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