Understanding Drug-Target Dynamics through Mathematical Formalism

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Abstract:

Evidence suggests G protein-coupled receptors heteromerize in both Central Nervous System and non-Central Nervous System regions, providing a framework for drug combination therapies. This study presents a heterodimer model using differential equations to represent the binding dynamics of two ligands (A and B) to a receptor heterodimer (R1R2). We prove the existence of a unique, biologically plausible equilibrium within a broad parameter space of rate constants, ensuring feasible pharmacological scenarios. The time dynamics of the biological response vary with the efficacies of the four heterodimeric species, aiding in the exploration of drug combinations.

References: