
Subject: How to customize Merge Equivalent Rows
Posted by [yuan](#) on Thu, 23 May 2024 04:44:03 GMT
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Hi Thomas,

Datawarrior is a very useful open-source cheminformatics tools. Thanks for sharing it.

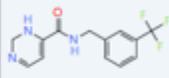
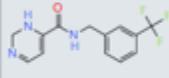
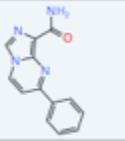
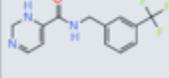
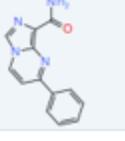
We wanted to use it organize experiment data by merging different assay results. When we used merge equivalent rows, we found that except for selected column(s) for equivalent check, other columns with the same values were also merged as a single value. Can we keep them individual or modify this function to let user determine whether merging equivalent values?

Many thanks!

Yuan

File Attachments

1) [merge equivalent rows 1.png](#), downloaded 434 times

Table							
	ID	Structure of Structure	Structure	MS Assay	Species	T1/2(min)	Experiment Date
1	cmpd001		<chem>O=C(C1=CC=NCN1)NCc1cccc(C(F)(F)F)c1</chem>	MS	mouse	584.74	2024/1/24
2	cmpd001		<chem>O=C(C1=CC=NCN1)NCc1cccc(C(F)(F)F)c1</chem>	MS	dog	427.44	2024/1/24
3	cmpd002		<chem>NC(c(ncn1cc2)c1nc2-c1ccc cc1)=O</chem>	MS	mouse	484.35	2024/1/24
4	cmpd001		<chem>O=C(C1=CC=NCN1)NCc1cccc(C(F)(F)F)c1</chem>	MS	monkey	153.73	2024/1/24
5	cmpd002		<chem>NC(c(ncn1cc2)c1nc2-c1ccc cc1)=O</chem>	MS	dog	484.35	2024/2/24

 Merge Equivalent Rows

Select column(s) to consider for equivalent rows
(use <CTRL> for multiple selection)

- ID
- Structure of Structure
- Structure
- MS Assay
- Species
- T1/2(min)
- Experiment Date

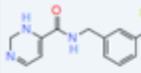
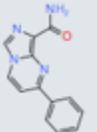
Case sensitive

Merge all rows

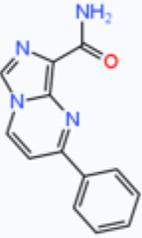
Current merge equivalent rows

What we want

2) [merge equivalent rows 2.png](#), downloaded 413 times

Table							
ID	Structure of Structure	Structure	MS Assay	Species	T1/2(min)	Experiment Date	
1		<chem>O=C(C1=CC=CC=C1)NC(=O)N1CCc1ccc(C(F)(F)F)cc1</chem>	MS	mouse dog monkey	584.74 427.44 153.73	2024/1/24	
2		<chem>NC(c1nc2c(c1)ccc2=O)c1ccc2-c1ccc2</chem>	MS	mouse dog	484.35	2024/1/24 2024/2/24	

MS

ID: cmpd002	Structure of Structure:		
			
MS Assay: MS	Species: mouse dog	T1/2(min): 484.35	Experiment Date: 2024/1/24 2024/2/24

2 of 2

What we wanted

- 3) [test data.xlsx](#), downloaded 416 times
- 4) [Test-keep individual.dwar](#), downloaded 430 times