
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

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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 753 times

Evolutionary_Library.dwar

File Edit Data Chemistry Database List Macro Help

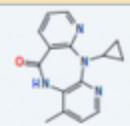
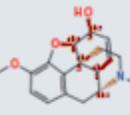
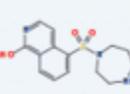
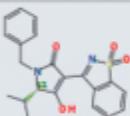
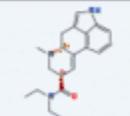
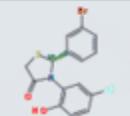
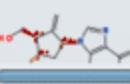
Structure	ID	Parent ID	Cycle	Generation	Parent Generation	Child No	Fitness
	1	-1	0	0	-1	1	1
	2	-1	0	0	-1	1	1
	3	-1	0	0	-1	1	1
	4	-1	0	0	-1	1	1
	5	-1	0	0	-1	1	1
	6	-1	0	0	-1	1	1
	7	-1	0	0	-1	1	1
	8	-1	0	0	-1	1	1

Table Structure Fitness Evolution

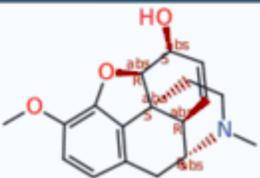
151 of 512 MB Selected: Visible:182 Total:274

Control Panel:

- ID: 1
- Parent ID: -1
- Cycle: 0
- Generation: 0
- Parent Generation: -1

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 367 times