

SBML Multi Package: Development Update and Discussion

Fengkai Zhang

Breakout session

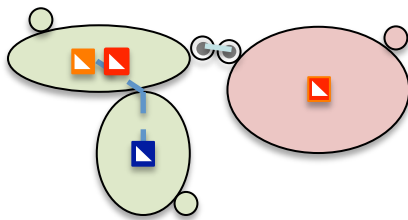
COMBINE 2015

Development Highlights

- The Multi Specification (v 1.0.4): *stable*
- Implementation of libsbml-multi: *complete*
 - Library functions
 - Reading and writing
 - Validation Rules:
 - Identifier
 - Consistency
 - Tests

Example Models Covered by Multi

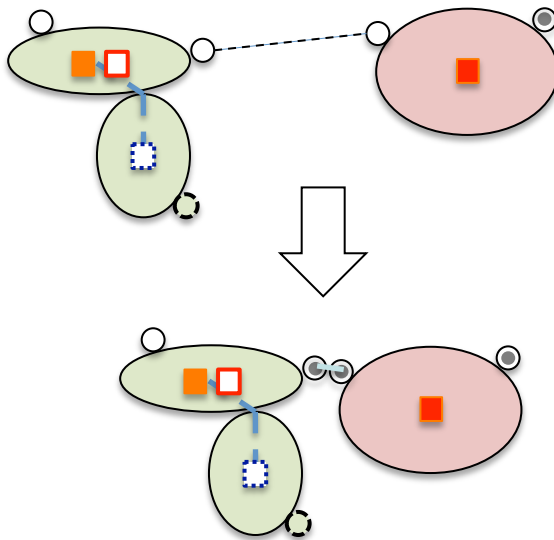
Complex Species:



Molecule type:

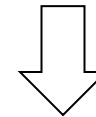
EGFR(L, CR1, Y1068~U~P)

Association (complex-complex):



Transformation (Phosphorylation)

EGFR(CR1!+,Y1068~U)



EGFR(CR1!+,Y1068~P)

libsbml: package implementation

- Package extension
 - <http://sbml.org/Software/libSBML/5.11.4/docs/formatted/cpp-api/libsbml-extending.html>
- Validation
 - http://sbml.org/SBML_Projects/libSBML/Implementing_validation_for_packages
- Reference to other implemented packages
“Comp”, “Group”, ...



libsbml-multi

- Multi library implementation:
 - Classes:
 - Extension (plugin) classes: **9**
 - New SBML Multi classes: **15**
 - Reading and writing functions
- Multi validation Rules: **163**
 - Identifier
 - At Read: **23**
 - Check: **9**
 - Consistency
 - At Read: **99**
 - Check: **32**
- Multi unit tests: **77**
- Core modification

libsbml-multi

- SBML core modification to support multi classes
 - **BindingSiteSpeciesType** and **IntraSpeciesReaction**
 - Changes of core classes: **SBase**, **SBasePlugin** and **ListOf**
 - **MultiASTPlugin**: ci element, multi:speciesReference
 - Changes of core class: **ASTBasePlugin**

To become “official”

- **Specification** 
- **libSBML-multi** 
- **Software support:** ?

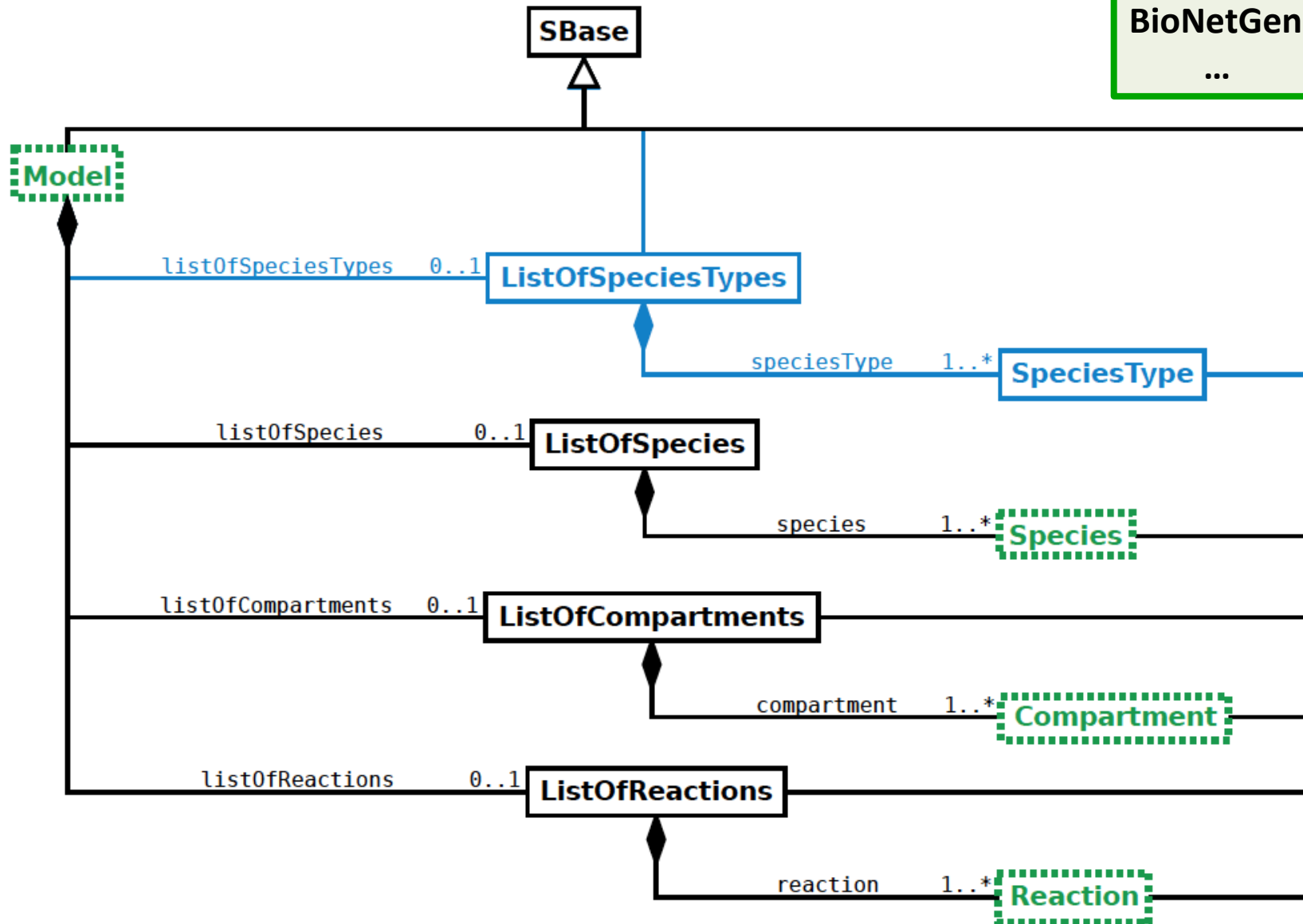
** At least two different software packages implement 'most' of the spec.*

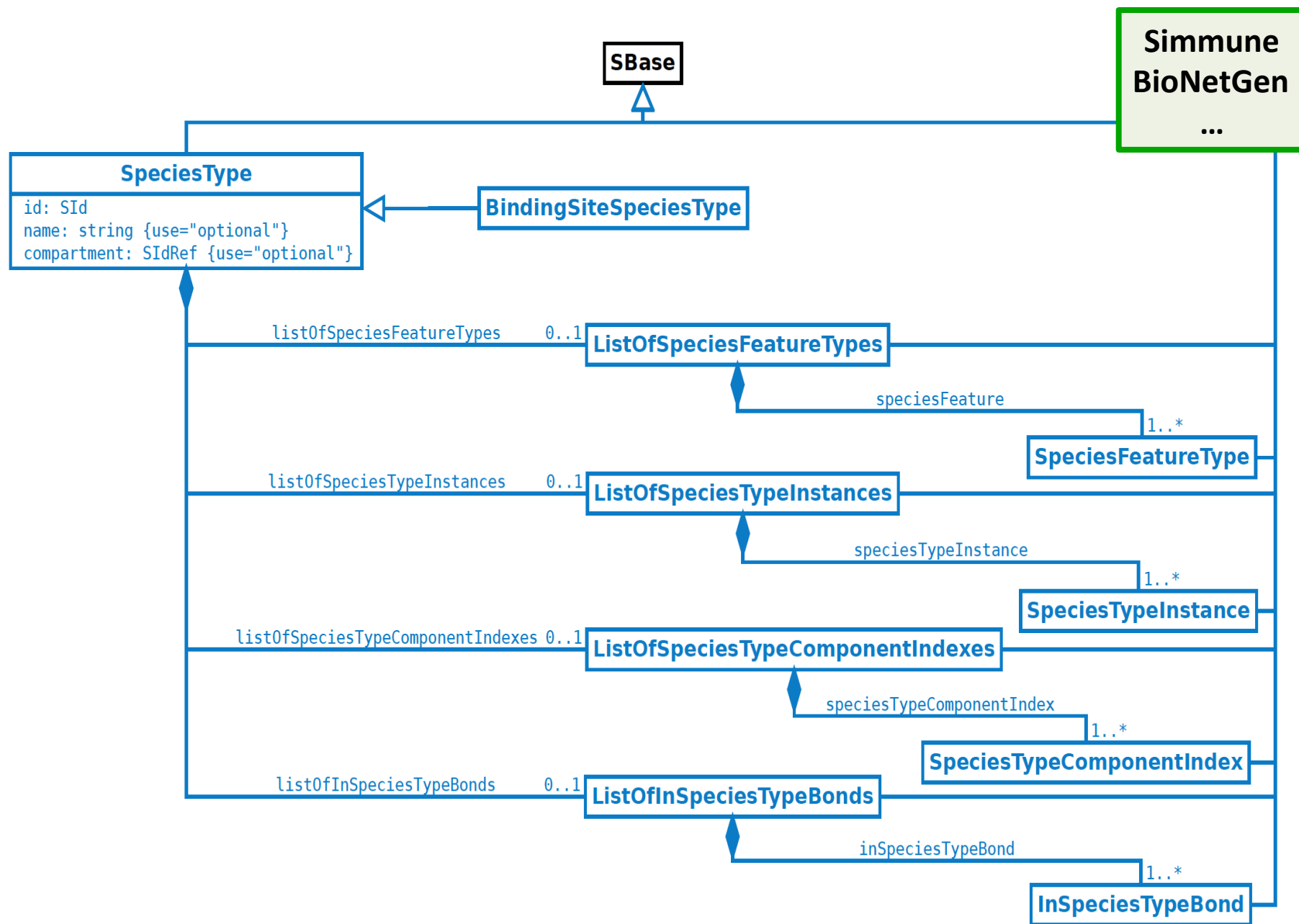
** Each part of the spec is implemented by at least one software package.*

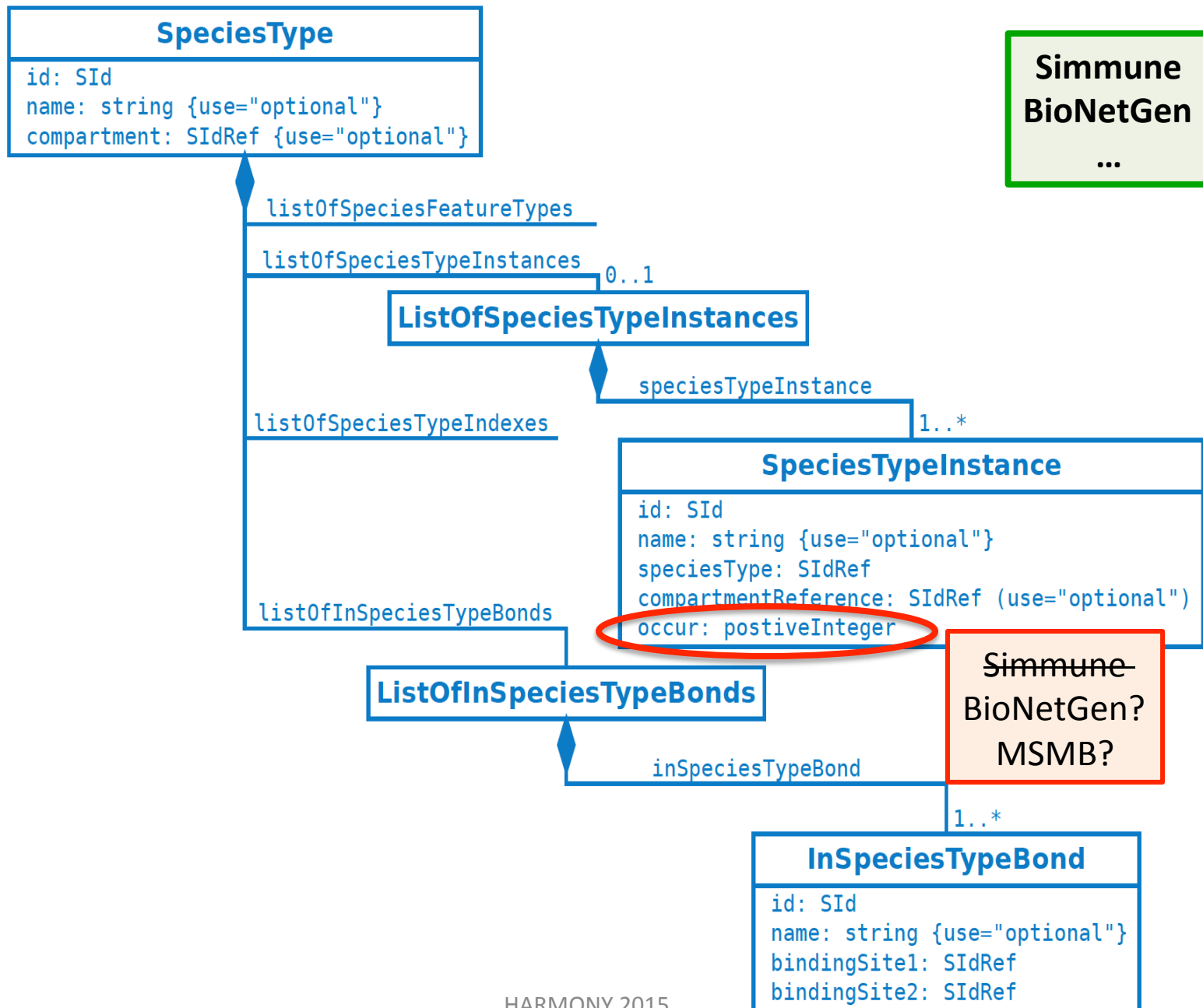
Software Support

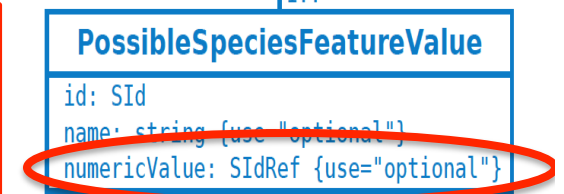
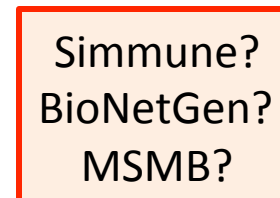
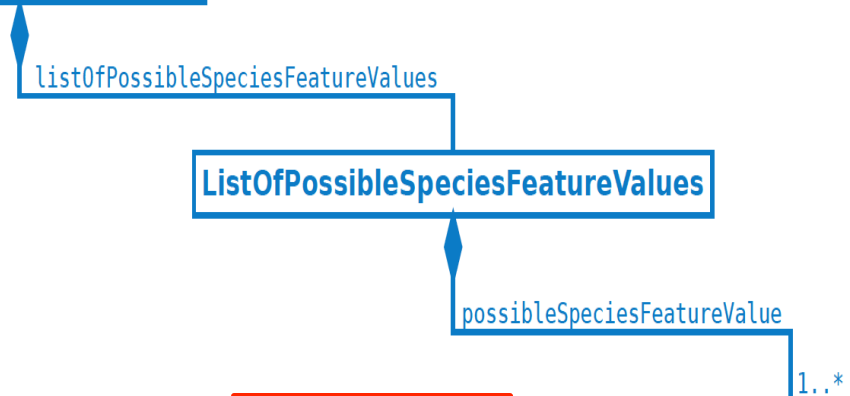
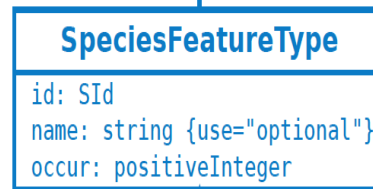
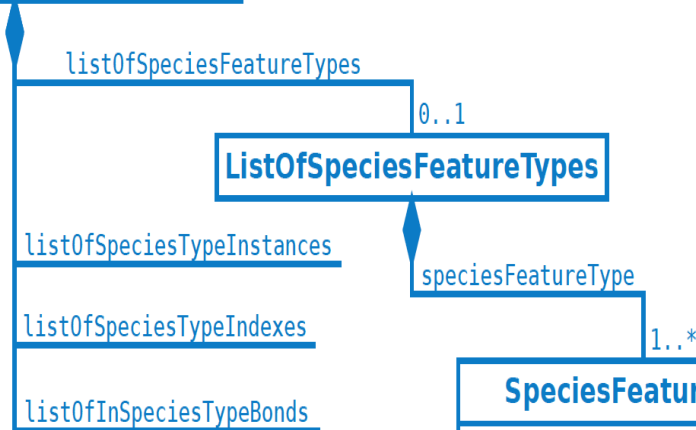
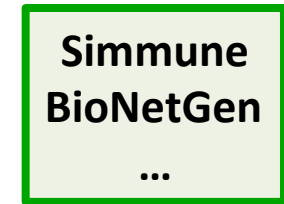
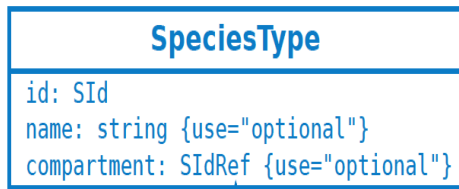
- Simmune
 - Export ✓
 - Import: under development
- BioNetGen
- MSMB
- ...

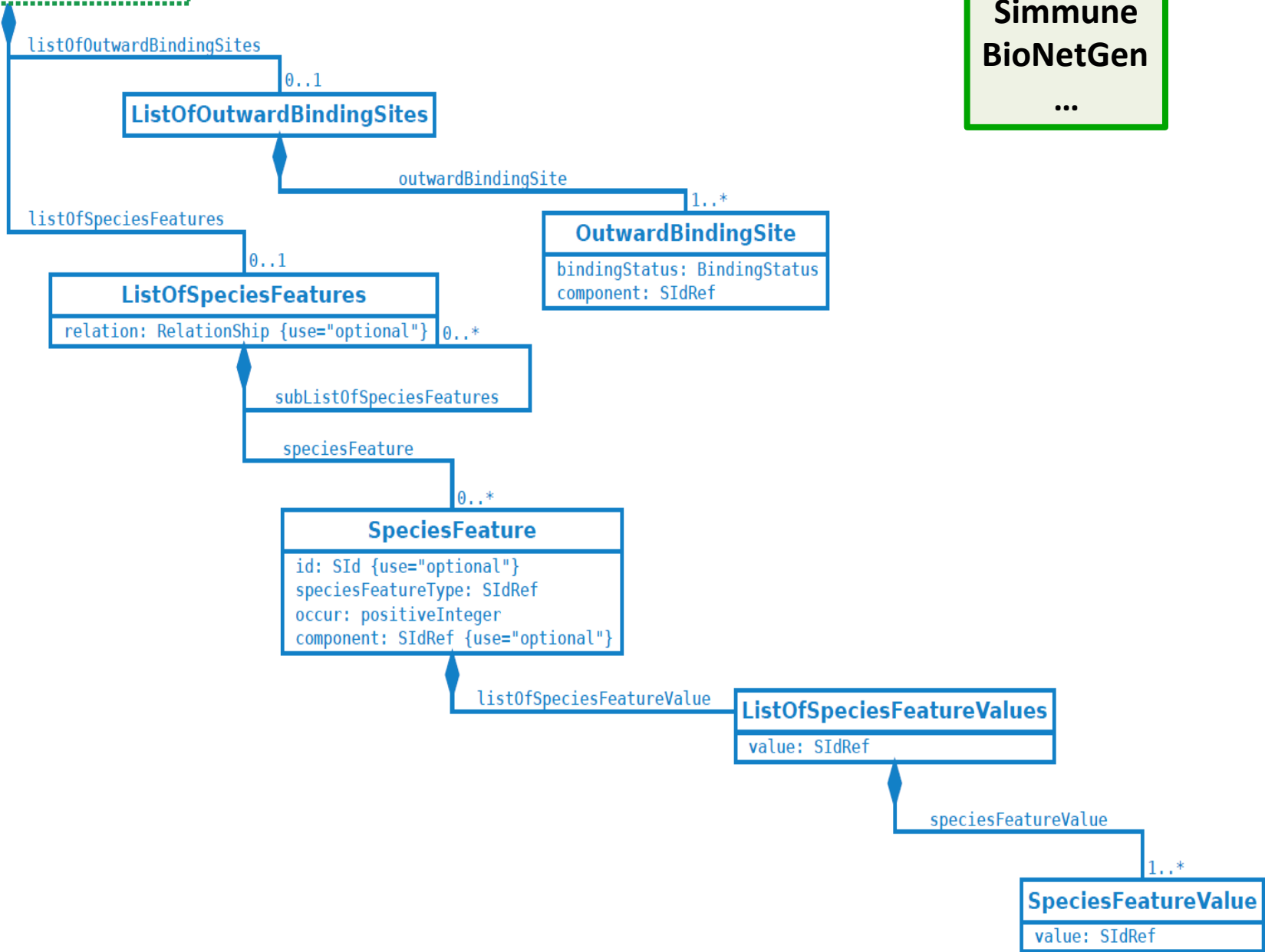
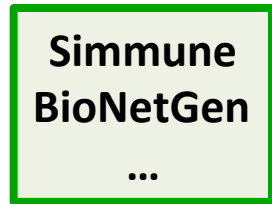
Simmune
BioNetGen
...

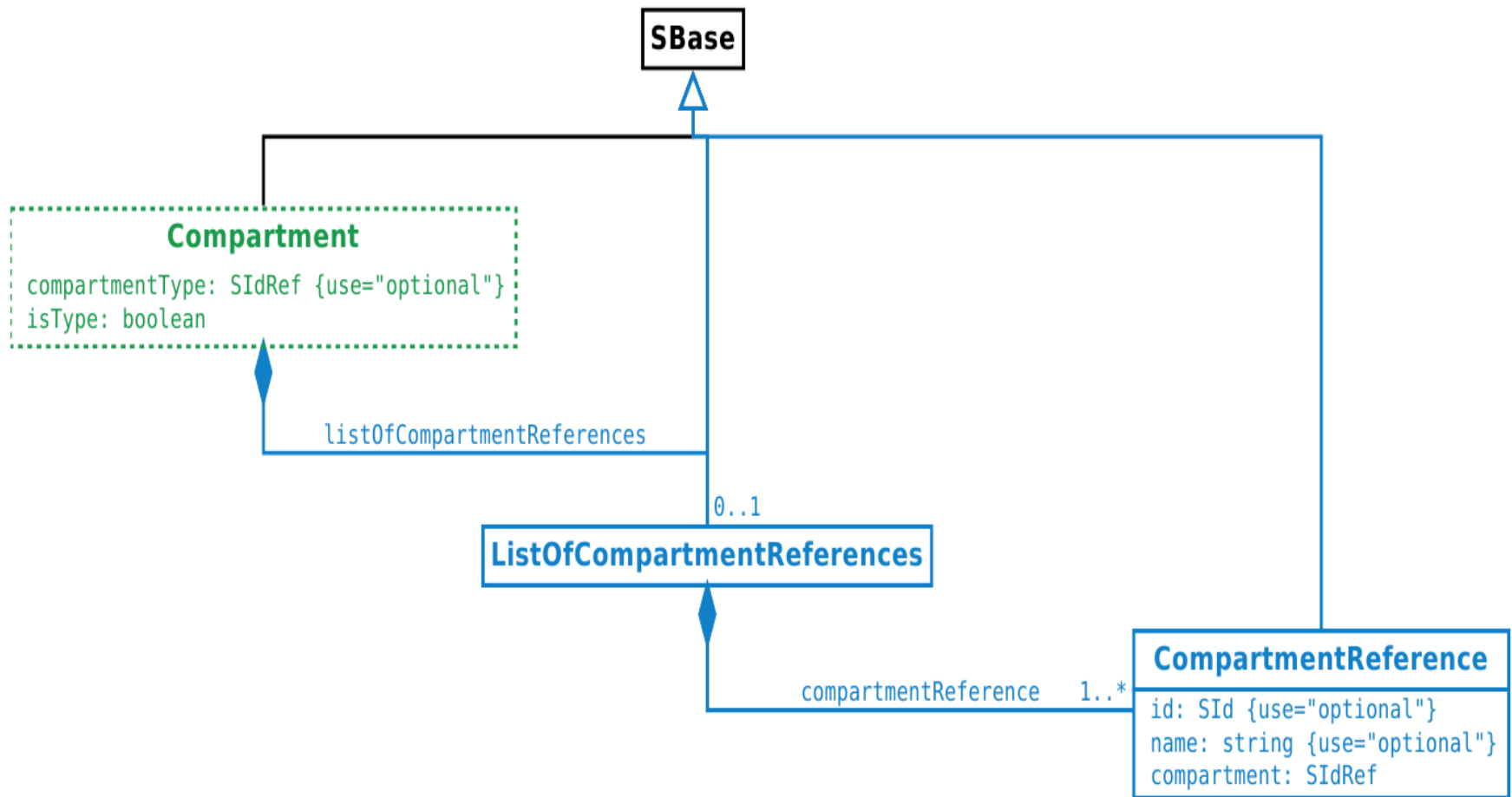
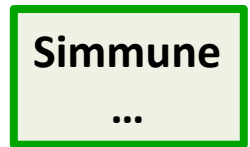


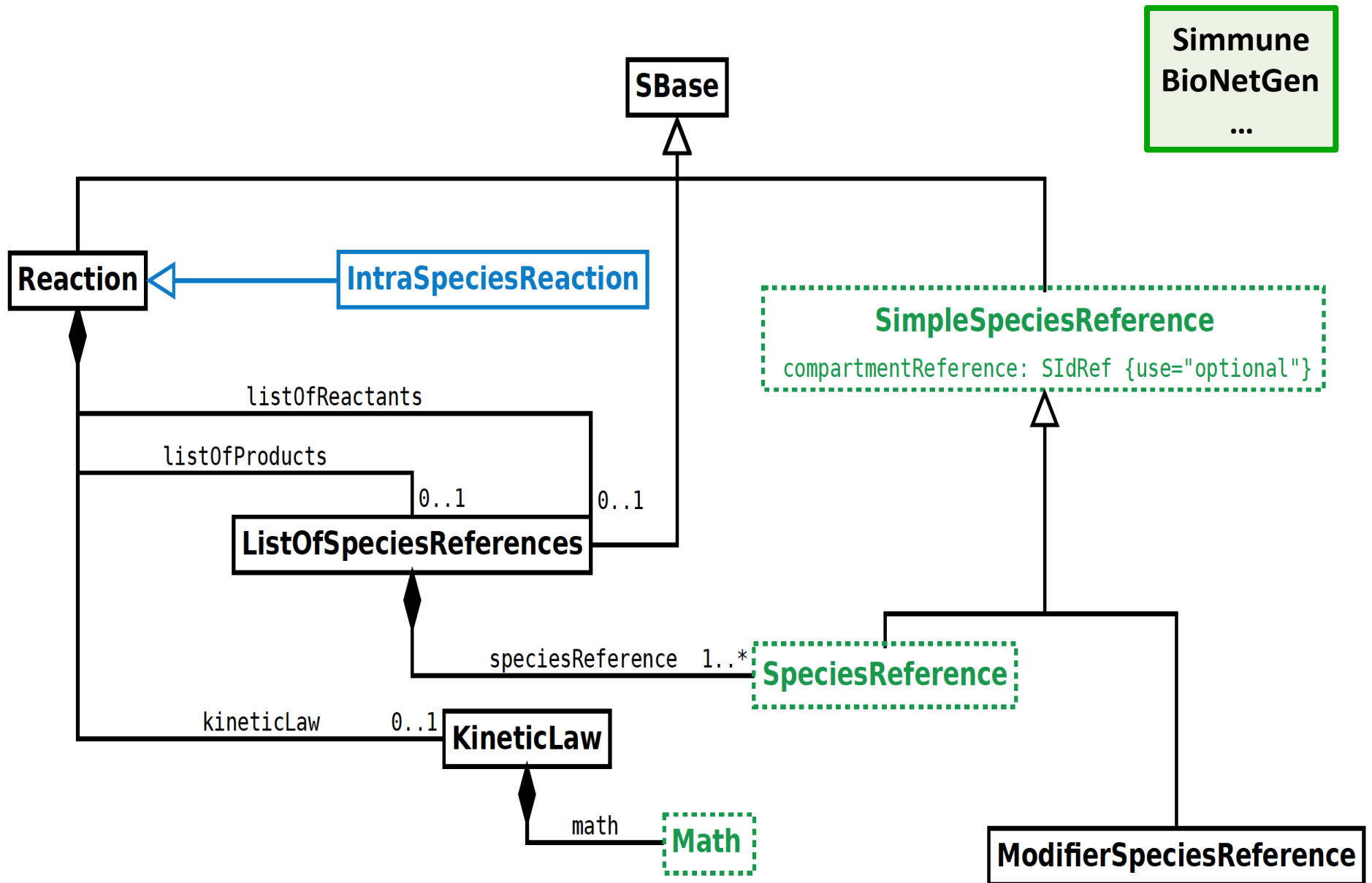


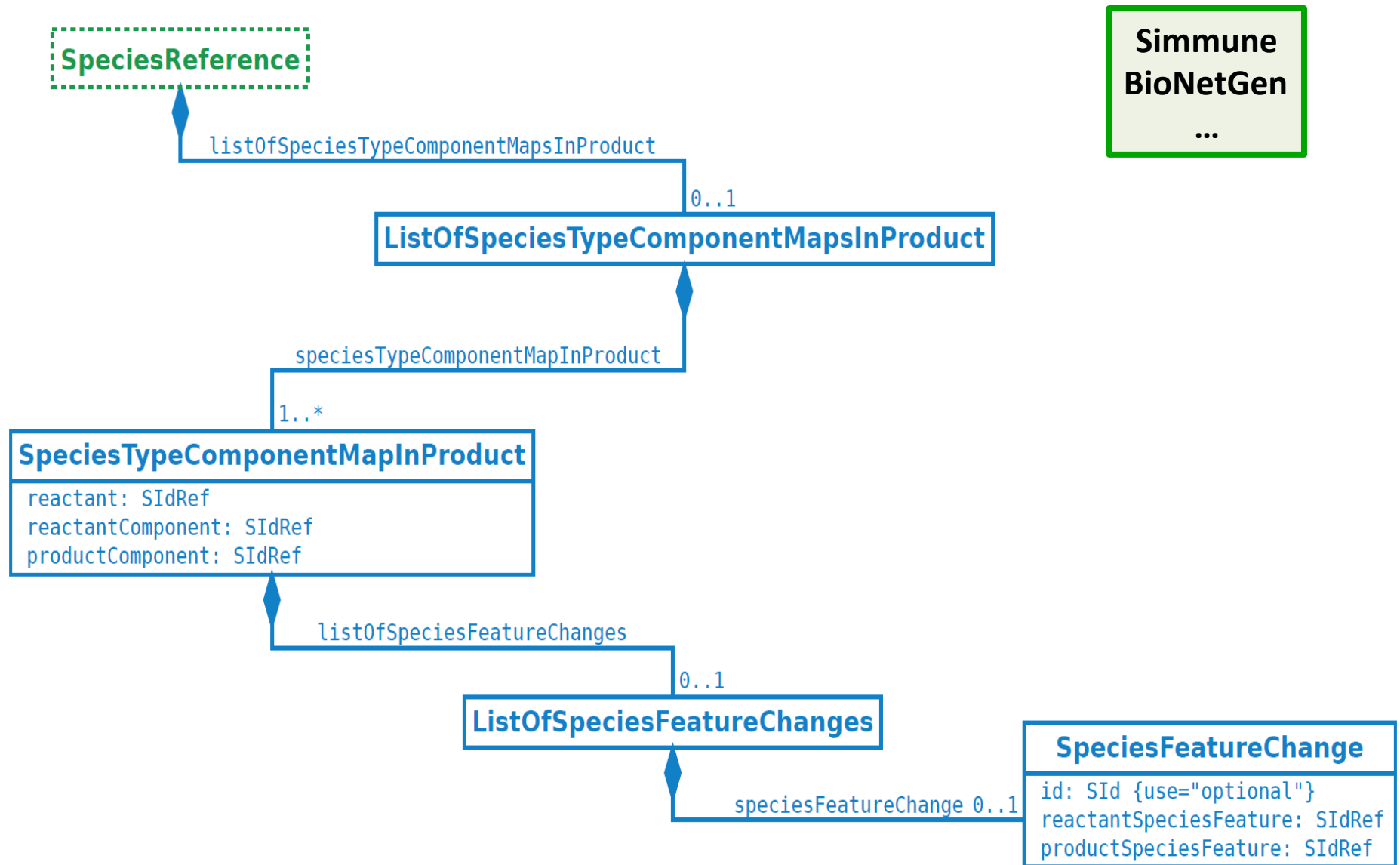












Features may not be supported by any tool

- “Occur” attribute in **SpeciesTypeInstance**
- “Occur” attribute in **SpeciesTypeComponentIndex**
- **DenotedSpeciesTypeComponentIndex** ?

Keep or Drop?

Challenges in tool support

- Model export: No issue identified
 - All issues have been resolved.
- **Model import**
 - Simmune
 - Multi **SpeciesType** to Simmune “Complex Species, Molecule, Component and Binding site”
 - Automatic graphic layout
 - BioNetGen?
 - Multi **SpeciesType** to BioNetGen data structure?
 - Other tools?

Next...