

## Supplemental Information

### Salt Bridges Govern the Structural Heterogeneity of Heme Protein Interactions and Porphyrin Networks: Microperoxidase-11

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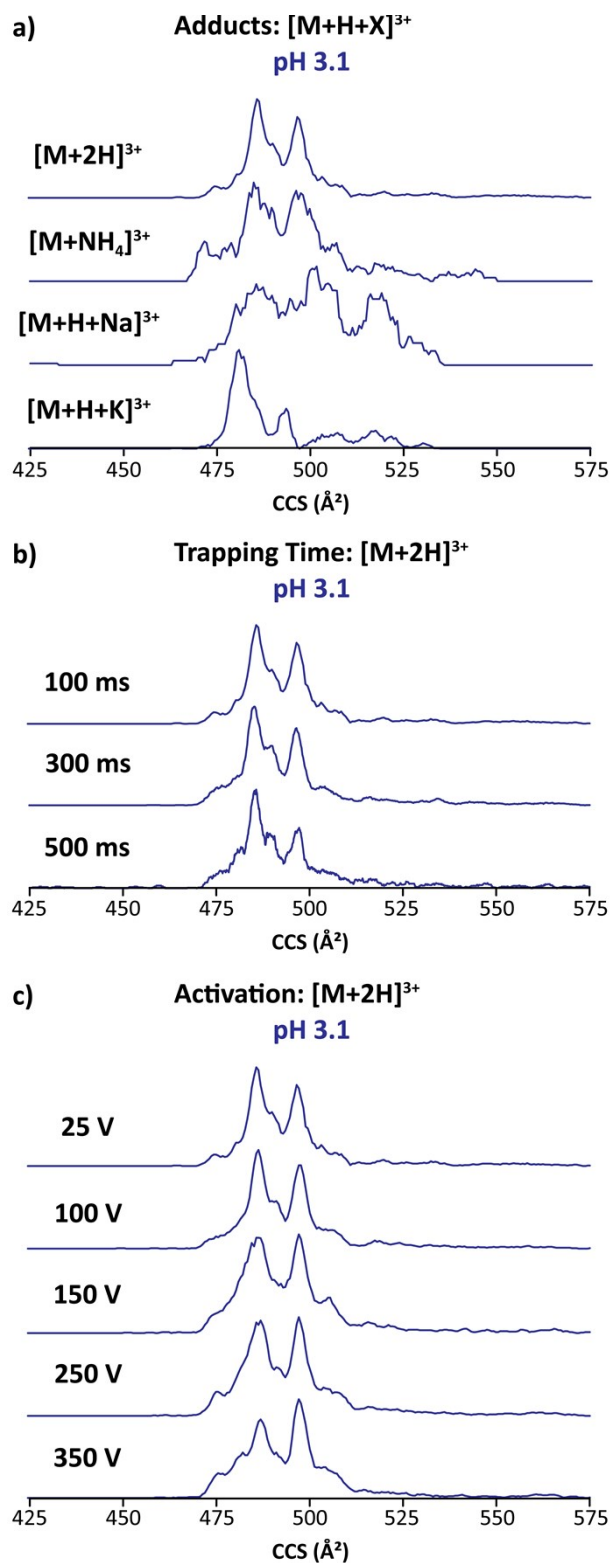
**Figure S1.** TIMS profiles of MP-11 triply-charged monomers at pH 3.1 as a function of adducts, trapping time and collisional activation.

**Figure S2.** TIMS profiles of MP-11  $[M]^+$ ,  $[M+H]^{2+}$ ,  $[2M]^{2+}$  and  $[2M+H]^{3+}$  ions at pH 6.6, 4.5 and 3.1 as a function of trapping time.

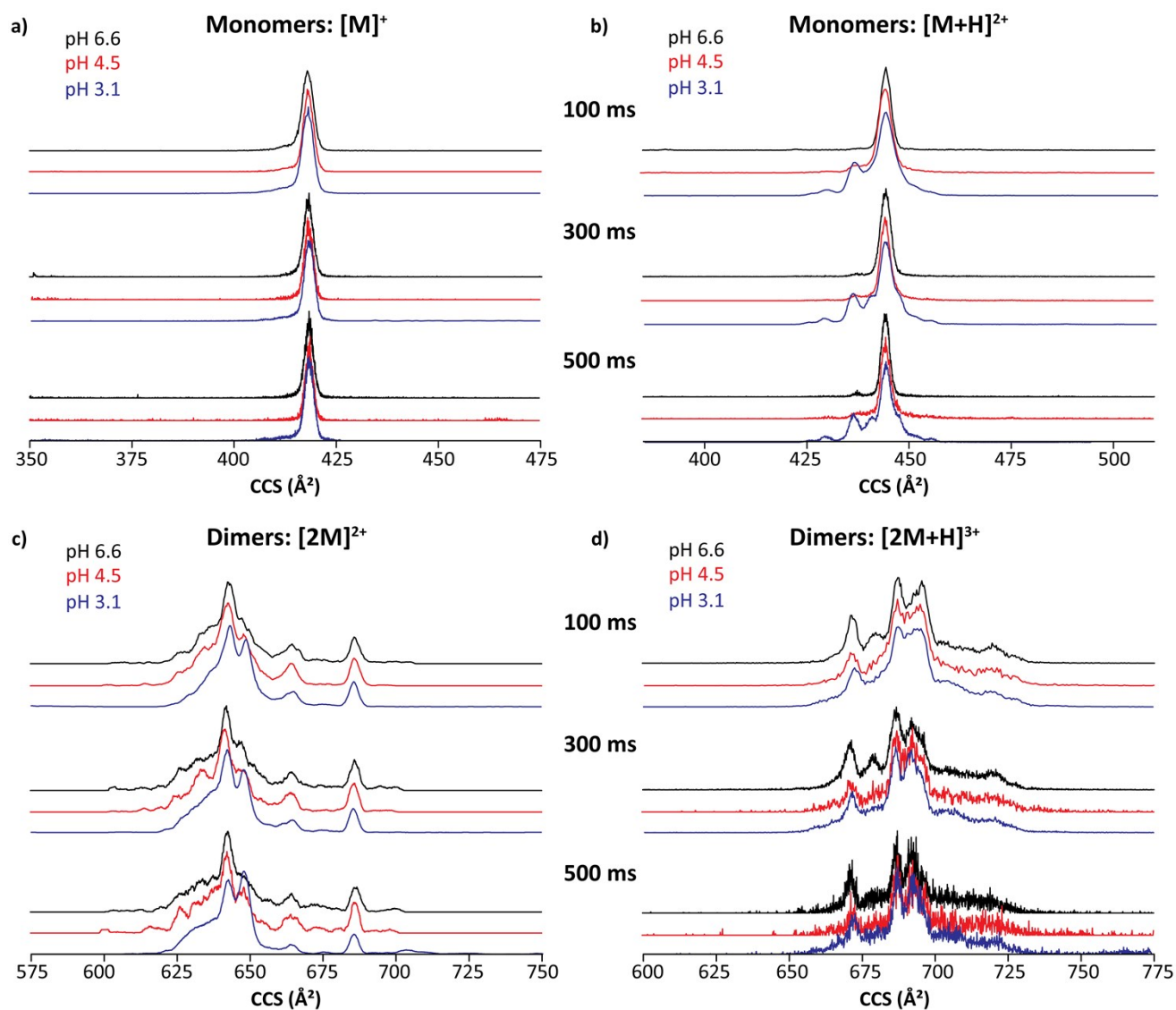
**Figure S3.** TIMS profiles of MP-11  $[M]^+$ ,  $[M+H]^{2+}$ ,  $[2M]^{2+}$  and  $[2M+H]^{3+}$  ions at pH 6.6, 4.5 and 3.1 as a function of collisional activation.

**Figure S4.** TIMS profiles of MP-11  $[M]^+$ ,  $[M+H]^{2+}$ ,  $[2M]^{2+}$  and  $[2M+H]^{3+}$  ions at pH 6.6, 4.5 and 3.1 as a function of the ionization process.

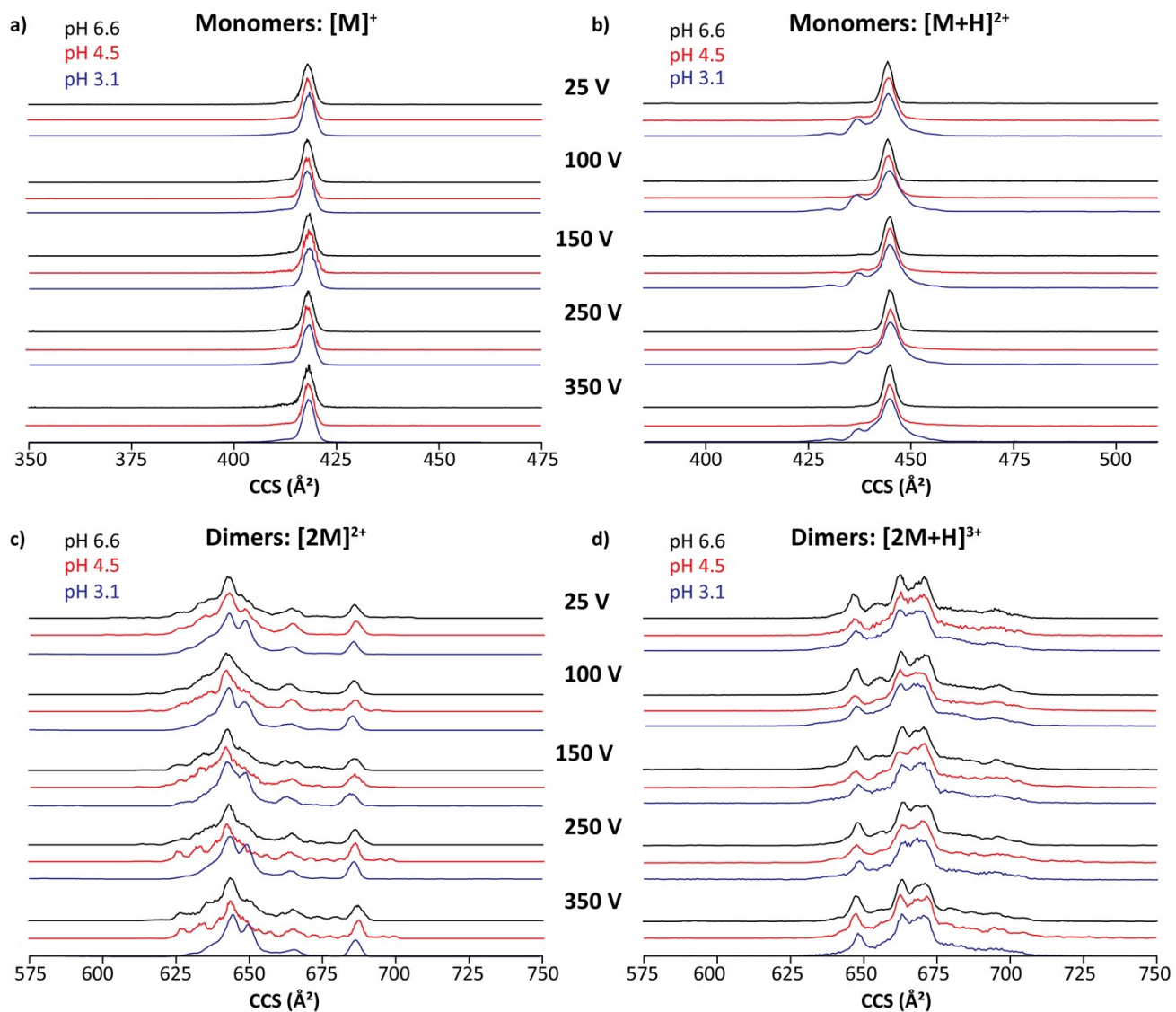
**Figure S5.** MS spectra of the  $[2M+H]^{3+}$  as a function of the collision energy and plots representing the relative abundances of the  $[2M+X]^{3+}$  ions as a function of collision energy.



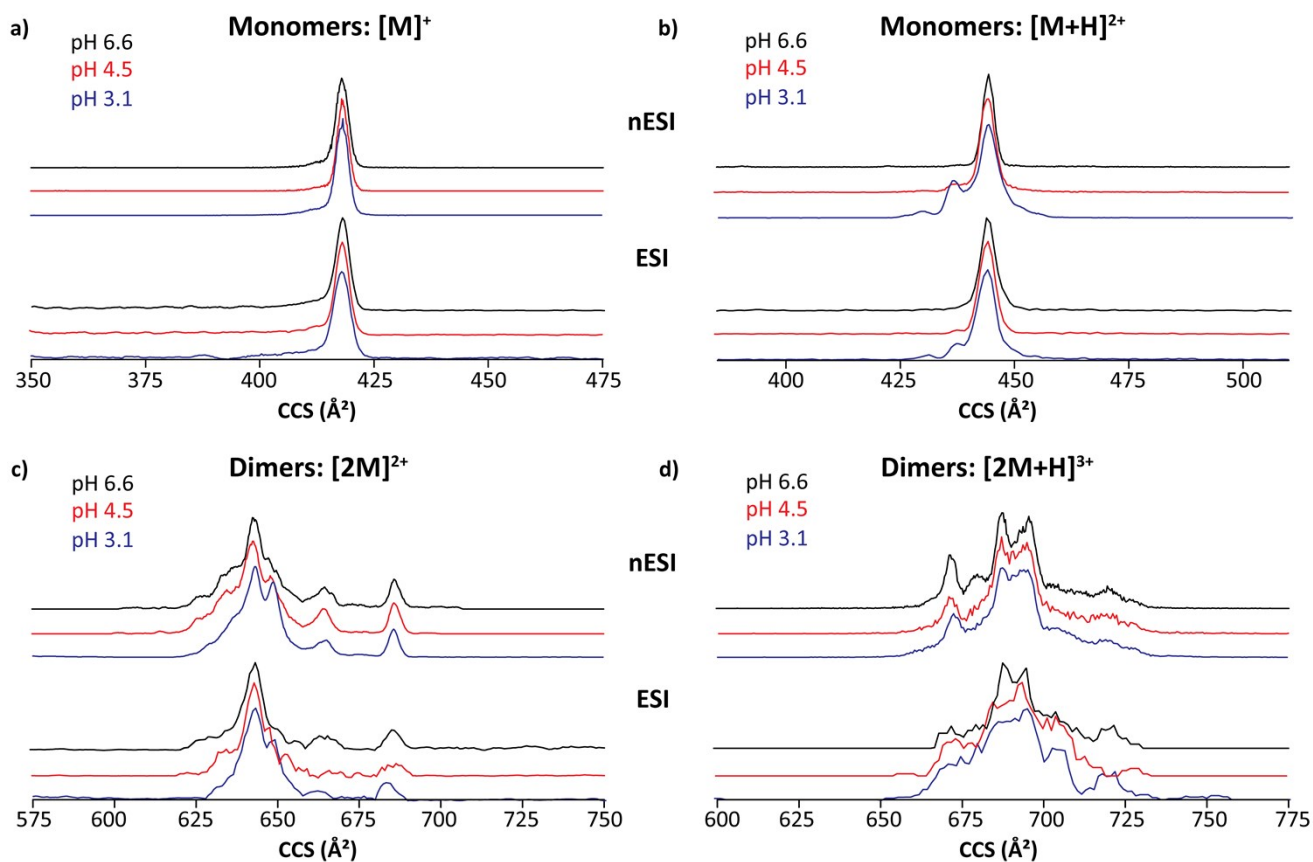
**Figure S1.** TIMS profiles of MP-11 triply-charged monomers at pH 3.1 (blue traces) as a function of (a) adducts  $[M+H+X]^{3+}$ , (b) trapping time and (c) collisional activation.



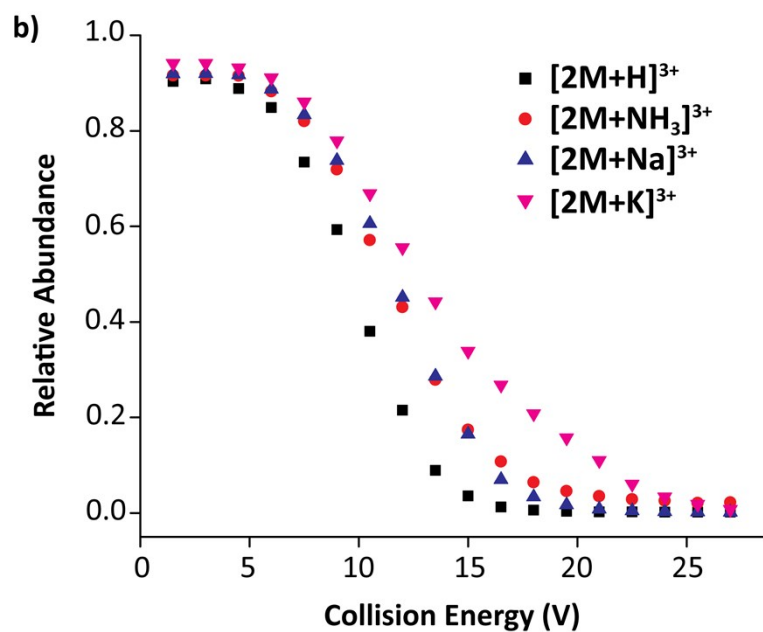
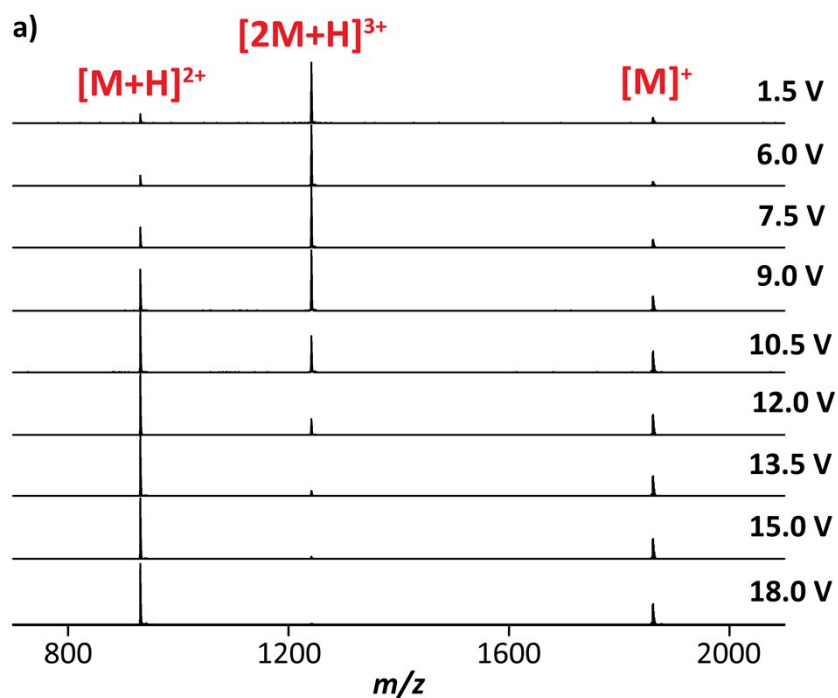
**Figure S2.** TIMS profiles of MP-11 (a)  $[M]^+$ , (b)  $[M+H]^{2+}$ , (c)  $[2M]^{2+}$  and (d)  $[2M+H]^{3+}$  ions at pH 6.6 (black traces), 4.5 (red traces) and 3.1 (blue traces) as a function of trapping time.



**Figure S3.** TIMS profiles of MP-11 (a)  $[M]^+$ , (b)  $[M+H]^{2+}$ , (c)  $[2M]^{2+}$  and (d)  $[2M+H]^{3+}$  ions at pH 6.6 (black traces), 4.5 (red traces) and 3.1 (blue traces) as a function of collisional activation.



**Figure S4.** TIMS profiles of MP-11 (a)  $[M]^+$ , (b)  $[M+H]^{2+}$ , (c)  $[2M]^{2+}$  and (d)  $[2M+H]^{3+}$  ions at pH 6.6 (black traces), 4.5 (red traces) and 3.1 (blue traces) as a function of the ionization process (nESI vs ESI).



**Figure S5.** (a) MS spectra of the  $[2M+H]^{3+}$  as a function of the collision energy and (b) plots representing the relative abundances of the  $[2M+X]^{3+}$  ions as a function of collision energy.