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Subject: Re: can you give an example on how to use refvalue()...

Posted by [chemist69](#) on Thu, 02 Jul 2015 07:07:39 GMT

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Dear Thomas,

thanks a lot for coming back to me, DataWarrior is a great project!  
refvalue takes four parameters. In the example that you give above, what would be the call to the function?

My concrete case involves a set of compounds which are categorized into scaffold fragments. Every compound belongs only to one fragment and the fragments are uniquely named and hierarchically dependent on each other:

| Hierarchy | scaf_smiles      | cpd_smiles                 | cpd_id | Activity |
|-----------|------------------|----------------------------|--------|----------|
| 12        | C1CC=CN1         | Cc1cc[nH]c1                | 1      | 5        |
| 12        | C1CC=CN1         | O=C(O)c1cc[nH]c1           | 2      | 7        |
| 012_013   | c1ccc2[nH]ccc2c1 | O=C(O)c1c[nH]c2ccccc12     | 3      | 6        |
| 012_013   | c1ccc2[nH]ccc2c1 | NC(=O)c1c[nH]c2ccccc12     | 4      | 8        |
| 012_013   | c1ccc2[nH]ccc2c1 | COc2ccc1[nH]cc(C(N)=O)c1c2 | 5      | 9        |

I would like to display the data in a tree-like way so that the scaffold fragments (column Hierarchy) are displayed as nodes and the individual compounds are leaves in the tree.  
Would that be possible?

Many thanks again for your help!

Kind regards,  
Axel

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