

# Biochemical Space: A framework for formal description and annotation of complex biological processes

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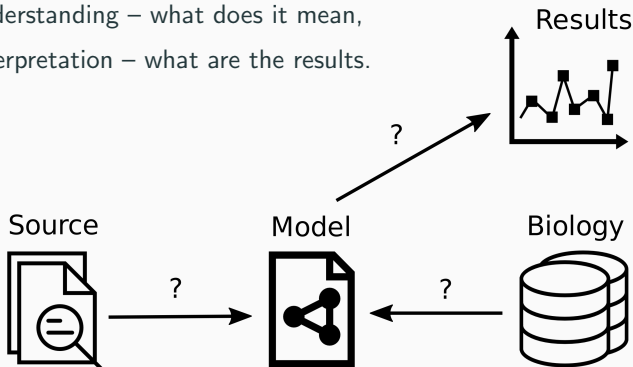
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# Motivation

Frequent issues with models:

- reconstruction – get it working,
- understanding – what does it mean,
- interpretation – what are the results.



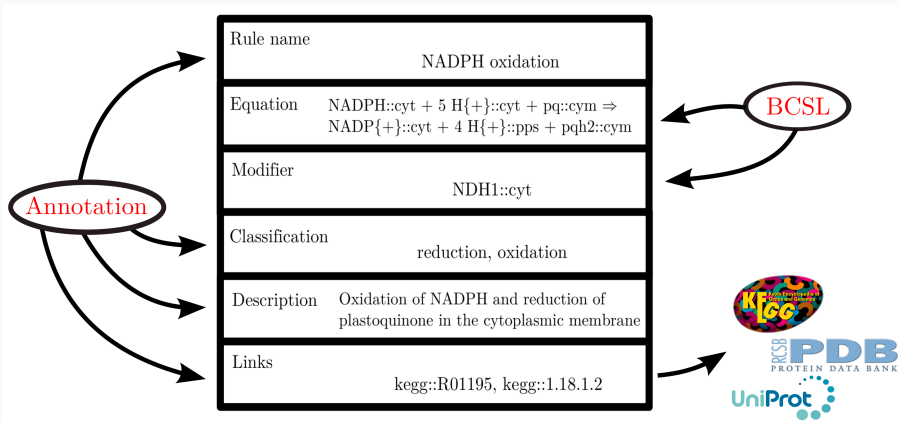
**Biochemical Space** (BCS) is a semi-formal knowledge-base providing

- description,
- annotation,
- public sharing

of domain-specific biological models.

**Motto:** *formalization of biological description while annotating models.*

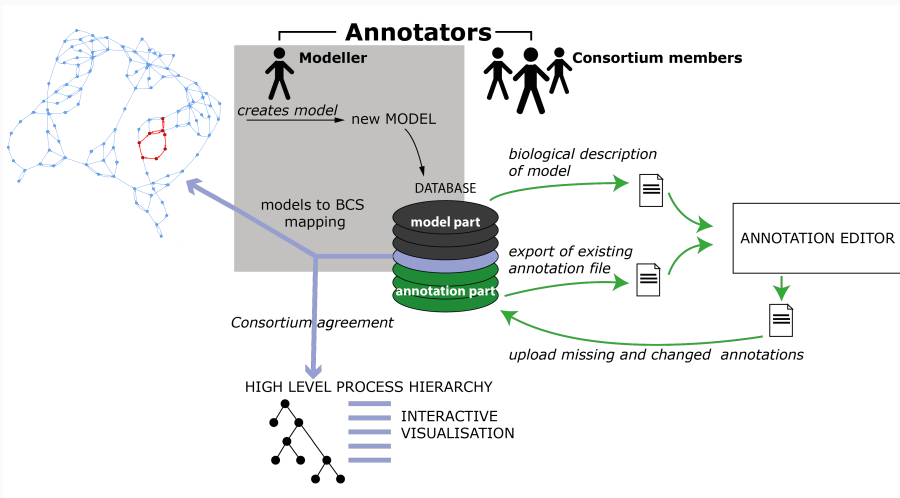




## Biochemical Space **Language** (BCSL)

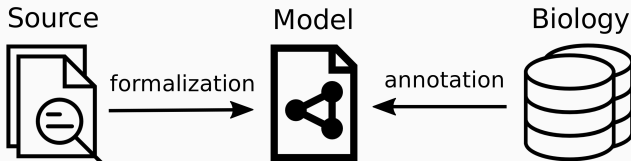
- internal representation easily editable and manageable,
- rule-based – decrease size of the space,
- completely textual – no graphical representation,
- human-readable – direct interpretation to the user,
- not just a notation – operational semantics suitable for analysis (translation to Kappa).

# How it works



# Advantages

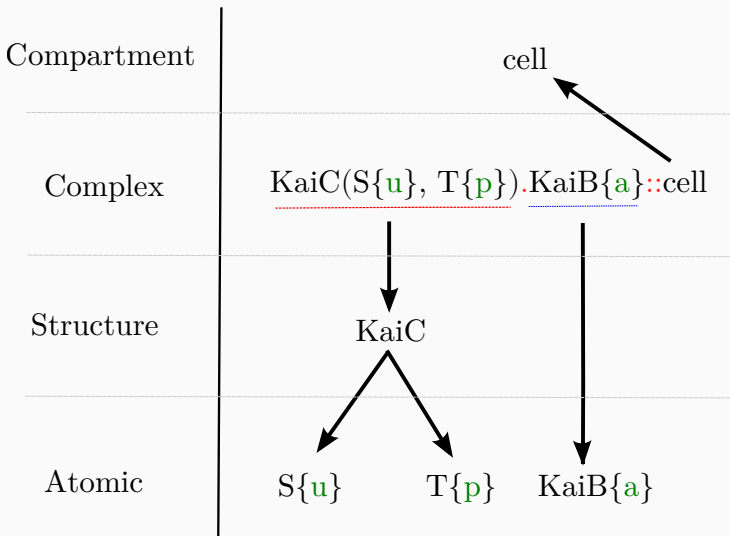
- gives the model back its biological meaning
  - individual annotation for entities/reactions easily accessible
  - implemented model available online
- relating to BCS produces model described in BCSL
  - allows further analysis
  - provides qualitative formal description



- helps to reveal differences between models



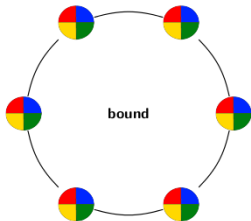
# Entities



# Abstraction of the complex

## Biology

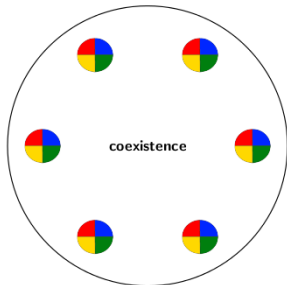
- graph "isomorphism"
- 700 different deviations



- Unphosphorylated protein
- Serine residue phosphorylated protein
- Threonine residue phosphorylated protein
- Both residues phosphorylated protein

## BCS abstraction

- mixture  $\rightarrow$  order not important
- 84 different deviations



# Rules



# BCS domain allows further abstractions

Entity ID	KaiC
Entity name	KaiC protein
Composition	S, T
Type	structure
	...

Entity ID	KaiC6
Entity name	KaiC complex
Composition	KaiC.KaiC.KaiC.KaiC.KaiC.KaiC
Type	complex
	...

$$S\{u\}::KaiC::KaiC6::cyt \Rightarrow S\{p\}::KaiC::KaiC6::cyt$$

$$KaiC(S\{u\}).KaiC. \dots .KaiC::cyt \Rightarrow KaiC(S\{p\}).KaiC. \dots .KaiC::cyt$$

## Summary

- *Biochemical Space* – framework for process modeling
  - not strictly in the very same configuration
    - usage of alternative representation
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## Future work

- independent operational semantics / improved representation
- custom analysis tool for BCSL models
  - efficient static analysis
- *BCS numbers* extension
  - annotation of parameters