Dimensionality of motion and binding valency govern receptor-ligand kinetics as revealed by agent-based modeling.

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Abstract

Mathematical modeling and computer simulations have become an integral part of modern biological research. The strength of theoretical approaches is in the simplification of complex biological systems. We here consider the general problem of receptor-ligand binding in the context of antibody-antigen binding. On the one hand, we establish a quantitative mapping between macroscopic binding rates of a deterministic differential equation model and their microscopic equivalents as obtained from simulating the spatio-temporal binding kinetics by stochastic agent-based models. On the other hand, we investigate the impact of various properties of B cell derived receptors – such as their dimensionality of motion, morphology and binding valency – on the

receptor-ligand binding kinetics. To this end, we implemented an algorithm that simulates antigen binding by B cell derived receptors with a Y-shaped morphology that can move in different dimensionalities, i.e. either as membrane-anchored receptors or as soluble receptors. The mapping of the macroscopic and microscopic binding rates allowed us to quantitatively compare different agent-based model variants for the different types of B cell derived receptors. Our results indicate that the dimensionality of motion governs the binding kinetics and that this predominant impact is quantitatively compensated by the bivalency of these receptors.

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