

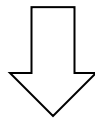
# SBML Multi Package

Breakout session

# Rule Based Model Examples

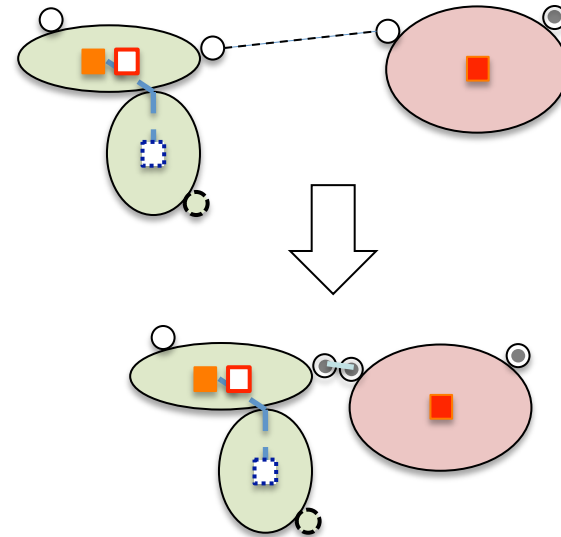
*Transformation (Phosphorylation)*

EGFR(CR1!+,Y1068~U)



EGFR(CR1!+,Y1068~P)

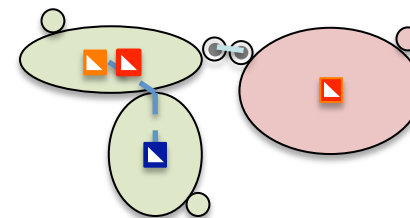
*Association (complex-complex):*



*Molecule type:*

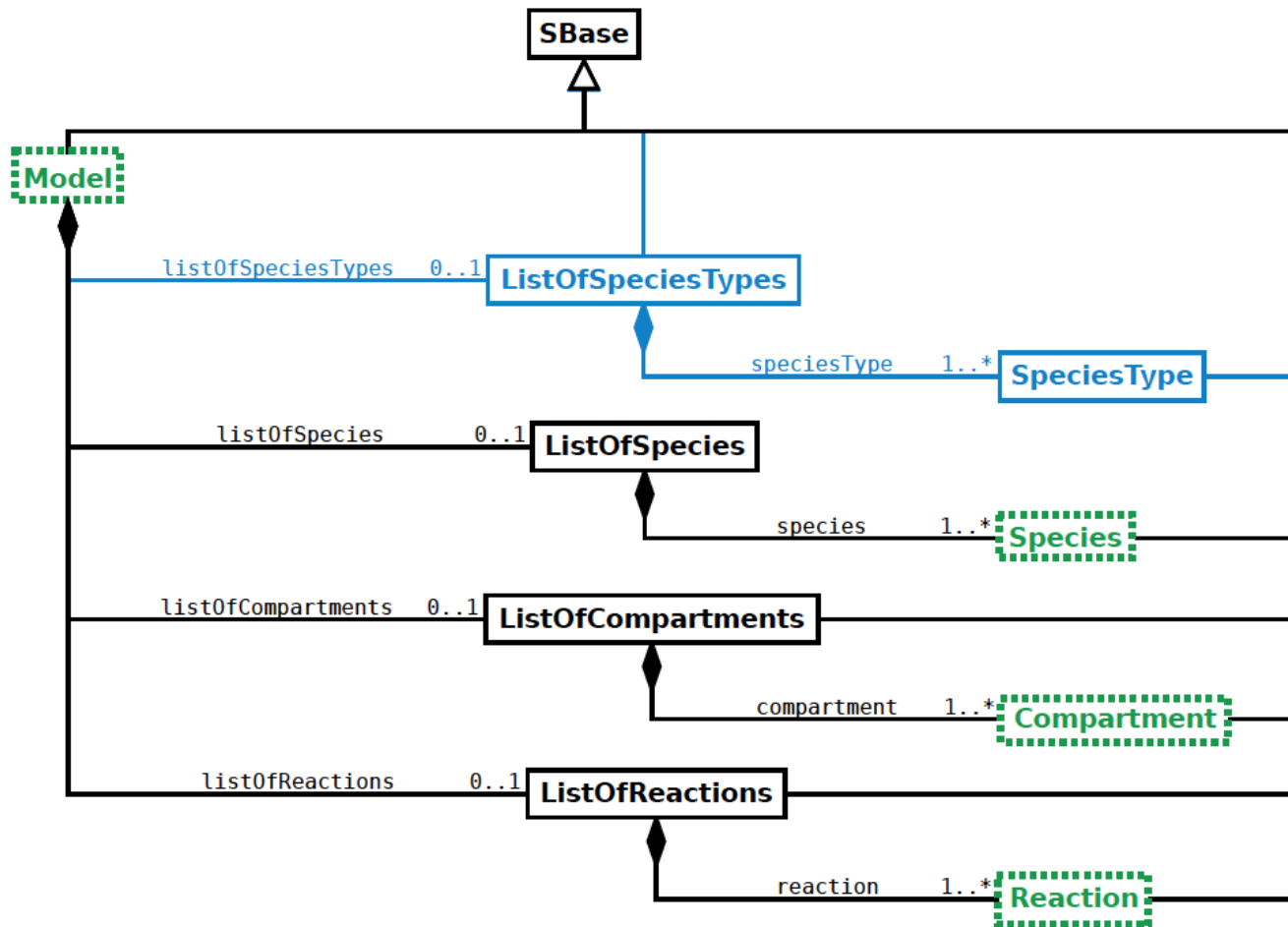
EGFR(L, CR1, Y1068~U~P)

*Complex Species:*



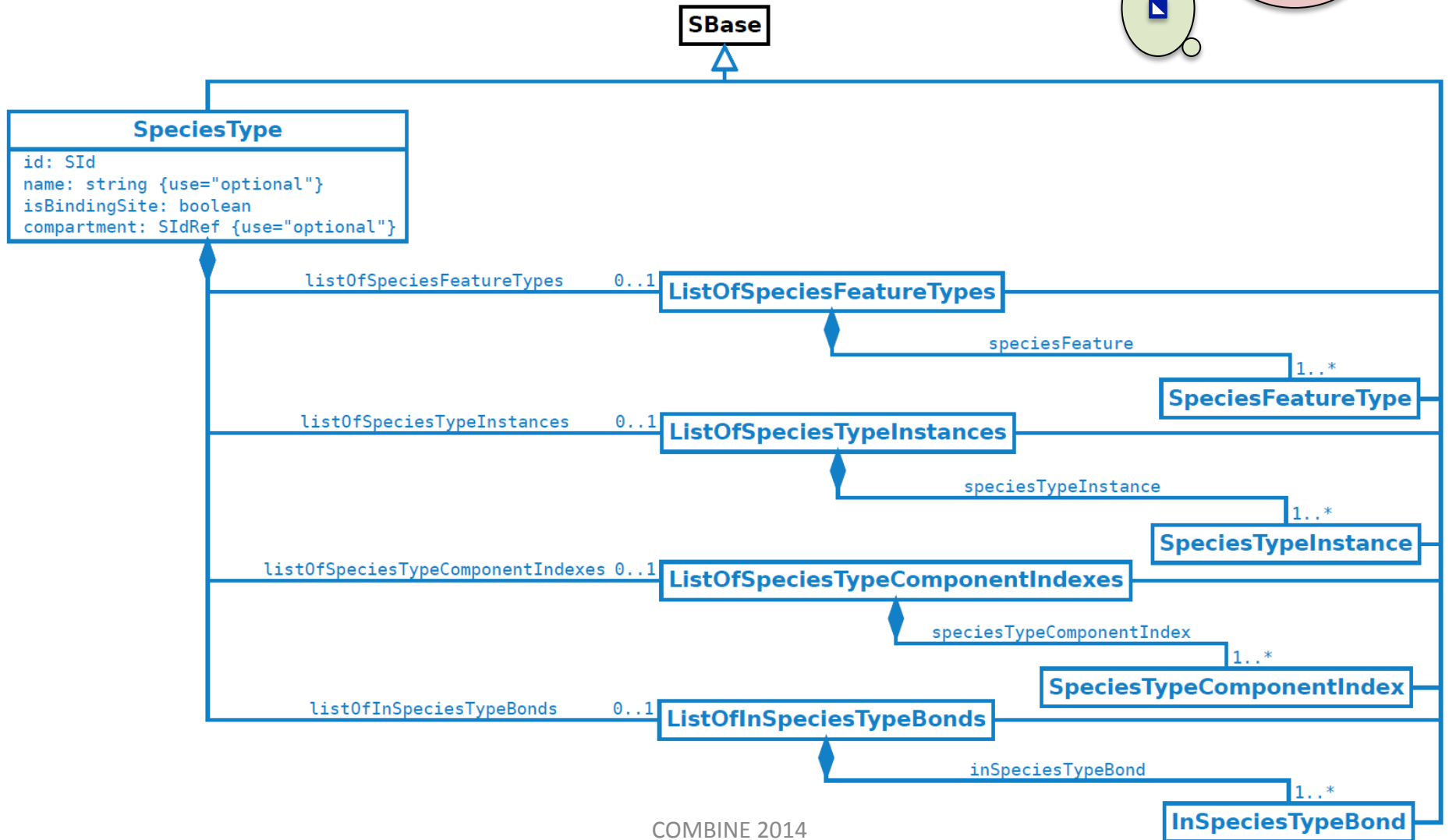
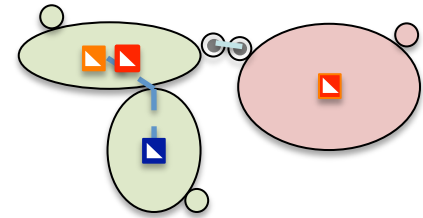
# Review of Current Multi

# Model

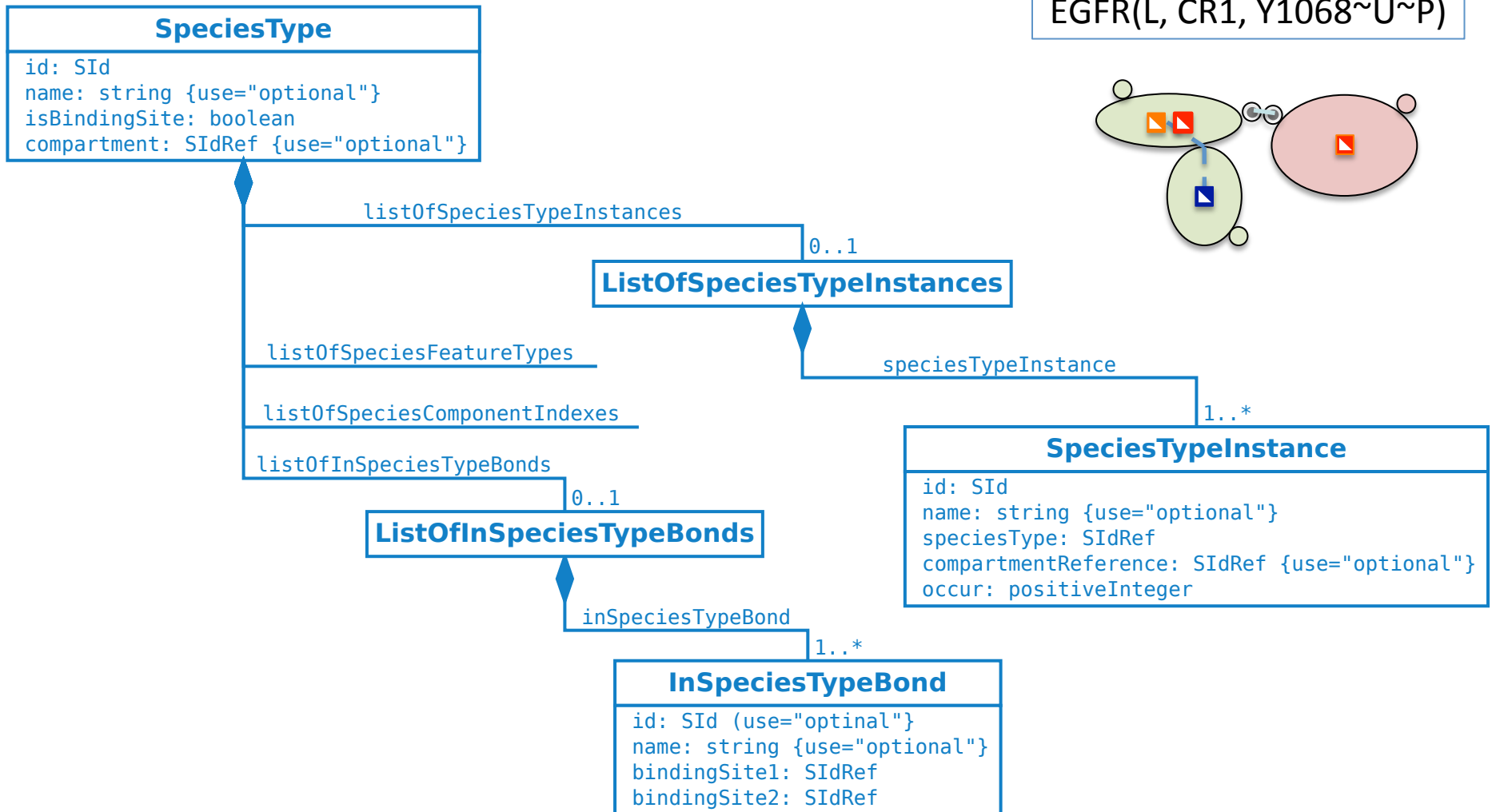


# SpeciesType

EGFR(L, CR1, Y1068~U~P)

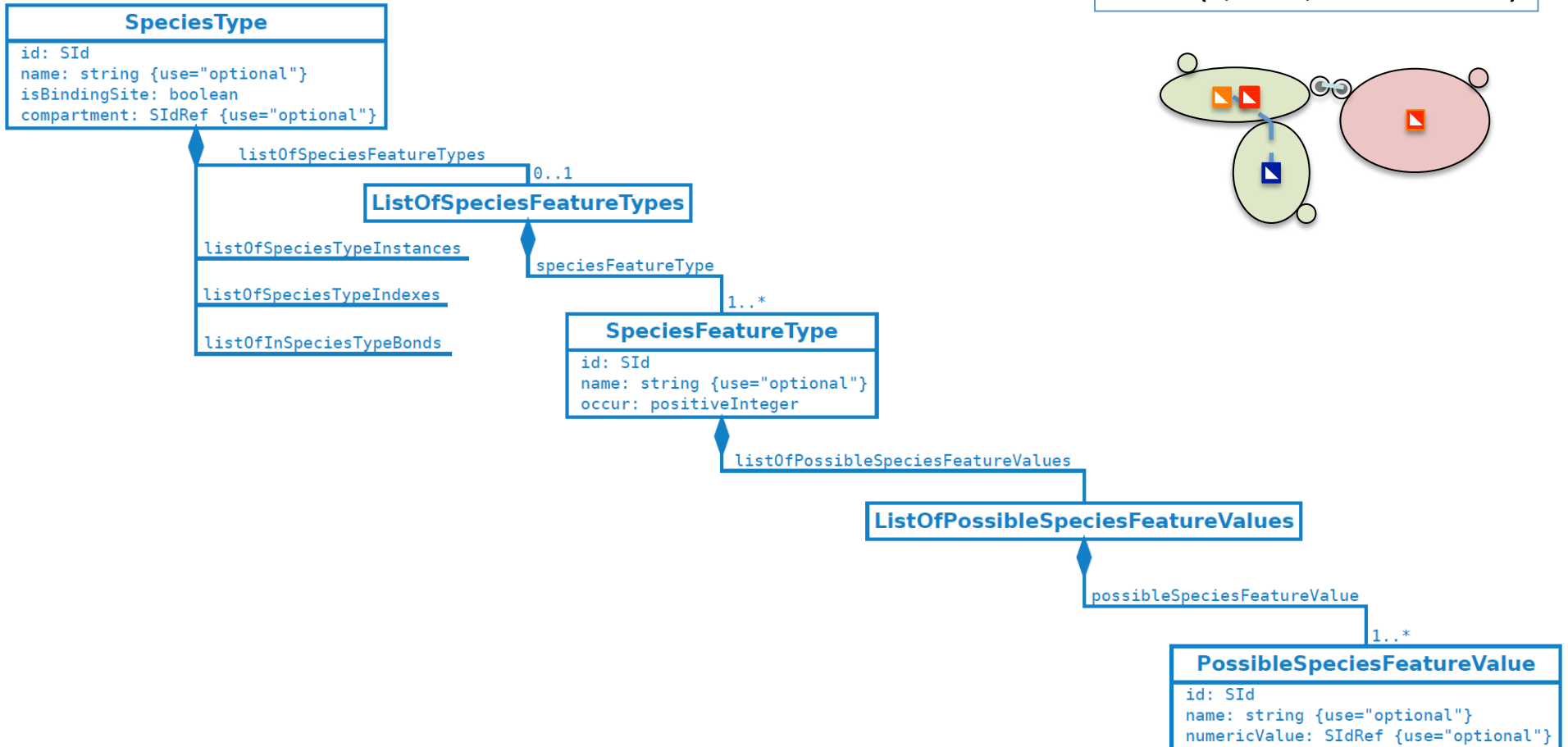


# SpeciesType: *SpeciesTypeInstance* and *InSpeciesTypeBond*

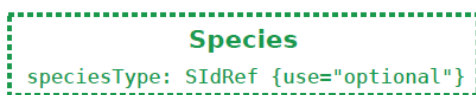


# SpeciesType: *SpeciesFeatureType*

EGFR(L, CR1, Y1068~U~P)

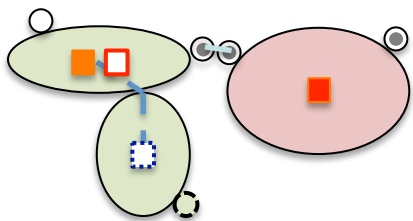
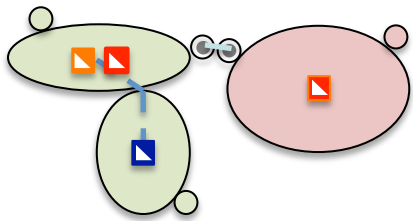
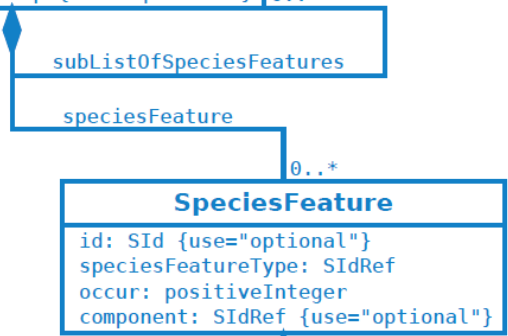


# Species



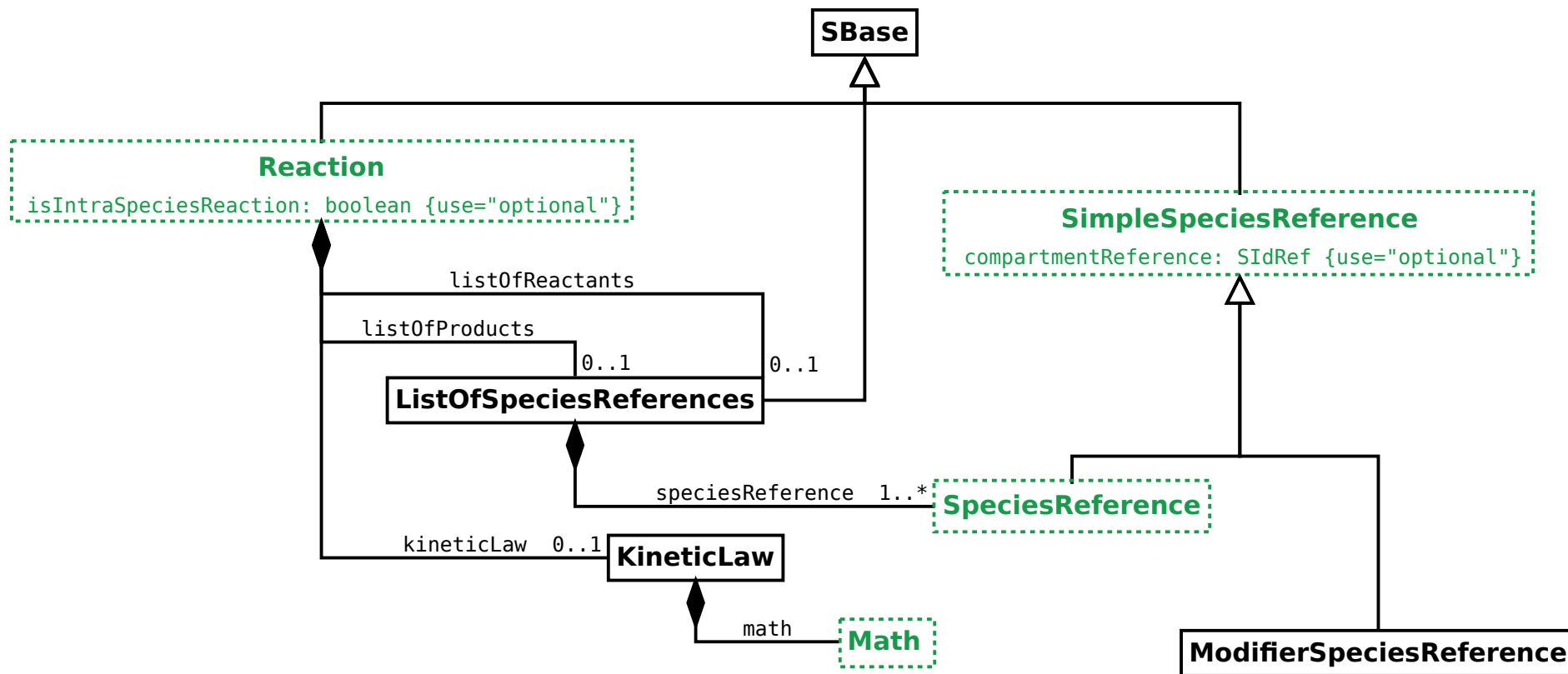
EGFR(L, CR1, Y1068~U~P)

EGFR(CR1!+,Y1068~P)  
EGFR(L!1,CR1).EGF(R!1)

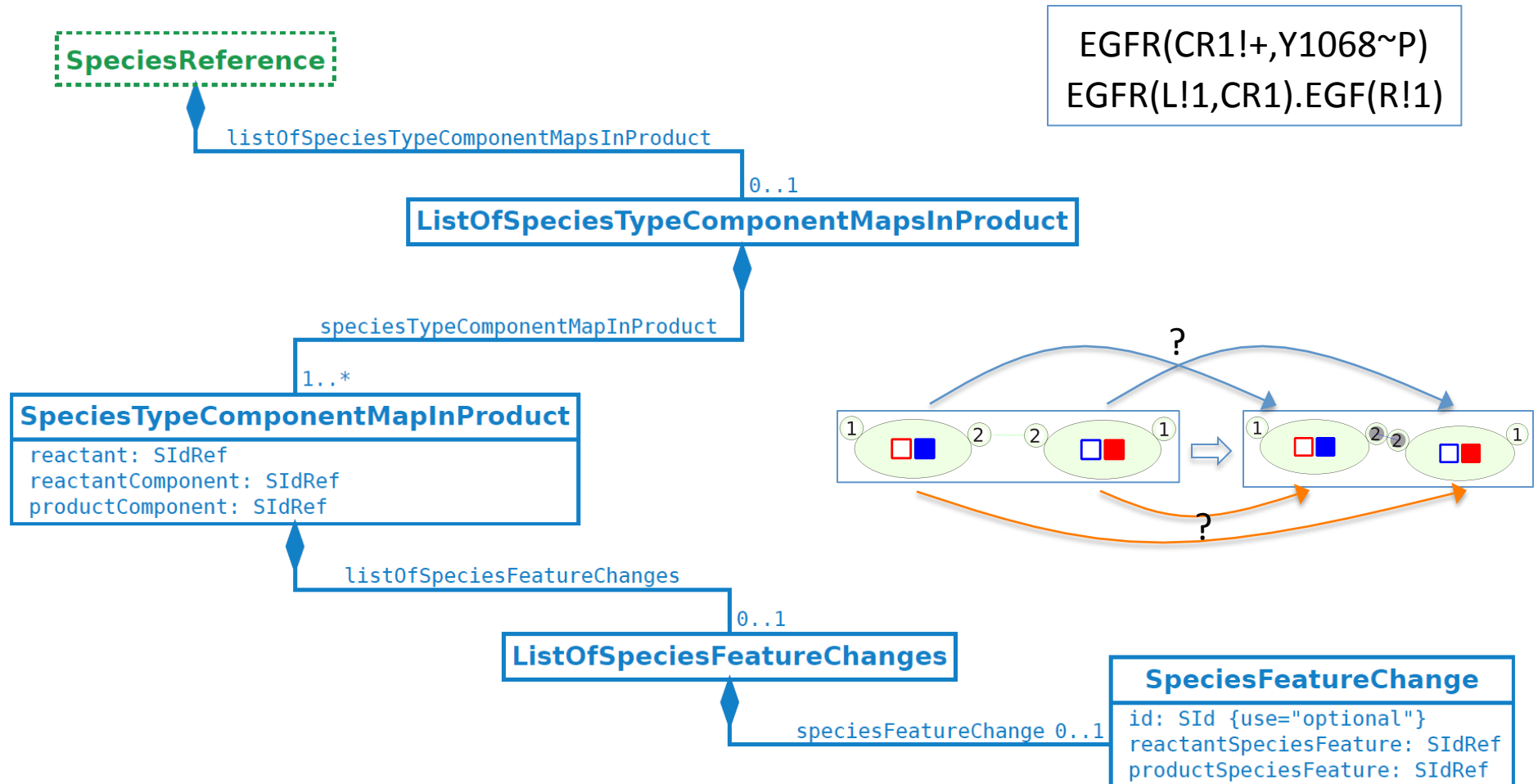




# Reaction



## Reaction: *SpeciesTypeComponentMapInProduct* and *SpeciesFeatureChange*



# Others (mainly discussed in COMBINE 2013)

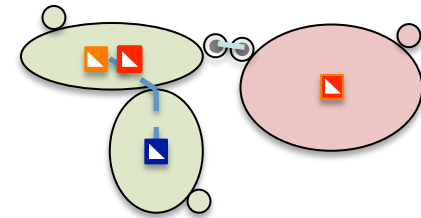
- Extended **Compartment** class
  - “*isType*” attribute
  - “**ListOfCompartmentReferences**” and “**CompartmentReference**” classes
- Under **SpeciesType** class
  - “**ListOfSpeciesTypeComponentIndexes**” and “**SpeciesTypeComponentIndex**” classes
    - Example usage: Multiple occurrences of identical components
- “**ci**” attributes under **kineticLaw** and **math**
  - “*speciesReference*”
    - **Species** id: concentration
    - **SpeciesFeature** id: *number Of appearances* or *numericValue*
  - “*representationType*”
    - “*sum*” - concentration
    - “*numericValue*”

# Questions for Discussion

- The current Multi specification has been developed to cover requirements from different modelers for model exporting, what is needed for **model importing**?

- Difficulties for Simmune

- Multiple occurrences of components and features
- Binding sites with child speciesTypeInstances
- Unlimited recursive relations of SpciesType and SpciesTypeInstance
- Feature for composite speciesTypes



- Potential issues for BioNetGen

- Compartment type?
- Multiple occurrences of components and features?
- Binding sites with child speciesTypeInstances
- Feature for composite speciesTypes

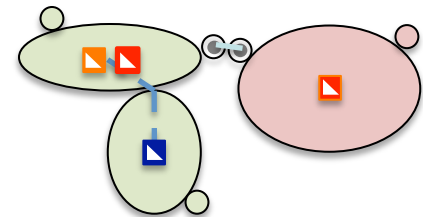
```
EGFR(CR1!+,Y1068~P)
EGFR(L!1,CR1).EGF(R!1)
```

- Other rule-based modeler?

# Proposed changes

- **SpeciesFeatureType** under **SpeciesType**
  - For a **composite** *speciesType* has at least one *inSpeciesTypeBond*
    - Can **NOT** have a *listOfSpeciesFeatureTypes*
- “*isBindingSite*” attribute of **SpeciesType** class
  - Can **NOT** be “true” for a **speciesType** has *listOfSpeciesTypeInstances*

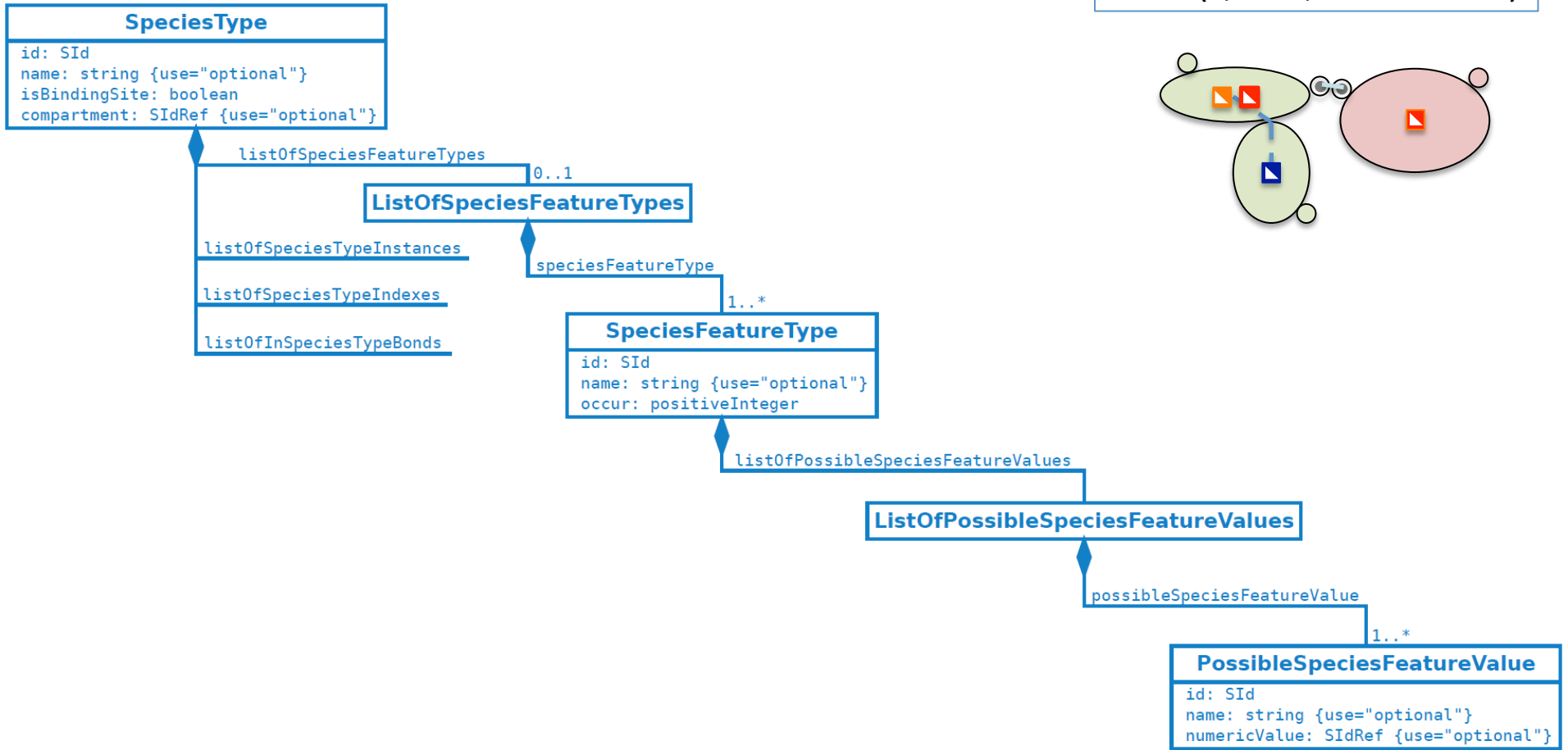
```
EGFR(CR1!+,Y1068~P)  
EGFR(L!1,CR1).EGF(R!1)
```



# Questions for Discussion

- **Compartment** class in Multi and other packages, such as Spatial?
  - Possible to integrate or cross reference(mapping)?
- **Species** class
  - Can multi species ids be referenced by “Core” or other packages?
    - “Fully defined” property: modeler function or attribute?
- Working with the Distribution package
  - Referencing a function id, or adding a variable for “occur” (as well other) attributes?

# SpeciesType: *SpeciesFeatureType*



# Identify things needed for package approval

*([http://sbml.org/Documents/SBML\\_Development\\_Process/SBML\\_Development\\_Process\\_for\\_SBML\\_Level\\_3#The\\_approval\\_of\\_the\\_specification](http://sbml.org/Documents/SBML_Development_Process/SBML_Development_Process_for_SBML_Level_3#The_approval_of_the_specification))*

- Specification: 1.01 (rev369)
  - a new version (1.02) will be available to reflect the discussion of this meeting
- libSBML-multi (Thanks to Sarah and the SBML team! Experimental release available from libSBML 5.9.0)
  - Enforce of validation rules
- Two software implementations
  - Simmune (model export✓, model import?)
  - BioNetGen(model export?, model import?)
  - Other?



# Things needed for requesting package approval

*([http://sbml.org/Documents/SBML\\_Development\\_Process/SBML\\_Development\\_Process\\_for\\_SBML\\_Level\\_3#The\\_approval\\_of\\_the\\_specification](http://sbml.org/Documents/SBML_Development_Process/SBML_Development_Process_for_SBML_Level_3#The_approval_of_the_specification))*

- “Every feature in the package specification must be supported and manipulated by at least one to the two tools”
  - “numericValue” attribute in PossibleSpeciesFeatureValue class?
    - Current Simmune: no support
    - Current BioNetGen:?
    - Other?
  - “occur” attribute in SpeciesFeatureType class?
    - Current Simmune: always “1”
    - Current BioNetGen:?
    - Other?
  - “occur” attribute in SpeciesTypeInstance class
    - Current Simmune: always “1”
    - Current BioNetGen:?
    - Other?
  - “occur” attribute in SpeciesTypeComponentIndex
    - Current Simmune: always “1”
    - Current BioNetGen:?
    - Other?

# Support SBML L3v1 and/or L3v2

- Id and name in SBase in L3v2
  - Different specification to support L3v2?
  - Or drop support to L3v1?