A disulfide bridge survey and library

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Disulfide bridges between cysteine sidechains are one of the more unusual features of protein macromolecules. They provide a strong, stabilizing, covalent connection between sequence-distant parts of a protein.

Previous efforts by the Richardson Lab to compile a comprehensive library of disulfide conformations were frustrated by our datasets being insufficiently large in the face of the huge conformational space afforded by disulfides' 5 chi torsions (more than lysine!). Now, enabled by the Top2018 dataset, we present our survey of disulfide bridges.

Disulfides have great conformational diversity. This diversity is matched by the diversity of proteins and structural contexts they appear in. Nevertheless, disulfide conformations are often conserved among proteins with similar functions. Some conformations are even unique to certain protein families. Others are conserved according to their position relative to secondary structure. This library will aid in selection of appropriate disulfides in model building and in MolProbity-style validation of experimental and predicted models.