Subject: Re: Defining columntype while appending columns Posted by helloWorld22 on Mon, 19 Feb 2024 09:58:24 GMT View Forum Message <> Reply to Message

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

Page 1 of 1 ---- Generated from openmolecules.org Forum