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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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