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Characterizing the statistical properties of protein surfaces[1] 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 the shapes of their surfaces. We take into account the high-resolution structures of E.coli non-DNA-binding cytoplasmic proteins, retrieved from the Protein Data Bank. We aim to characterize the statistical properties of the protein surfaces at two levels: First, we study the intrinsic dimensionality at the level of the ensemble of the surface objects. Second, at the level of the individual surfaces, we determine the scale of shape variation. We further discuss how the dimensionality of the shape space is linked to the statistical properties of individual protein surfaces.

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