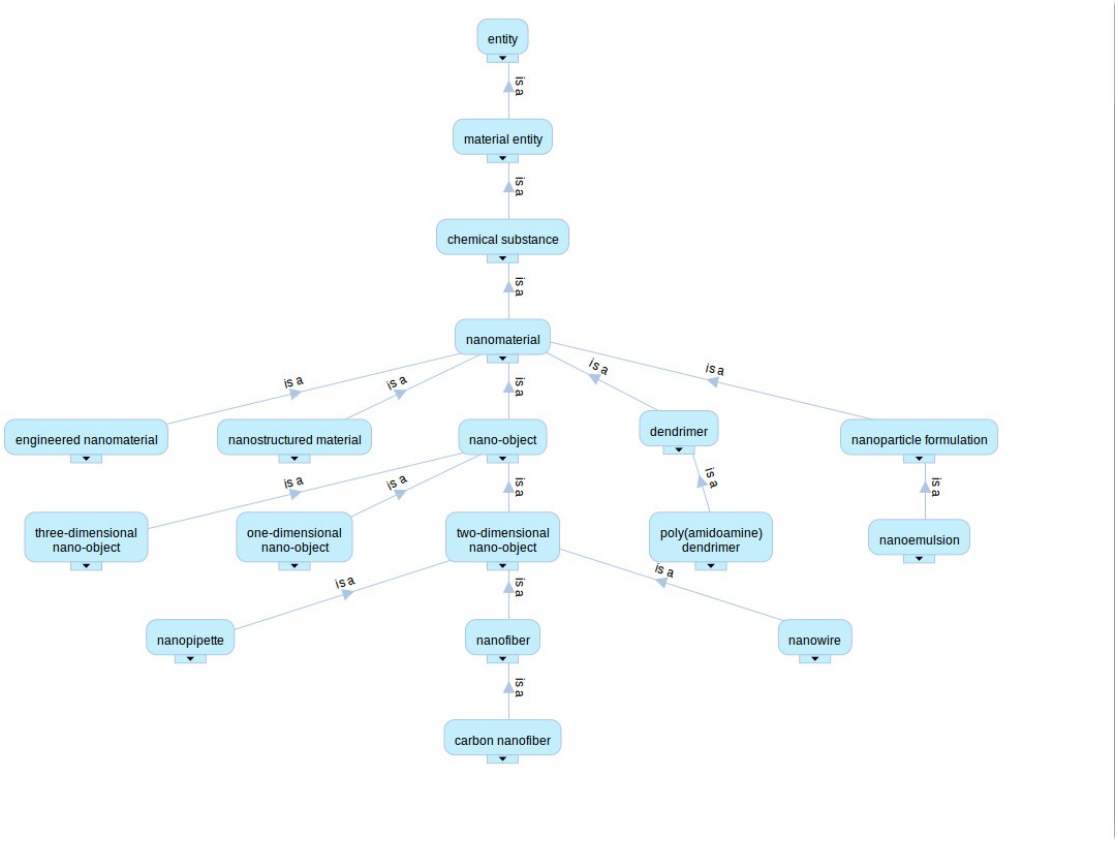
Aim/Hypothesis:

- **Found the following ontology three of a nano-materials on http://bioportal.bioontology.org/ontologies/ENM/**



- **Trying to implement the structure in the converter code.**

Description:

- **Tried different ways of adding the branches as shown on the figure.**
- **Created attributes and added them to properties and let appended the properties under the substance.**
- **Added the molecules of the substance under the last leaf node of properties.**

```
public CMLSubstance cdkSubstanceToCMLSubstance(ISubstance model) {
     CMLSubstance cmlSubstance = new CMLSubstance();
     cmlSubstance.setConvention("??");
     cmlSubstance.setDictRef("??:??");

     if(model.getID() != null)
           cmlSubstance.setId(model.getID());
     else
           cmlSubstance.setId("????");

     Map<Object, Object> props = model.getProperties();
     Iterator<Object> keys = props.keySet().iterator();
     CMLProperty  prevProp = null;
     CMLProperty  firstProp = null;
```

```
        while (keys.hasNext()) {
            Object key = keys.next();

            CMLAttribute att = new CMLAttribute((String)key,
(String)props.get(key));
            CMLProperty property = new CMLProperty();
            property.addAttribute(att);
            if (prevProp != null)
                  property.appendChild(prevProp);
            else
                  firstProp = property;
            prevProp = property;
        }


      for (int j = 0; j < model.getAtomContainerCount() ; j++){

                  IAtomContainer cdkAtomContainer = model.getAtomContainer(j);
                  CMLMolecule cmlMolecule =
cdkAtomContainerToCMLMolecule(cdkAtomContainer);

                  if(cdkAtomContainer.getID() != null)
                        cmlMolecule.setId(cdkAtomContainer.getID());

                  firstProp.appendChild(cmlMolecule);
            }

      cmlSubstance.appendChild(prevProp);
      return cmlSubstance;
    }
```

Results :

- **After a conversation with Egon I found out that what I did was not necessary at all and I just need to read of the npo values from :**
  http://bioportal.bioontology.org/ontologies/ENM/?p=classes&conceptid=http%3A%2F%2Fpurl.bioontology.org%2Fontology%2Fnpo%23NPO_1494&jump_to_nav=true
  For a substance which is a nano material and
  set the IDs for the molecules as the npo from :
  http://bioportal.bioontology.org/ontologies/ENM/?p=classes&conceptid=http%3A%2F%2Fpurl.bioontology.org%2Fontology%2Fnpo%23NPO_1895

- **Below you will see an example of the desired cml file :**

```
<?xml version="1.0" encoding="UTF-8"?>
<substance convention="??" dictRef="npo:NPO_1895" id="????"
   xmlns:npo="http://purl.bioontology.org/ontology/npo#"
   xmlns="http://www.xml-cml.org/schema">
   <molecule id="ID1" dictRef="npo:NPO_1494">
      <atomArray>
```

```
        <atom id="a1" elementType="S" formalCharge="0"/>
        <atom id="a2" elementType="O" formalCharge="0"/>
        <atom id="a3" elementType="O" formalCharge="0"/>
        <atom id="a4" elementType="O" formalCharge="0"/>
      </atomArray>
      <bondArray>
        <bond id="b1" atomRefs2="a1 a2" order="D"/>
        <bond id="b2" atomRefs2="a1 a3" order="D"/>
        <bond id="b3" atomRefs2="a1 a4" order="D"/>
      </bondArray>
    </molecule>
    <molecule id="ID2" dictRef="npo:NPO_1494">
      <atomArray>
        <atom id="a1" elementType="Xe" formalCharge="0"/>
        <atom id="a2" elementType="F" formalCharge="0"/>
        <atom id="a3" elementType="F" formalCharge="0"/>
        <atom id="a4" elementType="F" formalCharge="0"/>
        <atom id="a5" elementType="F" formalCharge="0"/>
      </atomArray>
      <bondArray>
        <bond id="b1" atomRefs2="a1 a2" order="S"/>
        <bond id="b2" atomRefs2="a1 a3" order="S"/>
        <bond id="b3" atomRefs2="a1 a4" order="S"/>
        <bond id="b4" atomRefs2="a1 a5" order="S"/>
      </bondArray>
    </molecule>
</substance>
```