Subject: Defining columntype while appending columns
Posted by helloWorld22 on Thu, 15 Feb 2024 15:25:54 GMT
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Hi,
In DW SDK, while I want to define a columntype after initializing new columns, it is throwing exception.

firstNewColumn = dwInterface.initializeNewColumns(result.get(t).toArray(new String[0]));
dwInterface.setColumnType(firstNewColumn,
IPluginHelper.COLUMN_TYPE_STRUCTURE_FROM_SMILES);

The logic is to check if the new column added has a column header "SMILES", if so, then append the column as COLUMN_TYPE_STRUCTURE_FROM_SMILES.

It works fine when setColumnType is not used. But smiles are shown as String and not structure.

The exception occurs in line
dwInterface.setColumnType(firstNewColumn,
IPluginHelper.COLUMN_TYPE_STRUCTURE_FROM_SMILES);
as nullpointer exception.

The exception occurs in com.actelion.research.datawarrior.plugin.PluginHelper line:
mCoordinateColumn[column] = mTargetTableModel.addNewColumns(1);

Since mCoordinateColumn is not set in initializeNewColumns, it is throwing nullpointer exception.

Is it possible to set up a column type while appending column?

Subject: Re: Defining columntype while appending columns
Posted by nbehrnd on Fri, 16 Feb 2024 05:33:07 GMT
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Hi helloworld22,

because a SMILES string is a sequence of printable characters, why wouldn't a new colum of type `text` defined via the GUI fit your needs here?

Regards,

Norwid

Subject: Re: Defining columntype while appending columns
Posted by helloWorld22 on Mon, 19 Feb 2024 09:58:24 GMT
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Hi Norwid,
The requirement is to add columns containing structures and my plugin retrieves the structures(SMILES or Mol File) from our internal database.
I can now append the column as a text as smiles. But I cant convert them as a structure. Unless I convert them as a structure column, I wont be able to do structure search on the existing data.

I tried : dwInterface.setColumnType and added IPluginHelper.COLUMN_TYPE_STRUCTURE_FROM_SMILES. But this doesnot work while appending column.

Is it possible to append column via SDK as structure and not text? I can also retrieve mol files, instead of SMILES, from DB, if that helps.

Thanks

Subject: Re: Defining columntype while appending columns
Posted by nbehrnd on Tue, 20 Feb 2024 05:52:20 GMT
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Hello helloWorld22,
I don't know if this is possible.
Norwid

Subject: Re: Defining columntype while appending columns
Posted by helloWorld22 on Tue, 20 Feb 2024 08:54:17 GMT
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Is it possible to make it available in the next release of SDK?
