Subject: Create structure image (idcode) from pasted SMILES
Posted by chemtv on Wed, 28 Jan 2026 20:26:17 GMT

Hello,

I want to paste a new structure with data into a large existing datawarrior file. I created a new empty row and pasted in the name, SMILES, IC50, etc, into the appropriate columns, but I can't get datawarrior to calc/show the structure (idcode) for the new smiles I pasted in. Is there a way to force dw to calc the idcode in the existing dw file?
BTW I did try this... I read the smiles file into an empty dw sheet and copied the idcode and was able to paste that into my other existing file, which seemed to work but is kludgy. Can't we force dw to calc/recalc the idcodes for a column of smiles?

Thanks,
Greg

Subject: Re: Create structure image (idcode) from pasted SMILES
Posted by nbehrnd on Wed, 28 Jan 2026 21:34:54 GMT

Hello Greg,

when pasting data into DataWarrior via Edit -> Paste Special -> New From Data With Header Row, the individual columns in the raw data to be copied need to be tabulator separated. As an illustration, see the attached .gif with a few dummy data. To let this work, it however was necessary to adjust the editor's preferences; pressing the tabulator key should not be converted into spaces. Here, this indicated by pale arrows of varying width between the columns.

On the other hand, if data are comma separated, it is better to save these into a .csv with subsequent access by File -> Open.

Best regards,

Norwid

Setup used: DW 06.05.02 published by September 8th, 2025 in an instance of Linux Debian

File Attachments
1) 2026-01-28_DW_copy_paste.gif, downloaded 141 times

DataWarrior

File Edit Data Chemistry Database List Macro Help

Column Name

58 of 512 MB   Selected: Visible: Total: