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?

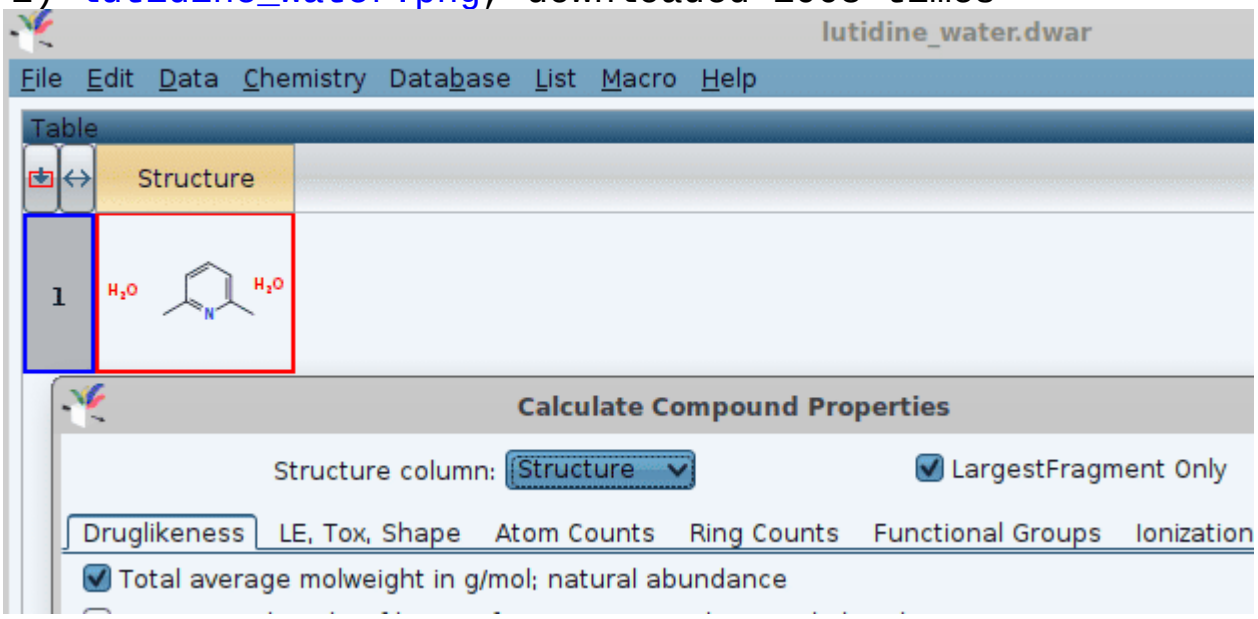
In the structure editor, 2,6-lutidine and a few molecules of water were defined. Subsequently, I launched the computation of the molecular weight while "Largest Fragment Only" was activated (via chemistry -> from chemical structure -> calculate properties, cf. screenphoto attached). Contrasting to my 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 1008 times



2) lutidine_water.dwar, downloaded 68 times