Challenges of Structural Genomics Two Decades Perspective

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Structural Genomics (SG) programs have developed many novel methodologies for faster and more accurate structure determination over the last two decades. The entire structural biology community used these new tools to generate enormous amounts of experimental data, which resulted in significant improvements in the understanding of many biological processes at molecular levels. The structural information obtained from structural genomics has been used for various purposes, including drug discovery, designing new proteins possessing specific functions, and predicting structures. One such tool, the Alpha FOLD2 system that revolutionized structure prediction, was trained on the vast amount of data deposited to the Protein Data Bank (PDB). However, the amount of data collected so far is so large that traditional analysis methods limit the extraction rate of biological and biochemical information from 3D models. Taking a 20 years perspective has prompted us to review the unmet SG challenges and those that can be significantly addressed by carefully looking into the details of the Protein Structure Initiative.