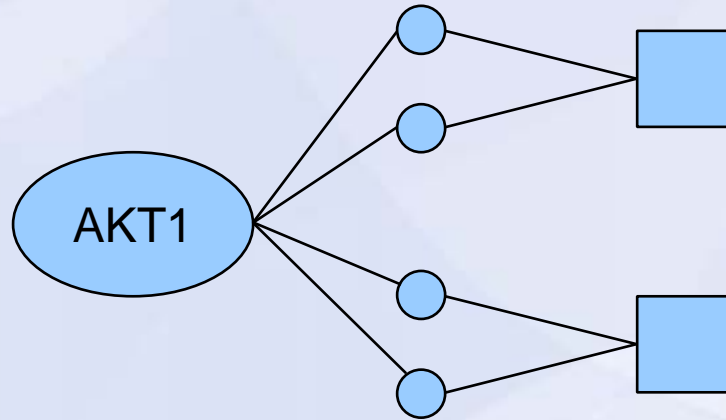


BioPAX Level 3: An overview of new features

Emek Demir
Memorial Sloan Kettering Cancer Center

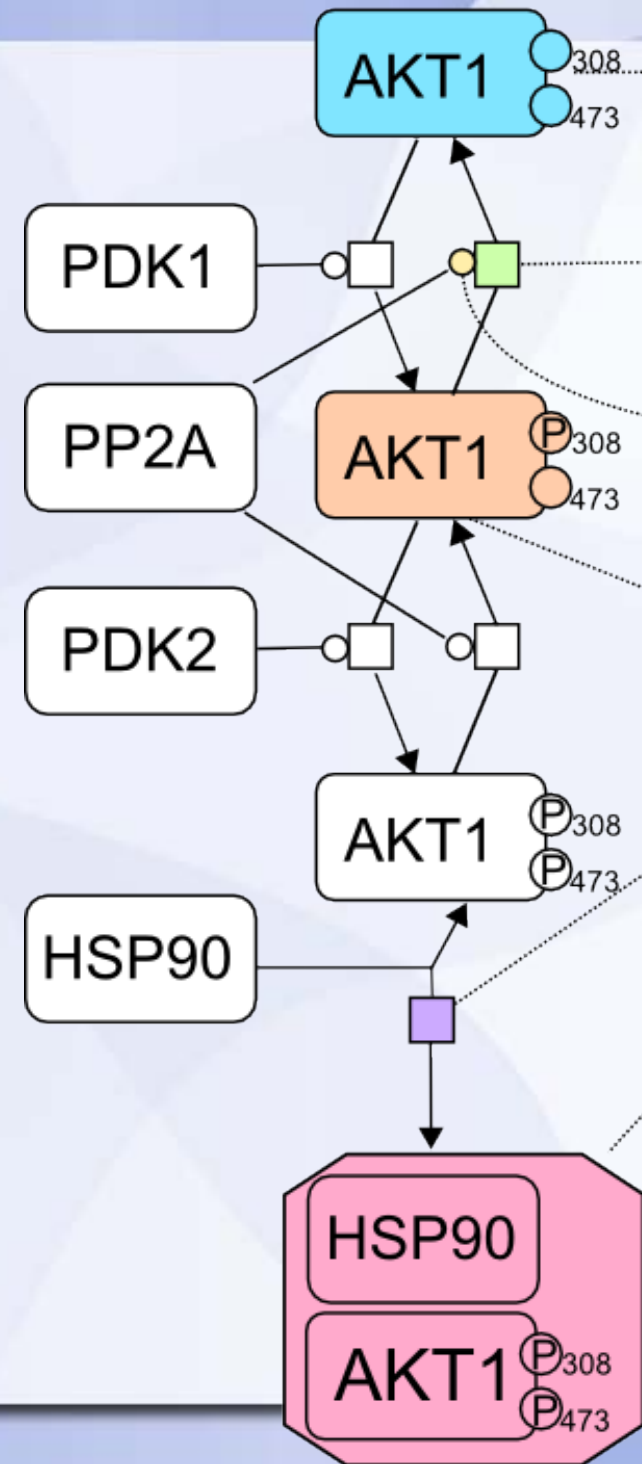
States in Level 2



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

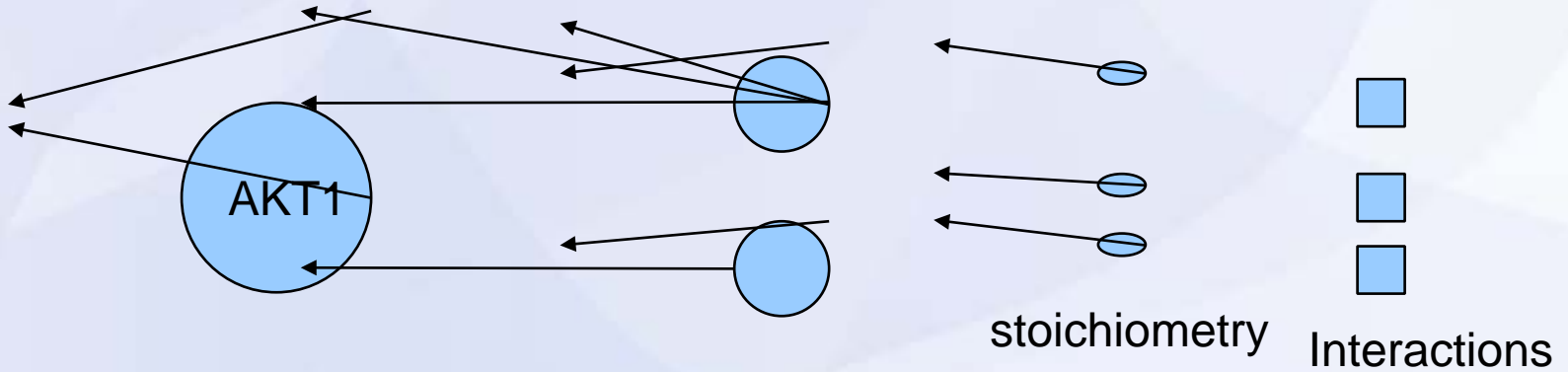
assem
has l
has l
has r
is re

comp
has
has

HSP
has
is bo

AKT
has
has
has
is bo

States in Level 3



Physical Entity Reference:
Name, Sequence,
etc

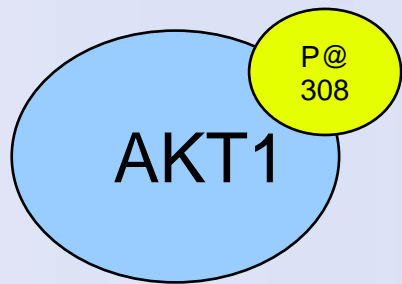
Physical Entity

State, location

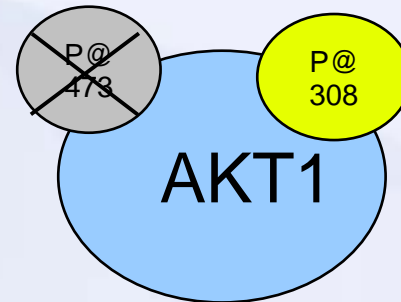
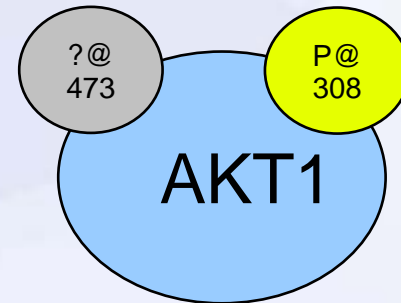
Features

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

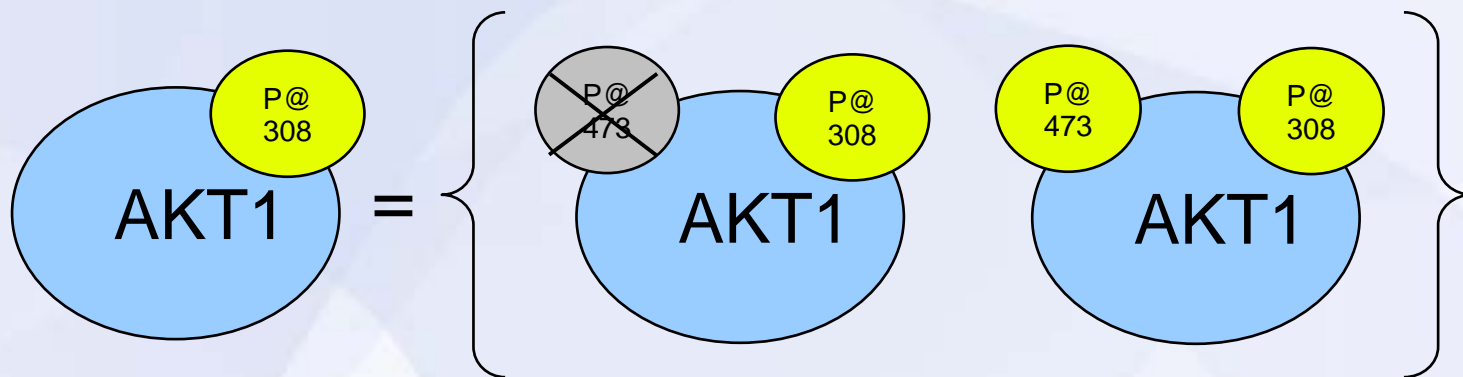
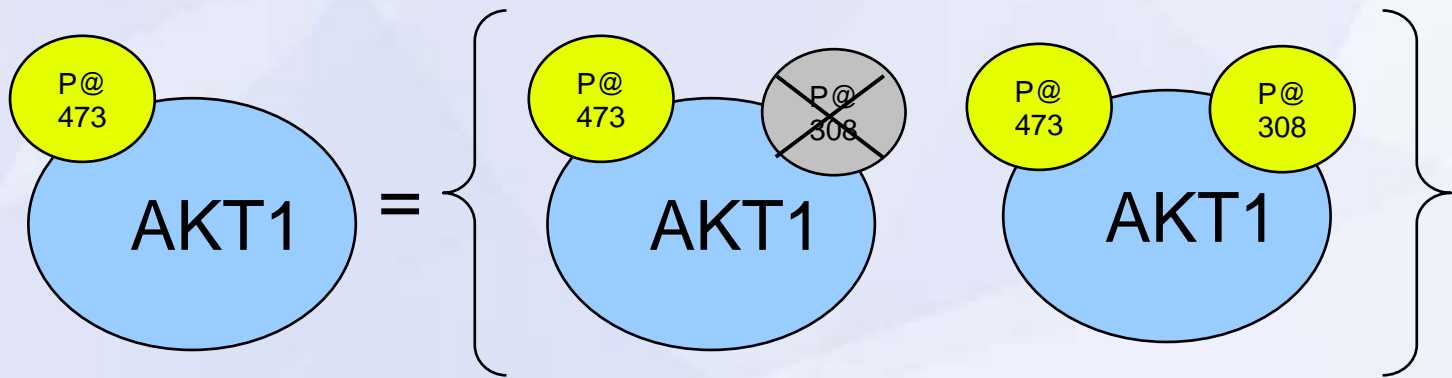
Features and Combinatorial Complexity



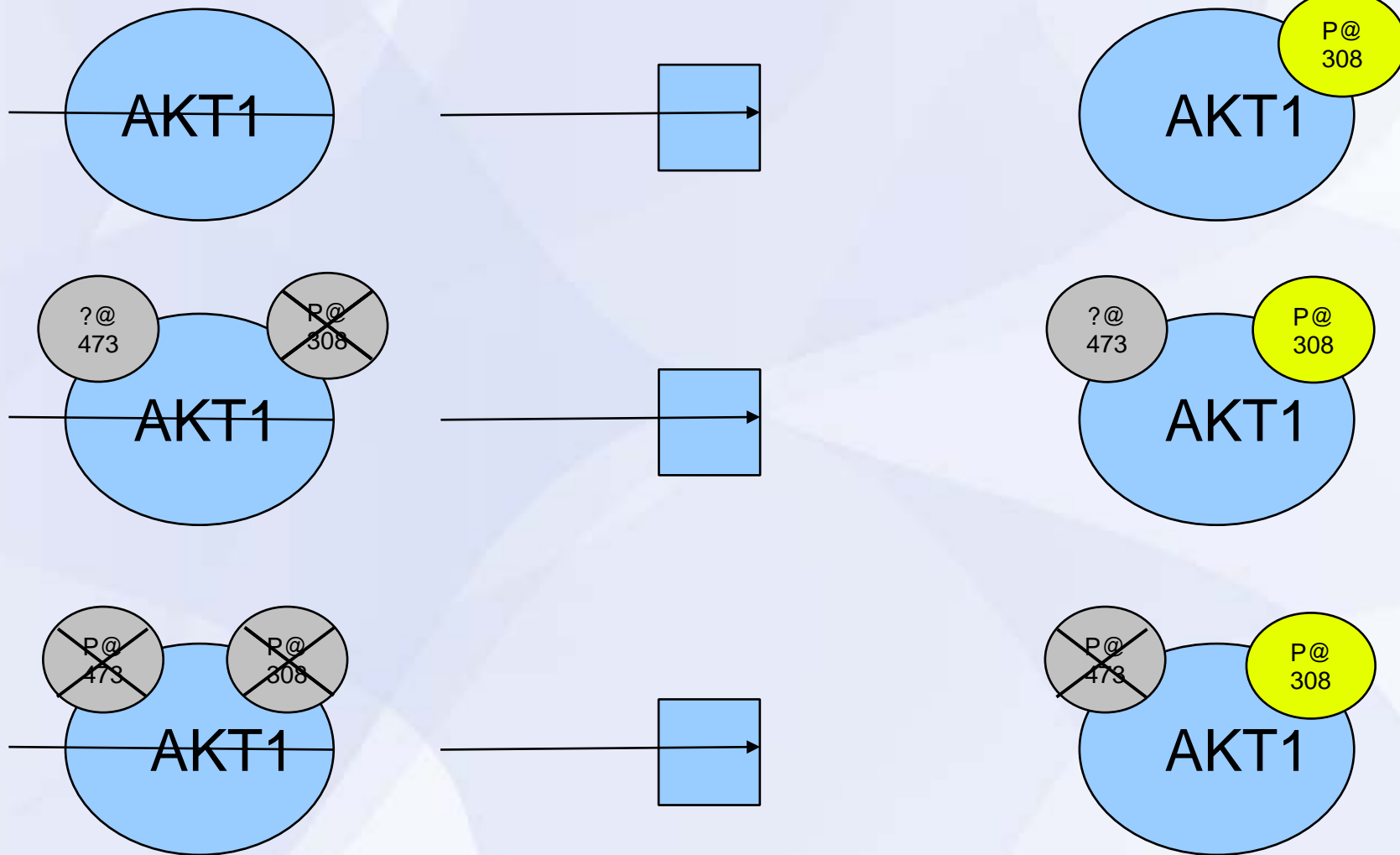
?



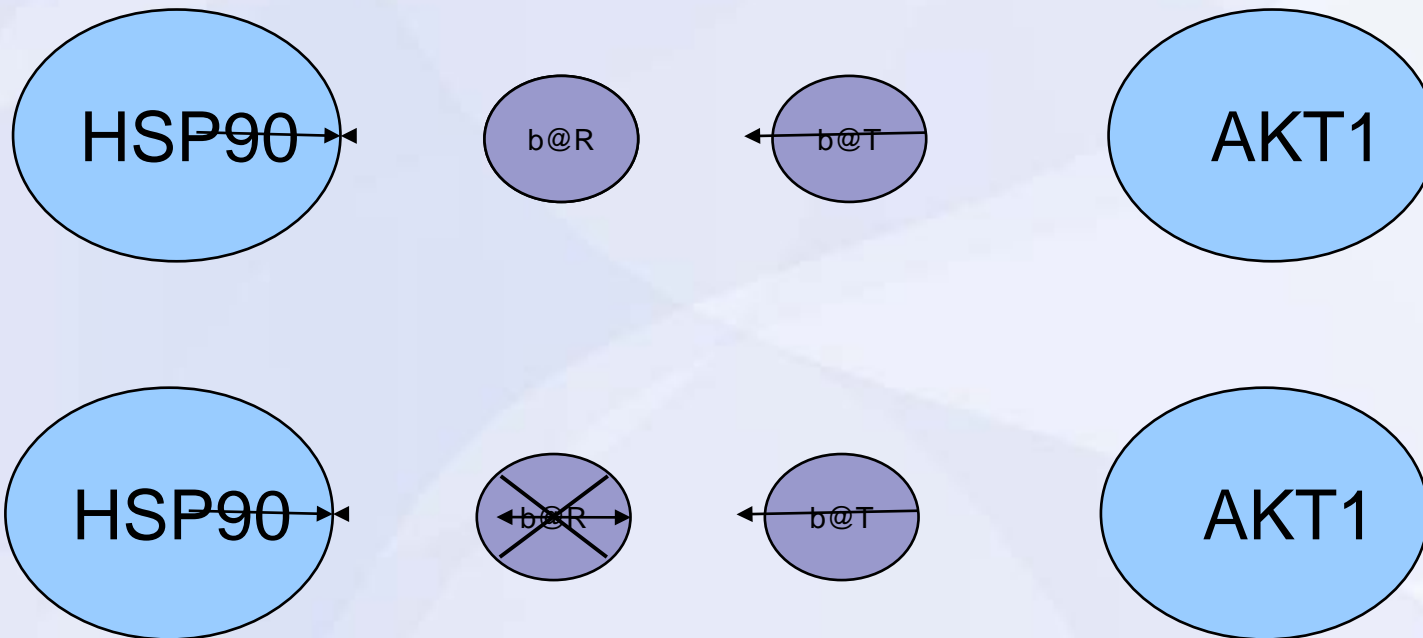
Features and Overlapping Pools



Features and not Features

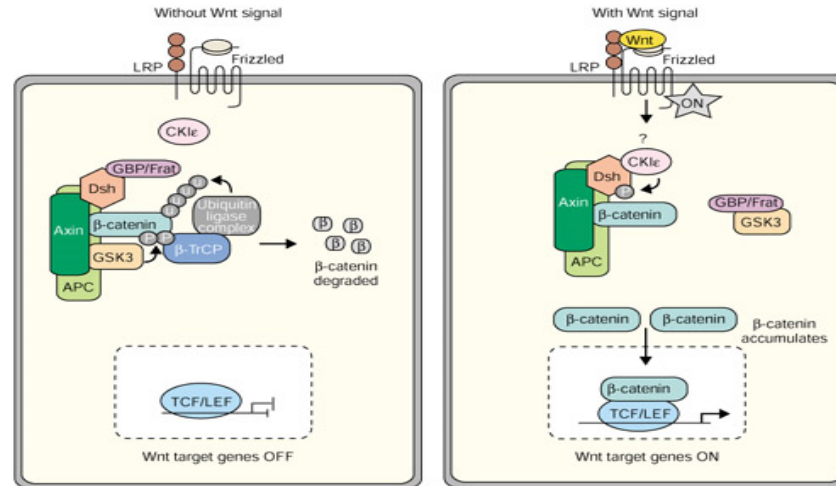


Binding Feature

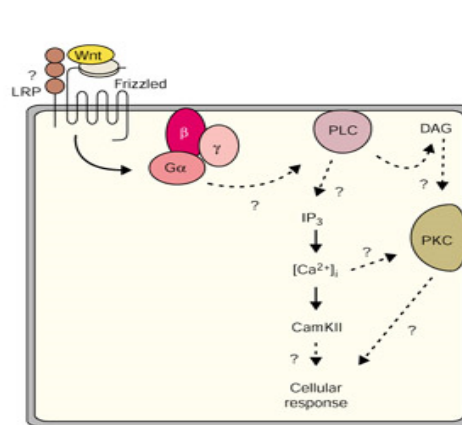


Generics

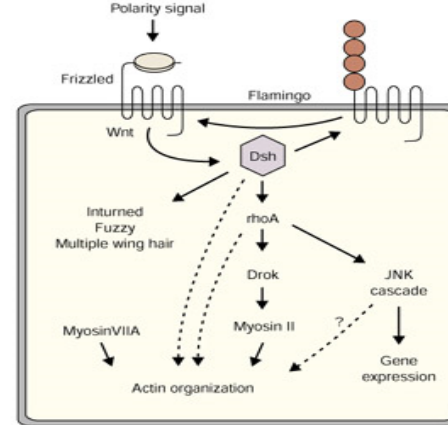
(a) Wnt/ β -catenin signaling pathway



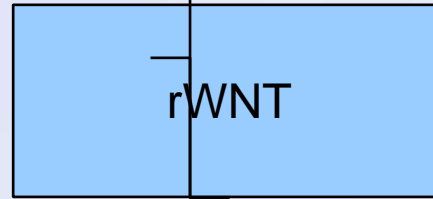
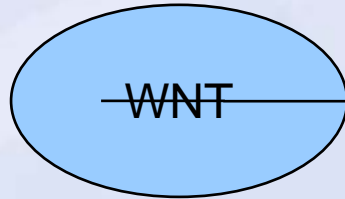
(b) Wnt/ Ca^{2+} pathway



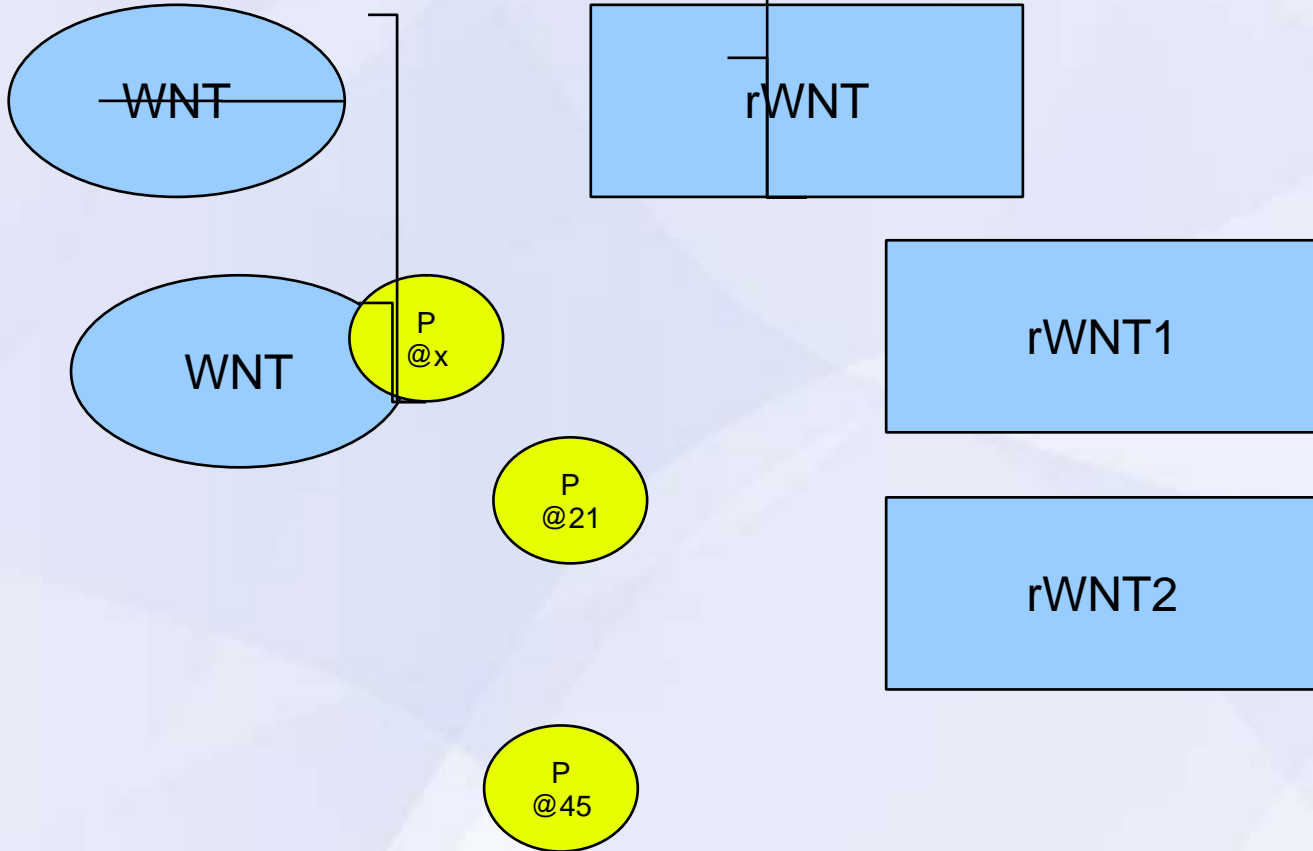
(c) Wnt/polarity pathway



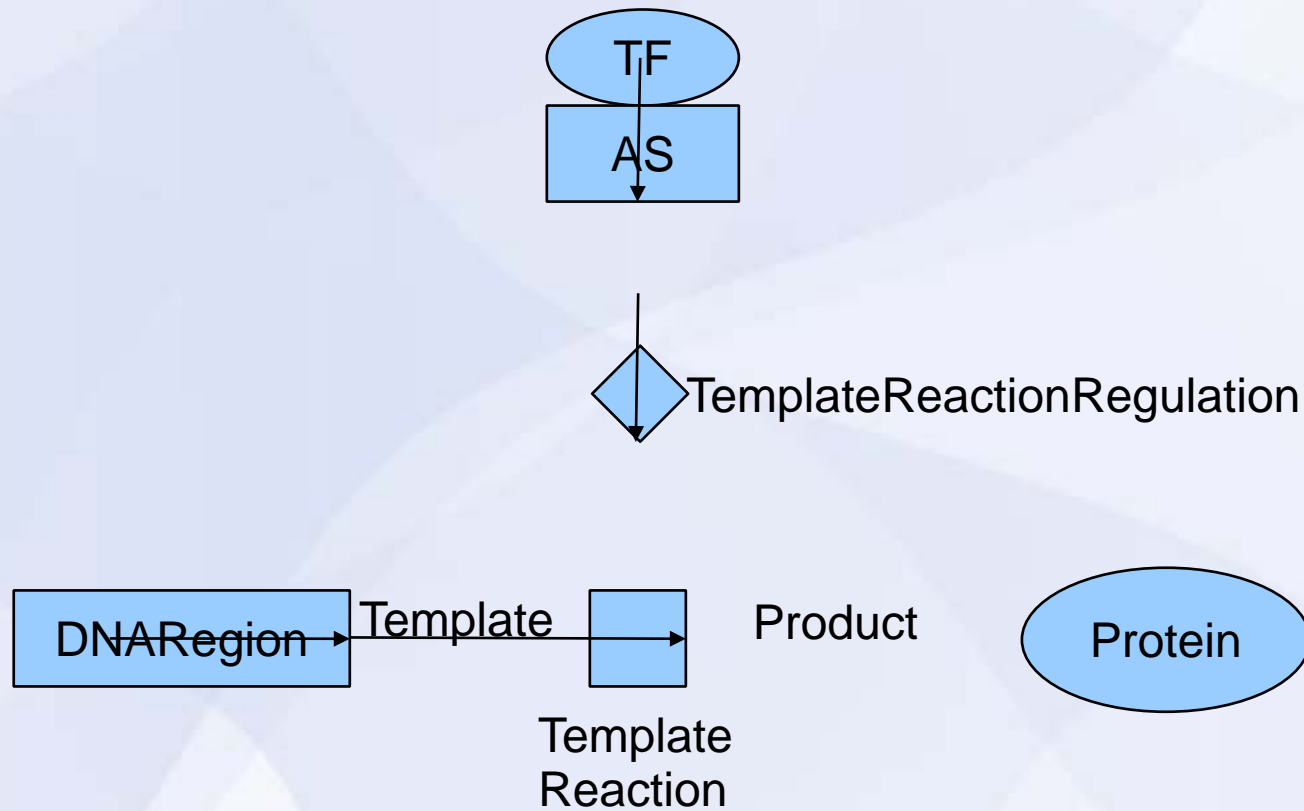
Generics



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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