Getting Started with libSBOLj 2.0

This beginner's guide introduces the creation and use of TopLevel SBOL 2.0 objects using libSBOLj 2.0. This guide is not meant to be a comprehensive documentation of the library but rather a simple introduction to the basic methods available. In particular, this document demonstrates the usage of the library's API through the creation of ComponentDefinition and Sequence entities for part of a genetic inverter. A similar approach can be taken for the other SBOL 2.0 TopLevel objects, such as ModuleDefinition, Model, Collection, and GenericTopLevel. Readers who are not familiar with Java are recommended to use other resources to learn about its basics.

Creating an SBOL Document

An SBOLDocument object is a container for TopLevel data objects. Therefore, the first step is to create an SBOLDocument to put our TopLevel objects into. This can be done by calling the SBOLDocument constructor as shown below.

```
String prURI="http://partsregistry.org";
SBOLDocument document = new SBOLDocument();
document.setDefaultURIprefix(prURI);
document.setTypesInURIs(true);
document.setComplete(true);
document.setCreateDefaults(true);
```

The method setDefaultURIprefix sets the default URI prefix to the value defined by the prURI string. All data objects created following this statement carry this default URI prefix. If we want to allow all top-level identity URIs to include their types, then we can call document.setTypesInURIs(true). The document.setComplete(true) statement sets the "complete" flag to true for the given document. It means that any URIs that cannot be dereferenced to a valid object in the current SBOLDocument object cause an exception to be thrown. Finally, the document.setCreateDefaults(true) statement sets the "createDefaults" flag to true for the given document. It means that when an object that must reference a ComponentInstance object cannot find the component, but it can find a ComponentDefinition object with the same displayId that it creates a default ComponentInstance object with this displayId and references it.

Creating SBOL Data Objects

The next step is to create TopLevel objects. All create methods take as parameters an optional URI prefix String, a display id String, and an optional version String. Each create method also has parameters for each required element of a TopLevel object. For a ComponentDefinition, the only required element is a set of type URIs. The code below creates ComponentDefinition objects for a promoter repressed by TetR, a coding sequence for the LacI repressor protein, and a cassette that includes them both. The types property creates a set of URIs to specify the biochemical or physical entity for each ComponentDefinition, which, in this case, is a double-stranded DNA. The first URI ComponentDefinition.DNA is a BioPAX ontology term defined as a constant in the ComponentDefinition class. The second URI is a Chemical Entities of Biological Interest (ChEBI) term specified by the given URI. Since only the display id is provided to the create functions below, the default URI prefix is used and no version is set.

The create sequence methods take an optional URI prefix String, a display id String, an optional version String, a String providing the elements of the sequence, and a URI specifying the encoding used by the sequence. The code below creates sequences for the TetR repressible promoter and LacI coding sequence.

```
Sequence seq_187 = document.createSequence(
                   "seq_187",
                   "tccctatcagtgatagagattgacatccctatcagtgatagagatactgagcac",
                  Sequence. IUPAC_DNA
String element2 = "atggtgaatgtgaaaccagtaacgttatacgatgtcgcagagtatgccggtgtc"
          + \ "tcttatcagaccgtttcccgcgtggtgaaccaggccacgtttctgcgaaaacgcggga"
          + \ \ "aaaagtggaagcggatggcggagctgaattacattcccaaccgcgtggcacaacaactgg"
          + "cgggcaaacagtcgttgctgattggcgttgccacctccagtctggccctgcacgcgccgtcg
          + \ \ "caa attgtcgcggcgattaaatctcgcgccgatcaactgggtgccagcgtggtggtgtcgat"
           + "ggtagaacgaagcggcgtcgaagcctgtaaagcggcggtgcacaatcttctcgcgcaacgcg"
          + \ "tcagtgggctgatcattaactatccgctggatgaccaggatgccattgctgtggaagctgcc"
          + \ "tgcactaatgttccggcgttatttcttgatgtctctgaccagacacccatcaacagtattat"
          + \ "tttctcccatgaagacggtacgcgactgggcgtggagcatctggtcgcattgggtcaccagc"
          + "cataaatatctcactcgcaatcaaattcagccgatagcggaacgggaaggcgactggagtgc"
          + \ " \verb|catgtccggttttcaacaaaccatgcaaatgctgaatgagggcatcgttcccactgcgatgc" \\
          + "tggttgccaacgatcagatggcgctgggcgcaatgcgcgccattaccgagtccgggctgcgc"
          + "gttggtgcggatatctcggtagtgggatacgacgataccgaagacagctcatgttatatccc"
          + "gccgttaaccaccatcaaacaggattttcgcctgctggggcaaaccagcgtggaccgcttgc"
           + "tgcaactctctcagggccaggcggtgaagggcaatcagctgttgcccgtctcactggtgaaa"
          + \ \ "agaaaaaccaccctggcgcccaatacgcaaaccgcctctccccgcgcgttggccgattcatt"
          + "aatgcagctggcacgacaggtttcccgactggaaagcgggcaggctgcaaacgacgaaaact"
          + "acgctttagtagcttaataa";
Sequence seq_153 = document.createSequence(
                  "seq_153",
                  element2,
                  Sequence.IUPAC_DNA
                  );
```

Setting and Editing Optional Fields

Next, we set and edit the optional fields for the TopLevel objects. For any optional field that is not a set or list, the library provides methods to set its value, unset its value, and check its value. The only exceptions where these methods are not available are the following three fields in the Identified class: persistentIdentity, displayId, and version. These fields cannot be edited, since they are crucial to maintaining compliant SBOL objects (see Section 11.2 "Compliant SBOL Objects" of the Specification (Data Model 2.0) for more details). The example code below first sets the name and description of the TetR repressible promoter and LacI repressor. Next, it checks if the name is set for TetR_promoter, then unsets it, and sets it to a new name.

```
TetR_promoter.setName("p tetR");
LacI_repressor.setName("lacI");
TetR_promoter.setDescription("TetR repressible promoter");
LacI_repressor.setDescription("lacI repressor from E. coli (+LVA)");
if (TetR_promoter.isSetName()) {
    TetR_promoter.unsetName();
    TetR_promoter.setName("p(tetR)");
}
```

For an optional field that is either a list or a set, the library provides methods for adding, removing, and checking if an element is contained in the list or set. The code below first adds roles to the TetR_promoter and LacI_repressor using constants in the SequenceOntology class that indicates that they are a promoter and coding sequence respectively. Next, it adds a second role to TetR_promoter, checks if the role is contained in the set of roles, then removes the role.

```
TetR_promoter.addRole(SequenceOntology.PROMOTER);
LacI_repressor.addRole(SequenceOntology.CDS);
URI TetR_promoter_role2 = URI.create("http://identifiers.org/so/SO:0000613");
TetR_promoter.addRole(TetR_promoter_role2);
if (TetR_promoter.containsRole(TetR_promoter_role2)) {
         TetR_promoter.removeRole(TetR_promoter_role2);
}
```

Fields that are a list or set of objects also include operations to clear, get, and set them. The example code below removes all roles at once by calling clearRoles(), gets the set of roles for the TetR_promoter, and checks if it is empty. Finally, it sets the entire set of roles (replacing any existing set) by calling setRoles(Set<URI> roles).

Creating and Editing References

TopLevel objects can refer to other TopLevel objects. For example, a ComponentDefinition object can refer to one or more sequences. This reference is created by calling the addSequence(URI) method. Note that since the "complete" flag is set to true, the library verifies that all objects referenced are present in this document. Methods available for manipulating references are similar to those for the optional fields. The code below adds one sequence for each of the ComponentDefinition objects, and then deletes all references for pikeleftCassette. Finally, if we include the last line, an exception is thrown because a sequence with the specified URI cannot be found.

```
TetR_promoter.addSequence(seq_187);
LacI_repressor.addSequence(seq_153);
pIKELeftCassette.addSequence(seq_187);
pIKELeftCassette.clearSequences();
//pIKELeftCassette.addSequence(
// URI.create("http://partsregistry.org/seq/partseq_154"));
```

Creating and Editing Child Objects

The ModuleDefinition and ComponentDefinition objects have child objects that can be created and edited. The code below creates a child object for pIKELeftCassette. Namely, it creates a child SequenceConstraint object that says the TetR_promoter precedes the LacI_repressor. A sequence constraint has a "subject" and an "object" reference that point to two different Component objects. They do not currently exist in our document and need to be created. With the "createDefaults" flag set to true, creation of these components is done automatically. Each component created has the same displayId as its corresponding ComponentDefinition object. They are added to pIKELeftCassette's set of components. This can be verified by calling the getComponent method. Finally, if we include the last line, it causes an exception, since the component being removed is used by a sequence constraint.

```
pIKELeftCassette.createSequenceConstraint(
    "pIKELeftCassette_sc",
    RestrictionType.PRECEDES,
    TetR_promoter.getDisplayId(),
    LacI_repressor.getDisplayId()
    );
if (pIKELeftCassette.getComponent("BBa_R0040")==null) {
    System.out.println("TetR_promoter component is missing");
}
if (pIKELeftCassette.getComponent("BBa_C0012")==null) {
    System.out.println("LacI_repressor component is missing");
}
//pIKELeftCassette.removeComponent(
// pIKELeftCassette.getComponent("BBa_R0040"));
```

Copying Objects

Finally, the library can make copies of TopLevel objects using the createCopy methods. There are several variations of this method. If only the object is provided, an identical copy is created. Note that this will cause an exception if it is copied into the same document, since it will not have a unique identity. Next, a new display id can be provided, which results in a copy with the display ids (and identities) updated accordingly. Similarly, a version can be provided as well, which results in a copy with the version (and identities) updated accordingly. Finally, a new URI prefix can also be provided, once again resulting in updated identities. The example below makes a copy of the TetR_promoter object by calling createCopy with a new display id, BBa_K137046. The identity URI for TetR_promoter_copy is changed to include the new display id, and this change also percolates through the identity URIs for any descendent objects. This example gives the new copy a new sequence, but it keeps all other properties the same.

The example used throughout this tutorial is listed as "GettingStartedExample.java" in the libSBOLj 2.0 examples directory. The RDF serialization for this example is shown below.

```
<?xml version="1.0" ?>
<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:dcterms="http://purl.org/dc/terms/" xmlns:prov="http://www.w3.org/ns/prov#"
    xmlns:sbol="http://sbols.org/v2#">
  <sbol:ComponentDefinition rdf:about="http://partsregistry.org/BBa_K137046">
   <sbol:persistentIdentity rdf:resource="http://partsregistry.org/BBa_K137046"/>
    <sbol:displayId>BBa_K137046</sbol:displayId>
    <prev:wasDerivedFrom rdf:resource="http://partsregistry.org/cd/BBa_R0040"/>
   <dcterms:title>p(tetR)</dcterms:title>
    <dcterms:description>TetR repressible promoter</dcterms:description>
   <sbol:type rdf:resource="http://identifiers.org/chebi/CHEBI:4705"/>
    <sbol:type rdf:resource="http://www.biopax.org/release/biopax-level3.owl#DnaRegion"/>
    <sbol:role rdf:resource="http://identifiers.org/so/S0:0000167"/>
    <sbol:sequence rdf:resource="http://partsregistry.org/seq/partseq_187"/>
    <sbol:sequence rdf:resource="http://partsregistry.org/seq/seq_K137046"/>
  </sbol:ComponentDefinition>
  <sbol:ComponentDefinition rdf:about="http://partsregistry.org/cd/BBa_C0012">
   <sbol:persistentIdentity rdf:resource="http://partsregistry.org/cd/BBa_C0012"/>
   <sbol:displayId>BBa_C0012</sbol:displayId>
    <dcterms:title>lacI</dcterms:title>
   <dcterms:description>lacI repressor from E. coli (+LVA)</dcterms:description>
    <sbol:type rdf:resource="http://identifiers.org/chebi/CHEBI:4705"/>
    <sbol:type rdf:resource="http://www.biopax.org/release/biopax-level3.owl#DnaRegion"/>
    <sbol:role rdf:resource="http://identifiers.org/so/S0:0000316"/>
    <sbol:sequence rdf:resource="http://partsregistry.org/seq/partseq_153"/>
  </sbol:ComponentDefinition>
  <sbol:ComponentDefinition rdf:about="http://partsregistry.org/cd/BBa_R0040">
   <sbol:persistentIdentity rdf:resource="http://partsregistry.org/cd/BBa_R0040"/>
   <sbol:displayId>BBa R0040</sbol:displayId>
    <dcterms:title>p(tetR)</dcterms:title>
   <dcterms:description>TetR repressible promoter</dcterms:description>
    <sbol:type rdf:resource="http://identifiers.org/chebi/CHEBI:4705"/>
    <sbol:type rdf:resource="http://www.biopax.org/release/biopax-level3.owl#DnaRegion"/>
    <sbol:role rdf:resource="http://identifiers.org/so/S0:0000167"/>
    <sbol:sequence rdf:resource="http://partsregistry.org/seq/partseq_187"/>
  </sbol:ComponentDefinition>
  <sbol:ComponentDefinition rdf:about="http://partsregistry.org/cd/pIKELeftCassette">
   <sbol:persistentIdentity rdf:resource="http://partsregistry.org/cd/pIKELeftCassette"/>
   <sbol:displayId>pIKELeftCassette
    <sbol:type rdf:resource="http://identifiers.org/chebi/CHEBI:4705"/>
    <sbol:type rdf:resource="http://www.biopax.org/release/biopax-level3.owl#DnaRegion"/>
   <sbol:component>
      <sbol:Component rdf:about="http://partsregistry.org/cd/pIKELeftCassette/BBa_R0040">
        <sbol:persistentIdentity</pre>
            rdf:resource="http://partsregistry.org/cd/pIKELeftCassette/BBa_R0040"/>
        <sbol:displayId>BBa_R0040</sbol:displayId>
        <sbol:access rdf:resource="http://sbols.org/v2#public"/>
        <sbol:definition rdf:resource="http://partsregistry.org/cd/BBa_R0040"/>
      </sbol:Component>
    </sbol:component>
    <sbol:component>
     <sbol:Component rdf:about="http://partsregistry.org/cd/pIKELeftCassette/BBa_C0012">
        <sbol:persistentIdentity</pre>
            rdf:resource="http://partsregistry.org/cd/pIKELeftCassette/BBa_C0012"/>
        <sbol:displayId>BBa_C0012</sbol:displayId>
        <sbol:access rdf:resource="http://sbols.org/v2#public"/>
        <sbol:definition rdf:resource="http://partsregistry.org/cd/BBa_C0012"/>
      </sbol:Component>
    </sbol:component>
    <sbol:sequenceConstraint>
     <sbol:SequenceConstraint</pre>
          rdf:about="http://partsregistry.org/cd/pIKELeftCassette/pIKELeftCassette_sc">
        <sbol:persistentIdentity</pre>
            rdf:resource="http://partsregistry.org/cd/pIKELeftCassette/pIKELeftCassette_sc"/>
        <sbol:displayId>pIKELeftCassette_sc</sbol:displayId>
        <sbol:restriction rdf:resource="http://sbols.org/v2#precedes"/>
        <sbol:subject rdf:resource="http://partsregistry.org/cd/pIKELeftCassette/BBa_R0040"/>
        <sbol:object rdf:resource="http://partsregistry.org/cd/pIKELeftCassette/BBa_C0012"/>
      </sbol:SequenceConstraint>
    </sbol:sequenceConstraint>
  </sbol:ComponentDefinition>
```

```
<sbol:Sequence rdf:about="http://partsregistry.org/seq/seq_K137046">
   <sbol:persistentIdentity rdf:resource="http://partsregistry.org/seq/seq_K137046"/>
   <sbol:displayId>seq_K137046</sbol:displayId>
   </sbol:elements>
   <sbol:encoding rdf:resource="http://www.chem.qmul.ac.uk/iubmb/misc/naseq.html"/>
 </sbol:Sequence>
 <sbol:Sequence rdf:about="http://partsregistry.org/seq/partseq_187">
   <sbol:persistentIdentity rdf:resource="http://partsregistry.org/seq/partseq_187"/>
   <sbol:displayId>partseq_187</sbol:displayId>
   < \verb|sbol|: elements| > \verb|tccctatcagtgatagagattgacatccctatcagtgatagagatactgagcac</ \verb|sbol|: elements| > \verb|tccctatcagtgatagagattgacatccctatcagtgatagagatactgagcac</ | |
   <sbol:encoding rdf:resource="http://www.chem.qmul.ac.uk/iubmb/misc/naseq.html"/>
 </sbol:Sequence>
 <sbol:Sequence rdf:about="http://partsregistry.org/seq/partseq_153">
   <sbol:persistentIdentity rdf:resource="http://partsregistry.org/seq/partseq_153"/>
   <sbol:displayId>partseq_153</sbol:displayId>
   <\!sbol: elements\!>\!atggtgaatgtgaaaccagtaacgttatacgatgtcgcagagtatgccggtgtctcttatcagaccgtttcccgcg
                tggtgaaccaggccagccacgtttctgcgaaaacgcggggaaaaagtggaagcggcgatggcggagctgaattacat\\
                {\tt tcccaaccgcgtggcacaacaactggcgggcaaacagtcgttgctgattggcgttgccacctccagtctggccctg}
                \verb|cacgcgccgtcgcaa| \verb|attgtcgcggcgattaa| \verb|atttcgcgccgatcaa| \verb|ctgggtgccagcgtggtggtgtcgatgg| \\
                taga acga agcgg cgtcg aagcctg taa agcgg cggtg caca atcttctcg cgca acgcgt cagtggg ctg atcat \\
                \tt gtctctgaccagacacccatcaacagtattattttctcccatgaagacggtacgcgactgggcgtggagcatctgg
                \verb|ctggcataaatatctcactcgcaatcaaattcagccgatagcggaacgggaaggcgactggagtgccatgtccggt| \\
                tgggcgcaatgcgcgctattaccgagtccgggctgcgcgttggtgcggatatctcggtagtgggatacgacgatac\\
                \verb|cgaagacagctcatgttatatcccgccgttaaccaccatcaaacaggattttcgcctgctggggcaaaccagcgtg|
                \tt gaccgcttgctgcaactctctcagggccaggcggtgaagggcaatcagctgttgcccgtctcactggtgaaaaggaa
                \tt ggtttcccgactggaaagcgggcaggctgcaaacgacgaaaactacgctttagtagcttaataa
   </sbol:elements>
   <sbol:encoding rdf:resource="http://www.chem.qmul.ac.uk/iubmb/misc/naseq.html"/>
 </sbol:Sequence>
</rdf:RDF>
```