Subject: Re: DWAR file format
Posted by thomas on Sat, 09 Mar 2019 20:33:06 GMT
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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.cColumnType3 DCoordinates, 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
  SDFileParser parser = new SDFileParser("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.cSpecifierNoRunt imeProperties, 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);
}
```