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Network analysis reveals the recognition mechanism for complex formation of mannose-binding lectins YIREN JIAN, YUNJIE ZHAO, CHEN ZENG, George Washington Univ — The specific carbohydrate binding of lectin makes the protein a powerful molecular tool for various applications including cancer cell detection due to its glycoprotein profile on the cell surface. Most biologically active lectins are dimeric. To understand the structure-function relation of lectin complex, it is essential to elucidate the short- and long-range driving forces behind the dimer formation. Here we report our molecular dynamics simulations and associated dynamical network analysis on a particular lectin, i.e., the mannose-binding lectin from garlic. Our results, further supported by sequence coevolution analysis, shed light on how different parts of the complex communicate with each other. We propose a general framework for deciphering the recognition mechanism underlying protein-protein interactions that may have potential applications in signaling pathways.

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