Subject: Re: Create a macro to split a .dwar file into multiple .dwar files
Posted by nbehrnd on Thu, 15 Aug 2024 18:16:22 GMT
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Hello,

for a one-at-a-time, DW very well can help you. Attached below the macro, raw data set and results, and a brief demo with DW 06.02.03

The idea is to check for the presence of a particular string in the column identifier. For this, the macro asks every line the same test question by the formula

```
if (identifier == askString("enter the identifier of interest"), "true", "false")
```

if a specific string is present at this intersection. The newly calculated column will contain an entry `true` if this is the case, or else the string `false`. (Of course you could opt-in for `active`, `inactive` to designate the two, too.) The flexibility you want is provided by DataWarrior's function `askString()` to allow to recycle the macro's function, to filter for records with an other string in this field. Watch out the pane to the right hand side: we now have a filter which allows to save the visible records per level `true`, or `false`.

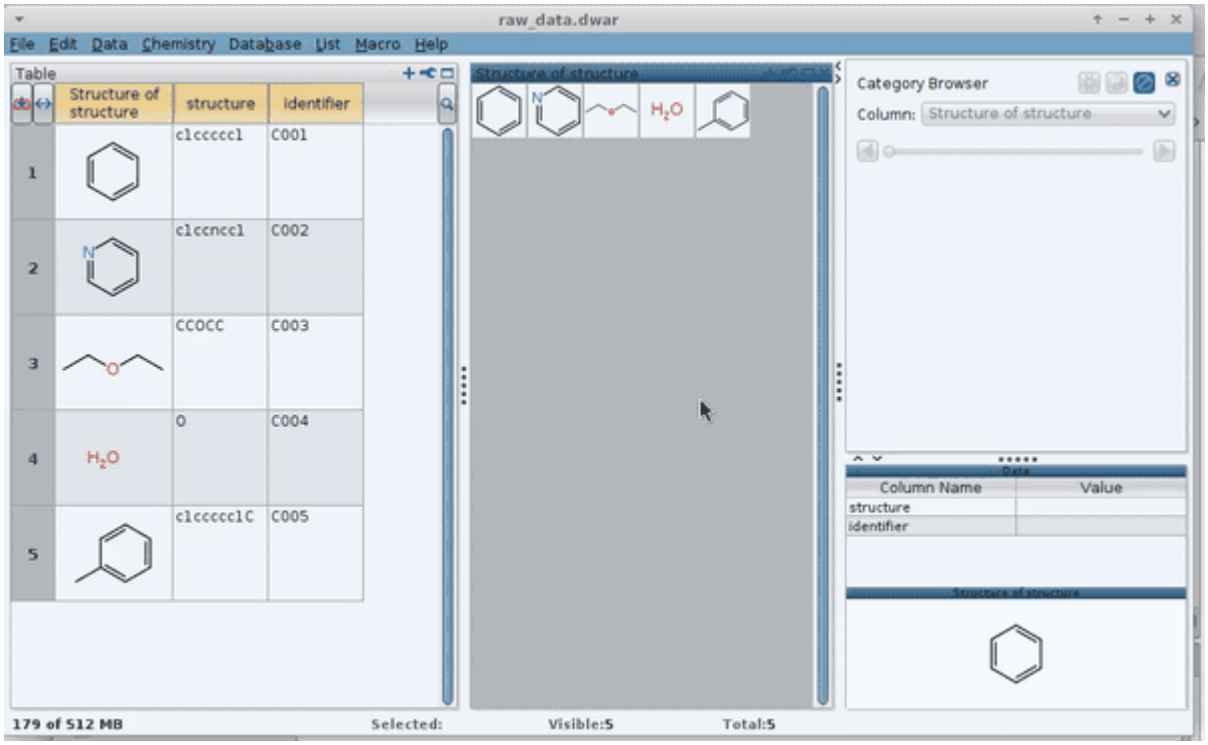
While running the macro editor, a double click on `save visible rows` allows you to toggle off the question to manually define the file name (for this sub set of data). This can be useful if i) raw data and the new files to be written are every time in the same location, and ii) the output should every time the same, e.g. `positive.dwar` and `negative.dwar`.

Best regards,

Norwid

File Attachments

1) filter_by_string.dwam, downloaded 500 times
2) raw_data.dwar, downloaded 426 times
3) true.dwar, downloaded 517 times
4) false.dwar, downloaded 507 times
5) demo.gif, downloaded 1072 times


raw_data.dwar
File Edit Data Chemistry Database List Macro Help
Table
Structure of structure
structure
identifier
1
c1ccccc1
C001
2
c1ccncc1
C002
3
CCOCC
C003
4
O
C004
5
c1ccccc1C
C005
Structure of structure
Category Browser
Column: Structure of structure
Data
Column Name
Value
structure
identifier
Structure of structure
179 of 512 MB
Selected:
Visible:5
Total:5