

The CDK data classes and change notifications

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Published April 12, 2006

Citation

Willighagen, E. (2006). The CDK data classes and change notifications. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/3xsm0-bt478>

Keywords

Cdk, Cheminf, Jchempaint

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chem-bla-ics

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 situations, 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.