
Subject: red slide rule after applying filtering macro on EL -- warning, or error?

Posted by [nbehrnd](#) on Tue, 23 Jul 2024 12:23:27 GMT

[View Forum Message](#) <> [Reply to Message](#)

Dear Thomas,

after the creation of a small EL with 279 entries, I applied a .dwam macro to remove entries containing the motif of the nitrile group. Though the number of structures retained is smaller, I observe DW's report of `visible: 182, total: 274` at the bottom of the frame. The export to .sdf via `save -> safe special -> sd` file exports 274 records. At the same time, the slide ruler «generation» turned red:

Is this an indicator of a warning, or of an error?

On other hand, I exported DW's evolutionary library right after its generation as .sdf. In a newly launched session of DW, the import of the filtering macro file and its application neither yields to a discrepancy of the numbers `visible` and `total` (both equate to 274), nor turns any of the slide rulers red.

The observations refer to current DW 06.02.01 for Linux used in Linux Debian 13/trixie.

Regards,

Norwid

File Attachments

1) [after_macro.png](#), downloaded 841 times

Evolutionary_Library.dwar

File Edit Data Chemistry Database List Macro Help

Table	Structure	ID	Parent ID	Cycle	Generation	Parent Generation	Child No	Fitness
1		1	-1	0	0	-1	1	1
2		2	-1	0	0	-1	1	1
3		3	-1	0	0	-1	1	1
4		4	-1	0	0	-1	1	1
5		5	-1	0	0	-1	1	1
6		6	-1	0	0	-1	1	1
7		7	-1	0	0	-1	1	1
8		8	-1	0	0	-1	1	1

Table Structure Fitness Evolution

151 of 512 MB Selected: Visible:182 Total:274

Control Panel:

ID: 1 (range 1-2)

Parent ID: -1 (range -1-2)

Cycle: 0 (range 0-2)

Generation: 0 (range 0-2)

Parent Generation: -1 (range -1-2)

Data Table:

Column Name	Value
ID	2
Parent ID	-1
Cycle	0
Generation	0
Parent Generation	-1
Child No	1

Structure:

2) [filter_on_EL.zip](#), downloaded 379 times

Subject: Re: red slide rule after applying filtering macro on EL -- warning, or error?
 Posted by [thomas](#) on Wed, 31 Jul 2024 14:23:23 GMT

[View Forum Message](#) <> [Reply to Message](#)

Dear Norvid,

this is a little tricky and it also involves a bug that I just fixed:

A range filter is turning red if it refers to a column that has empty entries. This is to make you aware that this filter hides rows even if it allows the full data range, because all empty-data rows are hidden by that filter.

In your case some of the generation values are empty. It took me a while to understand why: For evolutionary libraries the column 'Parent Generation' references the column 'Generation' in a 'topdown' direction. This reference is defined in the column properties section of the file. That information is, for instance, used by 2D-views to place arrows between markers. When DataWarrior deletes rows, which are reference by other rows, then it clears the referencing ID from rows if the referenced rows are deleted. This should happen in the 'Parent Generation' column. Due to a bug after introducing multiple runs, it wrongly removes IDs from the 'Generation' column, which I have fixed now.

There is no problem with your file, except that after deleting the Nitriles some generation numbers are missing and the filter turned red to make you aware of this fact.

You could fix your file 'Evolutionary Library.dwar' before deleting rows by changing `<columnName="Generation">` to `<columnName="Parent Generation">` that it looks as below:

```
<columnName="Parent Generation">  
<columnProperty="refColumn Generation">  
<columnProperty="refType topdown">
```

The deletion of the Nitriles causes then to remove some entries in the "Parent Generation" column, which is the expected behaviour.

Best wishes,

Thomas
