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 IDCODE. 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 IDCODE
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
    8.5487    6.4458    0.0000 C   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
    9.2625    6.8596    0.0000 O   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
    5.5365    5.0068    0.0000 O   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
    7.1210    6.4458    0.0000 C   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
    6.4686    6.9505    0.0000 O   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
    5.7843    6.4458    0.0000 C   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