Search Engine Cluster

Reaxys Architecture Diagram (simplified)



Reaxys Architecture Diagram (simplified)

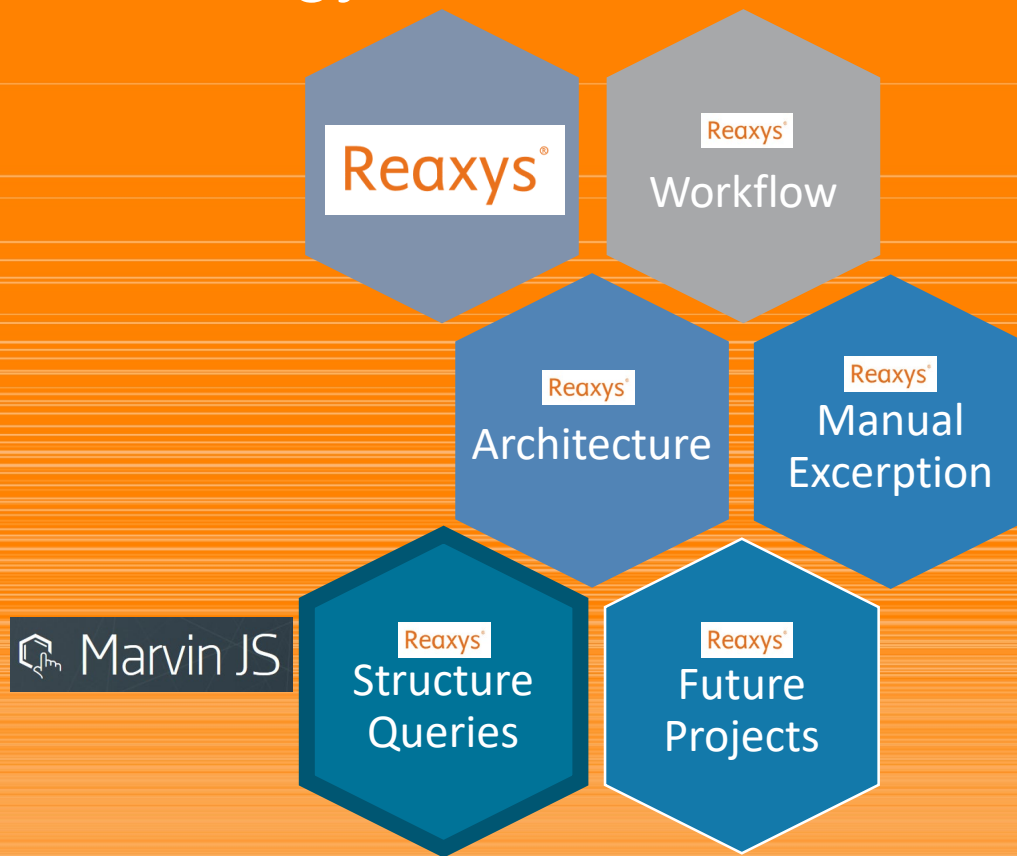


Marvin JS

JChem Web Services

MolPrinter

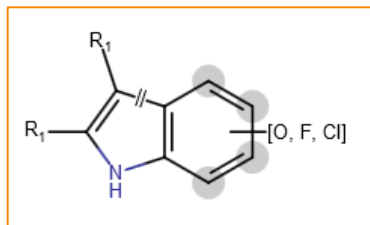
ChemAxon's technology in Reaxys



Key Reaxys Use Case: Reaction Searching and Synthesis Planning



- **Using MarvinJS to enter even complex reaction queries**
 - Find preparations for a substituted indole based on a sophisticated substructure query



Key Reaxys Use Case: Reaction Searching



Reaxys[®] Quick search Query builder Results Synthesis planner History Sign in ?

Structure editor

Create structure template from name

R Group Logic

R1 1, Rest H

Atom Mapping

Reaction center

R Groups

Atom lists

[O, F, Cl]

R1=

Position variation bond

Full-featured Java-Script Editor provided by ChemAxon allows to enter sophisticated structure and reaction queries

- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Clear Cancel Transfer to query

Feedback

Key Reaxys Use Case: Reaction Searching

MolPrinter

Reaxys[®] Quick search Query builder **Results** Synthesis planner History Sign in

117 Filters and Analysis

117 Reactions out of 71 Documents containing 224 Substances, 32 Targets

0 selected Limit To Exclude Export

Reaction ID: 9379493

1

Optimized results display with focus on reaction structures and context relevant filter & analysis tools

4 Conditions Find Similar

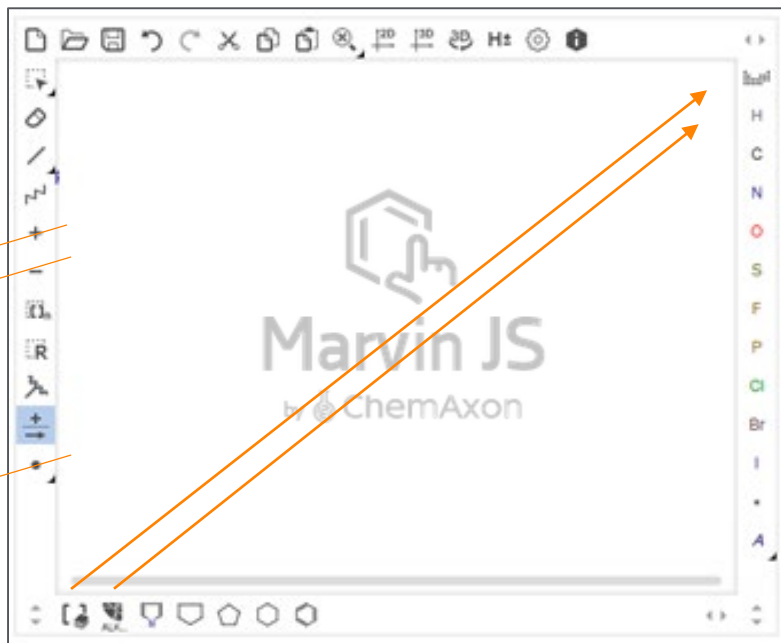
Yield	Conditions	References
36%	Stage #1: ethyl pyruvate; o-chlorophenylhydrazine hydrochloride With sulfuric acid in ethanol at 20°C; for 0.0833333h; Stage #2: With PPA for 24h; Heating;	Jablonowski, Jill A.; Grice, Cheryl A.; Chai, Wenyng; Dvorak, Curt A.; Venable, Jennifer D.; Kwok, Annette K.; Ly, Kev S.; (...) Lovenberg, Timothy W.; Carruthers, Nicholas I. - Journal of Medicinal Chemistry, 2003, vol. 46, # 19, p. 3957 - 3960 Full Text Cited 186 times Details Abstract
	With PPA; sodium bicarbonate; sulfuric acid in ethanol	Carruthers, Nicholas I.; Chai, Wenyng; Dvorak, Curt A.; Edwards, James P.; Grice, Cheryl A.; Jablonowski, Jill A.; Karlsson, Lars; (...) Wei, Jianmei; Xiao, Wei - US2003/207893, 2003, A1 Full Text Details Abstract
	With PPA; sulfuric acid in ethanol at 20°C; for 72h; Heating / reflux;	JANSSEN PHARMACEUTICA, N.V. - WO2004/22061, 2004, A1 Location in patent: Page/Page column 56-57 Full Text Details Abstract
	Stage #1: ethyl pyruvate; o-chlorophenylhydrazine hydrochloride With sulfuric acid in ethanol at 20°C; for 0.0833333h; Stage #2: In ethanol for 72h; Reflux;	Janssen Pharmaceuticals, Inc.; CARRUTHERS, Nicholas, I.; CHAI, Wenyng; DVORAK, Curt A.; EDWARDS, James, P.; GRICE, Cheryl, A.; JABLONOWSKI, Jill, A.; (...) WEI, Jianmei; XIAO, Wei - EP1373204, 2016, B1 Location in patent: Paragraph 0165

Feedback

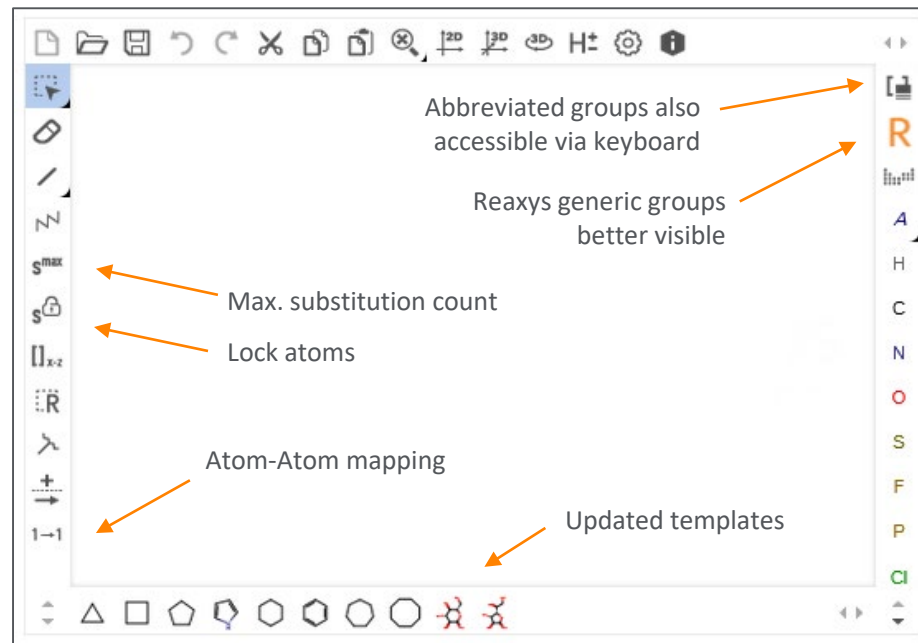
MarvinJS Usability Improvement Project



- **Originally integrated MarvinJS version was not optimized for Reaxys users**
 - ChemAxon and Elsevier exchanged end users feedback and came up with an improvement plan

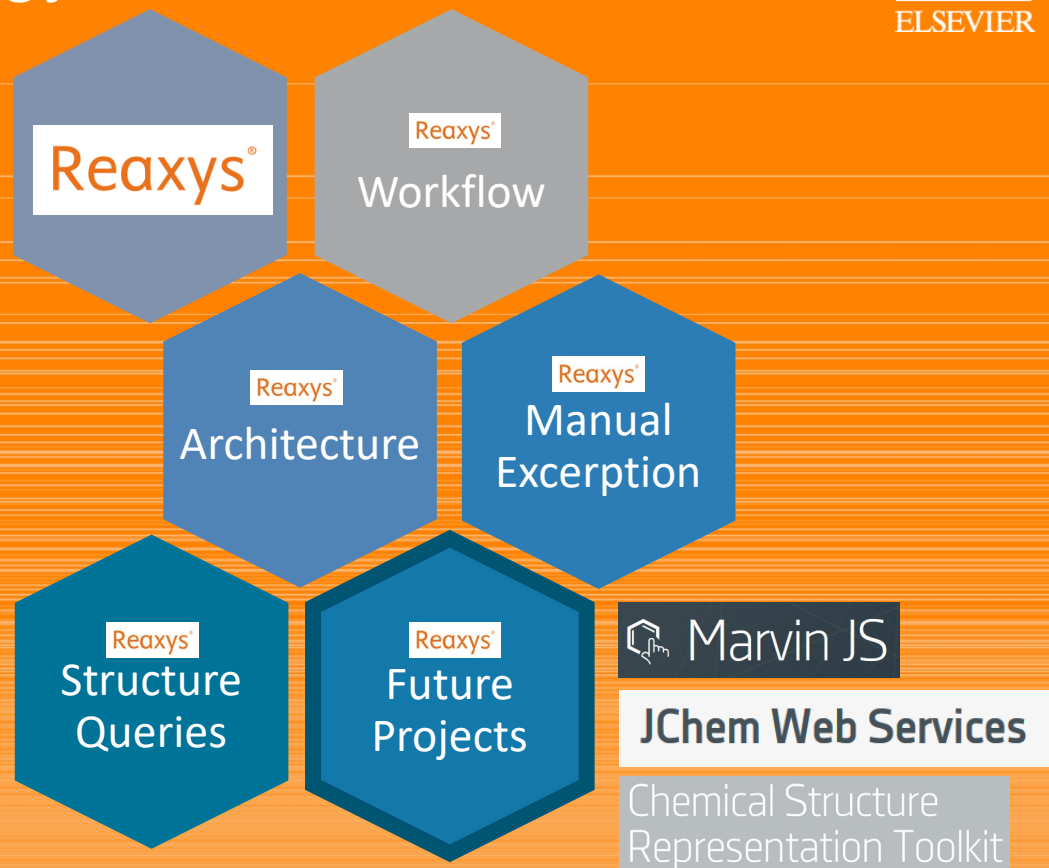


Old version



New version

ChemAxon's technology in Reaxys





MolPrinter

JChem Web Services

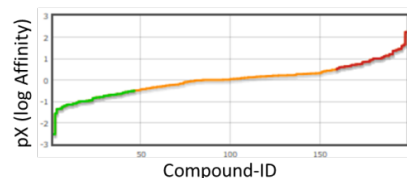
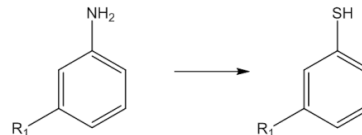
Chemical Structure
Representation Toolkit

Ongoing & Future Projects – Predictive Tools

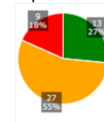
Using Reaxys Medicinal Chemistry bioactivity data to build predictive tools

➤ Bioisosteric replacements

- Enhance affinity
- Correct an ADME problem
- Overcome an IP issue



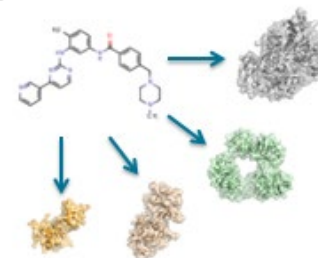
Compound Class



“What should we make next?”

➤ Target prediction

- Primary activity
- (un)favourable side effects
- Drug repurposing



“What can we expect from our compound?”

- Use of **Marvin JS** for rendering chemical structures and for formulating the chemical structure on the query page
- Use of **ChemAxon Server Tools** for transforming molecular sketches into SMILES and 3D structures, handling molecular topologies and creating molecular images



ELSEVIER

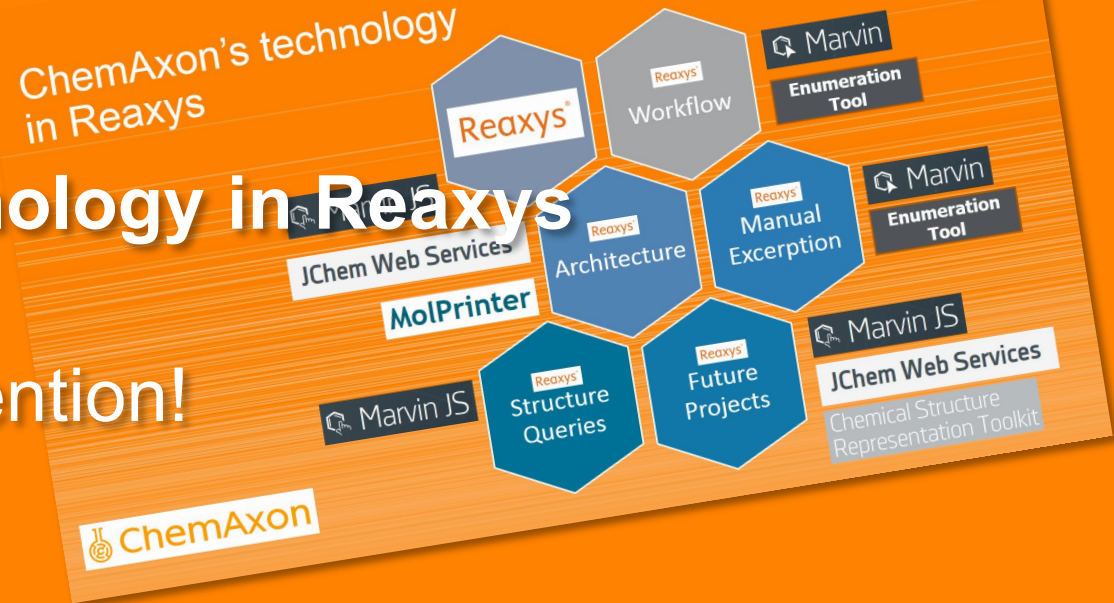


ELSEVIER

ChemAxon's technology
in Reaxys

ChemAxon's technology in Reaxys

Thanks for your attention!



Thanks to Elena Herzog, Stefan Roller, Olivier Barberan, Rosalind Sankey, Jürgen Swienty-Busch, and Pieder Caduff

Ralph Hössel



ChemAxon's technology in Reaxys

Next slide is the abstract

Abstract

ChemAxon's technology supporting Reaxys and Reaxys Medicinal Chemistry (RMC) production, searching and visualization workflows

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¹ Elsevier Information Systems, Frankfurt am Main, Germany, ² Elsevier Life Sciences IP Ltd, UK

Reaxys and Reaxys Medicinal Chemistry (RMC) is a first-class chemistry solution designed to support chemistry, pharma, environmental & material research. Its user-friendly and intuitive interface offers retrieval of a wide range of chemistry data which is stored & managed in a robust database. This is supported by a wide range of chemistry related search functionalities, including structure and reaction search, property search and NLP supported text search based on continuously updated and expanded taxonomies focused on chemistry and pharmacology disciplines.

Reaxys and RMC's end-to-end processing workflow embeds and employs ChemAxon's technology in various stages and processes; from supporting manual excerpting of factual data from full text publications (literature articles or patents), for chemical entity visualization, annotation and enumeration, and for advanced structure search and retrieval functionalities. ChemAxon's technology also provides presentation of structures and molecules to the end-user on the Reaxys and RMC's User Interface. The focus of the presentation will be on demonstration and usage of ChemAxon's cheminformatics tools and applications in Reaxys and Reaxys Medicinal Chemistry.

intuitive Excerpton Interface - iEI

- **iEI (intuitive Excerpton Interface) is a Windows-based, locally installed software for manual excerpton of chemistry and MedChem data**
- **iEI is embedded in the overall Reaxys and RMC workflow**
- **iEI ensures high data quality by...**
 - using **taxonomies** or completely fixed vocabularies (185) for nearly all text fields
 - well organized excerpton masks
 - More than 1000 check rules, 150 of them purely for Reaxys MedChem, 50 purely for chemical structure issues
- **iEI ensures high efficiency in excerpton by...**
 - providing hyperlinks between related objects (e.g. between assays and data points, or compounds and reactions etc)
 - providing several overviews from different angles (compounds, pharmacological data, physical data, reactions, etc)
 - providing tabular views for quick entry of similar data sets
 - various copy and paste features
- **iEI exports the final data set in a way that it can be loaded into the Reaxys data base, ensuring that all checks have been run**