Subject: Fragment cannot be converted to 2D structural
Posted by dreamfly on Tue, 03 Aug 2021 03:28:42 GMT
View Forum Message <> Reply to Message

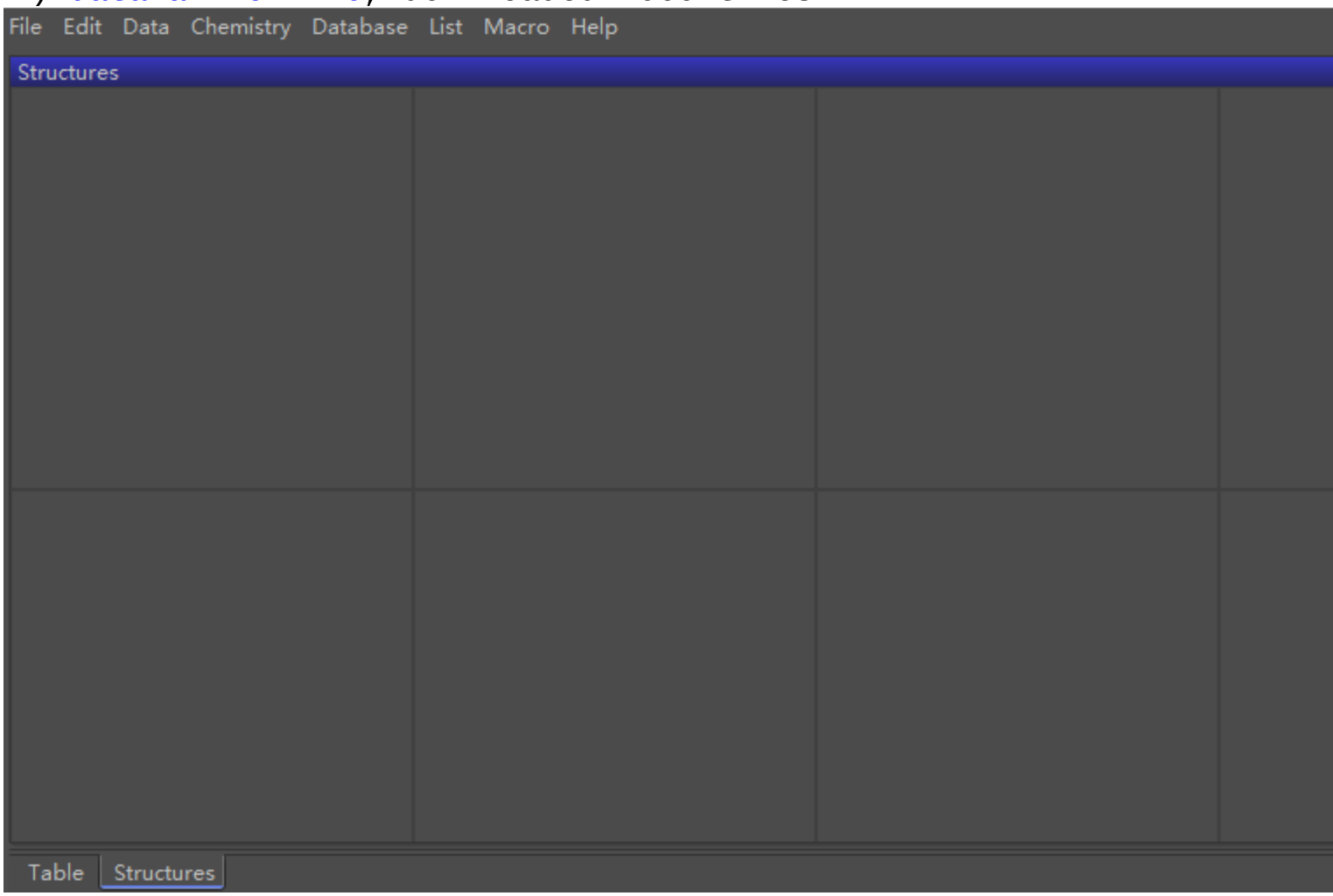
Hi,
When I converted fragment to 2D structural,the cell was blank. But the fragment can be converted to 2D structural rightly in the MarvinSketch19.21.The fragment smiles is "[*:1]Nc1cnc(OC)cc1C(=O)NC" and I've attached images of the error.

Thanks in advance!

Dreamfly

File Attachments

1) datawarrior.PNG, downloaded 1060 times



Subject: Re: Fragment cannot be converted to 2D structural
Posted by thomas on Thu, 19 Aug 2021 18:27:56 GMT
View Forum Message <> Reply to Message

till recently DataWarrior didn't support SMARTS features and it will never fully implements SMARTS, because some of DataWarrior's query features cannot be expressed in SMARTS and some SMARTS query features are not compatible with DataWarrior. However, very recently DataWarrior's SMILES support was extended to some SMARTS features. Soon exclude groups will be translated into negated recursive SMARTS. This will also work backwards.

When pasting your example "[*:1]Nc1cnc(OC)cc1C(=O)NC" into the DataWarrior 5.5.0, then I get one row with structure. If I paste it into the editor, then it is also correctly translated into a substructure with the exception that the ':'-bond converted into a single bond. With the SMARTS support ':'-bonds will be translated into an 'aromatic' bond query feature.

Expect this to happen very soon...

Thomas