Supplementary Table S1. An example BioPAX file describing the phosphorylation and activation of CHK2 by ATM in human. Data was originally obtained from the Reactome database[8].

```
<?xml version="1.0"?>
<rdf:RDF
    xmlns="http://www.biopax.org/examples/myExample#"
    xmlns:bp="http://www.biopax.org/release/biopax-level3.owl#"
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:xsd="http://www.w3.org/2001/XMLSchema#"
    xmlns:rdfs="http://www.w3.org/2000/01/rdf-schema#"
    xmlns:owl="http://www.w3.org/2002/07/owl#"
  xml:base="http://www.biopax.org/examples/myExample">
  <owl:Ontology rdf:about="">
    <owl:imports rdf:resource="http://www.biopax.org/release/biopax-level3.owl"/>
  </owl:Ontology>
  <rdf:Property rdf:about="http://www.biopax.org/release/biopax-
level3.owl#direction"/>
  <bp:Protein rdf:ID="Protein_5">
    <bp:dataSource>
      <bp:Provenance rdf:ID="Provenance_3">
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >Reactome (http://reactome.org)</bp:displayName>
        <bp:xref>
          <bp:PublicationXref rdf:ID="pubmed">
            <bp:year rdf:datatype="http://www.w3.org/2001/XMLSchema#int"
            >2003</bp:year>
            <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >pubmed</bp:db>
            <bp:title rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >The Genome Knowledgebase: a resource for biologists and
bioinformaticists.</bp:title>
            <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >15338623</bp:id>
          </bp:PublicationXref>
        </bp:xref>
      </bp:Provenance>
    </bp:dataSource>
    <bp:cellularLocation>
      <bp:CellularLocationVocabulary rdf:ID="CellularLocationVocabulary_6">
        <bp:term rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >nucleoplasm</bp:term>
        <bp:xref>
          <bp:UnificationXref rdf:ID="UnificationXref_7">
            <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >GENE ONTOLOGY</bp:db>
            <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >GO:0005654</bp:id>
          </bp:UnificationXref>
        </bp:xref>
      </bp:CellularLocationVocabulary>
    </bp:cellularLocation>
    <bp:entityReference>
      <bp:ProteinReference rdf:ID="CHK2">
        <bp:organism>
          <bp:BioSource rdf:ID="Homo_sapiens">
            <bp:taxonXref>
              <bp:UnificationXref rdf:ID="UnificationXref_10">
                <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >taxonomy</bp:db>
                <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >9606</bp:id>
              </bp:UnificationXref>
            </bp:taxonXref>
            <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Homo sapiens</bp:standardName>
            <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Human</bp:displayName>
          </bp:BioSource>
```

```
        </bp:organism>
        <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >Serine/threonine-protein kinase Chk2 (Cds1)</bp:standardName>
        <bp:xref>
          <bp:RelationshipXref rdf:ID="RelationshipXref_1">
            <bp:relationshipType>
              <bp:RelationshipTypeVocabulary rdf:ID="RelationshipTypeVocabulary_6">
                <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >EC Number</bp:comment>
                <bp:term rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >see-also</bp:term>
              </bp:RelationshipTypeVocabulary>
            </bp:relationshipType>
            <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >IUBMB</bp:db>
            <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >EC 2.7.1.37</bp:id>
          </bp:RelationshipXref>
        </bp:xref>
        <bp:xref>
          <bp:UnificationXref rdf:ID="UnificationXref_12">
            <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >O96017</bp:id>
            <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >uniprot</bp:db>
          </bp:UnificationXref>
        </bp:xref>
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >CHK2</bp:displayName>
        <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >CHEK2</bp:name>
      </bp:ProteinReference>
    </bp:entityReference>
    <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Serine/threonine-protein kinase Chk2 (Cds1)</bp:standardName>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >CHEK2</bp:name>
    <bp:xref rdf:resource="#UnificationXref_12"/>
    <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >CHK2</bp:displayName>
  </bp:Protein>
  <bp:PublicationXref rdf:ID="PublicationXref_24">
    <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >pubmed</bp:db>
    <bp:source rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >EMBO J 22:2860-71 </bp:source>
    <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Foray, N </bp:author>
    <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Jeggo, P </bp:author>
    <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >12773400</bp:id>
    <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Perricaudet, M </bp:author>
    <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Gabriel, A </bp:author>
    <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Ashworth, A </bp:author>
    <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Randrianarison, V </bp:author>
    <bp:title rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >A subset of ATM- and ATR-dependent phosphorylation events requires the BRCA1
protein.</bp:title>
    <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Carr, AM </bp:author>
    <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Marot, D</bp:author>
    <bp:year rdf:datatype="http://www.w3.org/2001/XMLSchema#int"
    >2003</bp:year>
  </bp:PublicationXref>
  <bp:SequenceSite rdf:ID="SequenceSite_20">
    <bp:positionStatus rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
```

```
      >EQUAL</bp:positionStatus>
      <bp:sequencePosition rdf:datatype="http://www.w3.org/2001/XMLSchema#int"
      >1981</bp:sequencePosition>
    </bp:SequenceSite>
    <bp:SmallMolecule rdf:ID="SmallMolecule_21">
      <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
      >Adenosine 5'-diphosphate</bp:standardName>
      <bp:cellularLocation rdf:resource="#CellularLocationVocabulary_6"/>
      <bp:dataSource rdf:resource="#Provenance_3"/>
      <bp:xref>
        <bp:UnificationXref rdf:ID="UnificationXref_22">
          <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
          >CHEBI:2342</bp:id>
          <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
          >ChEBI</bp:db>
        </bp:UnificationXref>
      </bp:xref>
      <bp:entityReference>
        <bp:SmallMoleculeReference rdf:ID="SmallMoleculeReference_23">
          <bp:xref rdf:resource="#UnificationXref_22"/>
          <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
          >ADP</bp:displayName>
          <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
          >Adenosine 5'-diphosphate</bp:standardName>
        </bp:SmallMoleculeReference>
      </bp:entityReference>
      <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
      >ADP</bp:displayName>
    </bp:SmallMolecule>
    <bp:ProteinReference rdf:ID="ATM">
      <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
      >Ataxia telangiectasia mutated) (A-T, mutated) </bp:name>
      <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
      >ATM</bp:displayName>
      <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
      >Serine-protein kinase ATM  (Ataxia telangiectasia mutated) (A-T,
mutated)</bp:standardName>
      <bp:xref rdf:resource="#RelationshipXref_1"/>
      <bp:xref>
        <bp:UnificationXref rdf:ID="UnificationXref_28">
          <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
          >Q13315</bp:id>
          <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
          >uniprot</bp:db>
        </bp:UnificationXref>
      </bp:xref>
      <bp:organism rdf:resource="#Homo_sapiens"/>
    </bp:ProteinReference>
    <bp:RelationshipXref rdf:ID="RelationshipXref_29">
      <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
      >GO:0016301</bp:id>
      <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
      >GENE ONTOLOGY</bp:db>
      <bp:relationshipType>
        <bp:RelationshipTypeVocabulary rdf:ID="GO_molecular_function">
          <bp:term rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
          >gene ontology term for cellular function</bp:term>
          <bp:xref>
            <bp:UnificationXref rdf:ID="UnificationXref_5">
              <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
              >PSI-MI</bp:db>
              <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
              >MI:0355</bp:id>
            </bp:UnificationXref>
          </bp:xref>
        </bp:RelationshipTypeVocabulary>
      </bp:relationshipType>
    </bp:RelationshipXref>
    <bp:Catalysis rdf:ID="Catalysis_1">
      <bp:dataSource rdf:resource="#Provenance_3"/>
      <bp:controlled>
        <bp:BiochemicalReaction rdf:ID="BiochemicalReaction_2">
```

```
        <bp:right>
          <bp:Protein rdf:ID="Protein_16">
            <bp:entityReference rdf:resource="#CHK2"/>
            <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >CHEK2</bp:name>
            <bp:xref rdf:resource="#UnificationXref_12"/>
            <bp:feature>
              <bp:ModificationFeature rdf:ID="ModificationFeature_17">
                <bp:featureLocation rdf:resource="#SequenceSite_20"/>
                <bp:modificationType>
                  <bp:SequenceModificationVocabulary
rdf:ID="SequenceModificationVocabulary_18">
                    <bp:xref>
                      <bp:UnificationXref rdf:ID="UnificationXref_19">
                        <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                        >PSI-MI</bp:db>
                        <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                        >MI:0176</bp:id>
                      </bp:UnificationXref>
                    </bp:xref>
                    <bp:term rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                    >o-phospho-serine</bp:term>
                  </bp:SequenceModificationVocabulary>
                </bp:modificationType>
              </bp:ModificationFeature>
            </bp:feature>
            <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Serine/threonine-protein kinase Chk2 (Cds1)</bp:standardName>
            <bp:dataSource rdf:resource="#Provenance_3"/>
            <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >CHK2</bp:displayName>
            <bp:cellularLocation rdf:resource="#CellularLocationVocabulary_6"/>
          </bp:Protein>
        </bp:right>
        <bp:xref rdf:resource="#PublicationXref_24"/>
        <bp:right rdf:resource="#SmallMolecule_21"/>
        <bp:participantStoichiometry>
          <bp:Stoichiometry rdf:ID="Stoichiometry_2">
            <bp:stoichiometricCoefficient
rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
            >1.0</bp:stoichiometricCoefficient>
            <bp:physicalEntity>
              <bp:Protein rdf:ID="Protein_27">
                <bp:dataSource rdf:resource="#Provenance_3"/>
                <bp:entityReference rdf:resource="#ATM"/>
                <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >Ataxia telangiectasia mutated) (A-T, mutated) </bp:name>
                <bp:standardName
rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >Serine-protein kinase ATM(Ataxia telangiectasia mutated) (A-T,
mutated)</bp:standardName>
                <bp:cellularLocation rdf:resource="#CellularLocationVocabulary_6"/>
                <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >"FUNCTION Involved in signal transduction, cell cycle control and DNA
repair. May function as a tumor suppressor. Necessary for activation of ABL1 and
SAPK"</bp:comment>
                <bp:xref rdf:resource="#UnificationXref_28"/>
                <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >ATM</bp:displayName>
              </bp:Protein>
            </bp:physicalEntity>
          </bp:Stoichiometry>
        </bp:participantStoichiometry>
        <bp:left rdf:resource="#Protein_5"/>
        <bp:left>
          <bp:SmallMolecule rdf:ID="SmallMolecule_13">
            <bp:entityReference>
              <bp:SmallMoleculeReference rdf:ID="SmallMoleculeReference_15">
                <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >ATP</bp:displayName>
                <bp:xref>
                  <bp:UnificationXref rdf:ID="UnificationXref_14">
```

```
                    <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                    >CHEBI:2359</bp:id>
                    <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                    >ChEBI</bp:db>
                  </bp:UnificationXref>
                </bp:xref>
                <bp:standardName
rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                  >Adenosine 5'-triphosphate</bp:standardName>
              </bp:SmallMoleculeReference>
            </bp:entityReference>
            <bp:xref rdf:resource="#UnificationXref_14"/>
            <bp:cellularLocation rdf:resource="#CellularLocationVocabulary_6"/>
            <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Adenosine 5'-triphosphate</bp:standardName>
            <bp:dataSource rdf:resource="#Provenance_3"/>
            <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >ATP</bp:displayName>
          </bp:SmallMolecule>
        </bp:left>
        <bp:participantStoichiometry>
          <bp:Stoichiometry rdf:ID="Stoichiometry_1">
            <bp:physicalEntity rdf:resource="#Protein_5"/>
            <bp:stoichiometricCoefficient
rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
            >1.0</bp:stoichiometricCoefficient>
          </bp:Stoichiometry>
        </bp:participantStoichiometry>
        <bp:xref>
          <bp:UnificationXref rdf:ID="UnificationXref_26">
            <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >REACT_69891</bp:id>
            <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >reactome</bp:db>
            <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >http://www.reactome.org </bp:comment>
          </bp:UnificationXref>
        </bp:xref>
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >Phosphorylation and activation of CHK2 by ATM</bp:displayName>
        <bp:conversionDirection rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >LEFT-TO-RIGHT</bp:conversionDirection>
        <bp:dataSource rdf:resource="#Provenance_3"/>
        <bp:participantStoichiometry>
          <bp:Stoichiometry rdf:ID="Stoichiometry_4">
            <bp:stoichiometricCoefficient
rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
            >1.0</bp:stoichiometricCoefficient>
            <bp:physicalEntity rdf:resource="#SmallMolecule_13"/>
          </bp:Stoichiometry>
        </bp:participantStoichiometry>
        <bp:xref>
          <bp:PublicationXref rdf:ID="PublicationXref_25">
            <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >McGowan, CH </bp:author>
            <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Laus, MC </bp:author>
            <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Luyten, WH </bp:author>
            <bp:title rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >A human homologue of the checkpoint kinase Cds1 directly inhibits Cdc25
phosphatase.</bp:title>
            <bp:source rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Curr Biol 9:1-10 </bp:source>
            <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Parker, AE </bp:author>
            <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >de Weyer, IV </bp:author>
            <bp:author rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Blasina, A </bp:author>
            <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >9889122</bp:id>
```

```
            <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >pubmed</bp:db>
            <bp:year rdf:datatype="http://www.w3.org/2001/XMLSchema#int"
            >1999</bp:year>
          </bp:PublicationXref>
        </bp:xref>
        <bp:participantStoichiometry>
          <bp:Stoichiometry rdf:ID="Stoichiometry_3">
            <bp:physicalEntity rdf:resource="#SmallMolecule_21"/>
            <bp:stoichiometricCoefficient
rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
            >1.0</bp:stoichiometricCoefficient>
          </bp:Stoichiometry>
        </bp:participantStoichiometry>
        <bp:spontaneous rdf:datatype="http://www.w3.org/2001/XMLSchema#boolean"
        >false</bp:spontaneous>
      </bp:BiochemicalReaction>
    </bp:controlled>
    <bp:controlType rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >ACTIVATION</bp:controlType>
    <bp:controller rdf:resource="#Protein_27"/>
    <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >ATM phosphorylates and activates CHK2</bp:displayName>
    <bp:xref rdf:resource="#RelationshipXref_29"/>
    <bp:availability rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Reactome is a free on-line resource, and Reactome software is open-source.
However, please take note of our disclaimer. (http://reactome.org/disclaimer.html)
</bp:availability>
    <bp:catalysisDirection rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >LEFT-TO-RIGHT</bp:catalysisDirection>
  </bp:Catalysis>
</rdf:RDF>

<!-- Created with Protege (with OWL Plugin 3.3.1, Build 430)
http://protege.stanford.edu -->
```

Supplementary Table S2. An example BioPAX file describing the two reactions involved in glucose metabolism in *Escherichia coli*. Data was originally obtained from the EcoCyc database[14].

```
<?xml version="1.0"?>
<rdf:RDF
    xmlns="http://www.biopax.org/examples/myExample#"
    xmlns:bp="http://www.biopax.org/release/biopax-level3.owl#"
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:xsd="http://www.w3.org/2001/XMLSchema#"
    xmlns:rdfs="http://www.w3.org/2000/01/rdf-schema#"
    xmlns:owl="http://www.w3.org/2002/07/owl#"
    xmlns:p1="http://www.owl-ontologies.com/assert.owl#"
  xml:base="http://www.biopax.org/examples/myExample">
  <owl:Ontology rdf:about="">
    <owl:imports rdf:resource="http://www.biopax.org/release/biopax-level3.owl"/>
  </owl:Ontology>
  <bp:Protein rdf:ID="Protein_54">
    <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >GLK</bp:standardName>
    <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >glucokinase</bp:displayName>
    <bp:xref>
      <bp:UnificationXref rdf:ID="SwissProtTrEMBL_P46880">
        <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >P46880</bp:id>
        <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >PMID: 15608167</bp:comment>
        <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >uniprot</bp:db>
      </bp:UnificationXref>
    </bp:xref>
    <bp:entityReference>
      <bp:ProteinReference rdf:ID="ProteinReference_15">
        <bp:sequence rdf:datatype="http://www.w3.org/2001/XMLSchema#string"

>MTKYALVGDVGGTNARLALCDIASGEISQAKTYSGLDYPSLEAVIRVYLEEHKVEVKDGCIAIACPITGDWVAMTNHTWAFSIAE
MKKNLGFSHLEIINDFTAVSMAIPMLKKEHLIQFGGAEPVEGKPIAVYGAGTGLGVAHLVHVDKRWVSLPGEGGHVDFAPNSEEEA
IILEILRAEIGHVSAERVLSGPGLVNLYRAIVKADNRLPENLKPKDITERALADSCTDCRRALSLFCVIMGRFGGNLALNLGTFGG
VFIAGGIVPRFLEFFKASGFRAAFEDKGRFKEYVHDIPVYLIVHDNPGLLGSGAHLRQTLGHIL</bp:sequence>
        <bp:xref rdf:resource="#SwissProtTrEMBL_P46880"/>
        <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >glucose kinase</bp:name>
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >glucokinase</bp:displayName>
        <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >GLK</bp:standardName>
        <bp:organism>
          <bp:BioSource rdf:ID="Escherichia_coli">
            <bp:taxonXref>
              <bp:UnificationXref rdf:ID="taxon_562">
                <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >562</bp:id>
                <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >taxonomy</bp:db>
              </bp:UnificationXref>
            </bp:taxonXref>
            <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Escherichia coli</bp:displayName>
          </bp:BioSource>
        </bp:organism>
      </bp:ProteinReference>
    </bp:entityReference>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >GLK_ECOLI</bp:name>
    <bp:cellularLocation>
      <bp:CellularLocationVocabulary rdf:ID="cytoplasm">
        <bp:xref>
          <bp:UnificationXref rdf:ID="GO_0005737">
```

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            <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >GO:0005737</bp:id>
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            >PMID: 11483584 </bp:comment>
            <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Gene Ontology</bp:db>
          </bp:UnificationXref>
        </bp:xref>
        <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >This example is meant to provide an illustration of how various BioPAX slots
should be filled; it is not intended to provide useful (or even accurate) biological
information  </bp:comment>
        <bp:term rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >cytoplasm</bp:term>
      </bp:CellularLocationVocabulary>
    </bp:cellularLocation>
    <bp:dataSource>
      <bp:Provenance rdf:ID="SwissProtTrEMBL">
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >Swiss-Prot/TrEMBL</bp:displayName>
      </bp:Provenance>
    </bp:dataSource>
    <bp:dataSource>
      <bp:Provenance rdf:ID="aMAZE">
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >aMAZE</bp:displayName>
        <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        ></bp:comment>
      </bp:Provenance>
    </bp:dataSource>
  </bp:Protein>
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    ></bp:comment>
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    >SMILES</bp:structureFormat>
    <bp:structureData rdf:datatype="http://www.w3.org/2001/XMLSchema#string"

>[CH]3(n1(c2(c(nc1)c(N)ncn2)))(O[CH]([CH](O)[CH](O)3)COP(=O)(O)OP(O)(=O)OP(O)(=O)O)</b
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            <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >PMID: 9847135</bp:comment>
            <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >C00668</bp:id>
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            >KEGG compound</bp:db>
          </bp:UnificationXref>
        </bp:xref>
        <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >b-D-glucose-6-phoshate</bp:name>
        <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >glucose-6-P</bp:name>
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >beta-D-glucose 6-phosphate</bp:displayName>
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            >260.14</bp:molecularWeight>
            <bp:chemicalFormula rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >C6H13O9P</bp:chemicalFormula>
```

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                <rdfs:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >beta-glucose-6-phosphate</rdfs:comment>
                <bp:structureFormat
rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >SMILES</bp:structureFormat>
              </bp:ChemicalStructure>
            </bp:structure>
            <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >beta-D-glucose 6-phosphate</bp:displayName>
            <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >b-D-glu-6-p</bp:standardName>
            <bp:xref rdf:resource="#KEGG_C00668"/>
          </bp:SmallMoleculeReference>
        </bp:entityReference>
        <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >D-glucose-6-P</bp:name>
        <bp:cellularLocation rdf:resource="#cytoplasm"/>
        <bp:dataSource>
          <bp:Provenance rdf:ID="KEGG">
            <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >Kyoto Encyclopedia of Genes and Genomes</bp:standardName>
            <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >KEGG</bp:displayName>
            <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            ></bp:comment>
          </bp:Provenance>
        </bp:dataSource>
        <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >a-D-glu-6-p</bp:standardName>
        <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >beeta-D-glucose-6-p</bp:name>
      </bp:SmallMolecule>
    </bp:physicalEntity>
  </bp:Stoichiometry>
  <bp:UnificationXref rdf:ID="KEGG_R01786">
    <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >kegg reaction</bp:db>
    <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >PMID: 9847135 </bp:comment>
    <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >R01786</bp:id>
  </bp:UnificationXref>
  <bp:BiochemicalReaction rdf:ID="phosphoglucoisomerase">
    <bp:eCNumber rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >5.3.1.9 </bp:eCNumber>
    <bp:participantStoichiometry>
      <bp:Stoichiometry rdf:ID="Stoichiometry_57">
        <bp:stoichiometricCoefficient
rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
        >1.0</bp:stoichiometricCoefficient>
        <bp:physicalEntity>
          <bp:SmallMolecule rdf:ID="beta-D-fructose_6-phosphate">
            <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >&lt;FONT FACE="Symbol"&gt;b&lt;/FONT&gt;-D-fructose-6-phosphate
      </bp:name>
            <bp:entityReference>
              <bp:SmallMoleculeReference rdf:ID="SmallMoleculeReference_14">
                <bp:structure>
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                    <bp:structureData
rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
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                    <rdfs:comment
rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                    >beta-fructose-6-phosphate</rdfs:comment>
                    <bp:structureFormat
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```
                    >SMILES</bp:structureFormat>
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                <bp:molecularWeight
rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
                >260.14</bp:molecularWeight>
                <bp:chemicalFormula
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                >C6H13O9P</bp:chemicalFormula>
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                >b-D-fru-6-p</bp:standardName>
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                    <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                    >C05345</bp:id>
                    <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                    >kegg compound</bp:db>
                  </bp:UnificationXref>
                </bp:xref>
              </bp:SmallMoleculeReference>
            </bp:entityReference>
            <bp:dataSource rdf:resource="#aMAZE"/>
            <bp:dataSource rdf:resource="#KEGG"/>
            <bp:xref rdf:resource="#KEGG_C05345"/>
            <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >b-D-fru-6-p</bp:standardName>
            <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >beta-D-fructose 6-phosphate</bp:displayName>
            <bp:cellularLocation rdf:resource="#cytoplasm"/>
          </bp:SmallMolecule>
        </bp:physicalEntity>
      </bp:Stoichiometry>
    </bp:participantStoichiometry>
    <bp:conversionDirection rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >REVERSIBLE</bp:conversionDirection>
    <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >beta-D-glu-6-p &lt;=&gt; beta-D-fru-6-p</bp:displayName>
    <bp:dataSource rdf:resource="#aMAZE"/>
    <bp:left rdf:resource="#alpha-D-glucose_6-phosphate"/>
    <bp:xref>
      <bp:UnificationXref rdf:ID="KEGG_R02740">
        <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >kegg reaction</bp:db>
        <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >R02740</bp:id>
        <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >PMID: 9847135 </bp:comment>
      </bp:UnificationXref>
    </bp:xref>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >beta-D-Glucose 6-phosphate =&gt; beta-D-Fructose 6-phosphate</bp:name>
    <bp:dataSource rdf:resource="#KEGG"/>
    <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >b-D-glu-6-p &lt;=&gt; b-D-fru-6-p</bp:standardName>
    <bp:right rdf:resource="#beta-D-fructose_6-phosphate"/>
    <bp:deltaG>
      <bp:DeltaG rdf:ID="DeltaG_12">
        <bp:deltaGPrime0 rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
        >0.4</bp:deltaGPrime0>
      </bp:DeltaG>
    </bp:deltaG>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >beta-D-Glucose 6-phosphate ketol-isomerase</bp:name>
    <bp:participantStoichiometry>
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        <bp:physicalEntity rdf:resource="#alpha-D-glucose_6-phosphate"/>
```

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        <bp:stoichiometricCoefficient
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      </bp:Stoichiometry>
    </bp:participantStoichiometry>
  </bp:BiochemicalReaction>
  <bp:SmallMoleculeReference rdf:ID="SmallMoleculeReference_10">
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      <bp:ChemicalStructure rdf:ID="ChemicalStructure_6">
        <bp:structureFormat rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >SMILES</bp:structureFormat>
        <bp:structureData rdf:datatype="http://www.w3.org/2001/XMLSchema#string"

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Data>
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    </bp:structure>
    <bp:xref>
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        <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >PMID: 9847135 </bp:comment>
        <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >kegg compound</bp:db>
      </bp:UnificationXref>
    </bp:xref>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >adenosine diphosphate</bp:name>
    <bp:chemicalFormula rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >C10H15N5O10P2</bp:chemicalFormula>
    <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >ADP</bp:standardName>
    <bp:molecularWeight rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
    >427.2</bp:molecularWeight>
    <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Adenosine 5'-diphosphate</bp:displayName>
  </bp:SmallMoleculeReference>
  <bp:PublicationXref rdf:ID="PublicationXref49">
    <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >2549346</bp:id>
    <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >PubMed</bp:db>
  </bp:PublicationXref>
  <bp:UnificationXref rdf:ID="Swiss-ProtTrEMBL_Q9KH85">
    <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >  PMID: 15608167</bp:comment>
    <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Q9KH85</bp:id>
    <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >UniProt</bp:db>
  </bp:UnificationXref>
  <bp:SmallMoleculeReference rdf:ID="SmallMoleculeReference_11">
    <bp:structure rdf:resource="#ChemicalStructure_9"/>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >adenosine triphosphate</bp:name>
    <bp:molecularWeight rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
    >507.18</bp:molecularWeight>
    <bp:chemicalFormula rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >C10H16N5O13P3</bp:chemicalFormula>
    <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >ATP</bp:standardName>
    <bp:xref>
      <bp:UnificationXref rdf:ID="KEGG_C00002">
        <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >C00002</bp:id>
        <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >kegg compound</bp:db>
        <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >PMID: 9847135 </bp:comment>
```

```
      </bp:UnificationXref>
    </bp:xref>
    <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
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  </bp:SmallMoleculeReference>
  <bp:SmallMolecule rdf:ID="ADP">
    <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Adenosine 5'-diphosphate</bp:displayName>
    <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >ADP</bp:standardName>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >adenosine diphosphate</bp:name>
    <bp:dataSource rdf:resource="#KEGG"/>
    <bp:entityReference rdf:resource="#SmallMoleculeReference_10"/>
    <bp:cellularLocation rdf:resource="#cytoplasm"/>
    <bp:dataSource rdf:resource="#aMAZE"/>
    <bp:xref rdf:resource="#KEGG_C00008"/>
    <bp:availability rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    ></bp:availability>
  </bp:SmallMolecule>
  <bp:BiochemicalPathwayStep rdf:ID="BiochemicalPathwayStep_3">
    <bp:stepDirection rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >LEFT-TO-RIGHT</bp:stepDirection>
    <bp:stepConversion rdf:resource="#phosphoglucoisomerase"/>
    <bp:stepProcess>
      <bp:Catalysis rdf:ID="phosphoglucose_isomerase_converts_alpha-D-gluc-6-
p_to_beta-D-fruc-6-p">
        <bp:controller>
          <bp:Protein rdf:ID="phosphoglucose_isomerase">
            <bp:xref rdf:resource="#Swiss-ProtTrEMBL_Q9KH85"/>
            <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >glucose-6-phosphate isomerase</bp:name>
            <bp:entityReference>
              <bp:ProteinReference rdf:ID="ProteinReference_16">
                <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >This example is meant to provide an illustration of how various
BioPAX slots should be filled; it is not intended to provide useful (or even accurate)
biological information    </bp:comment>
                <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >PHI</bp:name>
                <bp:sequence rdf:datatype="http://www.w3.org/2001/XMLSchema#string"

>KTFSEAIISGEWKGYTGKAITDVVNIGIGGSDLGPYMVTEALRPYKNHLNMHFVSNVDGTHIAEVLKKVNPETTLFLVASKTFTT
QETMTNAHSARDWFLKAAGDEKHVAKHFAALSTNAKAVGEFGIDTANMFEFWDWVGGRYSLWSAIGLSIVLSIGFDNFVELLSGAH
AMDKHFSTTPAEKNLPVLLALIGIWYNNFFGAETEAILPYDQYMHRFAAYFQQGNMESNGKYVDRNGNVVDYQTGPIIWGEPGTNG
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                >PGI</bp:standardName>
                <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >phosphohexose isomerase</bp:name>
                <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >phosphoglucose isomerase</bp:displayName>
                <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >glucose-6-phosphate isomerase</bp:name>
                <bp:organism rdf:resource="#Escherichia_coli"/>
                <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >GPI</bp:name>
              </bp:ProteinReference>
            </bp:entityReference>
            <bp:cellularLocation rdf:resource="#cytoplasm"/>
            <bp:dataSource rdf:resource="#KEGG"/>
            <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >PHI</bp:name>
            <bp:dataSource rdf:resource="#aMAZE"/>
            <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >phosphoglucose isomerase</bp:displayName>
            <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >phosphohexose isomerase</bp:name>
            <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >PGI</bp:standardName>
```

```
            <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >GPI</bp:name>
          </bp:Protein>
        </bp:controller>
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >catalysis of (beta-D-glu-6-p &lt;=&gt; beta-D-fruc-6-p)</bp:displayName>
        <bp:catalysisDirection rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >LEFT-TO-RIGHT</bp:catalysisDirection>
        <bp:controlled rdf:resource="#phosphoglucoisomerase"/>
        <bp:dataSource rdf:resource="#KEGG"/>
        <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >PGI -&gt; (b-d-glu-6-p &lt;=&gt; b-D-fru-6p)</bp:standardName>
        <bp:dataSource rdf:resource="#aMAZE"/>
        <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >The source of this data did not store catalyses of reactions as separate
objects, so there are no unification x-refs pointing to the source of these BioPAX
instances.   </bp:comment>
        <bp:availability rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        ></bp:availability>
        <bp:controlType rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >ACTIVATION</bp:controlType>
      </bp:Catalysis>
    </bp:stepProcess>
  </bp:BiochemicalPathwayStep>
  <bp:Stoichiometry rdf:ID="Stoichiometry_37">
    <bp:stoichiometricCoefficient
rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
    >1.0</bp:stoichiometricCoefficient>
    <bp:physicalEntity>
      <bp:SmallMolecule rdf:ID="alpha-D-glucose">
        <bp:xref>
          <bp:UnificationXref rdf:ID="KEGG_C00267">
            <bp:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >kegg compound</bp:db>
            <bp:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >C00267</bp:id>
            <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >PMID: 9847135 </bp:comment>
          </bp:UnificationXref>
        </bp:xref>
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >beta-D-glucose</bp:displayName>
        <bp:dataSource rdf:resource="#aMAZE"/>
        <bp:dataSource rdf:resource="#KEGG"/>
        <bp:cellularLocation rdf:resource="#cytoplasm"/>
        <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >b-D-glu</bp:standardName>
        <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >&lt;FONT FACE="Symbol"&gt;a&lt;/FONT&gt;-D-glucose </bp:name>
        <bp:entityReference>
          <bp:SmallMoleculeReference rdf:ID="SmallMoleculeReference_12">
            <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >b-D-glu</bp:standardName>
            <bp:structure>
              <bp:ChemicalStructure rdf:ID="ChemicalStructure_5">
                <rdfs:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >alpha-D-glucose</rdfs:comment>
                <bp:structureData
rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >C1(C(O)C(O)C(O)C(O1)CO)(O)</bp:structureData>
                <bp:structureFormat
rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
                >SMILES</bp:structureFormat>
              </bp:ChemicalStructure>
            </bp:structure>
            <bp:xref rdf:resource="#KEGG_C00267"/>
            <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >beta-D-glucose</bp:displayName>
            <bp:chemicalFormula rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
            >C6H12O6</bp:chemicalFormula>
            <bp:molecularWeight rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
            >180.16</bp:molecularWeight>
```

```
          </bp:SmallMoleculeReference>
        </bp:entityReference>
      </bp:SmallMolecule>
    </bp:physicalEntity>
  </bp:Stoichiometry>
  <bp:Stoichiometry rdf:ID="Stoichiometry_43">
    <bp:physicalEntity>
      <bp:SmallMolecule rdf:ID="ATP">
        <bp:xref rdf:resource="#KEGG_C00002"/>
        <bp:dataSource rdf:resource="#KEGG"/>
        <bp:dataSource rdf:resource="#aMAZE"/>
        <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >ATP</bp:standardName>
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >Adenosine 5'-triphosphate</bp:displayName>
        <bp:entityReference rdf:resource="#SmallMoleculeReference_11"/>
        <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >adenosine triphosphate</bp:name>
        <bp:cellularLocation rdf:resource="#cytoplasm"/>
      </bp:SmallMolecule>
    </bp:physicalEntity>
    <bp:stoichiometricCoefficient
rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
    >1.0</bp:stoichiometricCoefficient>
  </bp:Stoichiometry>
  <bp:BiochemicalReaction rdf:ID="glucokinase">
    <bp:xref rdf:resource="#KEGG_R01786"/>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >glucose ATP phosphotransferase     </bp:name>
    <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >beta-D-glu + ATP =&gt; beta-D-glu-6-p + ADP</bp:displayName>
    <bp:dataSource rdf:resource="#KEGG"/>
    <bp:conversionDirection rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >REVERSIBLE</bp:conversionDirection>
    <bp:participantStoichiometry rdf:resource="#Stoichiometry_43"/>
    <bp:participantStoichiometry rdf:resource="#Stoichiometry_37"/>
    <bp:left rdf:resource="#ATP"/>
    <bp:participantStoichiometry rdf:resource="#Stoichiometry_52"/>
    <bp:right rdf:resource="#ADP"/>
    <bp:eCNumber rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >2.7.1.1 </bp:eCNumber>
    <bp:left rdf:resource="#alpha-D-glucose"/>
    <bp:dataSource rdf:resource="#aMAZE"/>
    <bp:spontaneous rdf:datatype="http://www.w3.org/2001/XMLSchema#boolean"
    >true</bp:spontaneous>
    <bp:right rdf:resource="#alpha-D-glucose_6-phosphate"/>
    <bp:eCNumber rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >2.7.1.2 </bp:eCNumber>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >ATP:D-glucose 6-phosphotransferase </bp:name>
    <bp:participantStoichiometry>
      <bp:Stoichiometry rdf:ID="Stoichiometry_49">
        <bp:stoichiometricCoefficient
rdf:datatype="http://www.w3.org/2001/XMLSchema#float"
        >1.0</bp:stoichiometricCoefficient>
        <bp:physicalEntity rdf:resource="#ADP"/>
      </bp:Stoichiometry>
    </bp:participantStoichiometry>
    <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >b-D-glu =&gt; b-D-glu-6-p</bp:standardName>
  </bp:BiochemicalReaction>
  <bp:Pathway rdf:ID="Pathway50">
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >glucose degradation</bp:name>
    <bp:pathwayOrder rdf:resource="#BiochemicalPathwayStep_3"/>
    <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >glycolysis</bp:standardName>
    <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >This example is meant to provide an illustration of how various BioPAX slots
should be filled; it is not intended to provide useful (or even accurate) biological
information  </bp:comment>
    <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
```

```
    >Glycolysis Pathway</bp:displayName>
    <bp:availability rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >see http://www.amaze.ulb.ac.be/</bp:availability>
    <bp:organism rdf:resource="#Escherichia_coli"/>
    <bp:availability rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >All data within the pathway has the same availability</bp:availability>
    <bp:pathwayComponent rdf:resource="#phosphoglucose_isomerase_converts_alpha-D-
gluc-6-p_to_beta-D-fruc-6-p"/>
    <bp:pathwayComponent>
      <bp:Catalysis rdf:ID="glucokinase_converts_alpha-D-glu_to_alpha-D-glu-6-p">
        <bp:controlType rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >ACTIVATION</bp:controlType>
        <bp:displayName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >catalysis of (alpha-D-glu &lt;=&gt; alpha-D-glu-6-p)</bp:displayName>
        <bp:dataSource rdf:resource="#aMAZE"/>
        <bp:dataSource rdf:resource="#KEGG"/>
        <bp:controlled rdf:resource="#glucokinase"/>
        <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >The source of this data did not store catalyses of reactions as separate
objects, so there are no unification x-refs pointing to the source of these BioPAX
instances.   </bp:comment>
        <bp:controller rdf:resource="#Protein_54"/>
        <bp:standardName rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >GLK -&gt; (a-D-glu &lt;=&gt; a-D-glu-6-p)</bp:standardName>
        <bp:catalysisDirection rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >LEFT-TO-RIGHT</bp:catalysisDirection>
      </bp:Catalysis>
    </bp:pathwayComponent>
    <bp:pathwayComponent rdf:resource="#phosphoglucoisomerase"/>
    <bp:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    ></bp:comment>
    <bp:pathwayComponent rdf:resource="#glucokinase"/>
    <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
    >Embden-Meyerhof pathway</bp:name>
    <bp:xref rdf:resource="#PublicationXref49"/>
    <bp:dataSource rdf:resource="#KEGG"/>
    <bp:dataSource rdf:resource="#aMAZE"/>
    <bp:pathwayOrder>
      <bp:BiochemicalPathwayStep rdf:ID="BiochemicalPathwayStep_2">
        <bp:stepConversion rdf:resource="#glucokinase"/>
        <bp:nextStep rdf:resource="#BiochemicalPathwayStep_3"/>
        <bp:stepDirection rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
        >LEFT-TO-RIGHT</bp:stepDirection>
        <bp:stepProcess rdf:resource="#glucokinase_converts_alpha-D-glu_to_alpha-D-
glu-6-p"/>
      </bp:BiochemicalPathwayStep>
    </bp:pathwayOrder>
  </bp:Pathway>
</rdf:RDF>
```

Supplementary Table S3: BioPAX covers five main types of biological pathways and coverage has increased over time with new levels of the ontology.

Type of Biological Pathway	Main BioPAX Classes Used	Introduced
Metabolic pathways	All types of physical entities (most common use of protein, small molecule, complex), All types of conversion events (most common use of BiochemicalReaction, ComplexAssembly and Transport), Catalysis, Modulation and Pathway	Level 1
Signaling pathways	All types of physical entities (most common use of protein, complex), All types of conversion events (most common use of BiochemicalReaction, ComplexAssembly, Transport and Degradation), Control, Catalysis, Modulation, MolecularInteraction, Pathway	Level 2
Molecular interactions	All types of physical entities (most common use of protein, complex, small molecule), MolecularInteraction, Pathway	Level 2
Gene regulatory networks	All types of physical entities, TemplateReaction, TemplateReactionRegulation	Level 3
Genetic interactions	Gene, GeneticInteraction	Level 3

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Supplementary Table S4: Databases and software supporting BioPAX. Note, PSI-MI data sources can be converted to BioPAX Level 2 using the PSI-MI to BioPAX converter.

Database	Type	URL	Format	License	Statistics
BIND [1]	Protein interactions	http://tap.med.utoronto.ca/~bind/	PSI-MI Level 1	Free to all	>85,000 interactions
BioCyc databases [2,3]	Metabolic and signaling	http://biocyc.org	BioPAX Level 3	Free to all	~500 mostly computationally predicted pathway databases
BioGRID [4,5]	Protein-protein and genetic interactions	http://www.thebiogrid.org/	PSI-MI Level 1 and 2.5	Free to all	>265,000 interactions
BioModels [6]	Metabolic and signaling	http://biomodels.net/	SBML, BioPAX Level 2	Free to all	>450 pathways, >240 curated pathways, >40,000 interactions
Cancer Cell Map	Signaling Pathways	http://cancer.cellmap.org	BioPAX Level 2	Free to all	Pathways: 10 Interactions: 2,104 Physical Entities: 899
DIP [7,8]	Protein-protein interactions	http://dip.doe-mbi.ucla.edu/	PSI-MI Level 1	Free for Academics	>57,000 interactions
Ecocyc [9]	Metabolic and Signaling Pathways	http://ecocyc.org/	BioPAX, Level 3	Free to all	Pathways: 246 Regulatory interactions: 5,000 Metabolic reactions: 1400 Physical Entities: 3,606
HPRD [10]	Protein-protein interactions	http://hprd.org/	PSI-MI Level 2.5	Free for Academics	>38,000 interactions
IMID	Signaling	http://www.sbcny.org/data.htm	BioPAX Level 2	Free to all	>2000 interactions
INOH	Signaling	http://www.inoh.org/	BioPAX Level 2	Free to all	>60 pathways
IntAct [11]	Protein-protein interactions	http://www.ebi.ac.uk/intact	PSI-MI Level 1 and 2.5	Free to all	>200,000 interactions
KEGG Pathway [12]	Metabolic	http://www.genome.jp/kegg/	BioPAX Level 1	Free for Academics	>330 reference pathways
MetaCyc [13]	Metabolic and signaling	http://metacyc.org/	BioPAX Level 3	Free to all	1399 curated pathways, >8,100 reactions
MINT [14]	Protein-protein interactions	http://mint.bio.uniroma2.it/mint	PSI-MI Level 1 and 2.5	Free to all	>80,000 interactions
MIPS MPact [15]	Protein-protein interactions	http://mips.gsf.de/genre/proj/mpact/	PSI-MI Level 1 and 2.5	Free to all	>12,000 interactions
NCI/Nature Pathway	Signaling	http://pid.nci.nih.gov/	BioPAX Level 2	Free to all	>400 curated pathways >12800 interactions

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Interaction Database [16]					
NetPath [17]	Signaling	http://netpath.org/	BioPAX Level 2	Free to all	20 large curated pathways
OPHID [18]	Protein-protein interaction	http://ophid.utoronto.ca	PSI-MI Level 1	Free for Academics	>424,000 interactions
Pathway Commons	Pathways and interactions	http://www.pathwaycommons.org	BioPAX Level 2	Free to all	>1,400 collected pathways >421,000 interactions
Reactome [19]	Metabolic and Signaling Pathways	http://reactome.org/	BioPAX, Level 2	Free to all	>50 curated pathways
RegulonDB [20]	Regulatory Network	http://regulondb.ccg.unam.mx	BioPAX Level 3	Free to all	Regulatory interactions: 2,594 Physical Entities: 18,371 Pathways: 2,660
Rhea	Metabolic Reactions	http://www.ebi.ac.uk/rhea	BioPAX, Level 2	Free to all	>11,000 reactions
Software	Type	URL	Format	License	Language
BiNoM [21]	Editor/Converter	http://bioinfo-out.curie.fr/projects/binom/	BioPAX Level 1 and 2	Free to all (open source)	Java
BioPAX validator	Validator	http://www.ohsucancer.com/biopaxvalidator/index.html	BioPAX Level 1 and 2	Free to all (open source)	Java
BioPAX validator	Validator	http://www.biopax.org/biopax-validator/	BioPAX Level 3	Free to all (open source)	Java
BioUML	Editor/Simulator	http://www.biouml.org/	BioPAX Level 2	Free to all (open source)	Java
Biowarehouse	Biological data warehouse software	http://biowarehouse.ai.sri.com/	BioPAX Level 1 and 2	Free to all (open source)	C and Java
ChiBE [79]	Visualization and analysis	http://www.bilkent.edu.tr/~bcbi/chibe.html	BioPAX Level 1 and 2	Free for Academics	Java
cPath [22]	Pathway database software	http://cbio.mskcc.org/dev_site/cpath/	BioPAX Level 1 and 2	Free to all (open source)	Java
Cytoscape [23]	Visualization and analysis	http://cytoscape.org	BioPAX Level 1, 2, 3	Free to all (open source)	Java
ExPlain Analysis System	Pathway analysis	http://www.biobase-international.com/pages/index.php?id=286	BioPAX Level 1 and 2	Commercial	
GeneSpring GX	Pathway analysis	http://www.agilent.com/chem/genespring	BioPAX Level 1 and 2	Commercial	Java
Navigator [24]	Visualization and analysis	http://ophid.utoronto.ca/navigator/	BioPAX Level 1 and 2	Free for Academics	Java
Pathway Tools [25]	Pathway prediction,	http://bioinformatics.ai.sri.com/ptools/	BioPAX Level 3	Free for Academi	Lisp

	editing, visualization, network analysis, gene expression analysis			cs	
PATIKA [26]	Visualization and analysis	http://web.patika.org	BioPAX Level 1 and 2	Free for Academics	Java
Paxtools	BioPAX input/export library	http://www.biopax.org/paxtools/	BioPAX Level 1,2,3	Free to all (open source)	Java
PSI-MI to BioPAX converter	BioPAX translator		BioPAX Level 2,3	Free to all (open source)	Java
QPACA [27]	Gene expression analysis	https://cabig.nci.nih.gov/tools/QPACA	BioPAX Level 1 and 2	Free to all	Java
SBML tp BioPAX converter	BioPAX translator	http://www.ebi.ac.uk/compneur-srv/sbml/convertors/SBMLtoBioPax.html	BioPAX Level 2	Free to all (open source)	Java
SHARKview [28]	Pathway visualizer	http://www.bioinformatics.leeds.ac.uk/shark/	BioPAX Level 1 and 2	Free to all	Java
The Gateway to Biological Pathways	Pathway query web service	http://jlab.calumet.purdue.edu/theGateway/	BioPAX Level 1 and 2	Free to all	Java
VisANT [29,30]	Visualization and analysis	http://visant.bu.edu/	BioPAX Level 1 and 2	Free to all	Java

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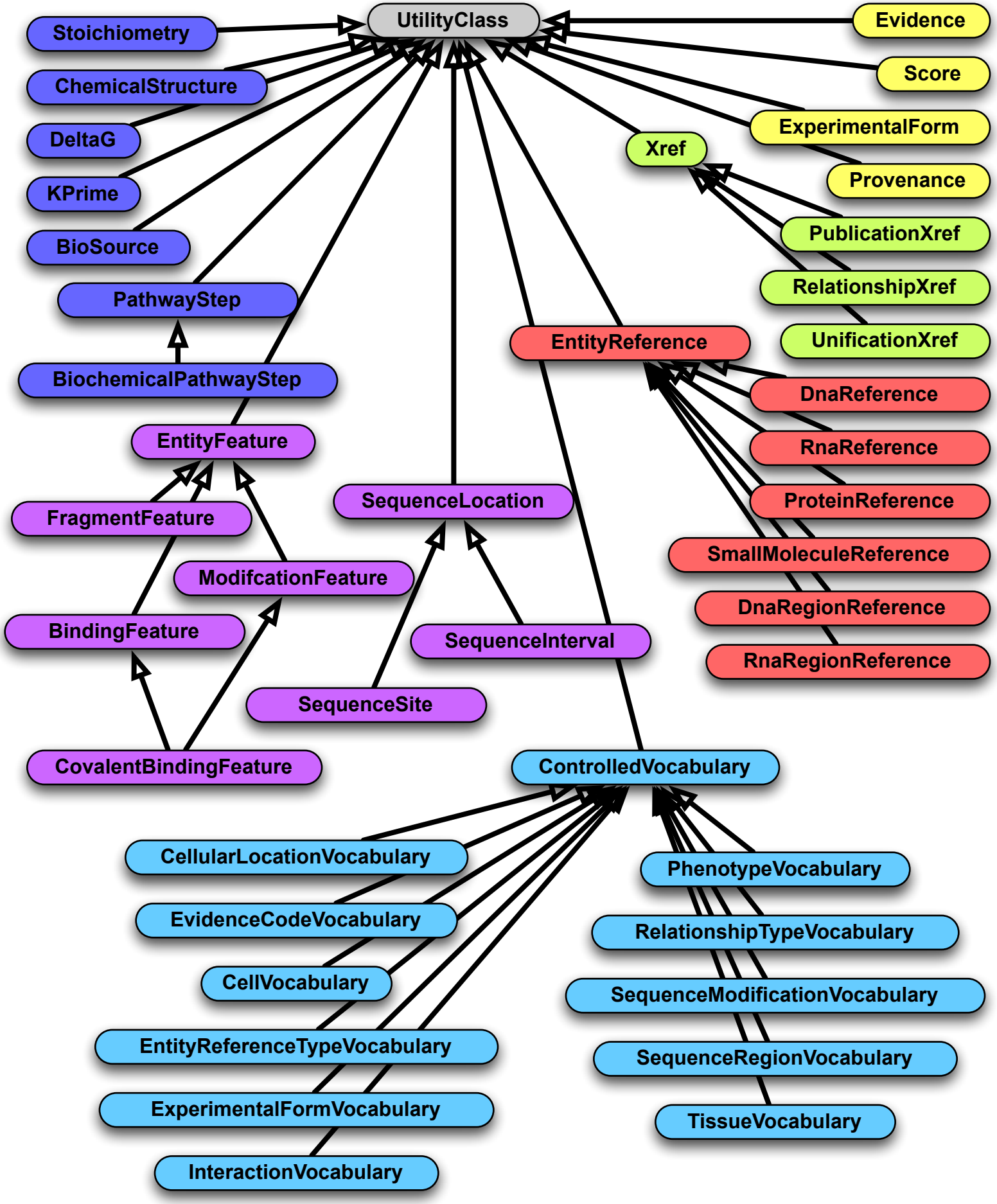

Supplemental Figure S1. Diagram of BioPAX Level 3 utility classes.

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