

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 this thesis we devise a program for automatic disulphide bond characterisation called Dibby. Dibby identifies fragments from the fragmentation spectra, and uses them to determine which cysteines were connected in the original protein. The identification algorithm is able to identify even complex fragments with multiple disulphide bonds that are unidentifiable 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 most of the disulphide bonds with minimal manual interventions.