

Subject: Re: Suggestion: add molecular weight calculation for individual compound
Posted by [nbehrnd](#) on Thu, 29 Jan 2026 14:32:50 GMT

[View Forum Message](#) <> [Reply to Message](#)

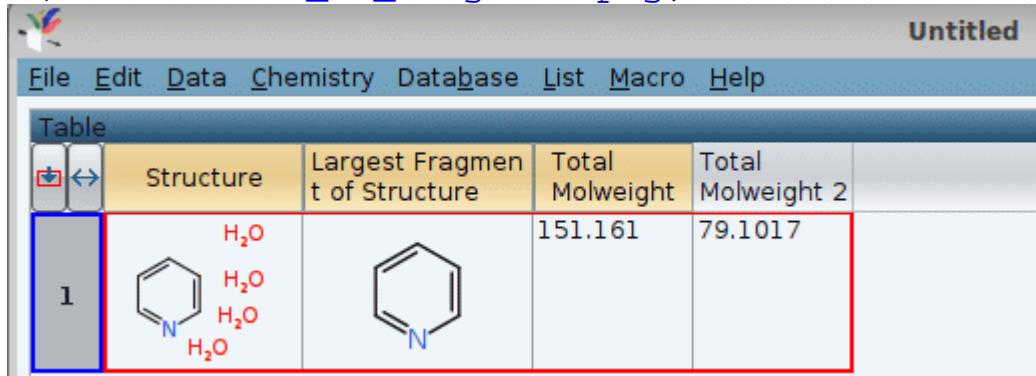
Hello Laurent

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?

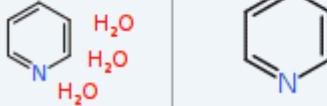
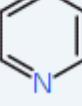
Best,
Norwid

File Attachments

1) [2026-01-29_DW_fragment.png](#), downloaded 6 times



The screenshot shows a software interface with a menu bar (File, Edit, Data, Chemistry, Database, List, Macro, Help) and a title bar (Untitled). Below the menu is a toolbar with a 'Table' icon. The main area displays a table with the following data:

	Structure	Largest Fragment of Structure	Total Molweight	Total Molweight 2	
1	 H ₂ O H ₂ O H ₂ O H ₂ O		151.161	79.1017	