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"Methods for Predicting Dimensions of Intrinsically Disordered Proteins."

Abstract: Intrinsically disordered proteins (IDPs) have recently drawn significant attentions, due to their emerging roles in biology systems, involvement in neurodegenerative diseases, and potential for designing biomimetic materials. In contrast to folded proteins, IDPs lack of a well defined three dimensional structures and therefore possible structural properties for capturing their functions. We have recently shown that the dimension of an IDP greatly impacts its amino acid interactions and ability of liquid-liquid phase separation. It is therefore of great interest to investigate the sequence determinants of IDP dimensions and ultimately make in silico predictions. However a data-driven approach is not possible solely from experimental inputs. We have therefore constructed an IDP dimension database using our coarse-grained model combining physical potential energy functions and existing experimental measurements. A machine learning method is then used to learn the relation between IDP sequences and their dimensions. We are able to extract most important sequence properties dominating IDP dimensions, shedding light upon IDP sequence-function relations and designing principles of IDP-like polymers.