Mass Spectrometry in Structural Biology

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Tertiary structural information is helpful in understanding functions of proteins which play critical roles in living cells. Moreover, structural information of target proteins at an atomic level can accelerate drug design. From such a viewpoint, structural biology has widely been carried out mainly by X-ray crystallography and NMR for various functional proteins. These methods can provide valuable structural information of proteins but have some limitations. If protein crystallization is unsuccessful, no information is available from X-ray crystallography. As for NMR, it is still difficult to characterize proteins with molecular masses of above 100 kDa.

Mass spectrometry is promising for characterization of large proteins or protein complexes which are difficult to crystallize. Although mass spectrometry requires sample preparation in volatile buffers, it enables characterization of whole protein complexes in the native state if appropriate experimental procedures are applied. It can provide not only masses of the whole protein complexes but also information of stabilities of the complexes. In the present paper, methodology of mass spectrometry in structural biology will be presented, and several examples of structural characterization of protein complexes which play important roles in transcription processes will also be demonstrated. Furthermore, novel technology in protein mass spectrometry will be presented.