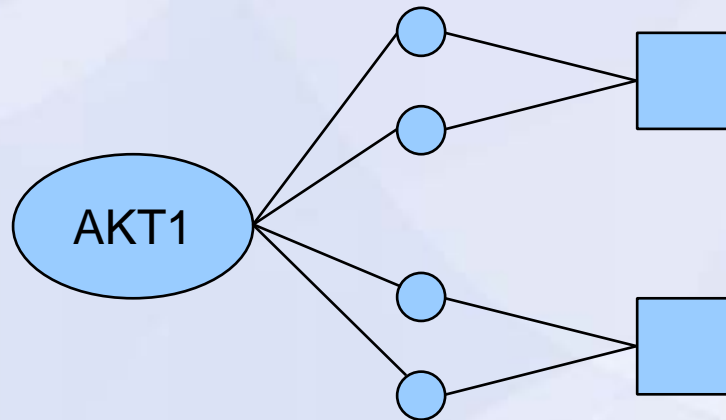


# **BioPAX Level 3: An overview of new features**

Emek Demir  
Memorial Sloan Kettering Cancer Center

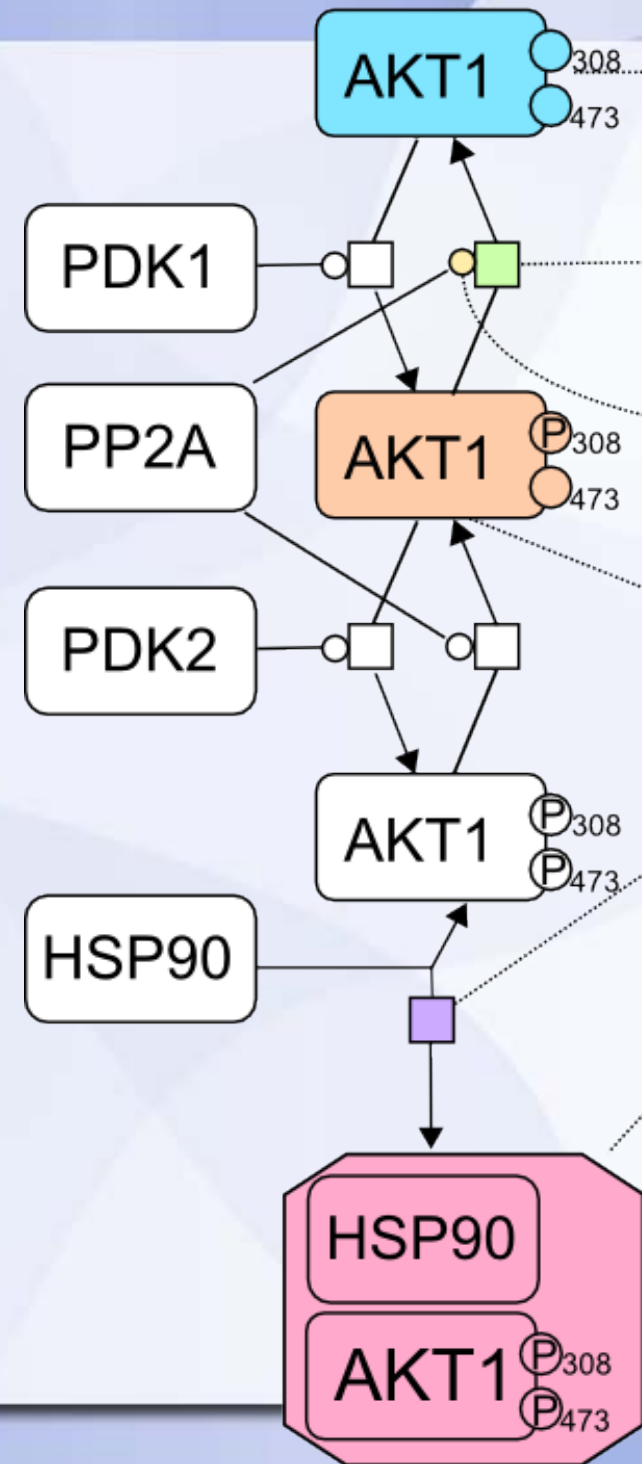
# States in Level 2



Physical Entity  
Name,  
Sequence  
etc.

Physical  
Entity  
Participant

Modifications  
Cellular location  
And  
**Stoichiometry**



AKT1  
has p  
has r  
has r

reacti  
has l  
has r  
is left

cataly  
has e  
has e  
has e

AKT1  
has p  
has t  
has s

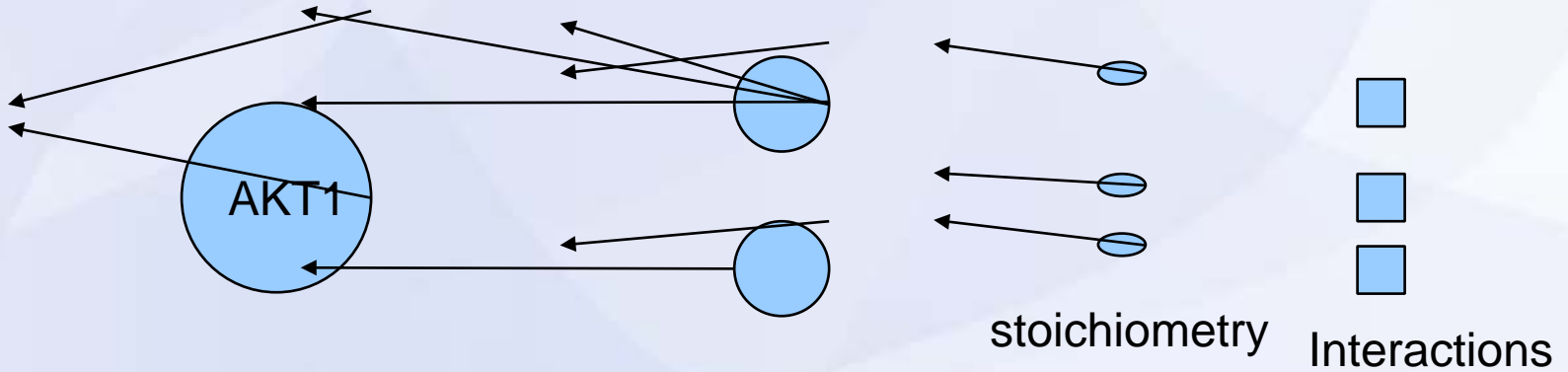
assem  
has l  
has l  
has r  
is re

comp  
has  
has

HSP  
has  
is bo

AKT  
has  
has  
has  
is bo

# States in Level 3



Physical Entity Reference:  
Name, Sequence,  
etc

Physical Entity

State, location

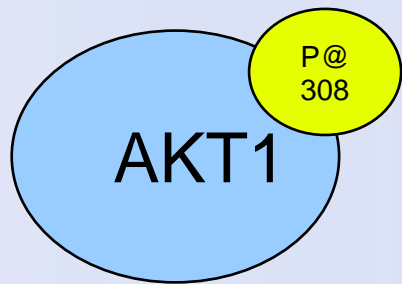
stoichiometry

Interactions

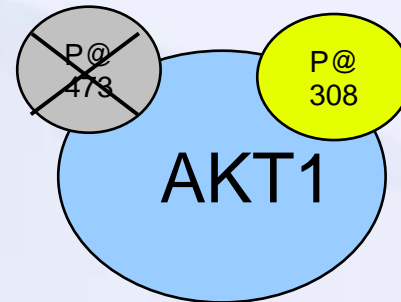
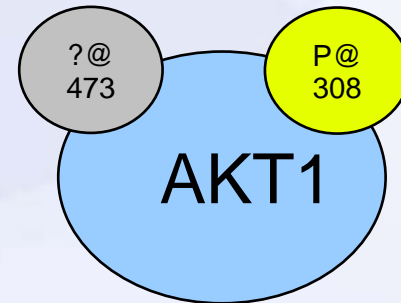
# Features

- Entity Feature
  - ModificationFeature
    - CovalentBindingFeature
  - BindingFeature
    - CovalentBindingFeature
  - FragmentFeature

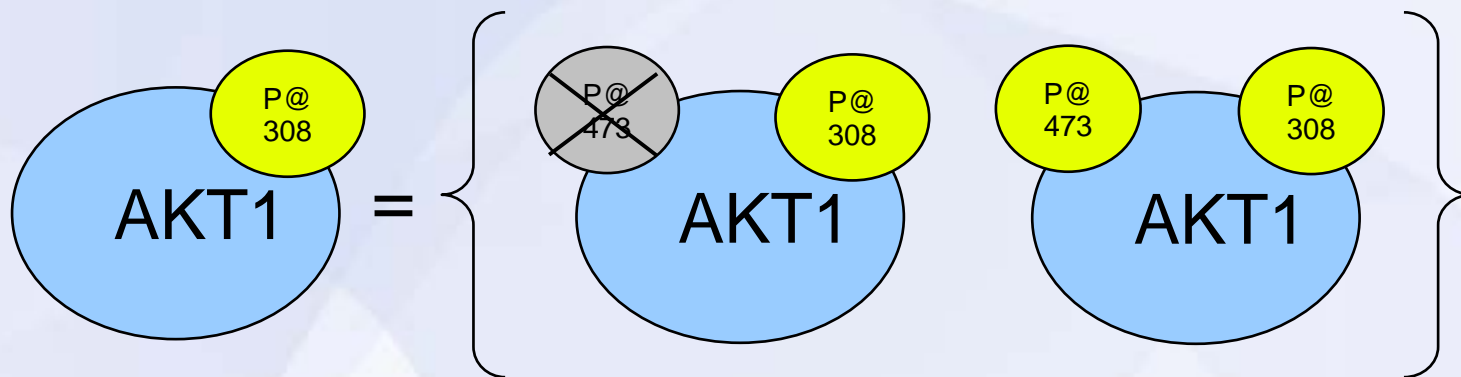
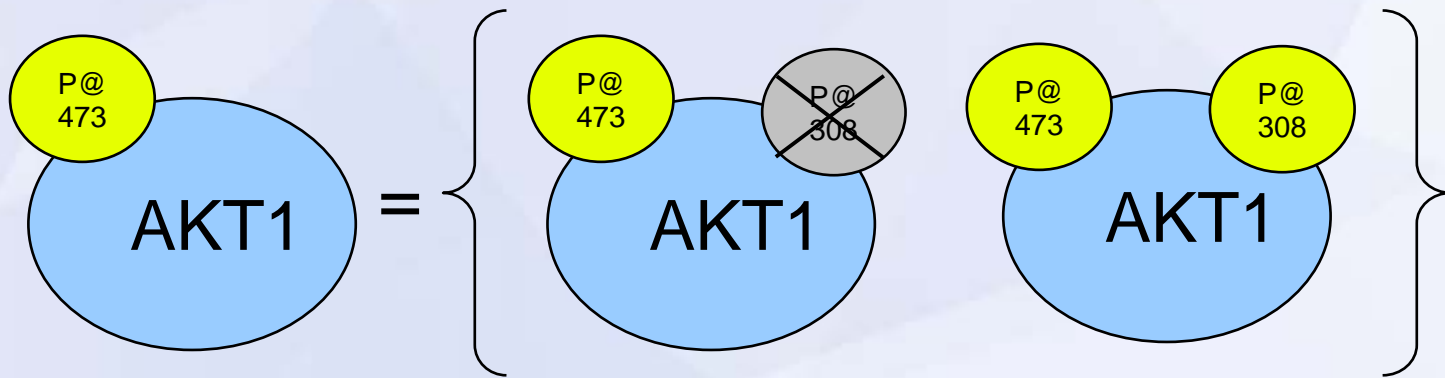
# Features and Combinatorial Complexity



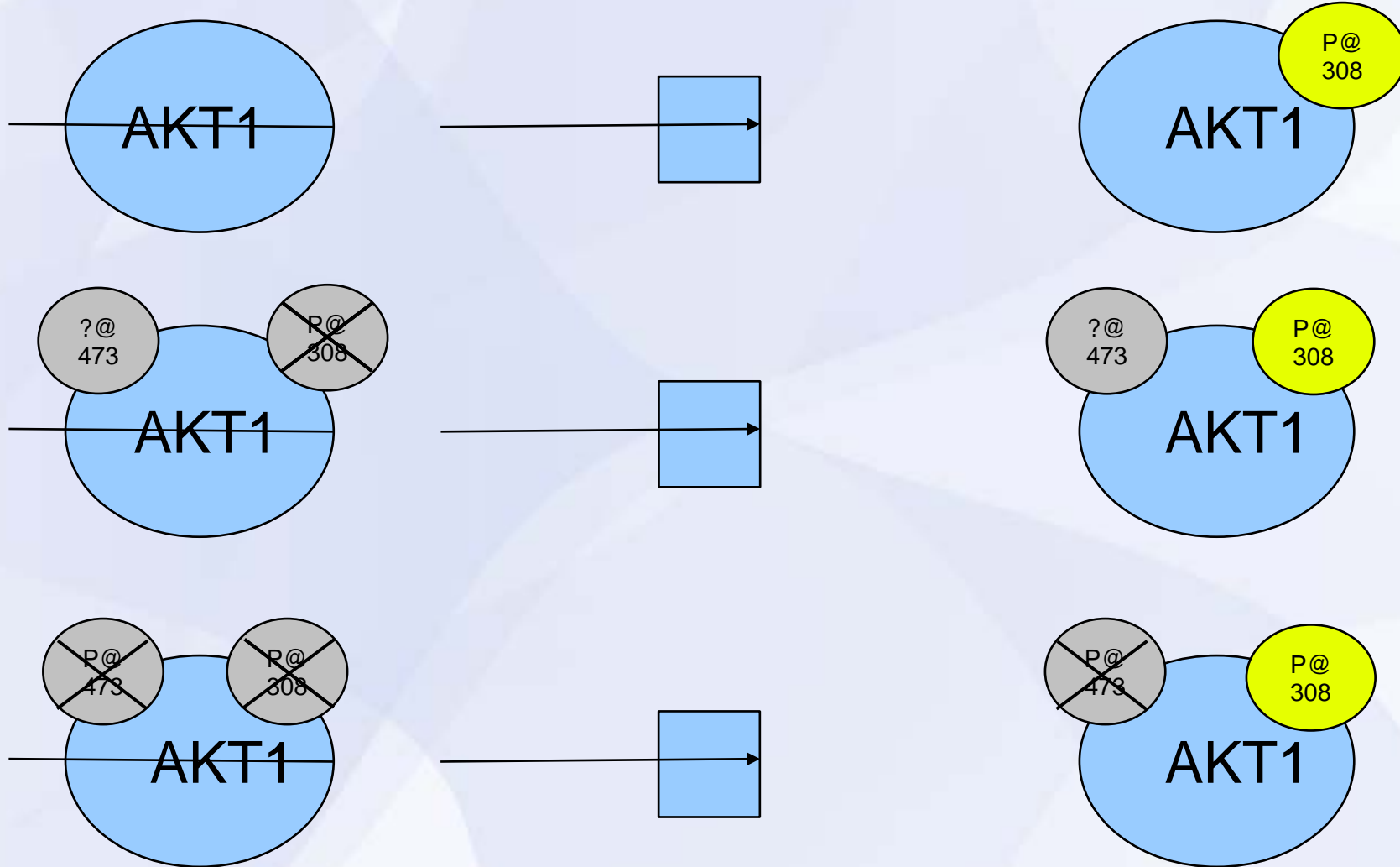
?



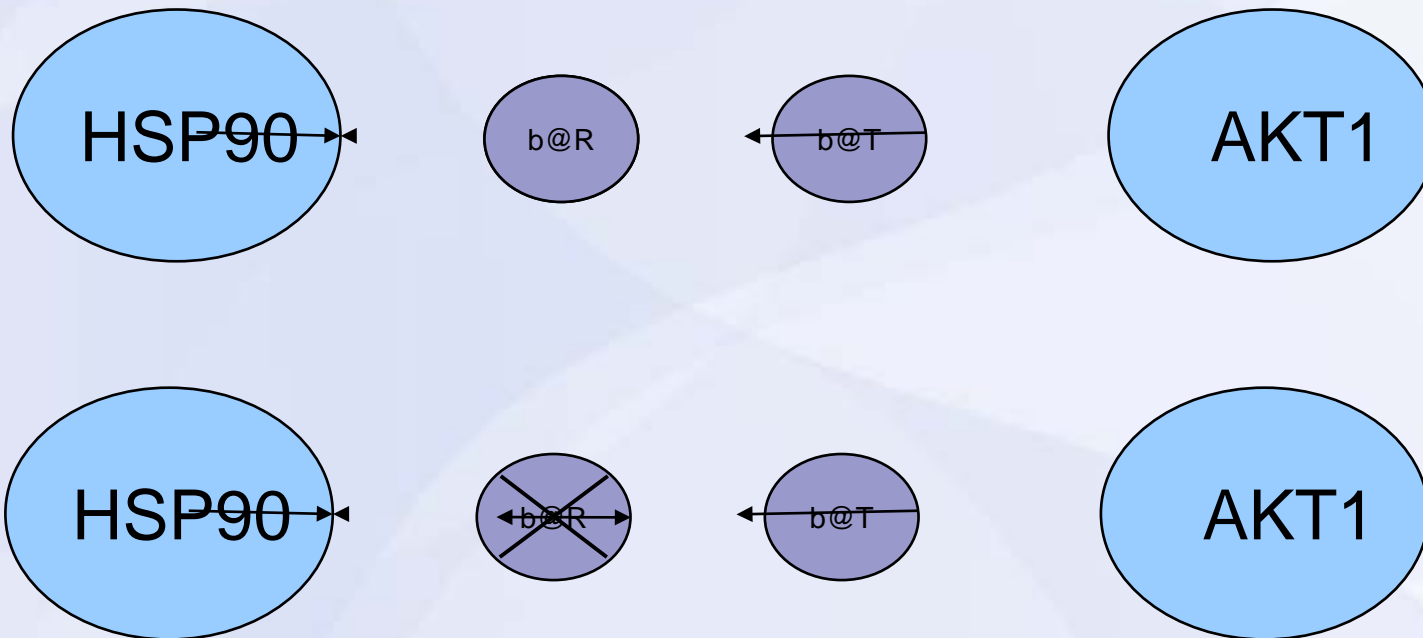
# Features and Overlapping Pools



# Features and not Features

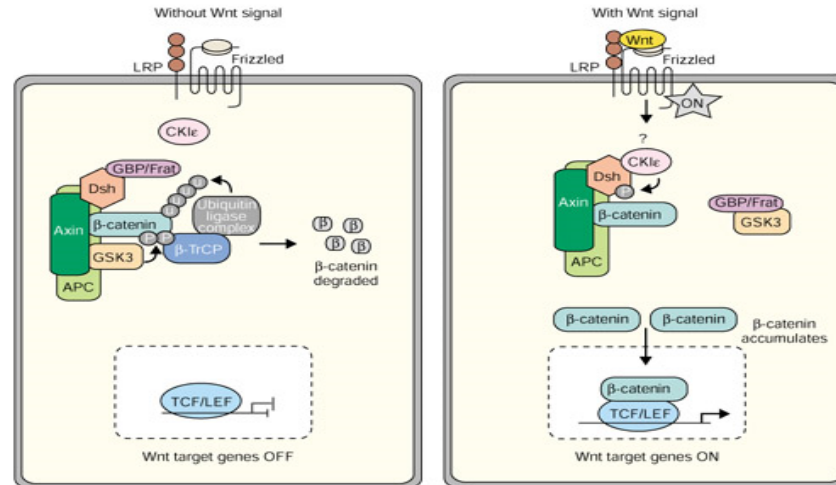


# Binding Feature

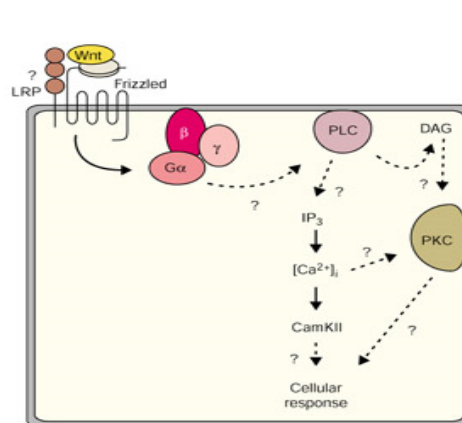


# Generics

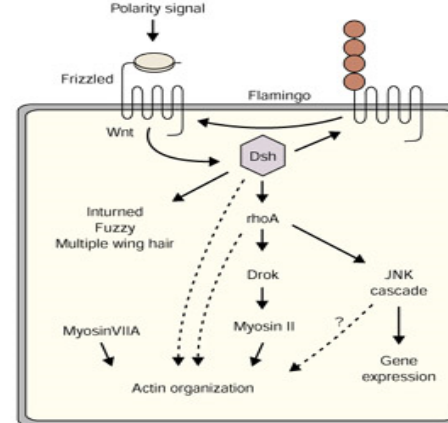
(a) Wnt/ $\beta$ -catenin signaling pathway



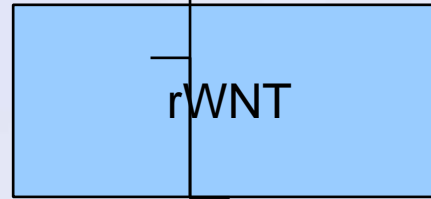
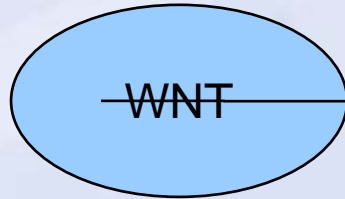
(b) Wnt/ $\text{Ca}^{2+}$  pathway



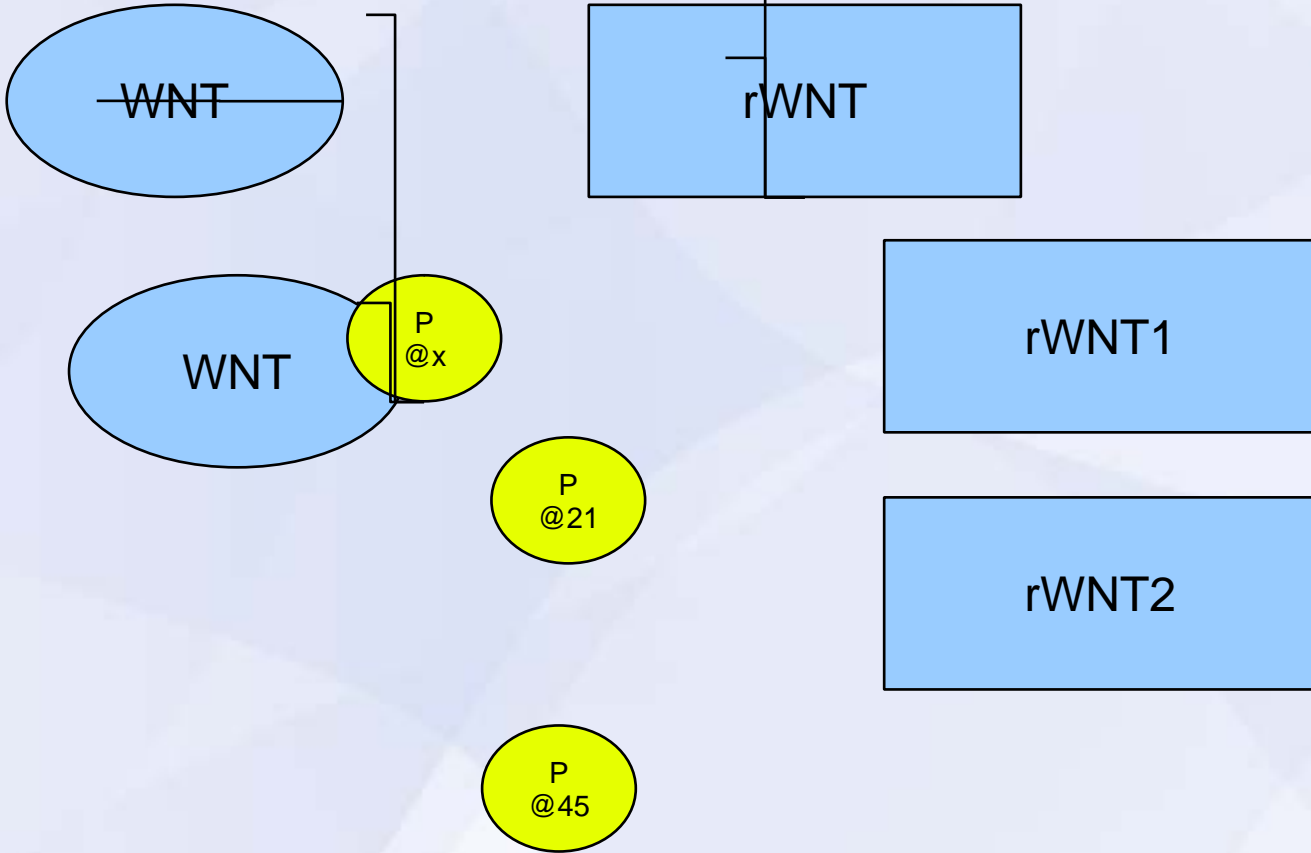
(c) Wnt/polarity pathway



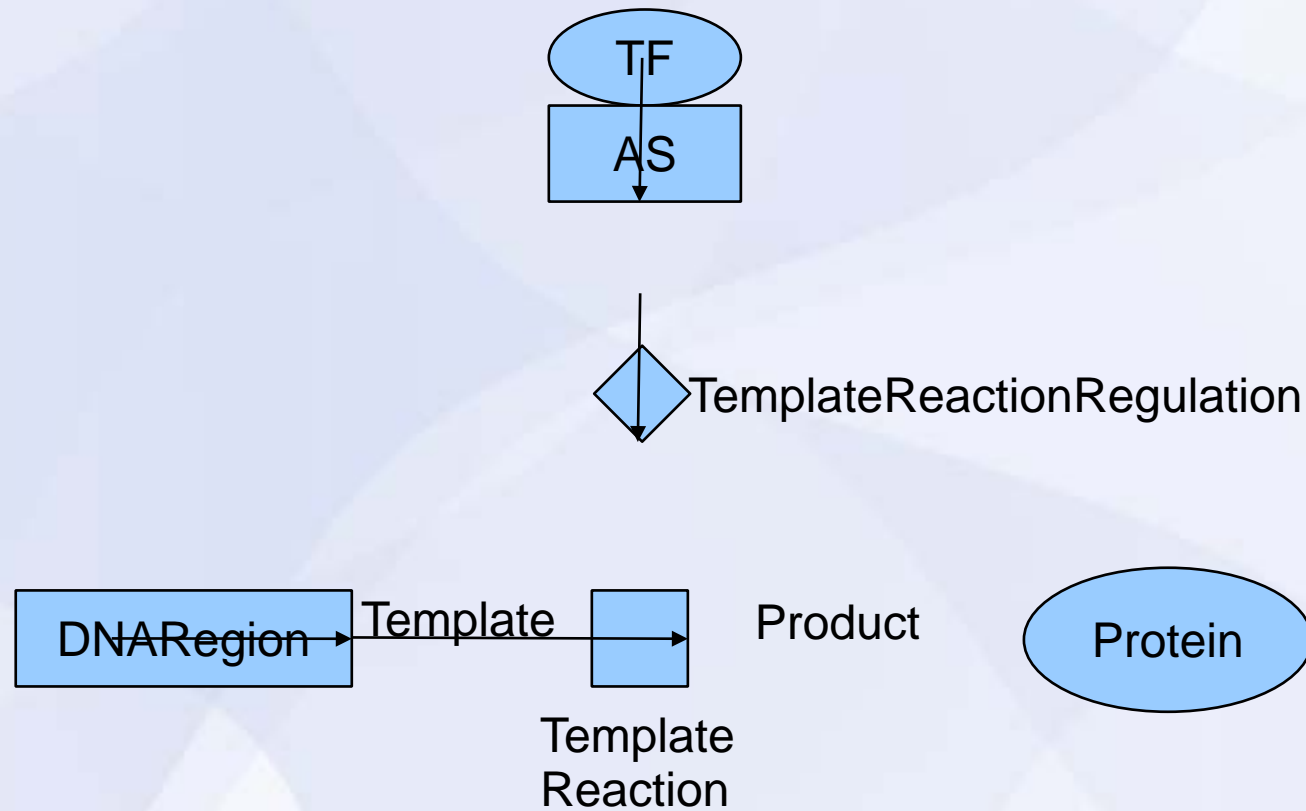
# Generics



# Generics



# Gene Regulation



# Genetic Interactions

- A separate non-causal, non-physical interaction : GeneticInteraction
- A separate non-physical entity : Gene
- Phenotype: e.g. viability
- InteractionScore: strength of interaction

# Controlled Vocabulary subclasses

- Cellular Location Vocabulary (GO)
- Relationship Type Vocabulary (Orphan)
- Sequence Modification Vocabulary (PSI-MI for protein, orphan for others)
- Experimental Form Vocabulary (PSI-MI for proteins, orphan for others)
- Tissue Vocabulary (BTO)

# Controlled Vocabulary subclasses

- Cell Vocabulary (CL)
- Evidence Code Vocabulary (PSI-MI for proteomics)
- Entity Reference Type Vocabulary ( Orphan)
- Phenotype Vocabulary ( PATO)
- Interaction Vocabulary ( PSI-MI)

# Refactorings

- All class names are now CamelCase
- All property names are now singular, lower case
- Some classes were renamed to better reflect biology/common terminology

# Refactorings

- Better handling of data source, method score, provenance
- Name, Standard Name, Display Name
- Pathways can now control reactions
- Pathway Step improved to cover context specific direction of reversible reactions.

# What is included in the release

Ontology specification	Web Ontology Language (OWL) XML file, developed using free Protégé ontology editor software[57].
Ontology documentation	Explanation of BioPAX entities, example documentation, best practice recommendations, use cases, how to.
Example files	Example files for biochemical pathway, protein and genetic interaction, protein phosphorylation, insulin maturation, gene regulation, generic molecules in OWL XML.
Graphical representation	Recommendations for graphical representation using Systems Biology Graphical Notation (SBGN) as a guide.
Paxtools software	Java programming library supporting import/export, conversion, validation. Can be used to add BioPAX support to software.
List of data sources & supporting software	Databases making data available in BioPAX format, software systems for storing, visualizing and analyzing BioPAX pathways.

## BioPAX – A community standard for pathway data sharing

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