

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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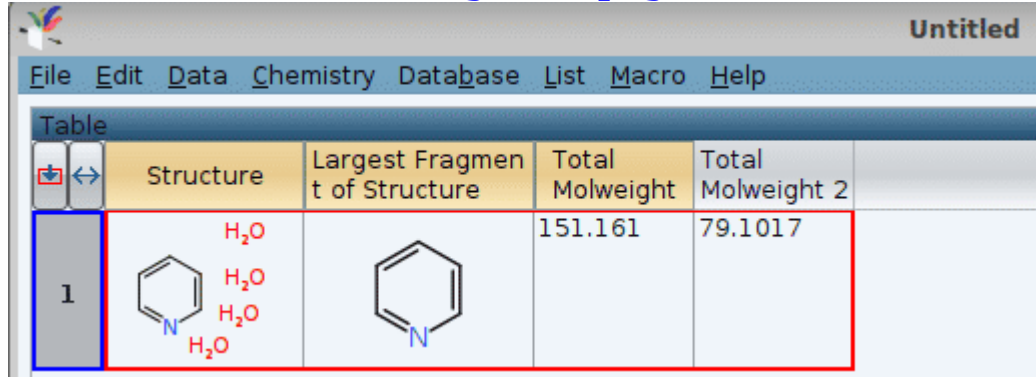
Hello Laurent

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?

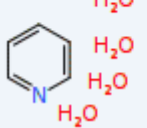
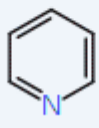
Best,  
Norwid

### File Attachments

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



The screenshot shows a software window titled "Untitled" with a menu bar (File, Edit, Data, Chemistry, Database, List, Macro, Help). Below the menu is a table with the following columns: "Structure", "Largest Fragment of Structure", "Total Molweight", and "Total Molweight 2". The table contains one row with the index "1". The "Structure" column shows a pyridine ring with four "H<sub>2</sub>O" labels. The "Largest Fragment of Structure" column shows a pyridine ring. The "Total Molweight" column shows "151.161". The "Total Molweight 2" column shows "79.1017".

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