Atomizer

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What’s in a model?

What’s in a model means...

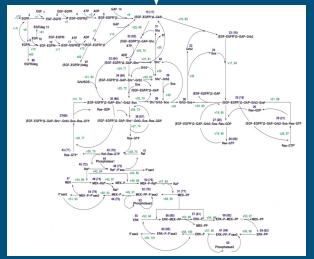
- I want to **understand** a model in the literature
- I want to **compare** a model against others in the literature
- I want to **reuse** models in the literature

What's in a model?

Model

Annotation information

Paper



The challenges of model understanding are...

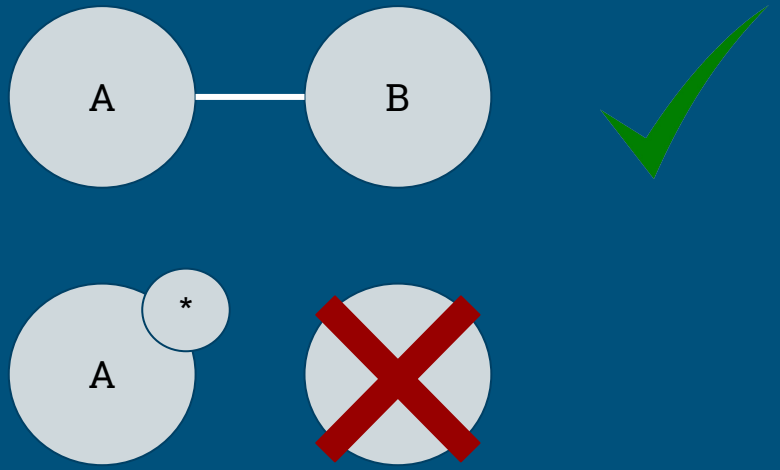
- How are elements inside a model related to each other?
- How do elements in a model compare to elements in other models?
- How do elements in a model compare to real-world objects?

The challenges of model understanding are...

- **How are elements inside a model related to each other?**
- How do elements in a model compare to elements in other models?
- How do elements in a model compare to real-world objects?

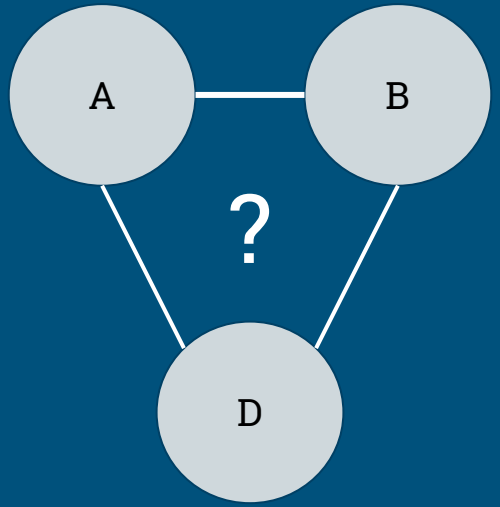
A pure RNM representation makes this a non-trivial problem...

A + B -> ~~C~~ A_B



It gets more interesting….

A_B + D -> A_B_D



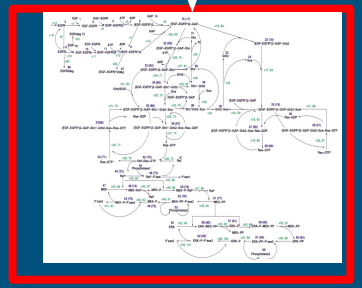
Some of these questions can be answered through model visualization

What's in a model?

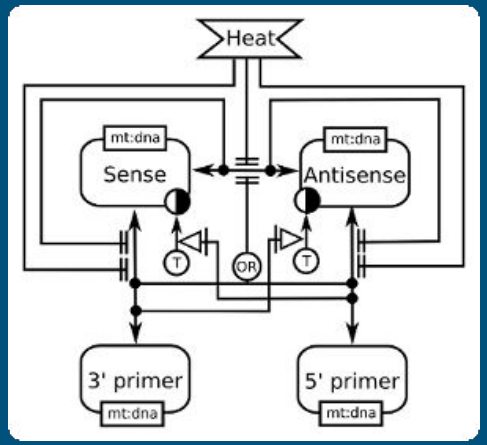
SBML

Annotation information

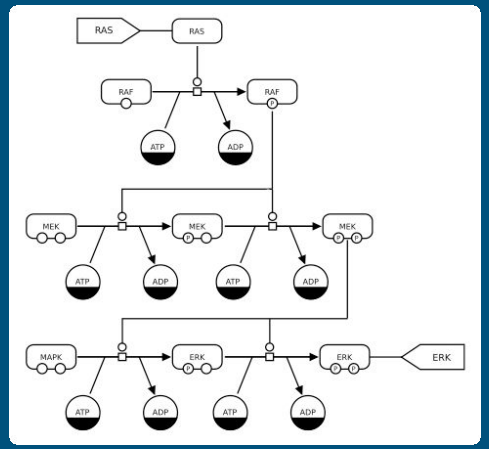
Paper



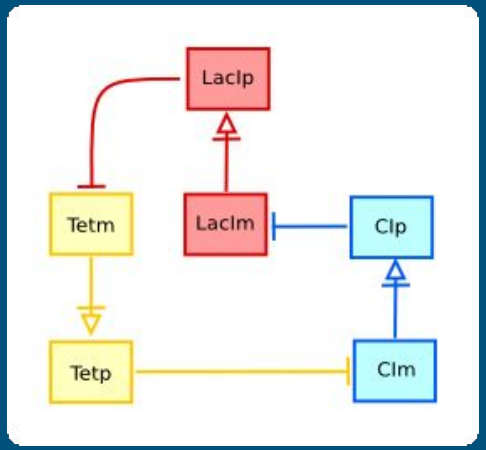
Standard visualization methodologies



Entity-relationship diagrams



Process diagrams



Activity flow diagrams

So we ask...

Does this scale for large models?

What happens if I want to understand and compare a large number of models?

Toward “model informatics”

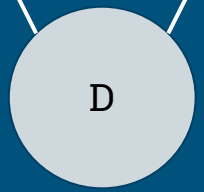
There’s a limit to what we can understand without computer assistance.

A model description should enable (semi) automated analysis of a single model and comparison with other models.

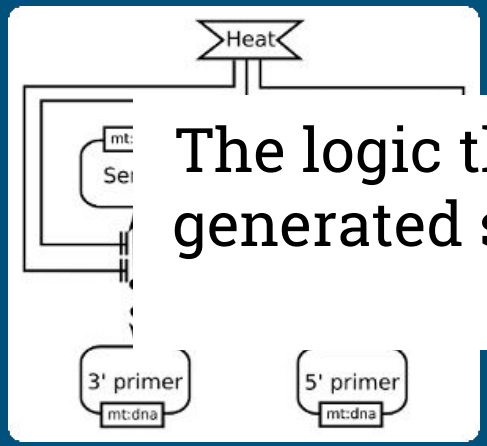
It gets more interesting….

A + B + D -> A + B + D

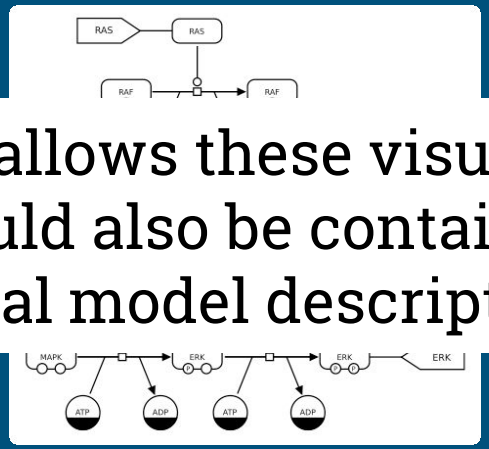
These questions should be answerable from the model description alone



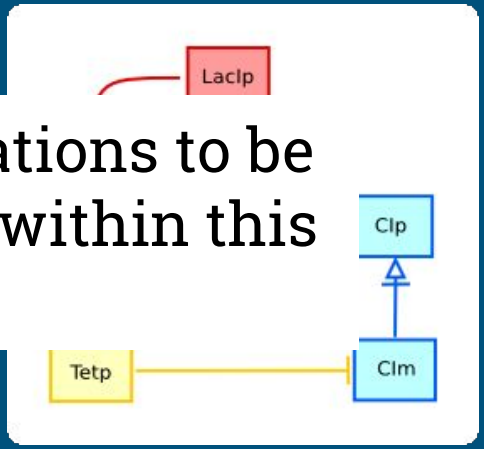
Standard visualization methodologies



Entity-relationship diagrams



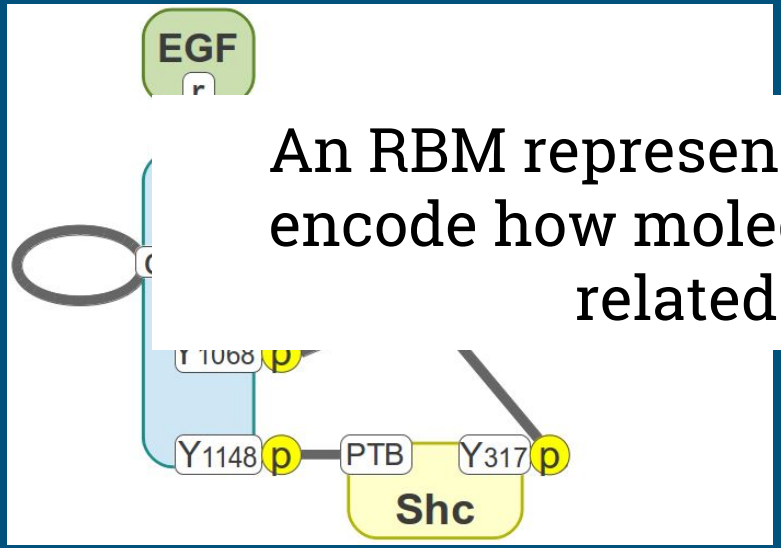
Process diagrams



Activity flow diagrams

The logic that allows these visualizations to be generated should also be contained within this ideal model description

Enter Rule-based modeling



An RBM representation allows the user to encode how molecules inside a model are related to each other

- Graph based representation

ins

interactions

- **Graph-based syntax allows a modeler to directly encode structural information**

Great… now I just need someone to rewrite my model as an RBM

Presenting...

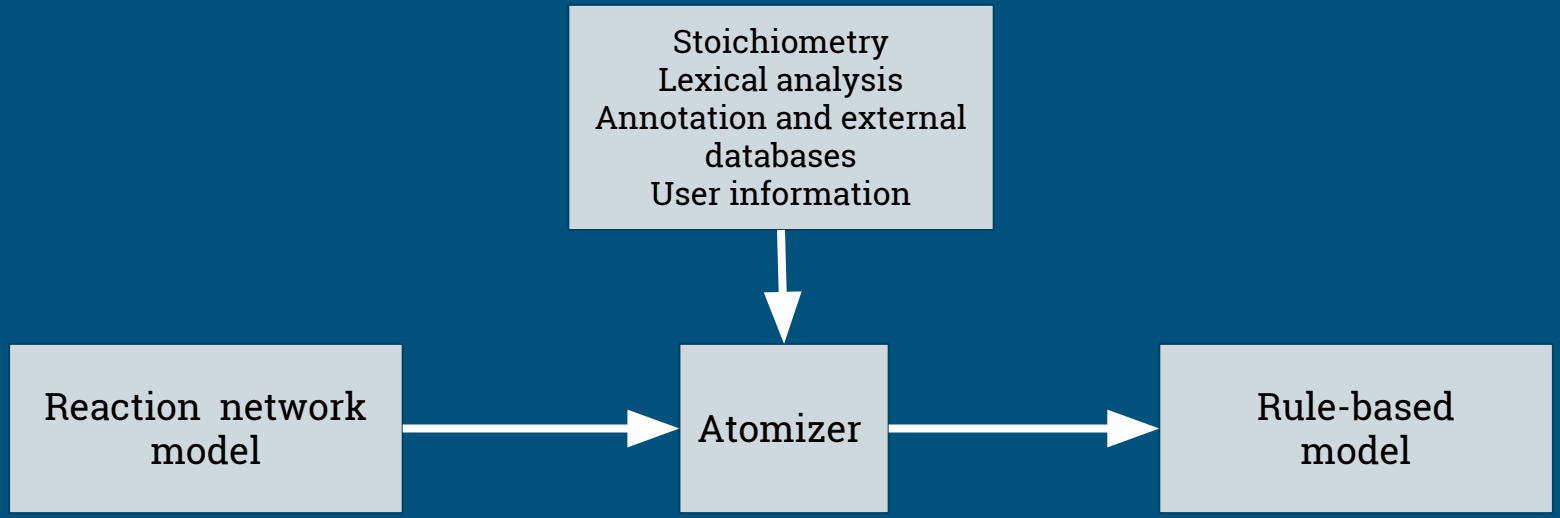
The

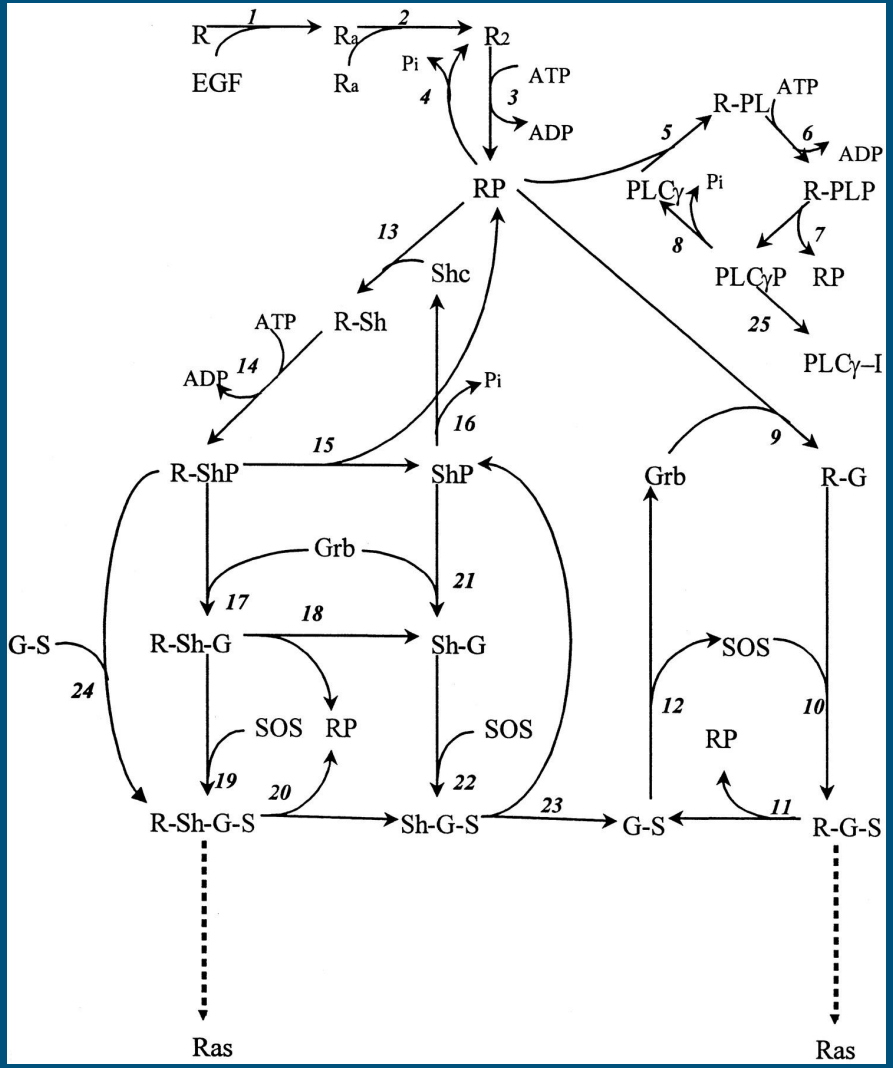
Atomizer

RBM

RNM

Now without the cats

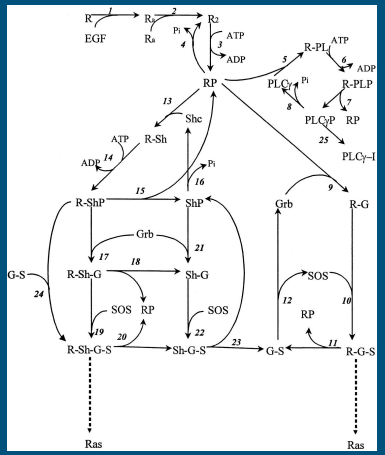


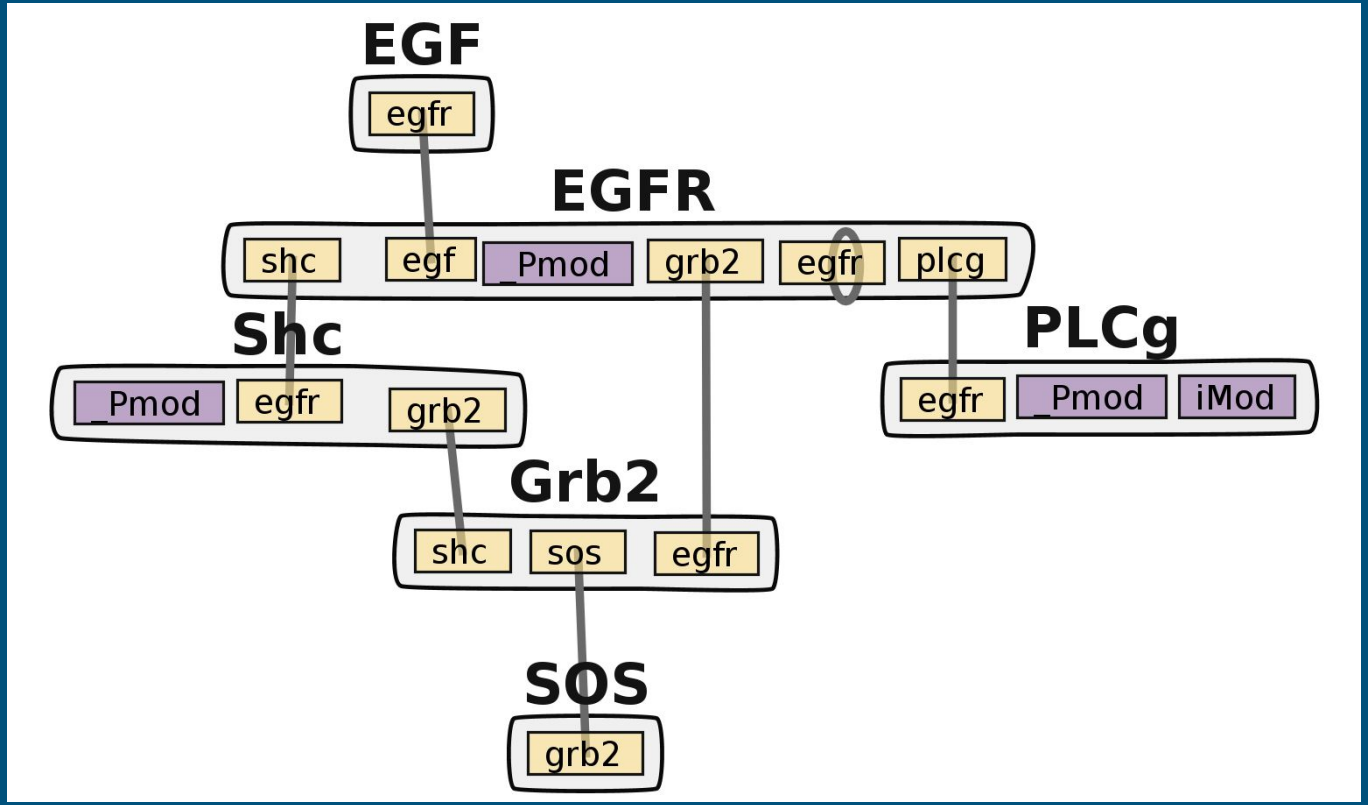


Motivational example

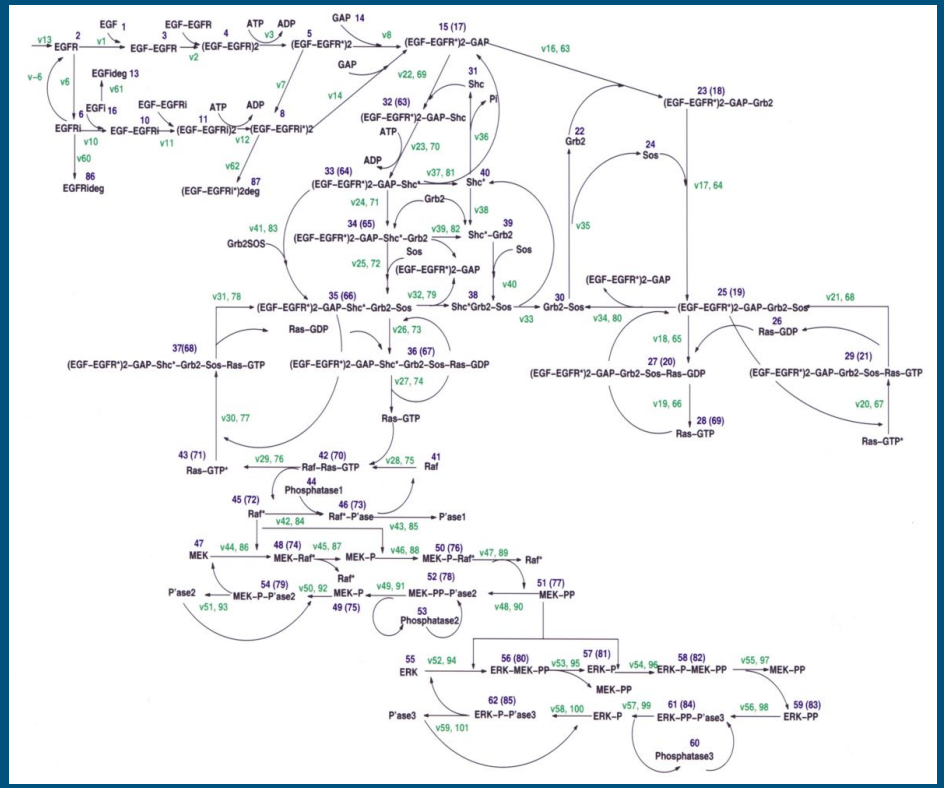
BIOMD48
(Kholodenko B. 1999)

Magic!


EGF
ATP
ADP
Pi
RP
Shc
R-Sh
R-ShP
Grb
R-G
R-Sh-G
Sh-G
SOS
R-Sh-G-S
Sh-G-S
G-S
R-G-S
R-PLP
PLCγP
PLCγ–I
Ras

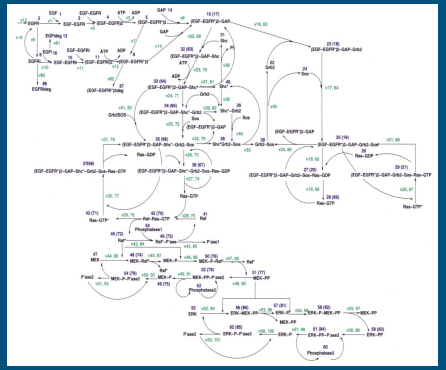

EGF
egfr
EGFR
shc
egf
_Pmod
grb2
egfr
plcg
Shc
_Pmod
egfr
grb2
PLCg
egfr
_Pmod
iMod
Grb2
shc
sos
egfr
SOS
grb2

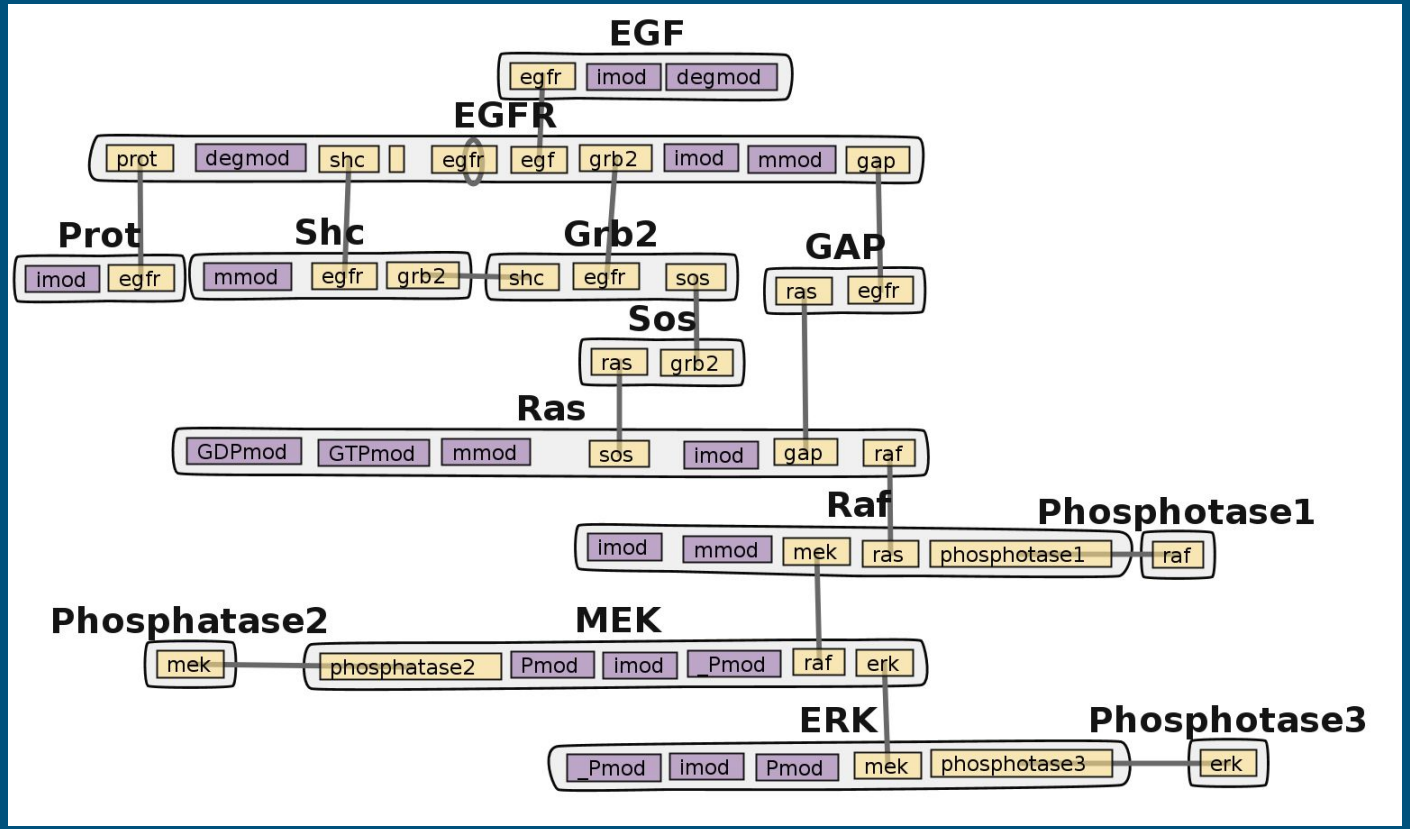
Motivational example (2)



Schoeberl et al.

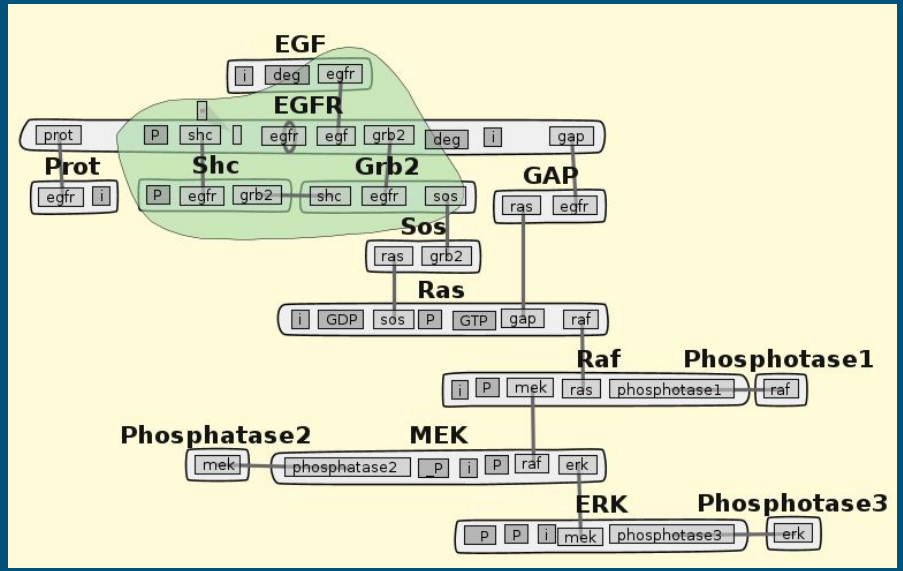
BIOMD19 atomized



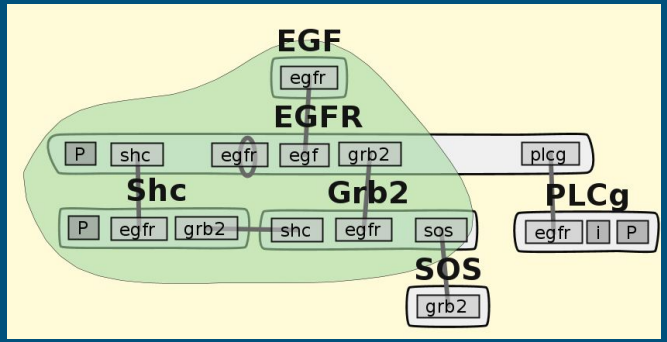


Comparison

BIOMD 19



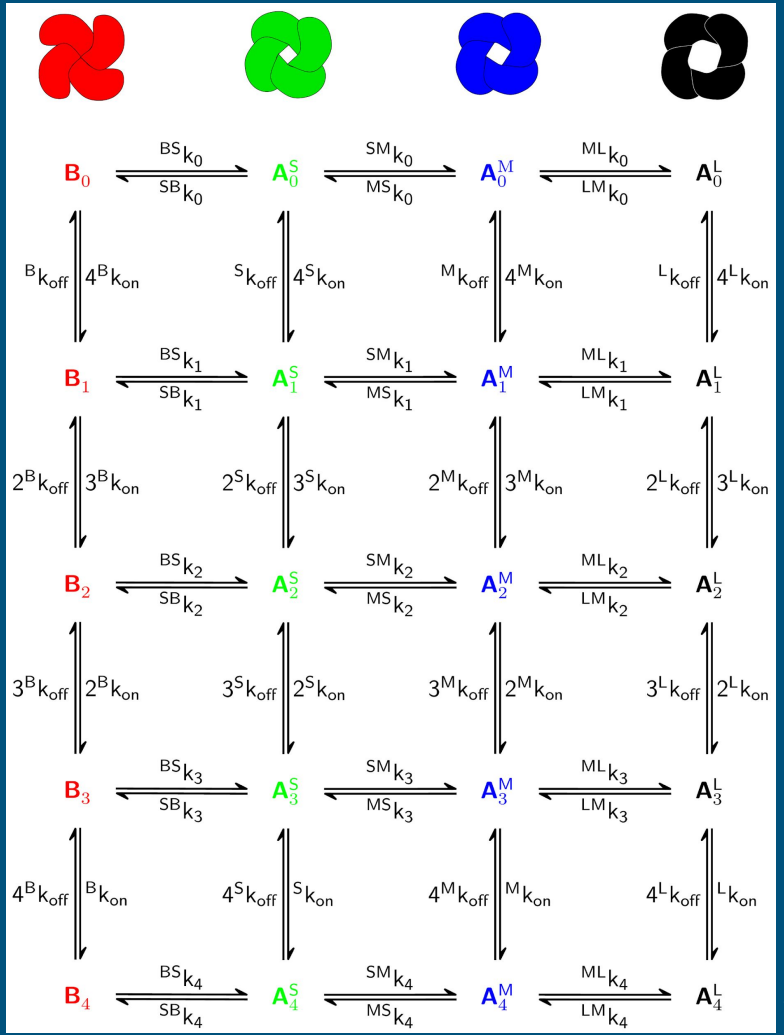
BIOMD 48



Demo

BMD 569

Ligand-Dependent Opening of the Multiple AMPA Receptor Conductance States: A Concerted Model



https://www.ebi.ac.uk/biomodels-main

Or Google for BioModels database