
Subject: Re: DWAR file format

Posted by [thomas](#) on Sat, 09 Mar 2019 20:33:06 GMT

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

you could use something like the following Java method, which reads conformers from an SD-File, creates a CompoundTableModel, populates it with the conformers, and uses a CompoundTableSaver to write the table model into a native DataWarrior file.

If you need to write much larger files, this method may not be the appropriate approach, because of the large memory footprint. I suggest that you contact me on my idorsia e-mail address (see openmolecules.org about page) to find an optimal solution.

(the following depends on some files of the DataWarrior source code):

```
public static void createConformerDWARDemo() {
    final int ROW_COUNT = 1000;

    CompoundTableModel tableModel = new CompoundTableModel();
    tableModel.initializeTable(ROW_COUNT, 3);

    // this is a hack to prevent nullpointer exception and won't be necessary in the future
    tableModel.setDetailHandler(new CompoundTableDetailHandler(tableModel));

    final String IDENTIFIER_COLUMN_NAME = "ID";
    final String STRUCTURE_COLUMN_NAME = "Structure";

    // first column will contain the structure name/ID
    tableModel.setColumnName(IDENTIFIER_COLUMN_NAME, 0);

    // define second column to contain idcodes
    tableModel.setColumnName(STRUCTURE_COLUMN_NAME, 1);
    tableModel.setColumnProperty(1, CompoundTableConstants.cColumnPropertySpecialType,
    CompoundTableConstants.cColumnTypeIDCode);

    // define third column to contain the 3D-coordinates and make it a child of the structure column
    tableModel.setColumnName(CompoundTableConstants.cColumnType3DCoordinates, 2);
    tableModel.setColumnProperty(2, CompoundTableConstants.cColumnPropertySpecialType,
    CompoundTableConstants.cColumnType3DCoordinates);
    tableModel.setColumnProperty(2, CompoundTableConstants.cColumnPropertyParentColumn,
    STRUCTURE_COLUMN_NAME);

    // read some molecules from an SD-File that should contain 3-dimensional atom coordinates
    SDFFileParser parser = new SDFFileParser("someFileName.sdf");
    for (int row=0; row<ROW_COUNT && parser.next(); row++) {
        StereoMolecule mol = parser.getMolecule();
```

```

Canonizer canonizer = new Canonizer(mol);
String id = "ID-"+(row+1);
String idcode = canonizer.getIDCode();
String coords = canonizer.getEncodedCoordinates();

tableModel.setTotalValueAt(id, row, 0);
tableModel.setTotalValueAt(idcode, row, 1);
tableModel.setTotalValueAt(coords, row, 2);
}
    tableModel.finalizeTable(CompoundTableEvent.cSpecifierNoRuntimeProperties, null);

// the new JFrame() is also a hack, which can be replaced by null very soon
CompoundTableSaver saver = new CompoundTableSaver(new JFrame(), tableModel, null);
saver.saveNative(null, new File("someFileName.dwar"), false, false);
}

```
