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Commentary

# Developing *In Silico* Models of Protein-Protein Interactions (PPIs)

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## DESCRIPTION

Proteins, biomolecules, or macromolecules perform a wide range of biological functions in organisms. Proteins must specifically recognize a wide variety of interaction partners for almost every cellular process. By interacting with other molecules like DNA, RNA, proteins, and small molecules, they can carry out their roles. The term "protein and protein interactions" (PPIs) refers to the deliberate physical contacts between two or more proteins caused by electrostatic forces, biochemical processes, or both.

The physical contacts between two or more proteins are known as protein-protein interactions, and they represent intricate biological functions. In order to investigate the complex pathways and discover the functions of unknown proteins, protein-protein interactions have been used to build protein-protein interactions networks. All biological processes in a cell are controlled by proteins, and while some proteins carry out their tasks on their own, the vast majority of proteins interact with one another to carry out their biological activity. Characterizing protein–protein interactions through methods such as Co-immunoprecipitation (Co-IP), pull-down assays, crosslinking, label transfer, and far–western blot analysis are all important for understanding the biology of the cell and the function of proteins.

The majority of a cell's biological processes, such as gene expression, cell growth, proliferation, nutrient uptake, morphology, motility, intercellular communication, and apoptosis, are facilitated by proteins. Protein expression is a dynamic process because cells respond to a variety of stimuli. It's possible that the proteins needed to carry out particular tasks won't always be expressed or activated. Additionally, many proteins are expressed in a cell type-dependent manner and all cells are not the same. When attempting to understand protein function within the proper biological context, these fundamental properties of proteins suggest a complexity that can be challenging to investigate.

### *In silico* models of protein–protein interactions

By catalyzing the covalent addition or subtraction of phosphate groups to serine and threonine or tyrosine residues in their substrates, protein kinases, also known as phosphatases, in eukaryotic cells are the primary fundamentals of signal transduction. This results in the rapid and reversible modification of proteins, allowing plants to quickly and precisely adapt to their surroundings. Mitogen-Activated Protein Kinase (MAPK, also known as MPK) is a crucial protein kinase that is essential for converting signals from the environment and during development into distinct nuclear responses. Through double phosphorylation on both conserved Threonine (T) and Tyrosine (Y) residues in the kinase activation loop, MAPKs are activated by their specific activator MAPK kinases (MAPKKs, MKKs). Dephosphorylation of cognate residues by a variety of tyrosine phosphatases and serine or threonine phosphatases, on the other side, causes MAPK inactivation (e.g., PP2C) and phosphatases with Dual Specificity (DUSPs)

Specific docking interactions typically result in the formation of a complex between MAPK and its connate activator, substrate, scaffold, or inactivator. All of the enzymatic reactions perform better as a result of the docking interactions, which may also help regulate the specificity of molecular recognition. A cluster of negatively charged amino acids in the C-terminal region outside the catalytic domain, which binds the basic residues at the N terminus of the Docking site (D-site) in MAPK-interaction proteins, was discovered to be present in MAPKs' Common Docking Domain (CD Domain). These D-sites encourage binding specificity and high affinity interactions with cognate MAPKs and have more consecutive positively charged amino acids. Additionally, MAPK-regulating proteins like MKKs, scaffold proteins, MAPK phosphatases, and substrates contain D-sites.

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