
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?

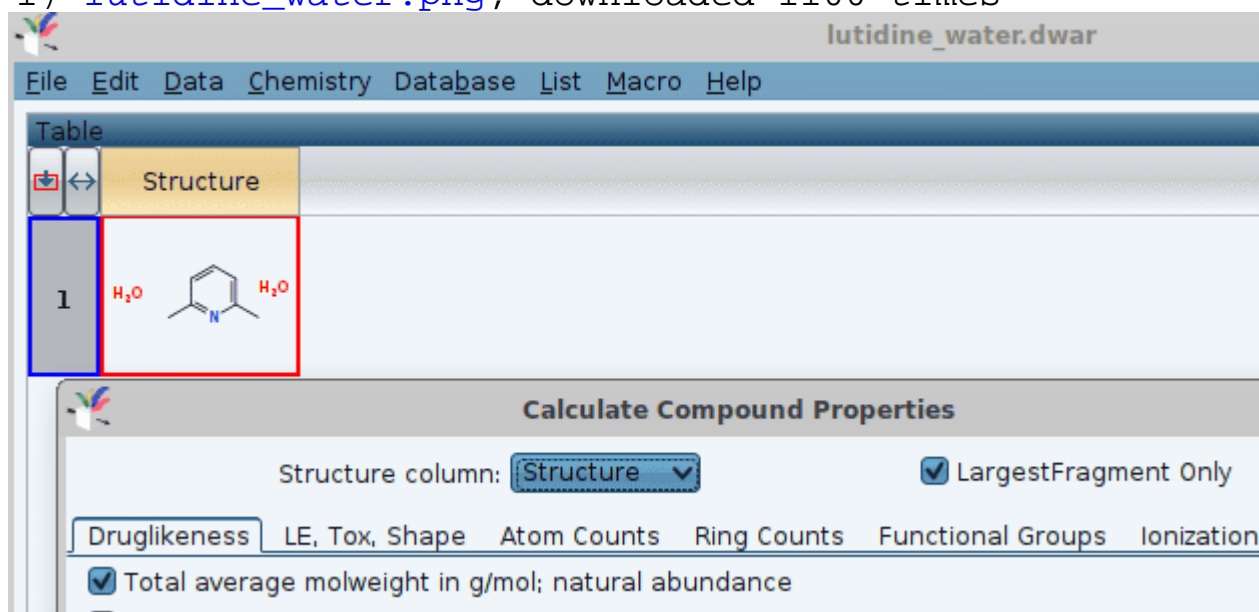
In the structure editor, 2,6-lutidine and a few molecules of water were defined. Subsequently, I launched the computation of the molecular weight while "Largest Fragment Only" was activated (via chemistry -> from chemical structure -> calculate properties, cf. screenphoto attached). Contrasting to my 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

1) [lutidine_water.png](#), downloaded 1100 times



The screenshot shows the OpenMolecules software interface. At the top, the title bar reads "lutidine_water.dwar". Below it is a menu bar with "File", "Edit", "Data", "Chemistry", "Database", "List", "Macro", and "Help". A "Table" window is open, showing a single row with the index "1" and a chemical structure of 2,6-lutidine with two water molecules (H₂O) attached. The structure is highlighted with a red border. Below the table is a "Calculate Compound Properties" dialog box. The "Structure column" is set to "Structure". The "LargestFragment Only" checkbox is checked. The "Total average molweight in g/mol; natural abundance" checkbox is also checked. The dialog box has tabs for "Druglikeness", "LE, Tox, Shape", "Atom Counts", "Ring Counts", "Functional Groups", and "Ionization".

2) [lutidine_water.dwar](#), downloaded 93 times
