

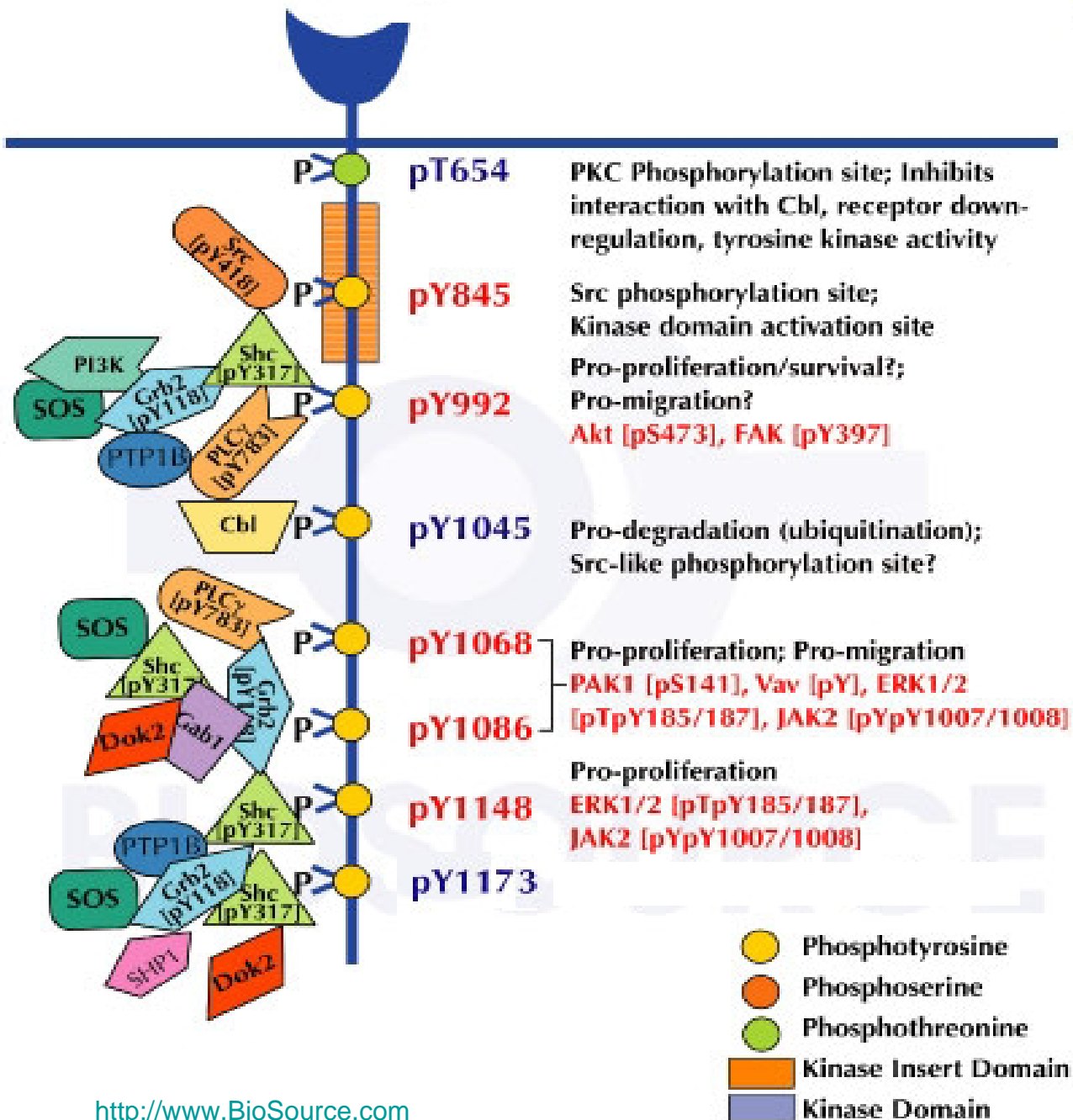
# BioNetGen: rule-based reaction networks generation

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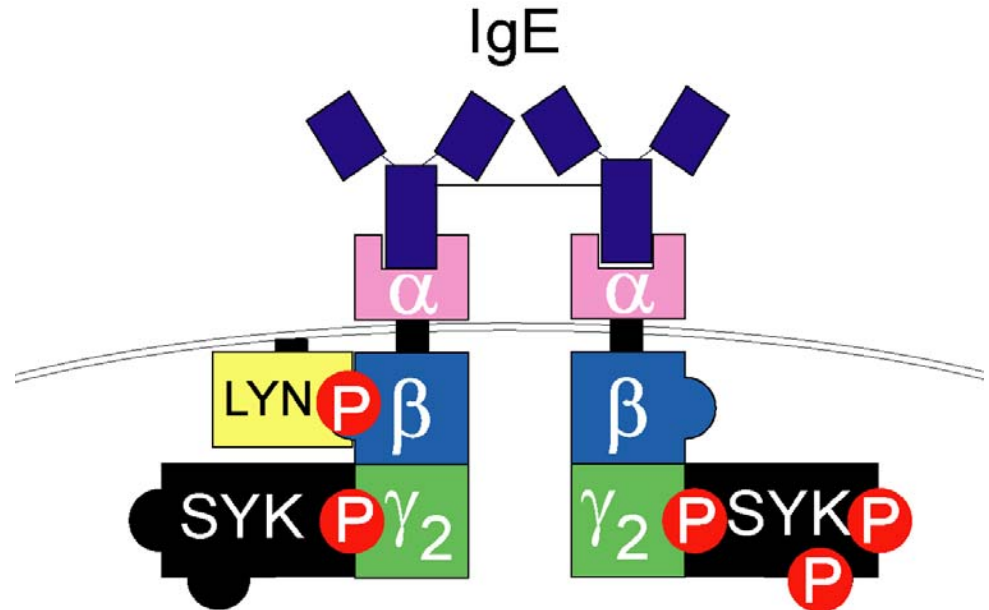
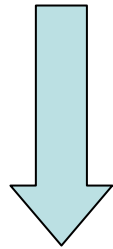
<http://cellsignaling.lanl.gov>



- Multi-state multi-component species
- Interactions specific to specific domains and sites of proteins

# Modeling, not simulation!

Describe your knowledge about the biological system



Let **BioNetGen** create a model for you

<http://cellsignaling.lanl.gov/bionetgen>

# Multi-state molecules: functional domains that can be in multiple states

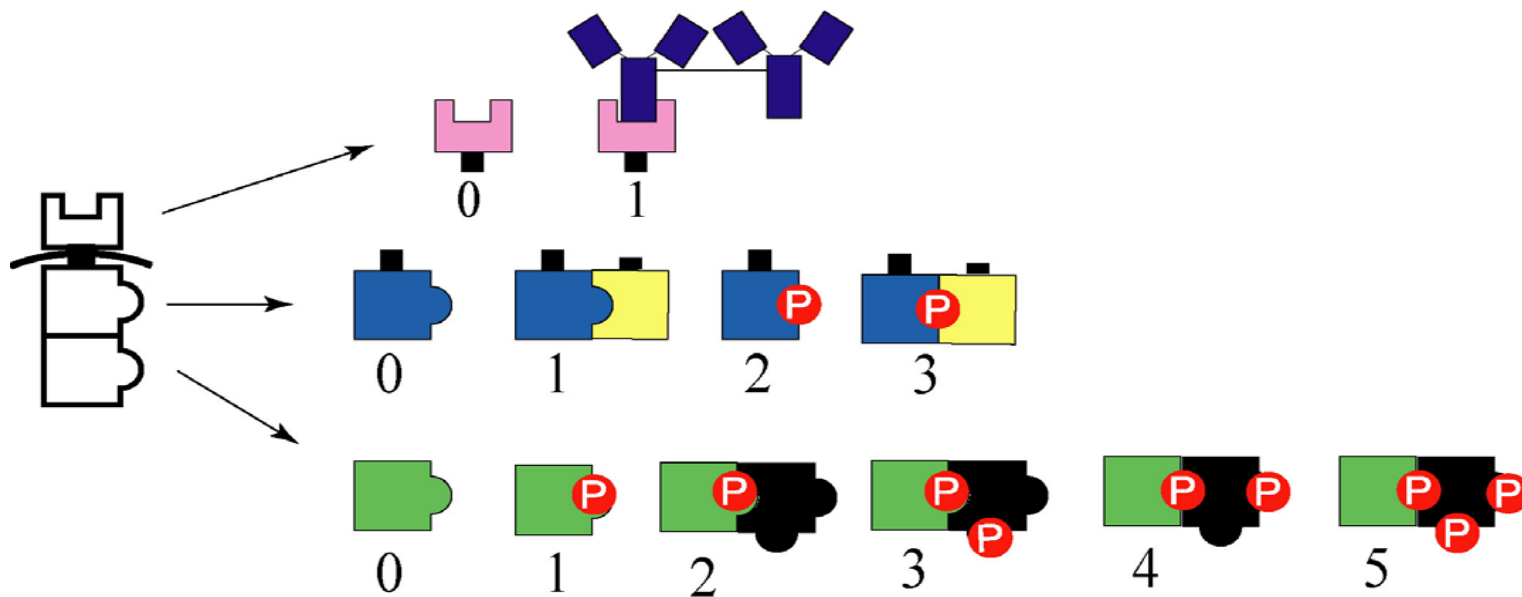
## Domain can be

- Binding domain, in multiple association states
- Modification domains, that undergoes conformational change, transphosphorylation etc
- Fictional domain, that represents being in a specific compartment, specific complex etc

# Multi-state molecules:

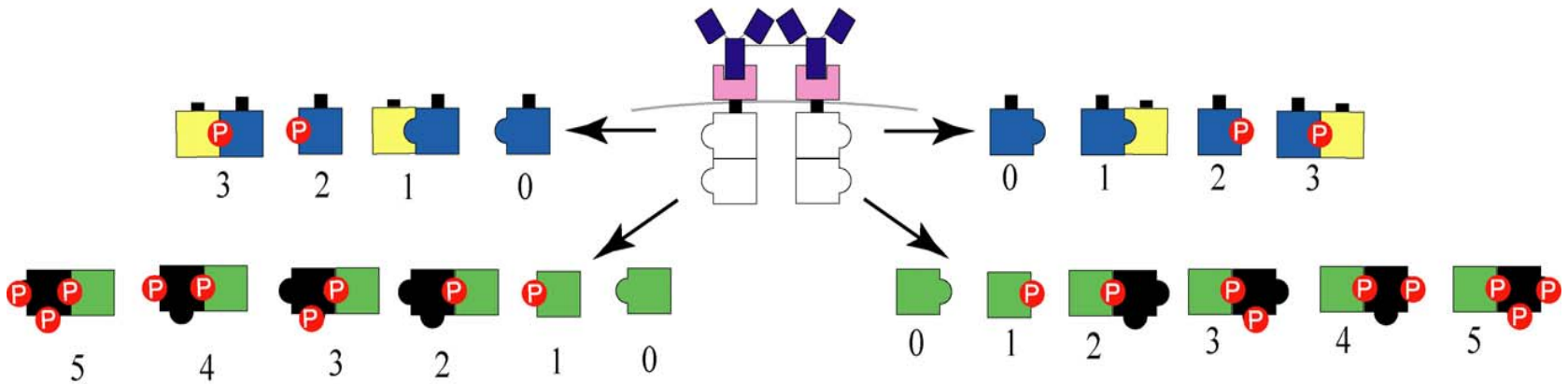
4 symbols specify 48 molecular species

**R 2,4,6**



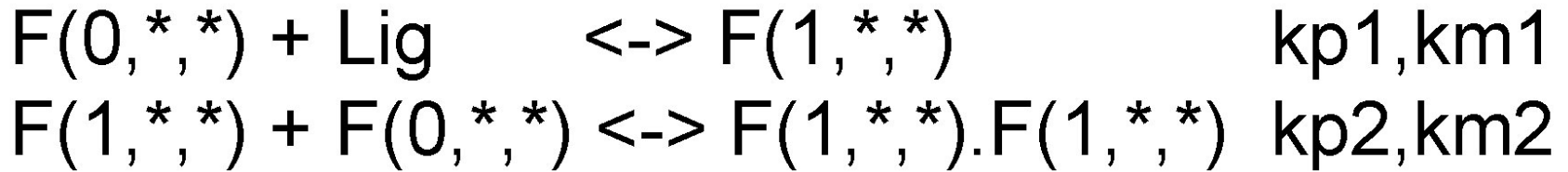
# Multi-component species

8 symbols specify 300 molecular species

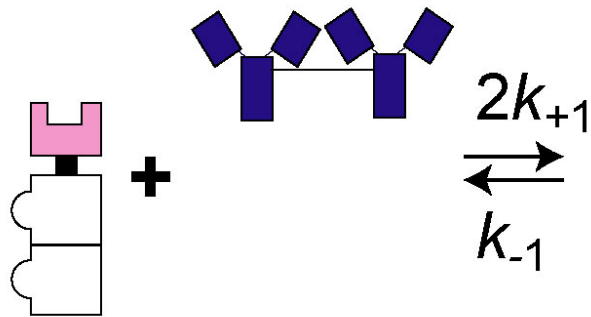
$$R(1, *, *) \cdot R(1, *, *)$$


Current version: binding of multi-state molecules is not domain-specific, but can be made such by introducing of fictional binding sites

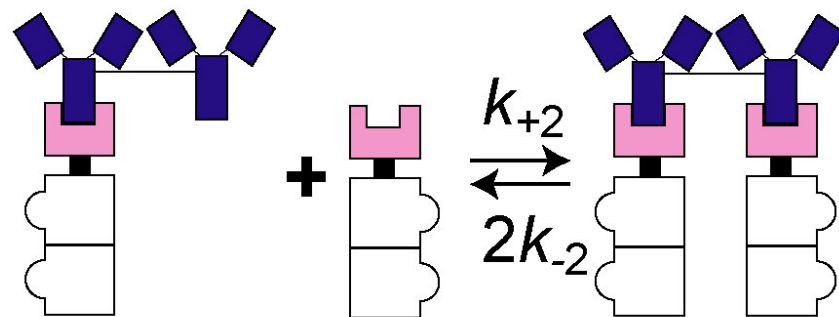
# Reaction rule declaration: 2 lines specify 1,200 elementary reactions



Ligand binding (48)

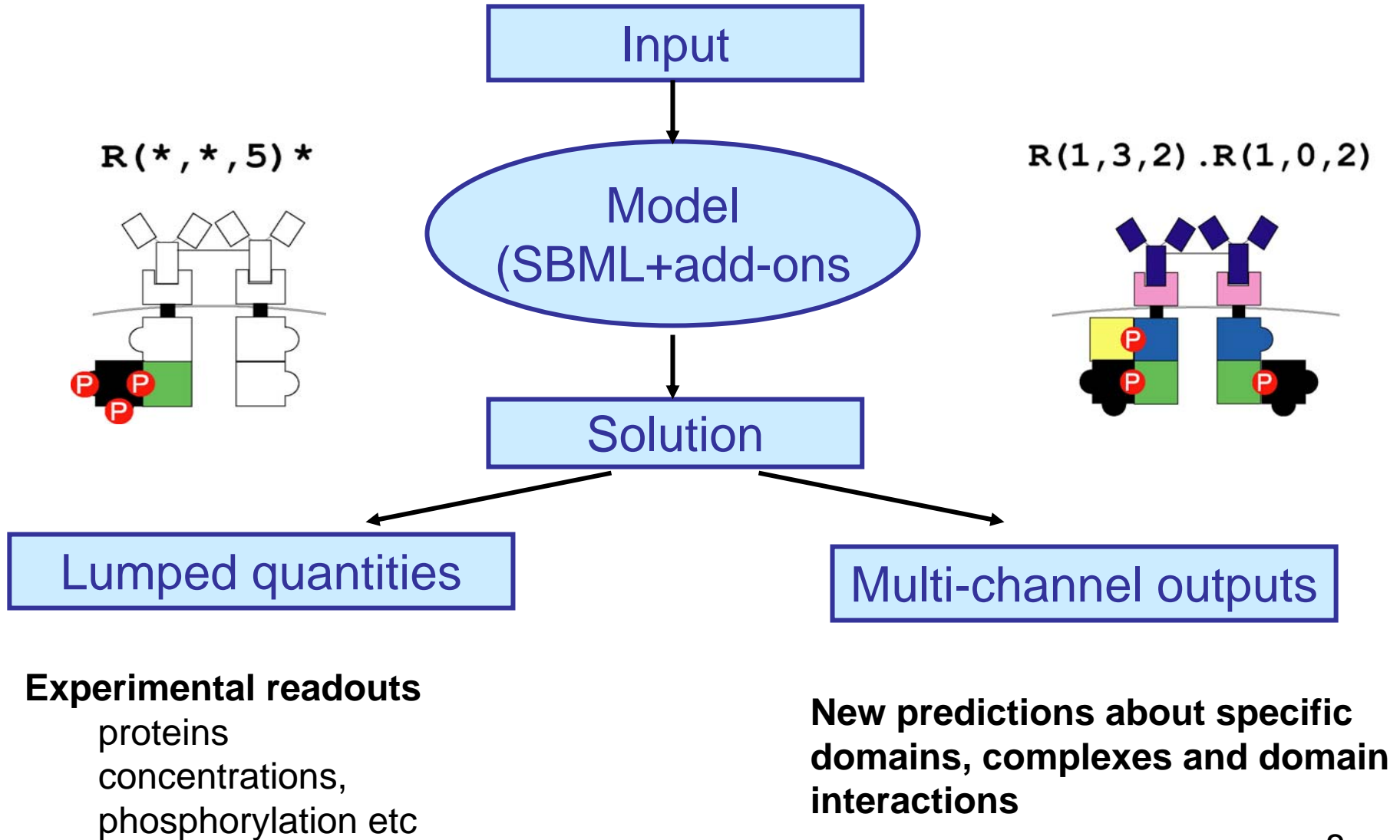


Receptor aggregation (1152)



**Different mechanistic assumptions!**

# Simulation



# Main research areas

- Signal transduction pathways
- Gene transcription factors

## Applications

- Modeling different mechanistic assumptions, domain knock-outs, over-expressions etc to
  - Test different hypothesis
  - Help design experiments
  - Find specific targets for drug intervention
  - Compare with protein complexes assays

# Advantages

- Very wide range of modeling capabilities

## Have to do

- Scripting language -> GUI
- Extend simulation and analysis capabilities

**Ready to collaborate!**  
**BioNetGen available**

- <http://cellsignaling.lanl.gov/bionetgen>