Subject: Re: extension of substructure definition
Posted by nbehrnd on Thu, 14 Sep 2023 20:31:39 GMT
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Dear Thomas,

I'm sorry to report the additional criterion to initiate the array with «substructure» instead of «structure» as first column represents an obstacle.

To venture out the new functionality, departing from a pristine installation of DW for Linux 5.5.0 (fetched 2022-05-18) in Linux Debian 13/trixie, I fetched the new update dw_wl_linux.zip. Under the assumption renaming file /opt/datawarrior/datawarrior would move it out of the way for the new files (of the update) to come, the content of the archive was moved into the folder. Lines 3--6 of the new shell script were understood as optional, and thus I retained the suggested defaults.

Case 1): Normal launch of DW, creating the array with «structure» as first column, no problem. Nor the generation of a library of random molecules and subsequent assignment of computed properties.

Case 2): Normal launch of DW, creating the array with «substructure» as first column. Now, the command shell became talkative. Shortly after, the message of «uncaught exception 3» on a widget appears which is above an other without a note (except the «cancel» button»). If I click on «cancel», this second widget claims to initiate some space cleaning. At this point, the task manager of the operational system does not show noticeable RAM allocated to DW. However leaving DW from its GUI is blocked, an exit possible the hard way by killing the corresponding PID.

Because of the noteworthy reorganization towards DW 5.6.0 and «it is a beta version, if something goes wrong, restore the old /opt/datawarrior/datawarrior file»), I equally gave this spin; in my case however it is on expense of new column type «substructure».

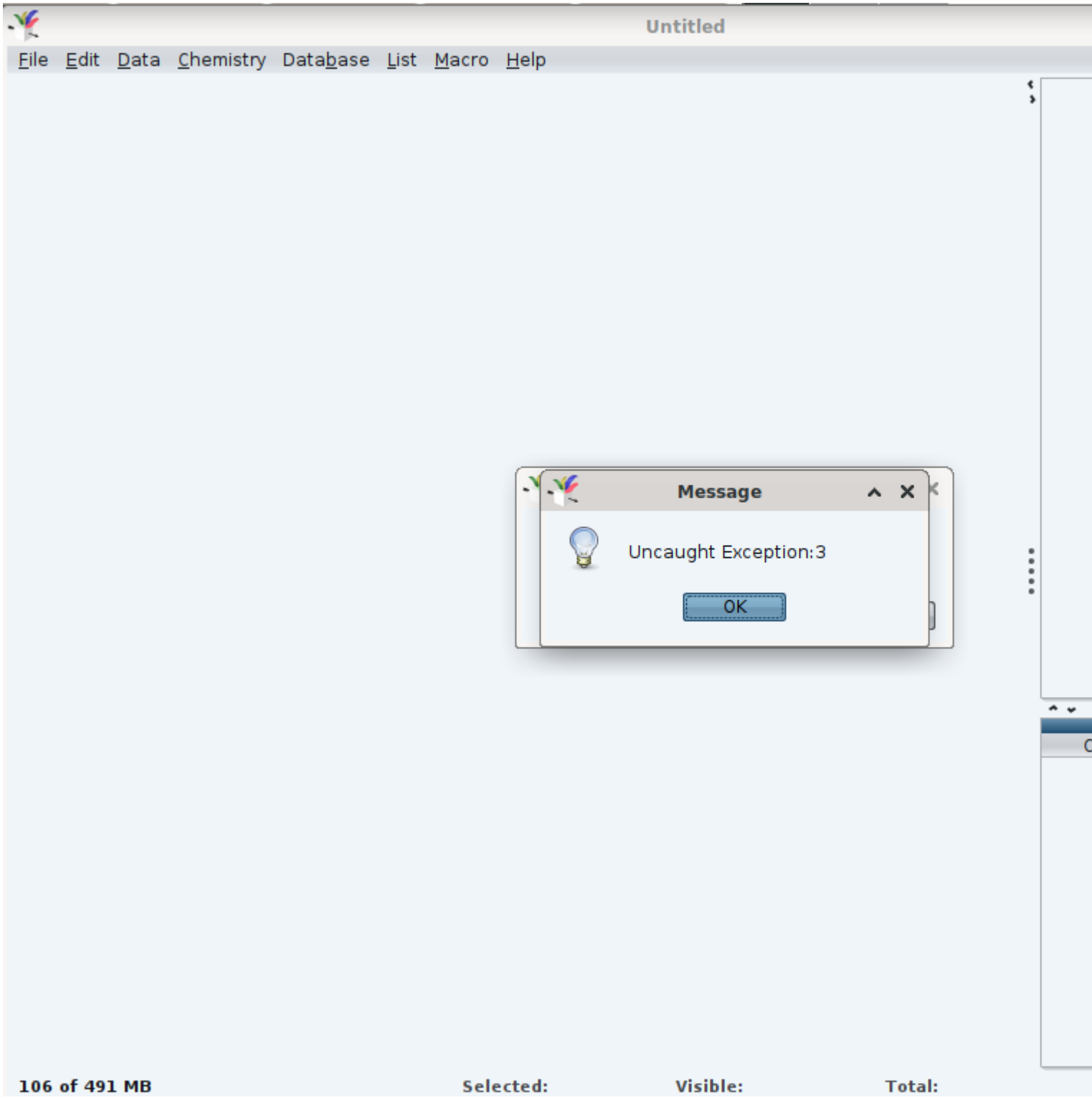
Attached below, screen photos recorded and what was logged via the shell (in this case, bash).

Best regards,

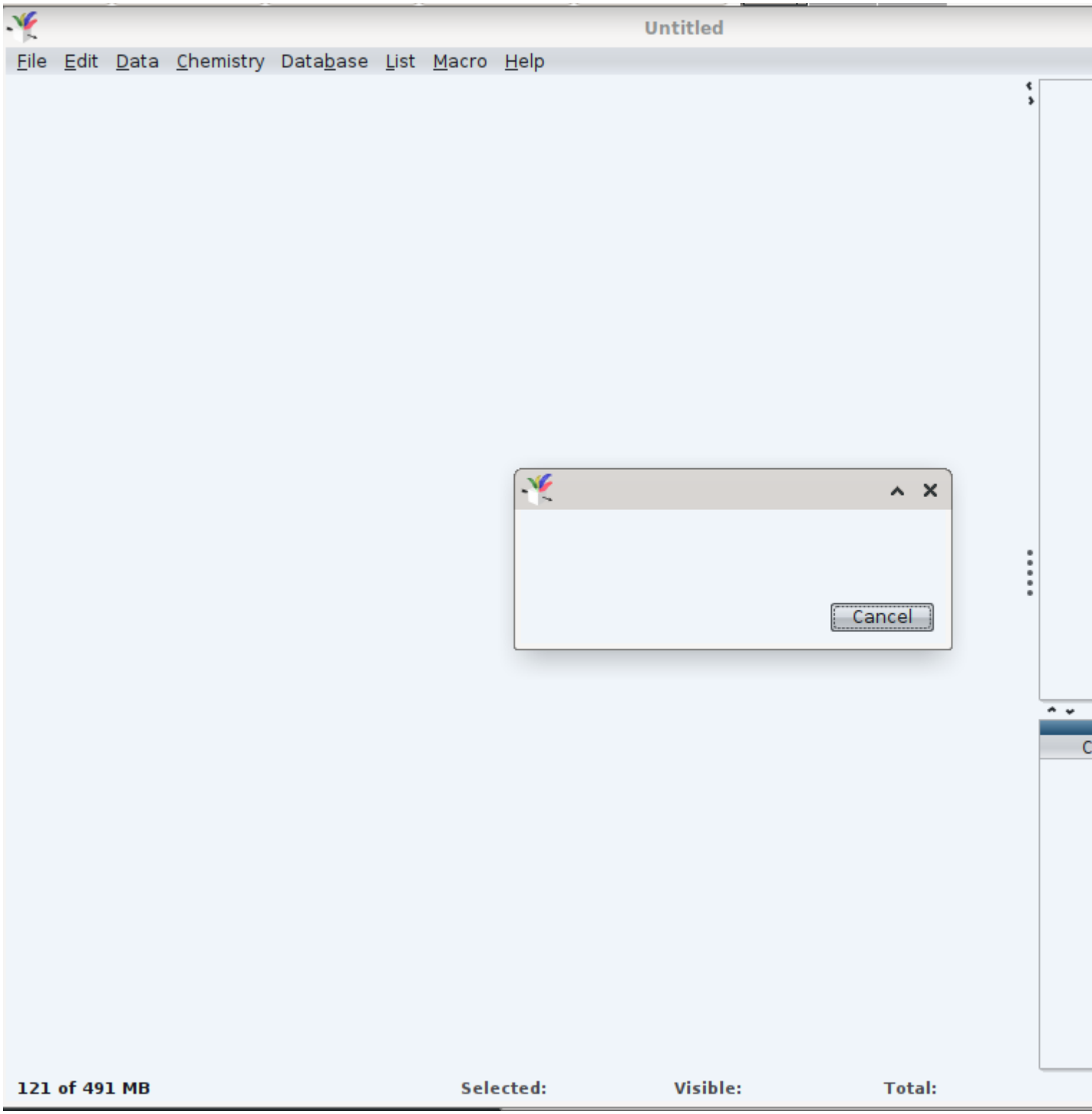
Norwid

File Attachments

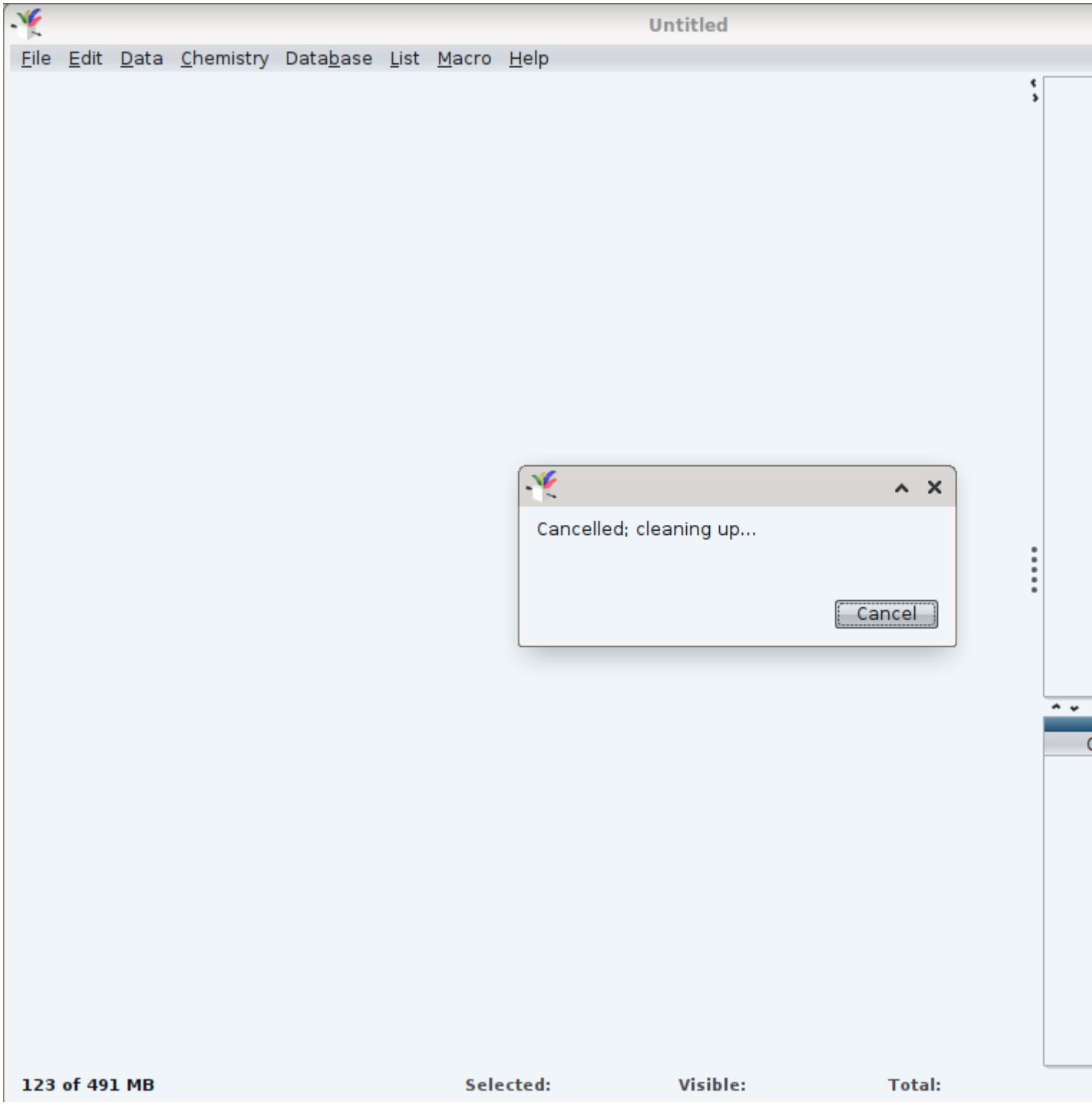
1) problem_01.png, downloaded 891 times



2) problem_02.png, downloaded 891 times



3) problem_03.png, downloaded 758 times



4) 2023-09-14_relevant_log -- dw.txt, downloaded 525 times