
Subject: Chemical Structure copy/paste issue for Linux v4.7.2

Posted by [bruno.b](#) on Mon, 19 Mar 2018 13:46:29 GMT

[View Forum Message](#) <> [Reply to Message](#)

I was very happy to see that the latest version support copy&paste and drag&drop.
I tried to paste a MOL, SMILES and IDCOD. Unfortunately, it does not work with MOL and SMILES. I am not sure this is a bug.

Here are the messages from the console:

GetClipboardData MDLCT

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Reaction

GetClipboardData MDL_MOL

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Reaction

GetClipboardData MDLSK

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Reaction

GetClipboardData MDLSK_EMBEDDED

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Reaction

GetClipboardData IDCOD

Pasted string 'VitC

```
13 13 0 0 1 0 0 0 0 0 1 V2000
 7.8349  6.8596  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 8.5487  6.4458  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 7.8349  7.6825  0.0000 O  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 9.2625  6.8596  0.0000 O  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 7.3256  5.0000  0.0000 O  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 5.5365  5.0068  0.0000 O  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 5.0000  6.7027  0.0000 O  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 7.1210  6.4458  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 6.8528  5.6752  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 6.4686  6.9505  0.0000 O  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 6.0230  5.6752  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 5.7843  6.4458  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
7.7507 5.9162 0.0000 H 0 0 0 0 0 1 0 0 0 0 0 0
1 2 1 0 0 0 0
1 3 1 1 0 0 0
1 8 1 0 0 0 0
2 4 1 0 0 0 0
5 9 1 0 0 0 0
6 11 1 0 0 0 0
7 12 2 0 0 0 0
8 9 1 0 0 0 0
8 10 1 0 0 0 0
8 13 1 1 0 0 0
9 11 2 0 0 0 0
10 12 1 0 0 0 0
11 12 1 0 0 0 0
M END
$$$$
'
```

returned Mol is null

Pasting a SMILES does not work:

GetClipboardData ACT_MOLECULE

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Reaction

Mol is null

GetClipboardData MDLCT

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Reaction

GetClipboardData MDL_MOL

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Reaction

GetClipboardData MDLSK

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion Reaction

GetClipboardData MDLSK_EMBEDDED

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Reaction

GetClipboardData IDCODE

Pasted string '[C@@H](CO)(O)[C@]1([H])C(O)=C(O)C(=O)O1'

NativeClipboardAccessor.pasteMolecule(): Exception java.lang.ArrayIndexOutOfBoundsException
returned Mol is null

Pasting an IDCODE works:

GetClipboardData ACT_MOLECULE

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Reaction

Mol is null

GetClipboardData MDLCT

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Reaction

GetClipboardData MDL_MOL

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Reaction

GetClipboardData MDLSK

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Reaction

GetClipboardData MDLSK_EMBEDDED

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Molecule

Exception in getClipboardData: java.awt.datatransfer.UnsupportedFlavorException: Actelion

Reaction

GetClipboardData IDCODE

Pasted string 'dcLF@@Rag\bbTVTILuSUTaSh@'

returned Mol is com.actelion.research.chem.StereoMolecule@7e9cbe66

Best regards,

Bruno

Subject: Re: Chemical Structure copy/paste issue for Linux v4.7.2

Posted by [thomas](#) on Sat, 21 Apr 2018 20:42:38 GMT

[View Forum Message](#) <> [Reply to Message](#)

Dear Bruno,

thank you for the suggestion. Indeed, it is not a bug. Pasting a SMILES or molfile is currently not supported. However, I have updated the clipboard handling code to automatically check for smiles and molfiles and convert, if possible. In addition I am looking into name to structure. IUPAC name to structure would be possible via the OPSIN library, other compound names would require a dictionary, which would make the DataWarrior installation substantially larger. I could use my name2structure remote service, but for privacy reasons should ask in advance, whether DataWarrior may send the name out to a server. I will think of a solution...

Regards, Thomas
