“Self-organization” and “molecular recognition” are two physicochemical processes essential for living bodies to maintain their life. Both processes may not proceed spontaneously in "vacuum" due to entropy preferences/barriers, but can occur spontaneously in a living body. Why? In this talk, a statistical mechanics theory called "3D-RISM/RISM" developed by us for past few decades will be introduced and discussed, with emphasis on two topics related to protein functions and drug discovery: (1) The oseltamivir binding efficiency with the wild-type and resistance-associated mutant forms of the viral influenza-B neuraminidase. (2) Theoretical and biochemical determination of ammonia pathway in the purine biosynthetic enzyme formylglycinamide ribonucleotide amidotransferase.