
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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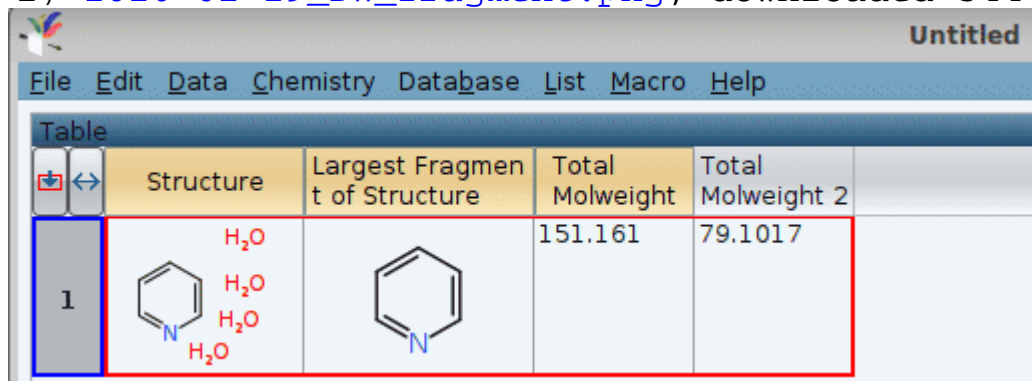
Hello Laurent

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?

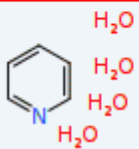
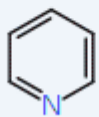
Best,
Norwid

File Attachments

1) [2026-01-29_DW_fragment.png](#), downloaded 344 times



The screenshot shows a software window titled "Untitled" with a menu bar (File, Edit, Data, Chemistry, Database, List, Macro, Help) and a table. The table has the following columns: "Structure", "Largest Fragment of Structure", "Total Molweight", and "Total Molweight 2". The first row (index 1) contains a chemical structure of a pyridine ring with four "H₂O" labels, a single pyridine ring structure, the value "151.161", and the value "79.1017".

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