

Supporting Information

Top-Down Characterization of Proteins with Intact Disulfide Bonds Using Activated-Ion Electron Transfer Dissociation

Matthew J.P. Rush^{1,2}, Nicholas M. Riley^{1,2}, Michael S. Westphall¹, and Joshua J. Coon^{1,2,3,4*}

¹Genome Center of Wisconsin, Madison, WI 53706, USA

²Department of Chemistry, University of Wisconsin–Madison, Madison, WI 53706, USA

³Department of Biomolecular Chemistry, University of Wisconsin–Madison, Madison, WI 53706,
USA

⁴Morgridge Institute for Research, Madison, WI 53715, USA

* Corresponding Author: jcoon@chem.wisc.edu

Figure S1.

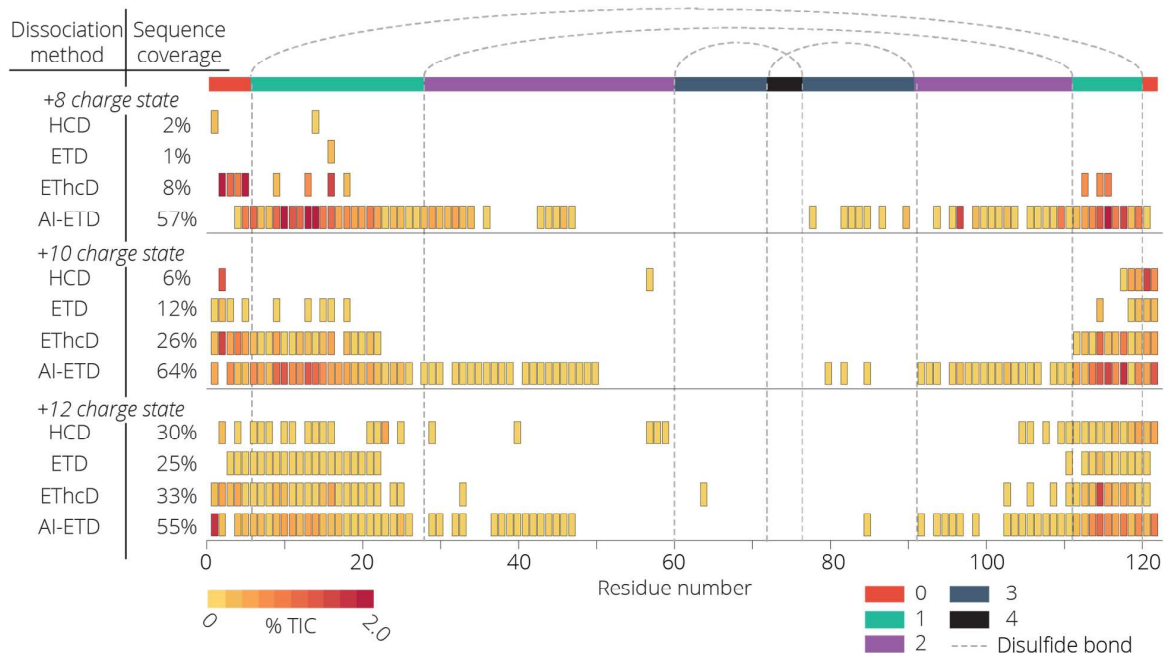


Figure S1. The sequence coverage map for α -lactalbumin precursor charge states $z = +8$, $z = +10$, and $z = +12$ is shown. The regions are codified by the number of disulfide bonds surrounding that portion of the protein backbone. The percent sequence coverage for each precursor charge state and dissociation method is shown in the table to the left.

Figure S2.

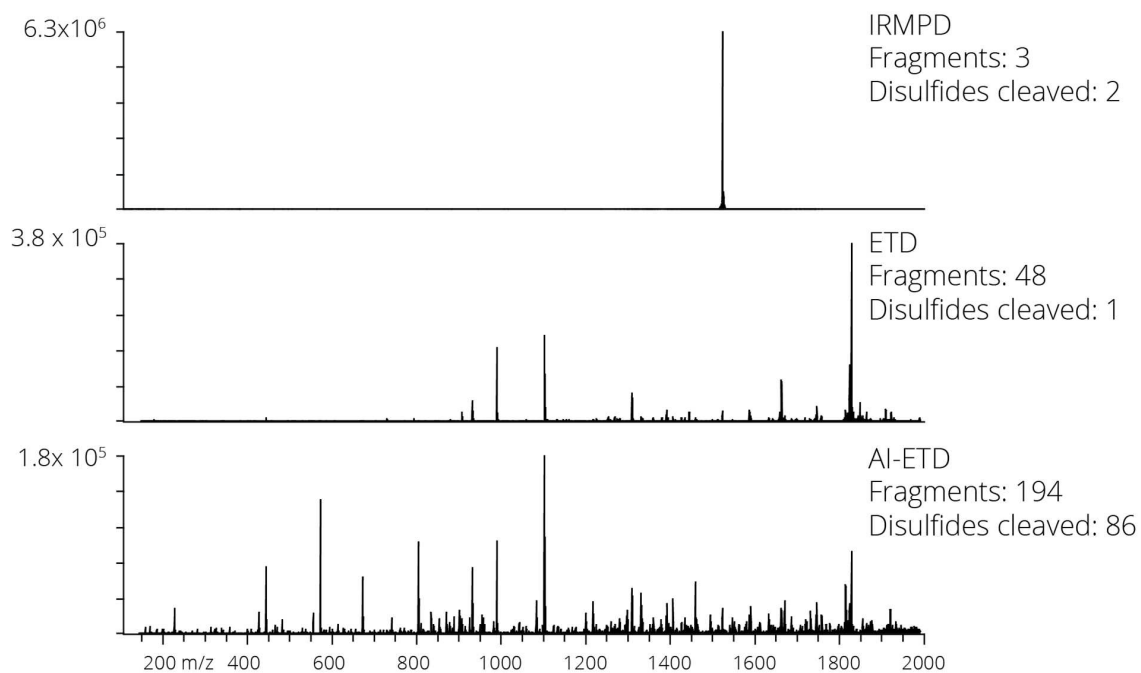


Figure S2. The IRMPD, ETD, and AI-ETD spectra for the $z=+12$ charge state of β -lactoglobulin is shown. IRMPD was performed in the high-pressure trap and the ions were irradiated at the same laser power (30 Watts) and time (35 ms) as the AI-ETD scan.

Figure S3.

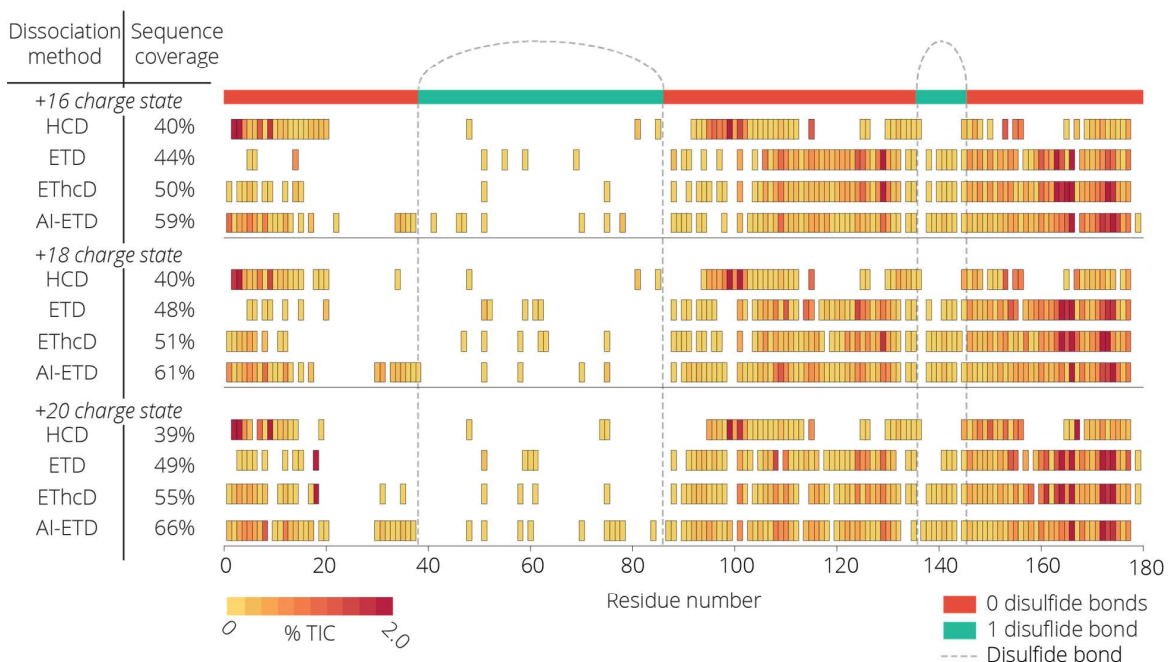


Figure S3. The sequence coverage map for trypsin inhibitor precursor charge states $z = +16$, $z = +18$, and $z = +20$ is shown. The regions are codified by the number of disulfide bonds surrounding that portion of the protein backbone. The percent sequence coverage for each precursor charge state and dissociation method is shown in the table to the left.

Figure S4.

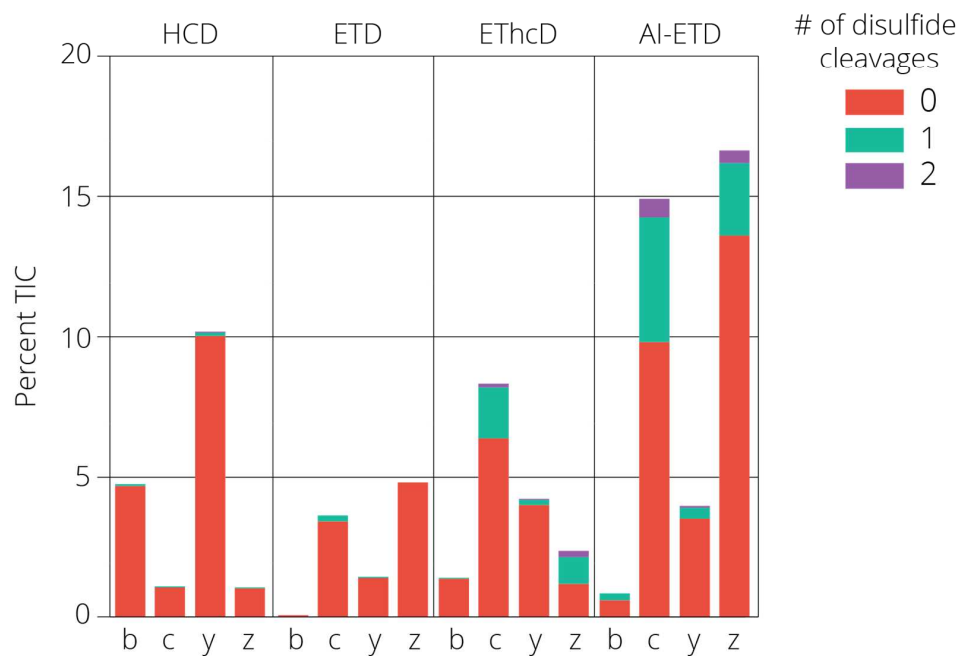


Figure S4. The intensity of fragment ions for each fragmentation method are summarized. The ions are grouped by fragment ion type and number of disulfide cleavages.