

Conformational kinetics study of MP-11 using TIMS-MS and molecular dynamics *by*

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Abstract Details

In the present work, we studied the conformational kinetics of microperoxidase 11 (MP-11), a digest fragment of cytochrome C that contains 11 amino acids with a covalently attached heme group. In particular, a novel technique recently developed at FIU in collaboration with Bruker Daltonics Inc. combined with theoretical calculation was used for the characterization of MP-11 conformational space [1-3]. Accurate ion-neutral collision cross sections were measured for all MP-11 generated charge states. Since MP-11 (like cytochrome C) undergoes conformational changes as a function of the solvent state, MP-11 ions were produced by electrospray ionization (ESI) in order to preserve the initial solution state structure and analyzed on the basis of size-to-charge, inside the Trapped Ion Mobility Spectrometer (TIMS) followed by mass identification using a time-of-flight mass analyzer (MS) [4-5]. TIMS-MS has the advantage that molecular ions can be trapped for several seconds which allow us to study the kinetics and stability of various isomers as a function of time, initial pH value (6.1, 4.5, 3.1), and molecular ion temperature. Results showed that MP-11 conformations vary with pH levels and trapping time, and multiple interconversion pathways were observed for $[M+2H]^+2$ and $[M+3H]^+3$ charge states. Candidate structures were proposed for each conformation observed and main molecular interactions responsible for the conformational changes are discussed.

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