A Helical Wheel Based Coiled Coil Prediction Algorithm and Its Application to Disease

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??-helical coiled coils are protein substructures that play important roles in a wide range of biological events. Some types of coiled coils are used by various viruses (eg SARS-CoV2) to enter the host cell, and overexpression of certain genes can be affected by DNA binding coiled coils causing diseases such as cancer. Coiled coil amino acid sequences and motifs vary according to the organism and protein to which they belong thus it is difficult to predict, based on sequence, whether and where a protein structure includes a coiled coil.. Coiled coils are typically shown with a {7/2} helical wheel. However, with the investigations we made on the coiled coils, we determined that the {18/5} helical wheel may be a more accurate model. Aminoacid interactions shown on the {7/2} helical wheel were projected onto {18/5} and new interaction representations were obtained. An LSTM-based coiled coil prediction algorithm was created using the obtained interaction representations and mathematical features. In the algorithm, the sequence data is threaded onto the {18/5} helical wheel and the amino acid in each corner of the helix is trained to the algorithm along with all the other residues in the same layer of the helix.. Various algorithms used for coiled coil prediction in the literature (Marcoil2, DeepCoil, PepCoil, COILS etc.) predict coiled coils based on only on the amino acid sequence. The algorithm we present offers higher precision than these existing algorithms as result of it taking into consideration the helical arrangement as well.

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