Subject: R-Decomp doesnt show R1
Posted by Santora V on Sat, 07 Mar 2026 21:39:31 GMT
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When I run an R-decomposition on the scaffold attached, the expected R1-R3 columns and most functional groups appear in the data table, but an R1 filter doesn't appear in the right panel. The scaffold, R2, and R3 selection lists appear as expected.
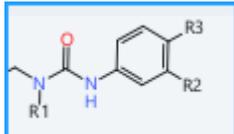
Also, hydrogen substituents at R1-R3 don't appear in the table (just empty cells), and the selection lists on the right do not show H as an option.

Any fixes appreciated.

VS

File Attachments
1) R1-R3 Substructure.png, downloaded 148 times

Subject: Re: R-Decomp doesnt show R1
Posted by thomas on Fri, 03 Apr 2026 15:23:18 GMT
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Hydrogen atoms are handled differently from other atoms by DataWarrior. Usually, they are not drawn. They are implicit. Infact, molecules in DataWarrior are processed without any hydrogen atoms, even if the structure contains some explicit hydrogen atoms. They also are not considered a substituent. An empty substituent means that open valences are always filled with hydrogens. Of course, non standard hydrogens are considered. For instance deuterium is treated like any other atoms and would show up as substituent.

I don't know, why you didn't get a filter for R1, but I assume that R1 is always hydrogen, i.e. empty. Then, there is nothing to select and you won't get a filter.

Subject: Re: R-Decomp doesnt show R1
Posted by Santora V on Thu, 09 Apr 2026 22:05:50 GMT
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Thanks for your help.

In my file, R1, R2, and R3 all have multiple groups (not just H). All three have columns in the

table, but only R2 and R3 appear as filters on the right, as shown in the attached pics.

File Attachments

Scaffold	R1	R2	R3