chem-bla-ics

Finding differences between IChemObjects #2

Egon Willighagen

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Abstract
CDK QSAR descriptors are not allowed to change the input [molecule|atom|bond], and I recently added a unit tests (rev 11138) for that to the abstract class AtomicDescriptorTest.

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CDK QSAR descriptors are not allowed to change the input [molecule|atom|bond], and I recently added a unit tests (rev 11138) for that to the abstract class AtomicDescriptorTest.

After some code clean up of the diff module code earlier this morning (in anticipation of the rain stopping), I applied this patch (rev 11269) that `noModification` unit test:

```
 public void testCalculate_NoModifications() throws Exception {
   IAtomContainer mol = someoneBringMeSomeWater();
   IAtom atom = mol.getAtom(1);
-  String priorString = atom.toString();
+  IAtom clone = (IAtom)mol.getAtom(1).clone();
   descriptor.calculate(atom, mol);
-  String afterString = atom.toString();
+  String diff = AtomDiff.diff(clone, atom);
   assertEquals(
-    "The descriptor must not change the passed bond in any respect.",
-    priorString, afterString
+    "The descriptor must not change the passed bond in any respect, but found
this diff: " + diff,
+    0, diff.length()
   );
 }
```

This is a nice example of where the new diff module is useful. Instead of dumping to long IAtom.toString()s, the output now gives output like:

```
AtomDiff(AtomTypeDiff(, NULL/H, NC:0/1, V:0/1))
```

This indicates (yes, a bit cryptic) that the formal neighbor count (NC) and the valence (V) fields have been modified, in addition to that first field, which I don't know what it refers too. Indeed, the output still needs a bit more tuning :)