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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.

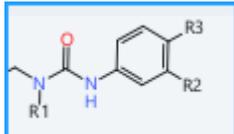
Also, hydrogen substituents at R1-R3 don't appear in the table (just empty cells), and the selection lists on the right do not show H as an option.

Any fixes appreciated.

VS

### File Attachments

1) [R1-R3 Substructure.png](#), downloaded 148 times



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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.

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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

1) [Screenshot 2026-04-09 150119.png](#), downloaded 51 times

The image shows a screenshot of a chemical structure filter interface. It is divided into two main sections: R2 and R3. Each section has a list of chemical structures on the right and a vertical column of checkboxes on the left. The R2 section contains five structures: a fluorine atom, a diene, a gem-difluoro ether, a trifluoromethyl group, and a diethylene glycol chain. The R3 section contains seven structures: a chlorine atom, a fluorine atom, a bromine atom, a methoxy group, a furan ring, a tetrahydrofuran ring, a tetrahydrofuran ring with a methyl group, and a diene. The interface includes window control icons (minimize, maximize, close) in the top right of each section.

**R2**

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**R3**

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2) Screenshot 2026-04-09 150033.png, downloaded 49 times

Scaffold	R1	R2	R3
	? /	?-F	?-O-CF3
	?-i-Pr	?-F	?-O-CF3
	?-Et	?-F	?-O-CF3
R2			