Subject: Re: Suggestion: add molecular weight calculation for individual compound
Posted by nbehrnd on Thu, 29 Jan 2026 14:32:50 GMT
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Hello Laurent

by the title of your question, I thought you refer to identify the largest fragment in a structure (chemistry -> from chemical structure -> extract unconnected fragment; note: singular) to the result a new column (cf. attached screen photo) eventually used as reference to compute for instance the molecular weight. The body however reads more like i) screen a .dwar file and compute e.g., the molecular weight only if ii) a predefined (sub)structure matches the an entry in the structure column. Can you amend your question with details?

Best,
Norwid

File Attachments

1) 2026-01-29_DW_fragment.png, downloaded 291 times