chem-bla-ics

Creating CMLReact from UsefulChem Ugi Reactions

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Cml, Cdk, Inchi

Abstract
Cameron, Jean-Claude and I were invited to Peter's place in Cambridge, where we are now hacking on CMLReact for the Ugi reactions Jean-Claude has been working on. I just finished a script that uses the CDK and Sam's interface to the InChI library to convert a list of four reactants and one Ugi product into CMLReact (doi:10.1021/ci0502698). The full BeanShell script looks like:

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Cameron, Jean-Claude and I were invited to Peter's place in Cambridge, where we are now hacking on CMLReact for the Ugi reactions Jean-Claude has been working on. I just finished a script that uses the CDK and Sam's interface to the InChI library to convert a list of four reactants and one Ugi product into CMLReact (doi:10.1021/ci0502698). The full BeanShell script looks like:

```
#!/usr/bin/bsh

import java.io.File;
import java.io.FileReader;
import java.io.BufferedReader;

import org.openscience.cdk.*;
import org.openscience.cdk.exception.*;
import org.openscience.cdk.inchi.*;
import org.openscience.cdk.interfaces.*;
import org.openscience.cdk.io.CMLWriter;

import org.openscience.cdk.libio.cml.Convertor;
import org.xmlcml.cml.element.CMLReaction;

import net.sf.jniinchi.INCHI_RET;

InChIGeneratorFactory factory = new InChIGeneratorFactory();
// Get InChIToStructure

File file = new File("inchi.ugi.txt"); // five inchis expected, last being the
product
BufferedReader reader = new BufferedReader(new FileReader(file));

String first = reader.readLine();
String second = reader.readLine();
String third = reader.readLine();
String fourth = reader.readLine();
String product = reader.readLine();

System.out.println("First: " + first);
IMolecule firstAC;
{
  InChIToStructure intostruct = factory.getInChIToStructure(first,
DefaultChemObjectBuilder.getInstance());

  INCHI_RET ret = intostruct.getReturnStatus();
```

```
  if (ret == INCHI_RET.WARNING) {
    // Structure generated, but with warning message
    System.out.println("InChI warning: " + intostruct.getMessage());
  } else if (ret != INCHI_RET.OKAY) {
    // Structure generation failed
    throw new CDKException("Structure generation failed failed: " +
ret.toString()
      + " [" + intostruct.getMessage() + "]");
  }

  firstAC = new Molecule(intostruct.getAtomContainer());
}

System.out.println("Second: " + second);
IMolecule secondAC;
{
  InChIToStructure intostruct = factory.getInChIToStructure(second,
DefaultChemObjectBuilder.getInstance());

  INCHI_RET ret = intostruct.getReturnStatus();
  if (ret == INCHI_RET.WARNING) {
    // Structure generated, but with warning message
    System.out.println("InChI warning: " + intostruct.getMessage());
  } else if (ret != INCHI_RET.OKAY) {
    // Structure generation failed
    throw new CDKException("Structure generation failed failed: " +
ret.toString()
      + " [" + intostruct.getMessage() + "]");
  }

  secondAC = new Molecule(intostruct.getAtomContainer());
}

System.out.println("Third: " + third);
IMolecule thirdAC;
{
  InChIToStructure intostruct = factory.getInChIToStructure(third,
DefaultChemObjectBuilder.getInstance());

  INCHI_RET ret = intostruct.getReturnStatus();
  if (ret == INCHI_RET.WARNING) {
    // Structure generated, but with warning message
    System.out.println("InChI warning: " + intostruct.getMessage());
  } else if (ret != INCHI_RET.OKAY) {
```

```
    // Structure generation failed
    throw new CDKException("Structure generation failed failed: " +
ret.toString()
      + " [" + intostruct.getMessage() + "]");
  }

  thirdAC = new Molecule(intostruct.getAtomContainer());
}

System.out.println("Fourth: " + fourth);
IMolecule fourthAC;
{
  InChIToStructure intostruct = factory.getInChIToStructure(fourth,
DefaultChemObjectBuilder.getInstance());

  INCHI_RET ret = intostruct.getReturnStatus();
  if (ret == INCHI_RET.WARNING) {
    // Structure generated, but with warning message
    System.out.println("InChI warning: " + intostruct.getMessage());
  } else if (ret != INCHI_RET.OKAY) {
    // Structure generation failed
    throw new CDKException("Structure generation failed failed: " +
ret.toString()
      + " [" + intostruct.getMessage() + "]");
  }

  fourthAC = new Molecule(intostruct.getAtomContainer());
}

System.out.println("Product: " + product);
IMolecule productAC;
{
  InChIToStructure intostruct = factory.getInChIToStructure(product,
DefaultChemObjectBuilder.getInstance());

  INCHI_RET ret = intostruct.getReturnStatus();
  if (ret == INCHI_RET.WARNING) {
    // Structure generated, but with warning message
    System.out.println("InChI warning: " + intostruct.getMessage());
  } else if (ret != INCHI_RET.OKAY) {
    // Structure generation failed
    throw new CDKException("Structure generation failed failed: " +
ret.toString()
      + " [" + intostruct.getMessage() + "]");
```

```
  }

  productAC = new Molecule(intostruct.getAtomContainer());
}

IReaction ugiReaction = new Reaction();
ugiReaction.addReactant(firstAC);
ugiReaction.addReactant(secondAC);
ugiReaction.addReactant(thirdAC);
ugiReaction.addReactant(fourthAC);
ugiReaction.addProduct(productAC);

StringWriter stringWriter = new StringWriter();
CMLWriter cmlWriter = new CMLWriter(stringWriter);

cmlWriter.write(ugiReaction);
cmlWriter.close();
System.out.println(stringWriter.toString());
```

My apologies for the code duplication, but never tried inline functions in BeanShell yet... You can monitor the efforts at Google Docs.