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

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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