
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.setColumnTypes(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.setColumnTypes(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 column 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 can't convert them as a structure. Unless I convert them as a structure column, I won't be able to do structure search on the existing data.

I tried : `dwInterface.setColumnType` and added `IPluginHelper.COLUMN_TYPE_STRUCTURE_FROM_SMILES`. But this does not 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?
