An assessment tool for determination of coiled-coil orientation

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The coiled-coil (CC) domain is a very important structural unit of proteins and plays critical roles in various biological functions. The major oligomeric state of CCs is a dimer, which could either be parallel or antiparallel. The orientation of each α-helix in a CC domain is critical for the molecular function of CC-containing proteins but cannot be determined easily using sequence-based prediction. We developed a biochemical method for assessing differences between parallel and antiparallel CC dimers and named it ACCORD (Assessment tool for Coiled-Coil ORientation Decision). To validate this technique, we applied it to 13 different CC proteins with known structures. Furthermore, the ACCORD was able to accurately determine the orientation of a CC domain of unknown directionality, which was confirmed by X-ray crystallography and small angle X-ray scattering. The ACCORD can be used as a general tool to determine CC directionality to supplement in silico prediction results.