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AlphaSS : Improving Protein Structure Prediction With Disulfide Bond Information

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Proteins are fundamental to life's molecular machinery, and understanding their structures can provide valuable insight into their functional mechanisms. Among the various types of covalent bonds in proteins, disulfide bonds –linkage between the sulfur atoms of two cysteine residues– play crucial roles in stabilizing a protein structure. Despite the impressive performance of AlphaFold2 in predicting protein structures, it often struggles with target proteins that have limited evolutionary information, i.e., their MSA(multiple sequence alignment) across various species. Inspired by methods such as AlphaLink, which incorporates distance information between two residues obtained from crosslinking mass spectrometry into predictions, we have developed AlphaSS. This modification of AlphaFold2 takes disulfide linkage information as its input to the machine learning network, enhancing the algorithm's capability to model protein folds more accurately than without MSA. Initial tests on monomer structures have shown promising results, and we anticipate that AlphaSS will also prove beneficial for predicting multimeric protein structures.