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Subject: largest fragment not recognized as such  
Posted by [nbehrnd](#) on Thu, 29 Jan 2026 14:50:48 GMT  
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Hello Thomas

Expanding from another question, DW processes fragments differently than expected by me -- does the following represent a bug?

In the structure editor, 2,6-lutidine and a few molecules of water were defined. Subsequently, I launched the computation of the molecular weight while "Largest Fragment Only" was activated (via chemistry -> from chemical structure -> calculate properties, cf. screenphoto attached). Contrasting to my anticipation, the result provided however is not 107 g/mol about lutidine alone, but 143 g/mol (i.e. including two molecules of water). To me, this is counterintuitive (though, as a bypass, I can split off the pyridine by "extract largest fragment" for an eventually referenced new column, too.)

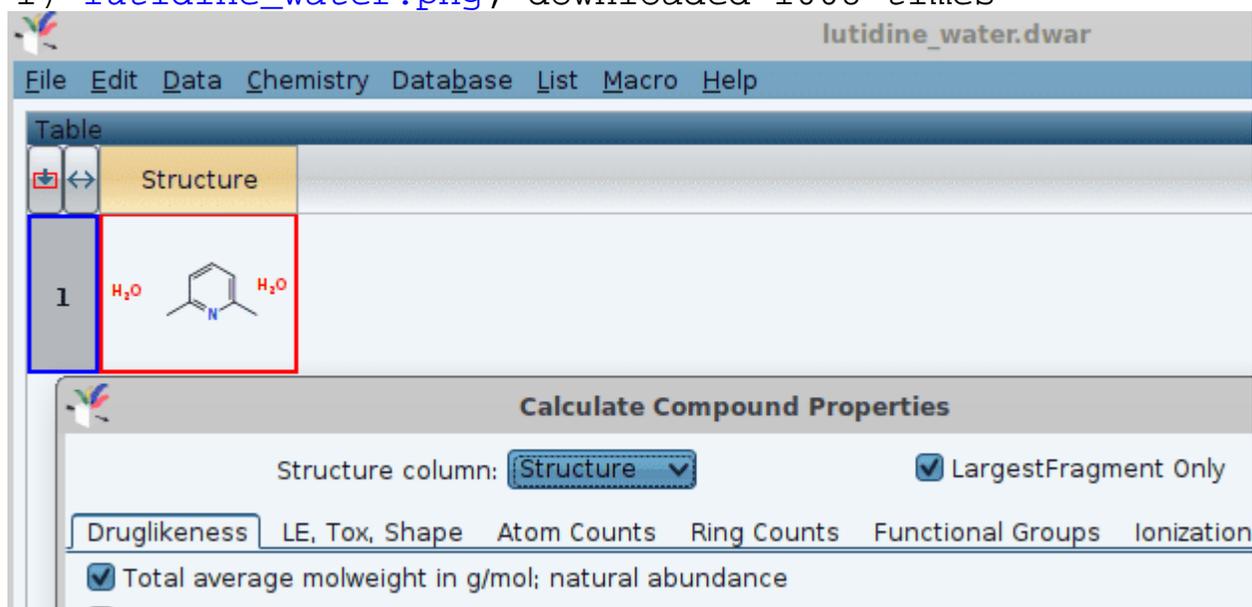
Best regards,  
Norwid

setup: DW 06.05.02 by September 2025

## File Attachments

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1) [lutidine\\_water.png](#), downloaded 1008 times



The screenshot shows a software window titled "lutidine\_water.dwar". The main area contains a table with one row. The first column of the table has the number "1". The second column contains a chemical structure of 2,6-lutidine (a pyridine ring with methyl groups at positions 2 and 6) with two water molecules (H<sub>2</sub>O) attached to it. Below the table is a dialog box titled "Calculate Compound Properties". The "Structure column:" dropdown is set to "Structure". The "LargestFragment Only" checkbox is checked. The "Total average molweight in g/mol; natural abundance" checkbox is also checked. Other tabs like "Druglikeness", "LE, Tox, Shape", "Atom Counts", "Ring Counts", "Functional Groups", and "Ionization" are visible.

2) [lutidine\\_water.dwar](#), downloaded 68 times

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