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Subject: How to enter custom core?

Posted by [Stacy R](#) on Fri, 18 May 2018 13:38:28 GMT

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I am new to using DataWarrior and have a question. I have a set of 100 compounds with activity data. The structures are fairly complex, but I want to analyze a pair of substituents by setting a defined core. Doing automatic SAR analysis selects one small ring of a larger substructure I want to use as a core. When I select Chemistry>Core-Based SAR Analysis the Structure column is the only one that can be selected. There is an area labelled "Define scaffold structures:" but there is no way to enter a structure or SMILES string. My question is: How can I enter the substructure I want to use as a Core? I am using DataWarrior4.7.2 on a Mac running MacOS 10.13.3. Thanks very much for any help.

Stacy

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Subject: Re: How to enter custom core?

Posted by [thomas](#) on Sat, 19 May 2018 15:09:22 GMT

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Hi Stacy, DataWarrior often uses the right mouse button for context specific functionality. When pressing that button within a main view or within the header of a main view, for instance, opens different popup menus. The structure list area beneath "Define scaffold structures" in another example. A popup gives you options to add individual sub-structures per editor, open structures from a file, save the list, etc.

On the Macintosh this may be less obvious, because many programs don't use the concept of a right mouse button. Depending on how your Mac is configured and whether you use a mouse or touchpad, you may press Ctrl-mouse, click the right bottom area of the touch pad, or something else. I have my MacBookPro setup to interpret right bottom area clicks on the touchpad as right mouse clicks.

Thomas

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