

A

```

<sbml>
  <model>
    <listOfCompartments>
      <compartment id="C1" name="Cytoplasm">
    </listOfCompartments>
    <listOfSpecies>
      <species id="M1" name="Glu"/>
      <species id="E1" name="hexokinase"/>
      ...
    </listOfSpecies>
    <listOfReactions>
      <reaction id="R1" name="reaction1">
        <listOfReactants>
          <speciesReference species="M1"/>
          ...
        </listOfReactants>
        <listOfProducts>
          <speciesReference species="M2"/>
          ...
        </listOfProducts>
        <listOfModifiers>
          <modifierSpeciesReference species="E1"/>
        </listOfModifiers>
      </reaction>
      ...
    </listOfReactions>
  </model>
</sbml>

```

Qualitative SBML model

B

```

<sbml>
  <model>
    <listOfUnitDefinitions>
      ...
    </listOfUnitDefinitions>
    <listOfCompartments>...</listOfCompartments>
    <listOfSpecies>
      <species id="M1" name="Glu" initialConcentration="10"/>
      <species id="E1" name="hvk" initialConcentration="3"/>
      ...
    </listOfSpecies>
    <listOfReactions>
      <reaction id="R1" name="reaction1">
        <listOfReactants>...</listOfReactants>
        <listOfProducts>...</listOfProducts>
        <listOfModifiers>...</listOfModifiers>
        <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
            ...
          </math>
          <listOfParameters>
            <parameter id="k1" value="2"/>
            ...
          </listOfParameters>
        </kineticLaw>
      </reaction>
      ...
    </listOfReactions>
  </model>
</sbml>

```

Parameterised SBML model

Parameterisation
workflow

Calibration
workflow

D

```

<sbrml>
  <ontologyTerms>
    <ontologyTerm id="term2" term="Steady State".../>
    ...
  </ontologyTerms>
  <model name="testmodel1" sourceURI="...">
    <operations>
      <operation id="op1" ontologyTerm="term2">
        <method ontologyTerm="term1"/>
        <software name=" COPASI" version="COPASI 4.5 Build"/>
        <result>
          <resultComponent id="component11">
            <dimensionDescription>
              <compositeDescription name="Metabolite"...>
                <tupleDescription>
                  <atomicDescription name="Concentration".../>
                  <atomicDescription name="Particle Numbers".../>
                </tupleDescription>
              </compositeDescription>
            </dimensionDescription>
            <dimension>
              <compositeValue indexValue="M1">
                <tuple>
                  <atomicValue>nan</atomicValue>
                  <atomicValue>nan</atomicValue>
                </tuple>
              </compositeValue>
            ...
          </resultComponent>
          ...
        </result>
      </operation>
    </operations>
  </model>
</sbrml>

```

SBRML simulation results

C

```

<sbml>
  <model>
    <listOfUnitDefinitions>
      ...
    </listOfUnitDefinitions>
    <listOfCompartments>...</listOfCompartments>
    <listOfSpecies>
      <species id="M1" name="Glu" initialConcentration="5"/>
      <species id="E1" name="hvk" initialConcentration="3"/>
      ...
    </listOfSpecies>
    <listOfReactions>
      <reaction id="R1" name="reaction1" ...>
        <listOfReactants>...</listOfReactants>
        <listOfProducts>...</listOfProducts>
        <listOfModifiers>...</listOfModifiers>
        <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
            ...
          </math>
          <listOfParameters>
            <parameter id="k1" value="4"/>
            ...
          </listOfParameters>
        </kineticLaw>
      </reaction>
      ...
    </listOfReactions>
  </model>
</sbml>

```

Calibrated SBML model

Simulation
workflow