Subject: how to associate detail information
Posted by chemist69 on Thu, 09 Jul 2015 10:03:33 GMT
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Dear Thomas,

could you please give an example on how to associate detail information to a table, as in the flyingObjects example?
I have a ChEMBL data set and would like to associate the cells in the <Chembl_Id> column with a link to the compound on the ChEMBL website
(https://www.ebi.ac.uk/chembl/compound/inspect/<Chembl_Id>)

Many thanks in advance for your help.

Kind regards,
Axel

Subject: Re: how to associate detail information
Posted by thomas on Fri, 10 Jul 2015 21:08:06 GMT
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Dear Axel,

if I understand you correctly, the solution to your problem is probably more defining a lookup URL rather than using the detail mechanism. Usually, we use details internally at Actelion, when we have some biological results that are extracted from a non-alphanumerical raw data or if we have more detailed information in the database. Typically the raw data is some SVG, PNG or JPEG and
further information is in HTML, plain text. In these cases the DataWarrior file contains links to the detail source, e.g. an Oracle CLOB or BLOB column, or a web service. When moving the mouse over
the result, the detail is fetched on-the-fly and shown in the detail area. When saving the DataWarrior
file, one can retrieve all details and store them within the DataWarrior file (compressed and text encoded). Details are always shown within the DataWarrior application, e.g. in the detail area (bottom right) or as part of the form view. Image data and plain text are rendered reasonable well, but the Swing based HTML viewer is rather simple and does not render modern websites well.

The URL lookup mechanism does not render HTML within DataWarrior itself, but offers with a right
mouse click to open an external website in the default web browser. If you add three simple column
properties to a file that has a column with ChEMBL-IDs then you get a new option in the popup menu
for every row like 'Open ChEMBL Page of 123456 in Web Browser'. For this to work you need to add
the following lines to the column properties section of the dwar file:

<columnName="ChEMBL-ID">
<columnProperty="lookupURL0 https://www.ebi.ac.uk/chembl/compound/inspect/%s">
<columnProperty="lookupName0 ChEMBL Page">
<columnProperty="lookupCount 1">

The DataWarrior upgrade, which is due very soon, will use this mechanisms for Wikipedia compound search and ChEMBL database access.

Hope this helps,

Thomas

Subject: Re: how to associate detail information
Posted by chemist69 on Mon, 13 Jul 2015 14:57:55 GMT
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Dear Thomas,

many thanks again for your help.

What you desctribe is exactly what I was looking for. However, when I try your example with the columnProperty lines, the .dwar file is not loaded and Java throws the following error:

java.lang.StringIndexOutOfBoundsException: String index out of range: -95
    at java.lang.String.substring(String.java:1955)
    at com.actelion.research.c.u.a(Unknown Source)
    at com.actelion.research.c.u.run(Unknown Source)
    at java.lang.Thread.run(Thread.java:745)

When I rename Chembl-Id to ChemblId, then the index is out of range at -94, etc.

Kind regards,
Axel

Subject: Re: how to associate detail information
Posted by thomas on Thu, 23 Jul 2015 06:24:38 GMT
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Dear Axel,

can you send me a sample file that produces the error? Ideally to my mail address shown on this page: http://openmolecules.org/about.html.

Kind regards,

Thomas

Subject: Re: how to associate detail information
Posted by chemist69 on Wed, 19 Aug 2015 07:17:38 GMT
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Dear Thomas,

could you make something out of the file that I sent you ?

Kind regards,
Axel

Subject: Re: how to associate detail information
Posted by thomas on Thu, 20 Aug 2015 19:02:57 GMT
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Dear Axel,

I may appologize, because I could not find your mail with the file. Can you please send it again or maybe upload it to the forum?

Kind regards, Thomas

Subject: Re: how to associate detail information
Posted by chemist69 on Mon, 07 Sep 2015 09:28:25 GMT
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Dear Thomas,

now it's my turn to apologize. I completely lost this out of focus, but I would still be interested in your help on this issue. I have mailed you the file again, I hope, it's not ending up in your spam filter.

Kind regards,
Axel