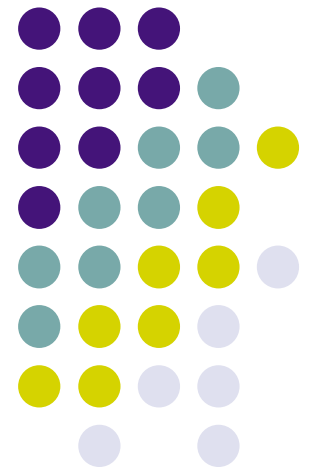
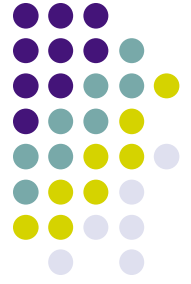


# Current status of CellDesigner and its extension of SBML

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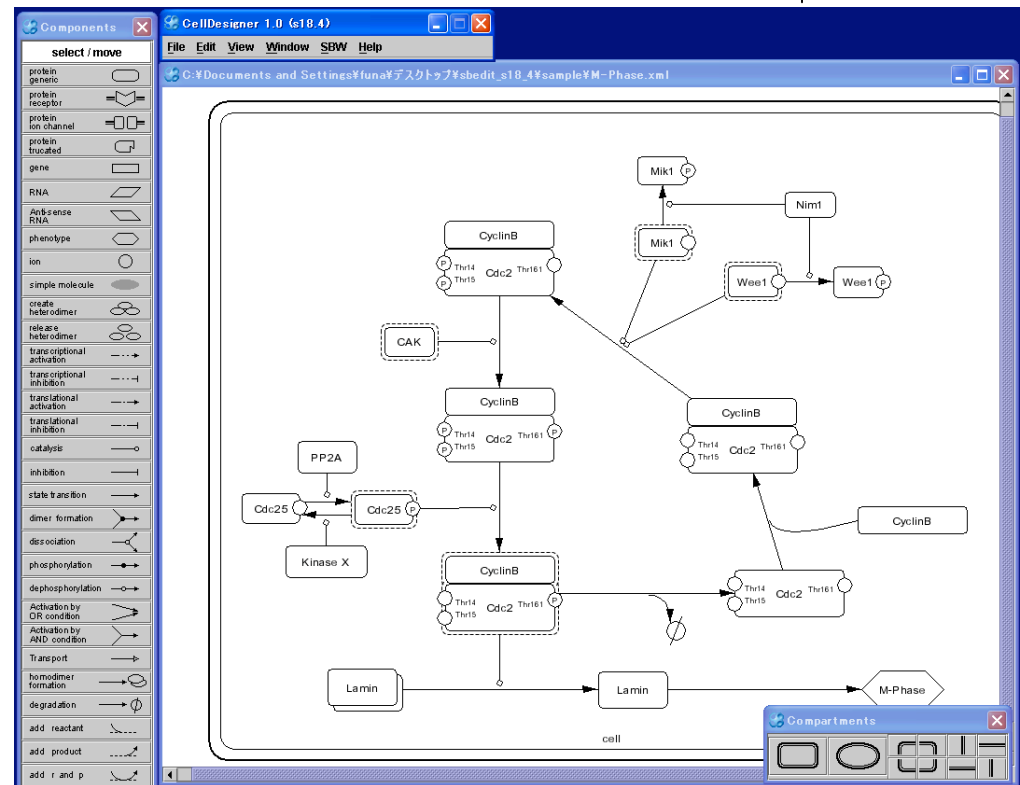
# Abstract

- Explanation of new tags for CellDesigner's editorial contents
  - The tags will be enclosed in annotation.
  - The tag's name will be under “cd:” name space.
  - Geometry information is placed in `<listOfSpeciesAliases>`
- Introduction of current status of CellDesigner
  - Read/Write pure SBML Level-1, 2 documents
  - Auto layout
  - SBW-enabled



# CellDesigner (SBEdit)

- Process network diagram editor
- Supports symbolic notation system
- Supports various types of species and reactions
  - Protein, Gene, RNA, Ion
  - Activation, Dimer formation, Dissociation, Catalysis, Inhibition
- SBW enabled
- Read/Write SBML L1, L2 document
- Written in Java (jdk1.3.1\_08)
- Tested on WindowsXP, Linux, FreeBSD



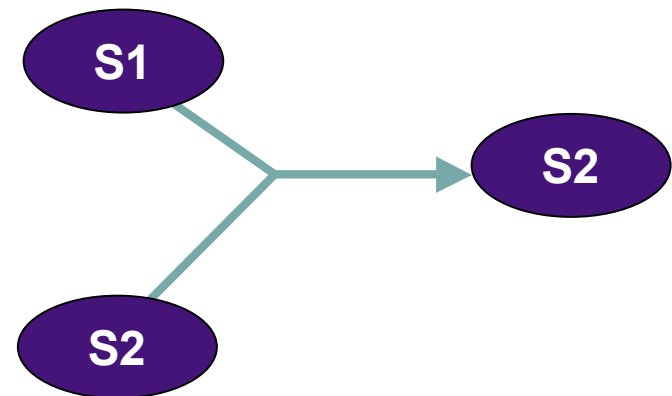
<http://www.symbio.jst.go.jp/~funa/CellDesigner/>



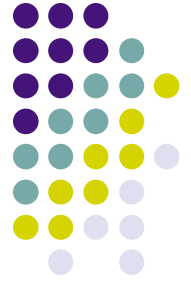
# Type Information

- Define **Class** tag in Species tag
- Define **reactionType** tag in Reaction tag

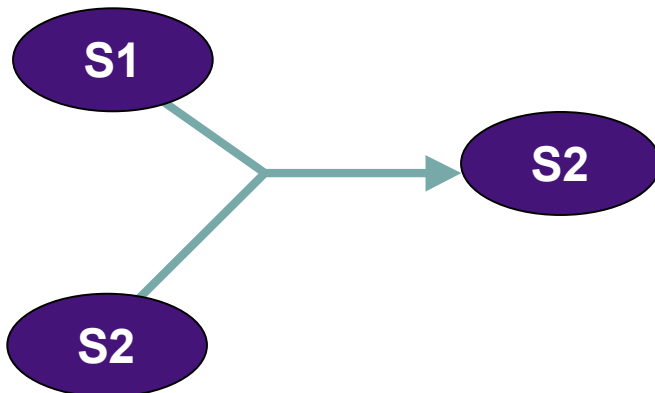
```
<specie name="s1" initialAmount="n" compartment="foo">  
  <cd:speciesIdentity>  
    <cd:class>PROTEIN</cd:class>  
  </cd:speciesIdentity>  
</specie>  
<reaction name="bar">  
  <listOfReactants>  
    list of specieReferences  
  </listOfReactants>  
  <listOfProducts>  
    list of specieReferences  
  </listOfProducts>  
  <cd:reactionType>DIMER_FORMATION</cd:reactionType>  
</reaction>
```



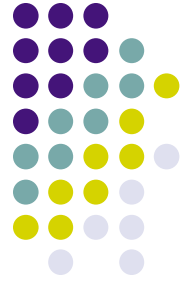
# Current implementation of CellDesigner



- The extension (new tags) are enclosed in annotation.
- The tag's name is under "cd:" name space.
- This notation rule is assumed in all tags in this presentation.

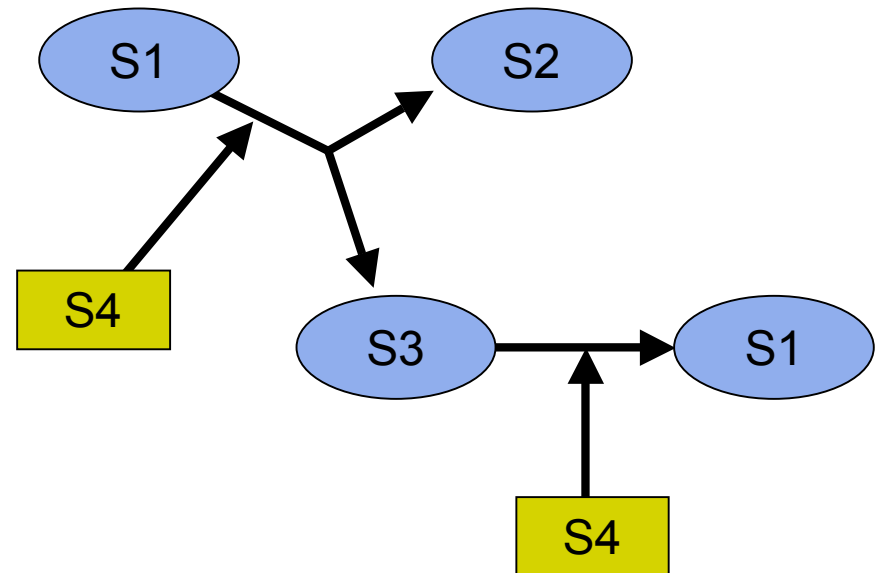


```
<reaction name="bar">
  <listOfReactants>
    list of specieReferences
  </listOfReactants>
  <listOfProducts>
    list of specieReferences
  </listOfProducts>
  <annotation>
    <cd:reactionType>DIMER_FORMATION
  </cd:reactionType>
  </annotation>
</reaction>
```



# Alias

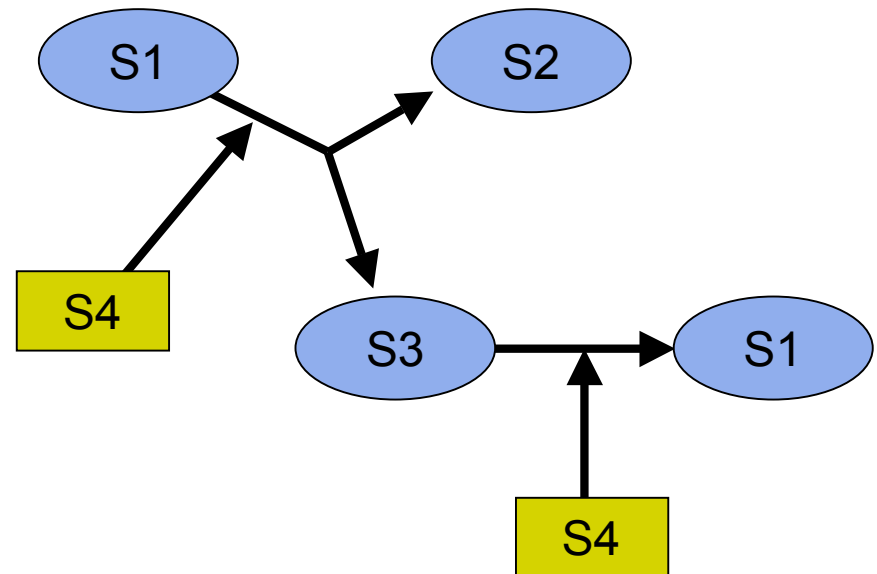
- Same species can appear more than once on a diagram.
- The view-information of appearing species on the diagram must be distinguished from their original information of the species.
- Alias tag contains all graphical information

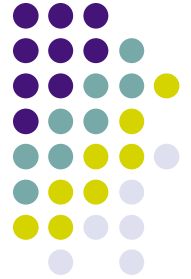




# Alias

```
<listOfSpecies>
  <specie name="s1" initialAmount="n" compartment="foo">
</listOfSpecies>
<reaction name="r1">
  <listOfReactants>
    <speciesReference species="s1">
      <cd:alias>a1</cd:alias>
    </speciesReference>
  </listOfReactants>
</reaction>
<reaction name="r2">
  <listOfProducts>
    <speciesReference species="s1">
      <cd:alias>a2</cd:alias>
    </speciesReference>
  </listOfProducts>
</reaction>
<cd:listOfSpeciesAliases>
  <cd:speciesAlias id="a1" species="s1" />
  <cd:speciesAlias id="a2" species="s1" />
</cd:listOfSpeciesAliases>
```





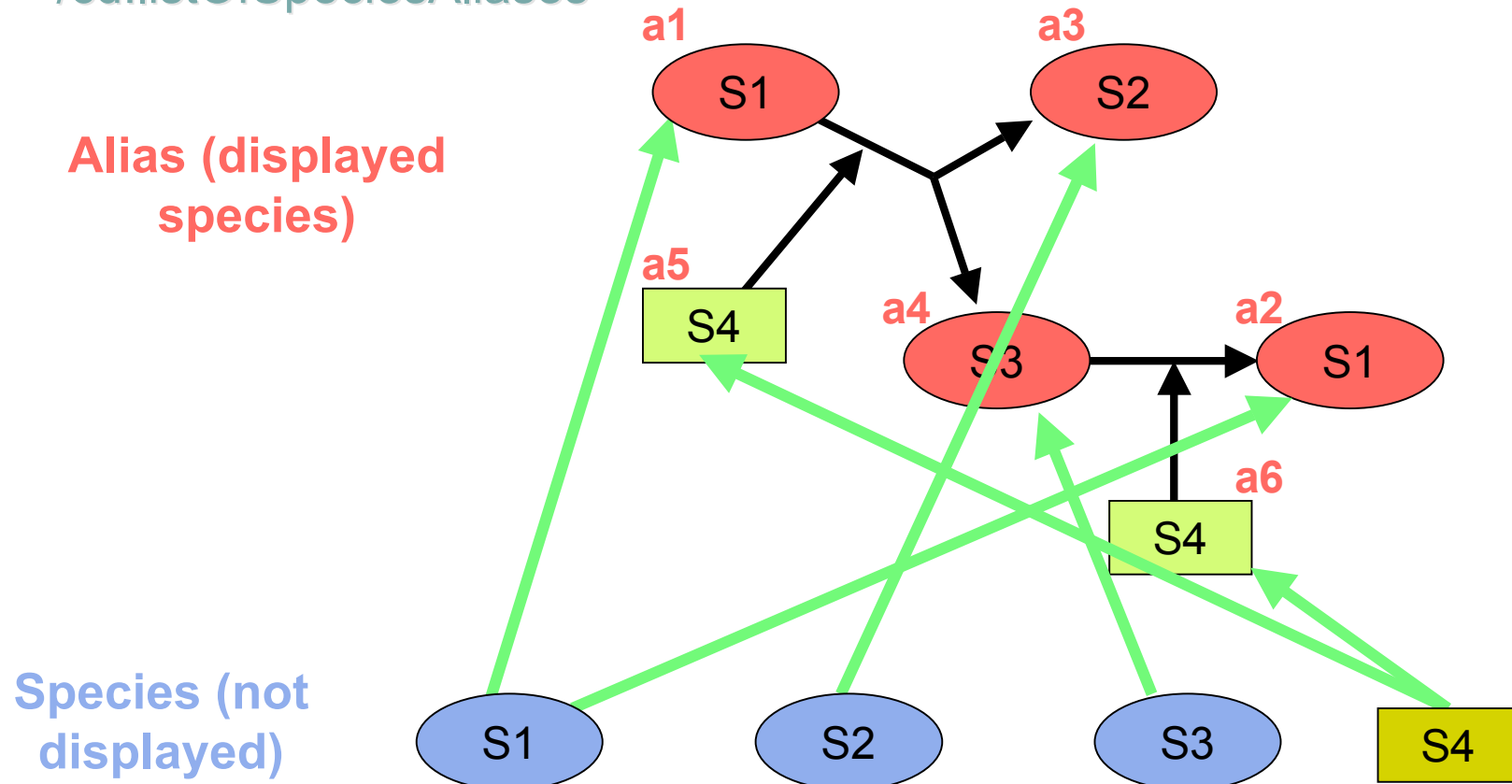
# Alias

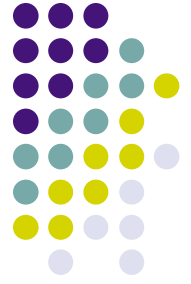
```
<cd:listOfSpeciesAliases>
```

```
  <cd:speciesAlias id="a1" species="s1" bounds="x1, y1, w1, h1">
```

```
  <cd:speciesAlias id="a2" species="s1" bounds="x2, y2, w2, h2">
```

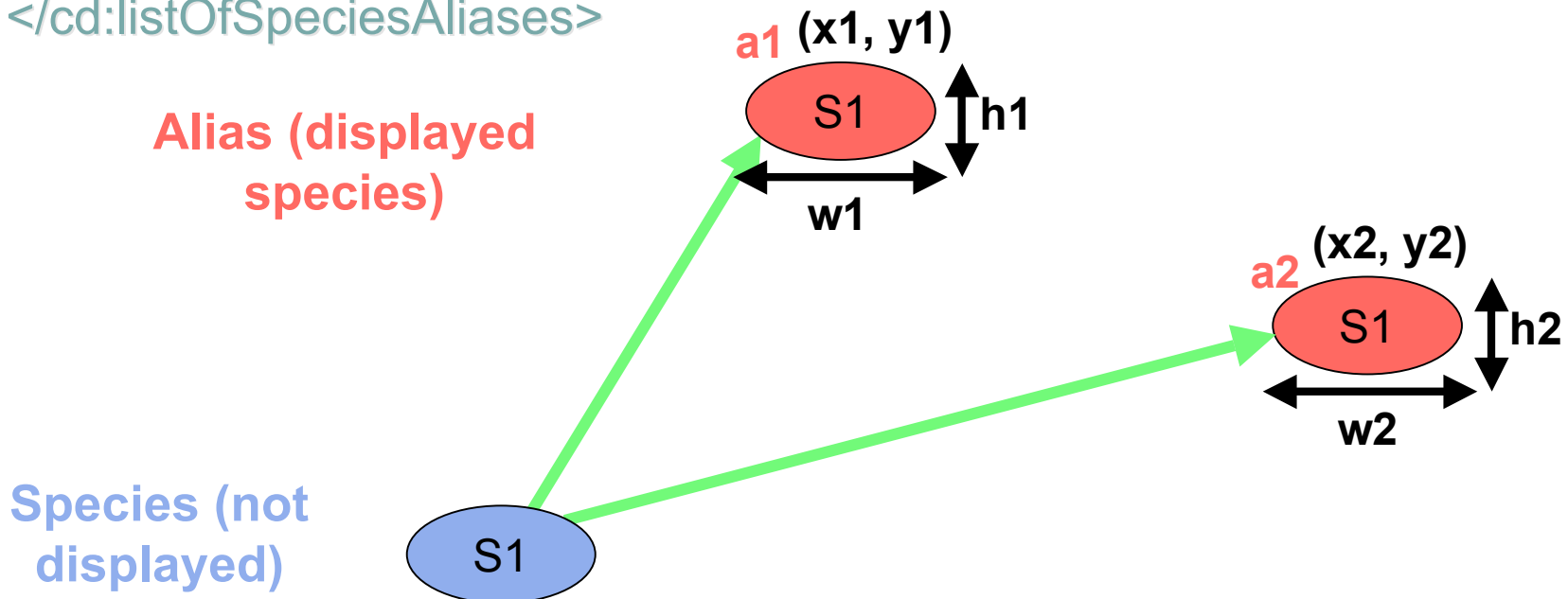
```
</cd:listOfSpeciesAliases>
```

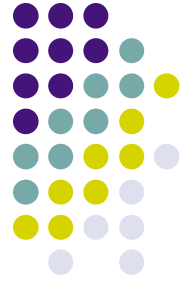




# Alias

```
<cd:listOfSpeciesAliases>  
  <cd:speciesAlias id="a1" species="s1">  
    <cd:bounds x="x1" y="y1" w="w1" h="h1"/>  
  </cd:speciesAlias>  
  <cd:speciesAlias id="a2" species="s1">  
    <cd:bounds x="x2" y="y2" w="w2" h="h2"/>  
  </cd:speciesAlias>  
</cd:listOfSpeciesAliases>
```





# Regulation

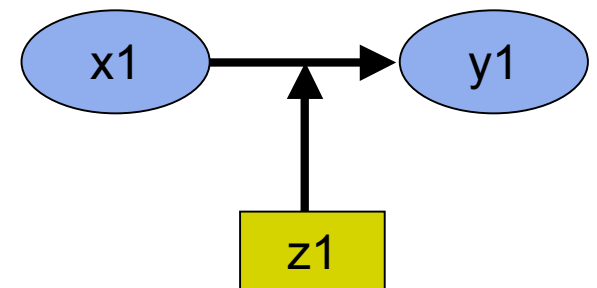
- CellDesigner uses `<listOfModifiers>` to represent regulators

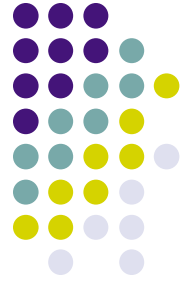
## SBEdit

```
<reaction>
  <listOfReactants>
    list of speciesReferences (x1,...,xn)
  </listOfReactants>
  <listOfProducts>
    list of speciesReferences (y1,...,yn)
  </listOfProducts>
  <listOfRegulations>
    <regulation>
      <listOfRegulators>
        list of speciesReferences (z1,...,zn)
      </listOfRegulators>
    </regulation>
  </listOfRegulations>
</reaction>
```

## CellDesigner

```
<reaction>
  <listOfReactants>
    list of speciesReferences (x1,...,xn)
  </listOfReactants>
  <listOfProducts>
    list of speciesReferences (y1,...,yn)
  </listOfProducts>
  <listOfModifiers>
    list of modifierSpeciesReferences (z1,...,zn)
  </listOfModifiers>
</reaction>
```

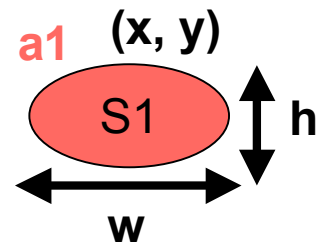




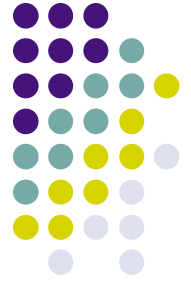
# Graphical Information

- Species
  - Graphical forms of symbols are pre-defined
  - Configuration of Bounding Box is required
- Reactions, Regulations
  - Arrows are automatically drawn
  - No need to specify the information of arrows

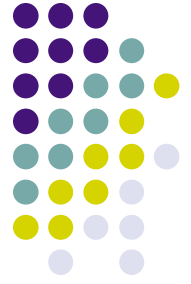
```
<model>
  <listOfCompartments>
  </listOfCompartments>
  <listOfSpecies>
  </listOfSpecies>
  <listOfReactions>
  </listOfReactions>
  <annotation>
    <cd:listOfCompartmentAliases>
    </cd:listOfCompartmentAliases>
    <cd:listOfSpeciesAliases>
    </cd:listOfSpeciesAliases>
  </annotation>
</model>
```



# Reading/Writing SBML document

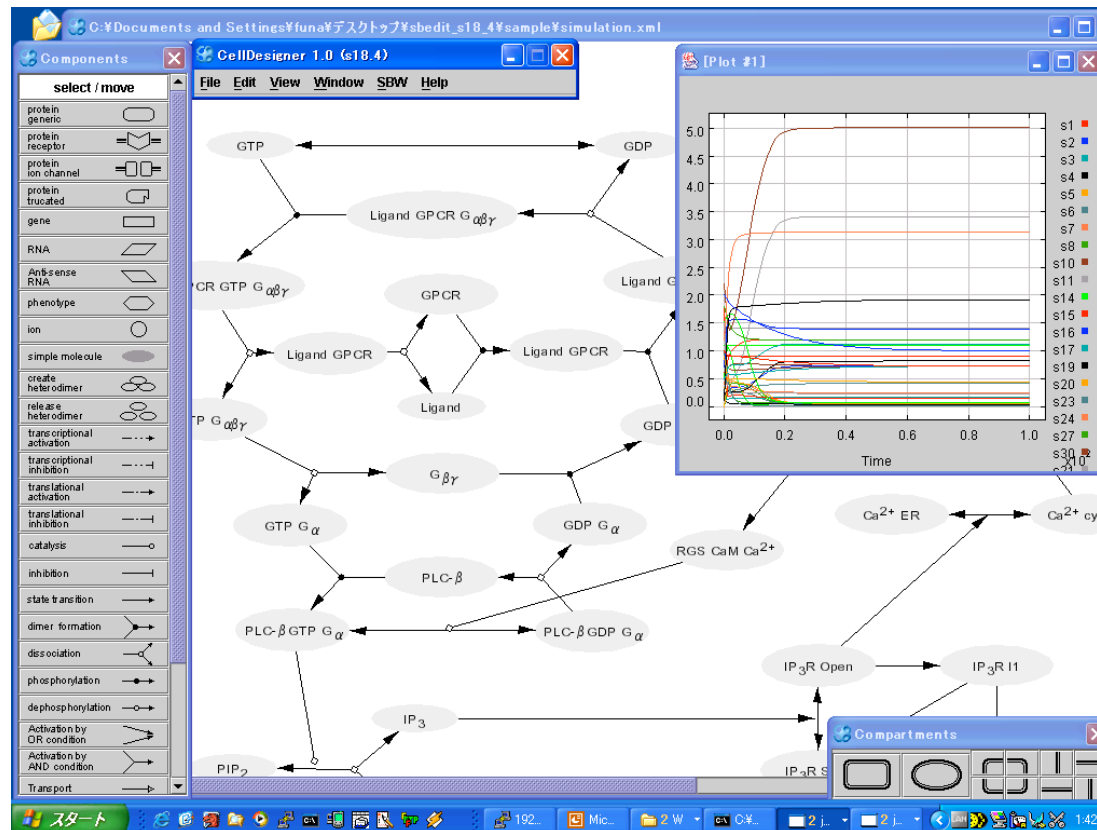


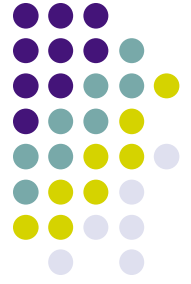
- CellDesigner supports:
  - Reading/Writing pure SBML Level-1
  - Reading/Writing pure SBML Level-2 (except MathML)
    - Auto layout
  - Reading SBML Level-1 + SBEdit annotation
  - Reading/Writing SBML Level-2 + CellDesigner annotation (except MathML)



# SBW enabled

- CellDesigner is *SBW-enabled* application
  - CellDesigner + Jarnac on WindowsXP
  - CellDesigner + Gibson on Linux





# Conclusion

- Explanation of CellDesigner's extension of SBML
  - Type information (`<cd:reactionType>`, `<cd:class>`)
  - Alias (`<cd:listOfSpeciesAliases>`, `<cd:alias>`)
  - Regulation (`<listOfModifiers>`, `<modifierSpeciesReference>`)
  - Graphical information (`<cd:bounds>`)
- Introduction of current status of CellDesigner.
  - Read/Write pure SBML Level-1, 2 documents
  - SBW-enabled

<http://www.symbio.jst.go.jp/~funa/CellDesigner/>