Reaxys®

Release notes for July 2023

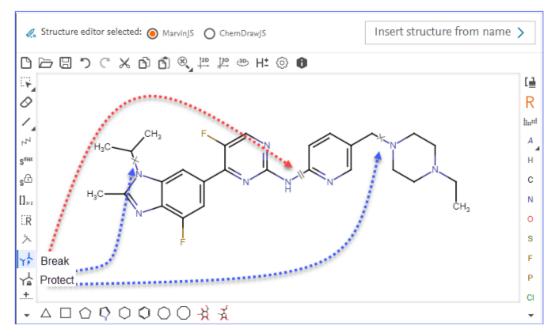
This release focuses on some feature improvements on Reaxys Predictive Retrosynthesis.

Using Break or Protect Bond definitions for Retrosynthesis Projects

Reaxys predictive retrosynthesis supports the definition of break and/or protect bond. The bond definitions can be entered via the structure editor with the following limitations:

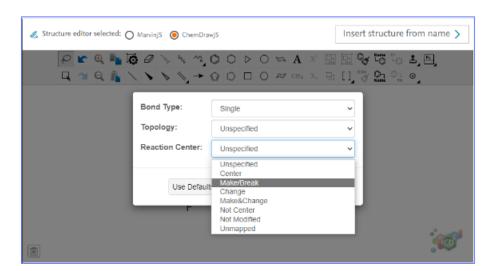
- One break feature per target molecule is allowed and will be applied as post-processing filter on last step reactions
- There is no limit on the number of protect bond features per target molecules, but it is recommended to use not more than 5, because processing time will take longer and the risk that no results will be found is increased
- Bond that has been defined as protect will be protected (not broken) throughout the synthesis tree
- It is possible to combine one break bond with many protect bond features

In MarvinJS, the features are available through the tool bar using the following buttons:



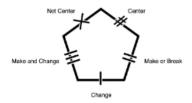


In ChemDraw the features are available via the Bond Properties menu:



The bond properties are interpreted and encoded in Molfiles as follows:

MarvinJS Reaction Center Depictions



MDL MolBlock (Reaction Centre Names in Italics)

	МJ	211	300																				
	5	5	0	0	0	0	0	0	0	0	999	V20	00										
	-	4.6	763		4.	250	8	0	.00	00	C	0	0	0	0	0	0	0	0	0	0	0	0
	-	5.3	437		3.	765	8	0	.00	00	C	0	0	0	0	0	0	0	0	0	0	0	0
	-	5.0	888		2.	98	12	0	.00	00	C	0	0	0	0	0	0	0	0	0	0	0	0
	-	4.2	638		2.	983	12	0	.00	00	C	0	0	0	0	0	0	0	0	0	0	0	0
	-	4.0	089		3.	765	58	0	.00	00	C	0	0	0	0	0	0	0	0	0	0	0	0
	1	2	1	0	0	0	-1	N	ot	ce	nte.	r											
	1	5	1	0	0	0	1	C	ent	er													
	2	3	1	0	0	0	12	M	ake	a	nd	Chan	ge										
	3	4	1	0	0	0	8	C	han	ge													
	4	5	1	0	0	0	4	M	ake	0.	r B	reak											
М	E	ND																					

Reaction Center Summary

Reacting Center Name	Reacting Center Number	Bond Preference
Not Center	-1	Protect
Center	1	Break
Make and Change	12	Break
Change	8	Break
Make or Break	4	Break

Please note that 'not modified' or 'unmapped' is not supported by Reaxys and will be ignored.

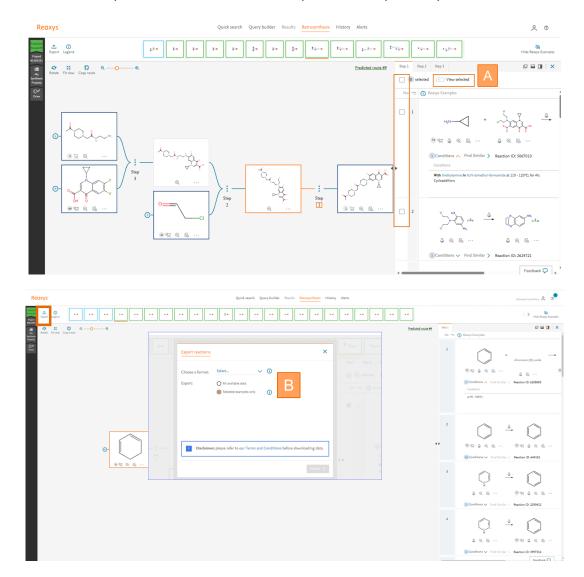


View and export selected set of examples in Tree View of Retrosynthesis

Users often want to review only specific examples of predicted synthesis routes and have the possibility to keep the selection and view for each step even if they leave the page and return to their project.

With this new feature, it is possible to (A) select and limit the view to selected examples.

In addition, the export feature supports this new functionality: a new radio button is available in the dialog box of the export of TreeViews (B) "Export selected examples only". The radio button becomes available and is checked if the user has examples selected. It is disabled if no examples are selected. If no examples are selected, then all examples will be exported by default.





Note:

while you can select also conditions in published retrosynthesis or in customized routes and limit the view to only those selected, it is not possible to export the selection for that type of retrosynthesis plans. The support of this feature for published retrosynthesis and customized routes is planned for future releases.

