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

Posted by [chemist69](#) on Tue, 30 Jun 2015 14:40:40 GMT

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...in order to be able to create tree-like structures?

Many thanks in advance.

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

Posted by [thomas](#) on Wed, 01 Jul 2015 19:43:11 GMT

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could you please a little more specific with the question. I realize also that my description of the refvalue()

function is not really clear. I try again:

If a dataset has three columns:

'A' with some category assignments (e.g. and experiment date)

'B' with row specific IDs that are unique within every category, but repeat throughout the categories (e.g. compound IDs)

'C' any values, e.g. measured numerical values

If one compound with ID xxxx serves as a reference compound in all experiments and if we wanted to use its

measured value as a reference value to be used for all compounds in the same experiment, then we use the refvalue()

function.

I this what you had in mind?

Kind regards, Thomas

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

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

Posted by [thomas](#) on Thu, 02 Jul 2015 19:56:56 GMT

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Dear Axel,

the refvalue(ref-ID-column, category-column, value-column, ref-ID) syntax would be:
refvalue("B","A","C","xxxx")

Your second question is more difficult to answer: DataWarrior out-of-the-box doesn't have a simple solution.

But with a little programming it should be possible to even generate such a tree of hierarchical increasing scaffolds contained in a dataset and to attach all compounds as leaves.

Currently, DataWarrior does support graph data, which includes tree structures. Various functions generate

such data, e.g. the evolutionary library and most prominent the similarity analysis. Last week I used an

unpublished and still experimental extension to layout a graph from a few thousand diseases connected over

their similarities, which were estimated by commonly mentioned genes in the literature.

But DataWarrior does not allow from the user interface to define a column to contain references to other rows.

If you want to construct a dwar file from tabular data in a way that DataWarrior recognized graph relationships, then you have to do it manually. First you need a column with unique row identifiers.

Second you need another column that contains references of the respective row to one or more other rows.

This is done by putting unique IDs from the first row into the second one, one ID per reference, delimited

by "; ". Third you need to define the second row as 'referencing column' and state whether references are

bi-directional or only one way. This is done by adding column properties to the file; Example:

```
<columnName="child">
```

```
<columnProperty="refColumn ID">
```

```
<columnProperty="refType topdown">
```

I have created a small dwar file from your example that illustrates the options. The file contains three different tree views: one with static coordinates of all structures and two dynamic one, which always use the selected molecule as root, both use a kind of forcefield approach for the layout (circular and standard vertical tree)

Kind regards,

Thomas

File Attachments

1) [fragmentHierarchy.dwar](#), downloaded 1012 times

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

Posted by [chemist69](#) on Mon, 06 Jul 2015 12:22:39 GMT

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Dear Thomas,

thanks a lot for the extensive answer and the work you put into creating the extremely helpful example!!

This is exactly what I was looking for!

Kind regards,

Axel
