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.

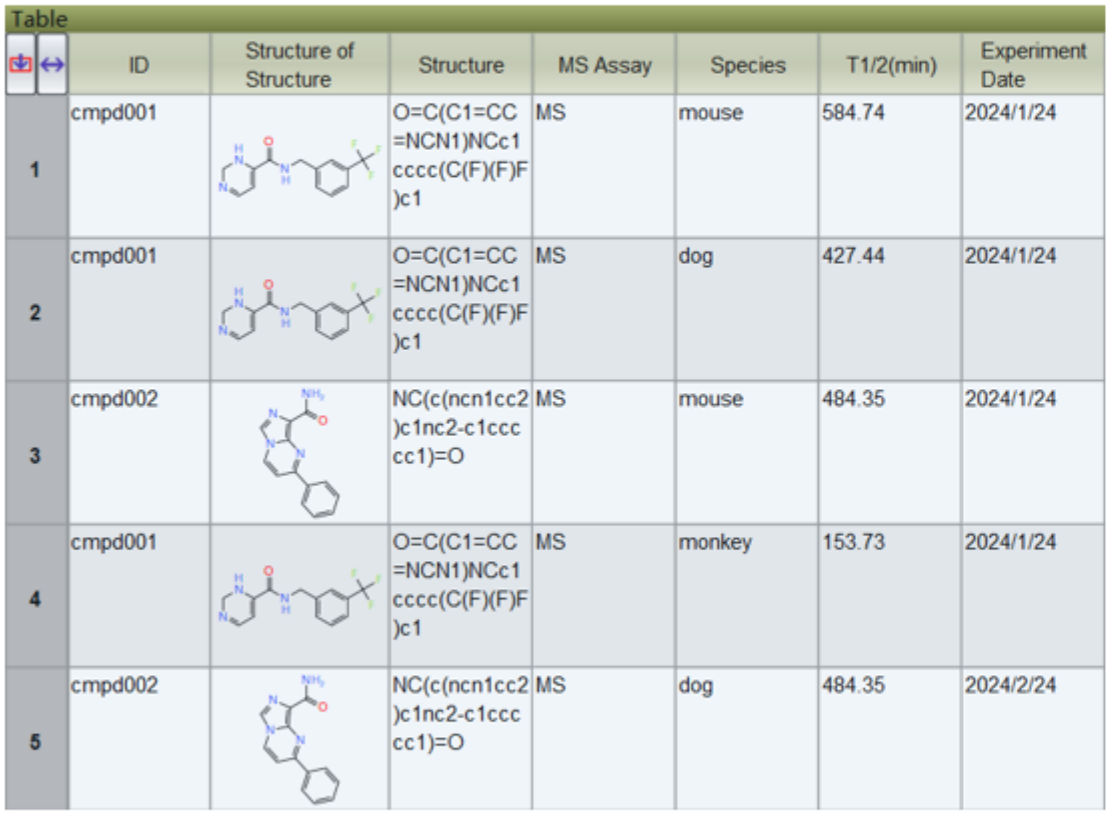
We wanted to use it organize experiment data by merging different assay results. When we used merge equivalent rows, we found that except for selected column(s) for equivalent check, other columns with the same values were also merged as a single value. Can we keep them individual or modify this function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

Many thanks!

Yuan

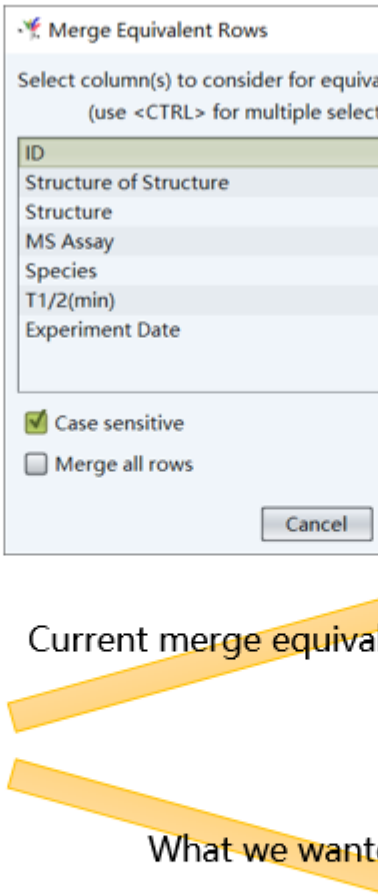
## File Attachments

1) merge equivalent rows 1.png, downloaded 897 times



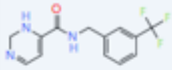
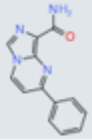
Table

| | ID | Structure of Structure | Structure | MS Assay | Species | T1/2(min) | Experiment Date |
|---|---|---|---|---|---|---|---|
| 1 | cmpd001 | | O=C(C1=CC=NCN1)NCc1cccc(C(F)(F)F)c1 | MS | mouse | 584.74 | 2024/1/24 |
| 2 | cmpd001 | | O=C(C1=CC=NCN1)NCc1cccc(C(F)(F)F)c1 | MS | dog | 427.44 | 2024/1/24 |
| 3 | cmpd002 | | NC(c(ncn1cc2)c1nc2-c1ccccc1)=O | MS | mouse | 484.35 | 2024/1/24 |
| 4 | cmpd001 | | O=C(C1=CC=NCN1)NCc1cccc(C(F)(F)F)c1 | MS | monkey | 153.73 | 2024/1/24 |
| 5 | cmpd002 | | NC(c(ncn1cc2)c1nc2-c1ccccc1)=O | MS | dog | 484.35 | 2024/2/24 |




2) merge equivalent rows 2.png, downloaded 802 times

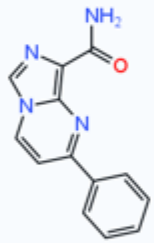
Table

| | ID | Structure of Structure | Structure | MS Assay | Species | T1/2(min) | Experiment Date |
|---|---|---|---|---|---|---|---|
| 1 | cmpd001 |  | O=C(C1=CC=NCN1)NCc1cccc(C(F)(F)F)c1 | MS | mouse<br>dog<br>monkey | 584.74<br>427.44<br>153.73 | 2024/1/24 |
| 2 | cmpd002 |  | NC(c(ncn1cc2)c1nc2-c1ccccc1)=O | MS | mouse<br>dog | 484.35 | 2024/1/24<br>2024/2/24 |

MS

**ID:**
cmpd002

**Structure of Structure:**



| MS Assay: | Species: | T1/2(min): | Experiment Date: |
|---|---|---|---|
| MS | mouse<br>dog | 484.35 | 2024/1/24<br>2024/2/24 |

2 of 2

Table MS

What we wanted

3) test data.xlsx, downloaded 549 times
4) Test-keep individual.dwar, downloaded 596 times