chem-bla-ics

The CDK data classes and change notifications

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ZCBjaGFuZ2Ugbm90aWZpY2F0aW9ucy4gPGk+Q2hlbS1ibGEtaWNzPC9pPi4gaHR0cHM6Ly9kb2ku
b3JnLzEwLjU5MzUwLzN4c20wLWJ0NDc4

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Abstract

The data classes of the Chemistry Development Kit are mutable, unlike those of Octet. This means that other classes may need to respond when the content updates. For example, a render class. CDK's ChemObject provides a notifyChanged() and addListener() methods for this.

The data classes of the Chemistry Development Kit are mutable, unlike those of Octet. This means that other classes may need to respond when the content updates. For example, a render class. CDK's ChemObject provides a `notifyChanged()` and `addListener()` methods for this. However, as was recently pointed out, while this is useful in editors, such as JChemPaint, this is a performance killer in high-throughput sitations, such as descriptor calculation, or structure diagram generation runs.

To address this, the IChemObject interface has been extended with the methods `setNotification(boolean)` and `getNotification()`, which allow to temporarily disable change notifications. There are no helper methods yet to disable it for a complete data structure, like `ChemModelManipulator.setNotification(ChemModel, boolean)`, but I expect these to be written soon.

Alternatively, special data classes may be used if notification is never needed for a special setup, for example, in case the QSAR descriptor calculation. In such cases, the new NoNotificationChemObjectBuilder can be used:

```
IChemObjectReader reader = new MDLReader(new FileInputStream(new
File("some.mol")));
IChemObjectBuilder builder = NoNotificationChemObjectBuilder.getInstance();
IMolecule molecule = reader.read(builder.newMolecule());
// then perform some operation in which the molecule changes a lot
```

The advantage is that you do not have to manually disable notification for each class you instantiate. This should give a considerable speed up, and I hope soon to give some statistics.