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Subject: macro comments

Posted by [juliocoll](#) on Tue, 06 Aug 2024 11:35:09 GMT

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dear Thomas,

I missed in the Macro Editor any reference to helpful non-coding commentaries, similar to those existing in other computational languages. Did I missed the information in some other place?

...

Just in case, I tested: //, /\*..\*/ , # and ' (used in other programs), but none of them worked in DW macros.

In case they are not yet considered, Would it be possible to include that possibility for DW macros?

It would be a great help for long codings...

Thank you for your attention

sincerly Julio

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Subject: Re: macro comments

Posted by [juliocoll](#) on Wed, 23 Oct 2024 10:23:57 GMT

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After trying many alternatives, the best way to include non-coded information on long DW macros may be to insert comments on "show message" tasks.

It may slow down the macro execution but have no other alternative to be somehow self-explanatory.

For example:

```
<task name="showMessage">
message= NOW THE VISIBLE ROWS WILL BE SAVED TO C:/....
</task>
```

Another example of use is included into the NTN macro for semi-automatically save all information on raw dwar and toxicity-filtered and mmff94s+ conformer sdf files for Vina, after running a DW Build Evolutionary Library

Hope it may serve to other DW macro-designers !

### File Attachments

1) [NTN.dwam](#), downloaded 26 times

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Subject: Re: macro comments

Posted by [nbehrnd](#) on Thu, 24 Oct 2024 19:50:28 GMT

I support Julio's request with preference for a single-character to start a line comment. Percent sign, ! and C didn't work either. The attempt to introduce visual indentation (because renaming the task name in an editor renders the block useless), either with two explicit spaces per level of indentation like

```
<macro name="test">
<task name="addSmilesCodes">
structureColumn=Structure
</task>
<task name="calculateCompoundProperties">
  propertyList=totalWeight logP
  structureColumn=Structure
</task>
</macro>
```

or with tabulator breaks everything in this indented block, too (a subsequent block without indentation will perform well).

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Subject: Re: macro comments

Posted by [thomas](#) on Sat, 26 Oct 2024 20:56:48 GMT

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Dear Julio,

sorry, I have missed this issue for today's update. But it will be in the next one. Macro task comments will look like the following. They are preceded by '#' and follow the task name tag. If you manually add a macro file and add comments at another position, they are moved automatically to the position where they belong. I will also add a user interface to edit task comments. From your point of view does that make sense?

```
<macro name="scaffoldReplacement">
<task name="replaceScaffoldAndLink">
# some comment
# more comment
# comment within properties
maxEVRMSD=0.15
atomsMore=10
maxEVDivergence=30.0
minPhesaFlex=0.5
  query=fasqr@DXT@UoQRWT@dsJrkO~wLxYsSMTuUTuTRbdcQt@•dDsdC}fRf TvuvL
#qMuyMo_oLLndsZj?PexZoGsSI_YzAltBDxkdmJHv_YzkL?VDJDYzGvmlo]
NykaIPWzRbHIGNMLXTKw~IMMxCWU_IWAjAEKrRSJFd^AqSq_yDz` @ @eyz?tz
AD}cG]B[\@GniCFI?nCbkuzHfkWW_CY[h]`tgx`dB|@xL?vVP{^GZyfe
PxjXyDOpeTQe@tFvP^kAS~|svKW~lg?XbNREsryUnKDGyI[p?GmMeawJuw\
```

fR}bvD{ \_HQi`i}`htj~QoKgiwfABqNogOydGkOi\Asf|yCnr~~Skw|UmBCkg  
eBqhetK{XLz{[^fBWUQnttLrrCRdfI~zh`@R@Aw@@@  
atomsLess=5  
inFile=/home/thomas/data/cod/cod-fragments\_4to16.dwar  
</task>  
</macro>

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Subject: Re: macro comments  
Posted by [nbehrnd](#) on Sun, 27 Oct 2024 15:39:38 GMT  
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Dear Thomas,

wonderful to see this as prospective pattern in future releases.

Best regards,

Norwid

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