

Supporting Information

Understanding the thermal denaturation of myoglobin with IMS-MS: evidence for multiple stable structures and trapped pre-equilibrium states

Daniel W. Woodall,^a Lucas W. Henderson,^a Shannon A. Raab,^a Kenji Honma,^b and David E. Clemmer^{a,*}

^aDepartment of Chemistry, Indiana University, Bloomington, Indiana, 47405

^bGraduate School of Material Science, University of Hyogo, 3-2-1 Kohto, Kamigori, Hyogo 678-1297, Japan

*Corresponding author:

David E. Clemmer

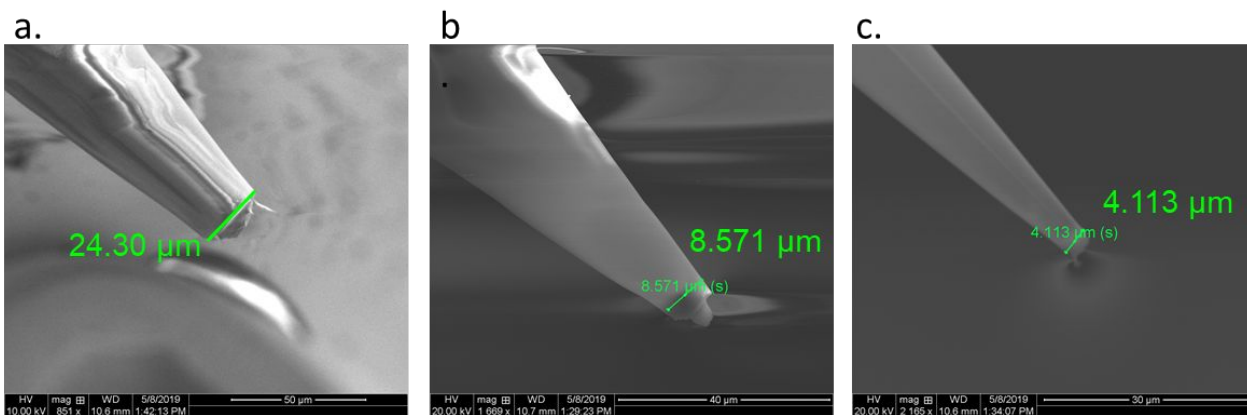


Figure S1. Scanning electron microscopy images of ESI capillary tips used in laser droplet heating experiments. Three different tip sizes were used, having diameters of 24.3 μm (a.), 8.60 μm (b.), and 4.10 μm (c.).

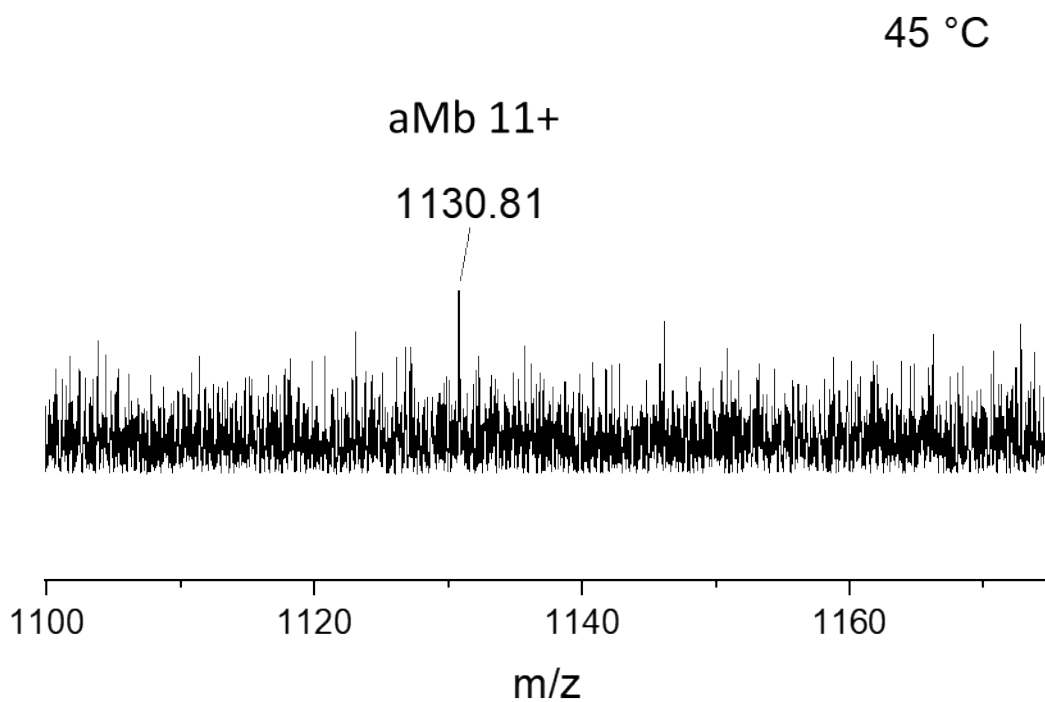


Figure S2. Zoomed mass spectra of holomyoglobin acquired at a solution temperature 45 °C in pH = 9.0 ammonium acetate. Peaks corresponding to apomyoglobin (aMb) begin to appear in the mass spectrum at temperatures above 45 °C. The 11+ aMb species is annotated in the mass spectrum.

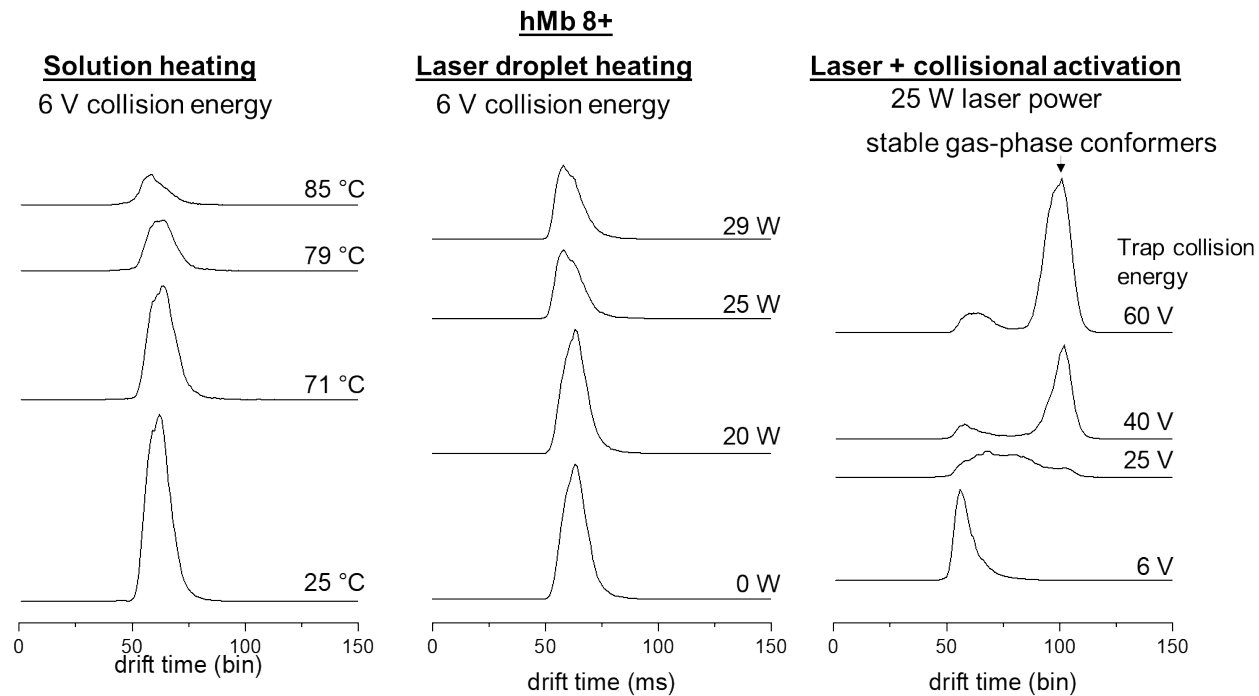


Figure S3. Drift time distributions of hMb 8⁺ ions at increasing temperatures (25, 71, 79, and 85 °C (left)), laser power (0, 20, 25, 29 W (middle)) and collisional activation 6, 25, 40, and 60 V (right)). All samples were prepared in 10 mM ammonium acetate (pH = 9), and electrosprayed from ~ 8 μm emitters.

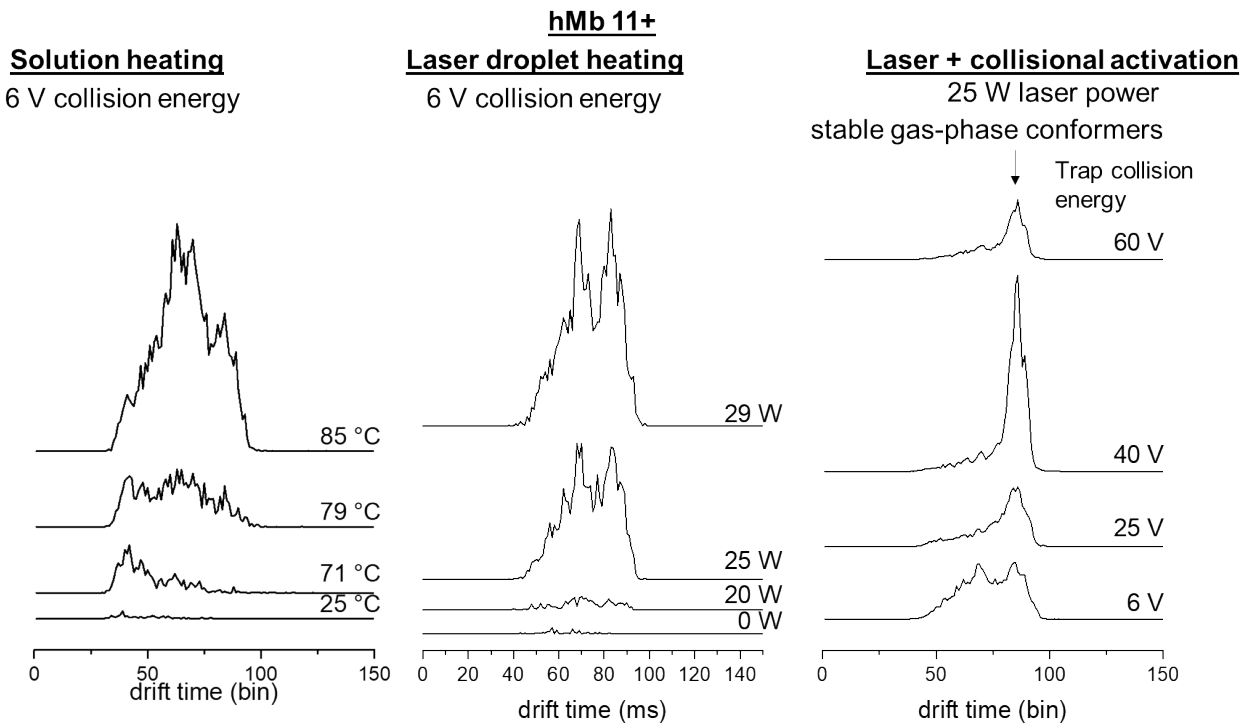


Figure S4. Drift time distributions of hMb 11+ ions at increasing temperatures (25, 71, 79, and 85 °C (left)), laser power (0, 20, 25, 29 W (middle)) and collisional activation 6, 25, 40, and 60 V (right)). All samples were prepared in 10 mM ammonium acetate (pH = 9), and electrosprayed from ~ 8 μm emitters.

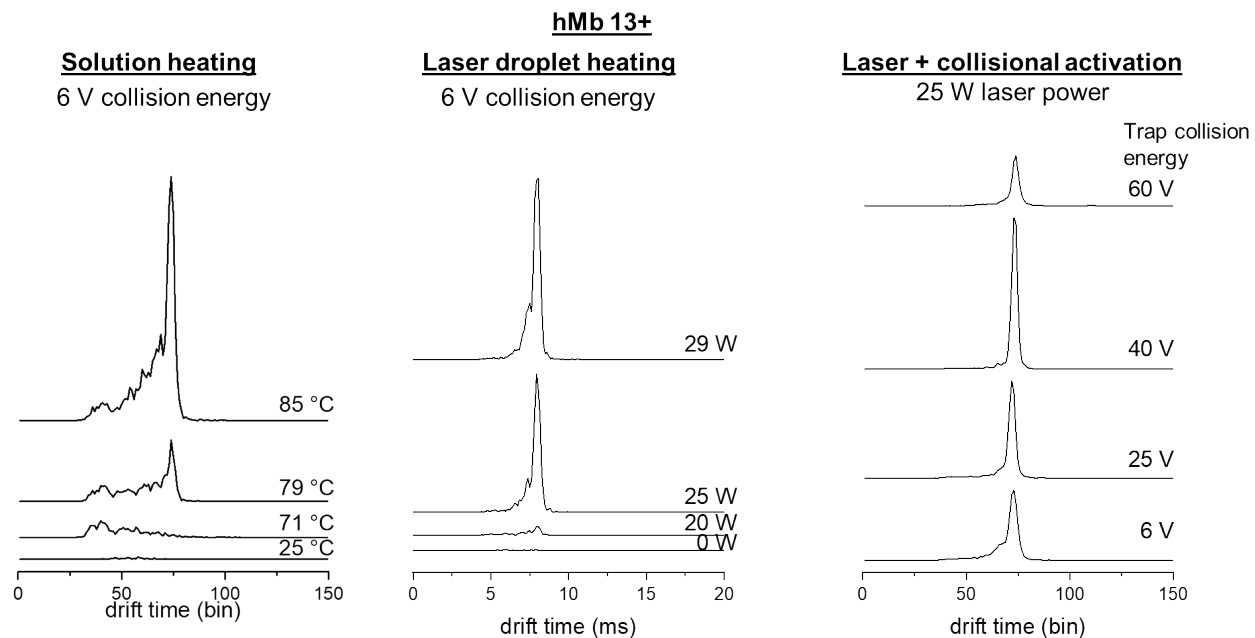


Figure S5. Drift time distributions of hMb 13+ ions at increasing temperatures (25, 71, 79, and 85 °C (left)), laser power (0, 20, 25, 29 W (middle)) and collisional activation 6, 25, 40, and 60 V (right)). All samples were prepared in 10 mM ammonium acetate (pH = 9), and electrosprayed from ~ 8 μm emitters.