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Characterizing the statistical properties of protein surfaces JI HYUN BAK, ANNE-FLORENCE BITBOL, WILLIAM BIALEK, Princeton University — Proteins and their interactions form the body of the signaling transduction pathway in many living systems. In order to ensure the accuracy as well as the specificity of signaling, it is crucial that proteins recognize their correct interaction partners. How difficult, then, is it for a protein to discriminate its correct interaction partner(s) from the possibly large set of other proteins it may encounter in the cell? An important ingredient of recognition is shape complementarity. The ensemble of protein shapes should be constrained by the need for maintaining functional interactions while avoiding spurious ones. To address this aspect of protein recognition, we consider the ensemble of proteins in terms of their three-dimensional shapes, more precisely in terms of their solvent-excluded surfaces. We take into account all high-resolution structures from E.coli non-DNA-binding cytoplasmic proteins that can be retrieved from the Protein Data Bank. We aim to characterize the statistical properties of the ensemble of protein surfaces, including the dimensionality of the space of surfaces.

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