

Disulphide bonds are crucial to correct protein folding, and heavily influence protein function. Tandem mass spectrometry protein analysis is often used for the determination of disulphide bond positions, in combination with manual or computational interpretation methods. In this thesis we devise a program for automatic disulphide bond characterization called Dibby. Dibby identifies protein fragments in the fragmentation spectra, and uses the identified fragments to determine which cysteines were connected in the protein. The identification algorithm is able to identify even complex fragments with multiple disulphide bonds that are often missed by other methods. To reduce the fragment search space, we employ divide and conquer and branch and bound techniques. We evaluate Dibby on both measured and in-silico generated datasets, and find that it correctly identifies large portion of the present disulphide bonds with minimal manual interventions.