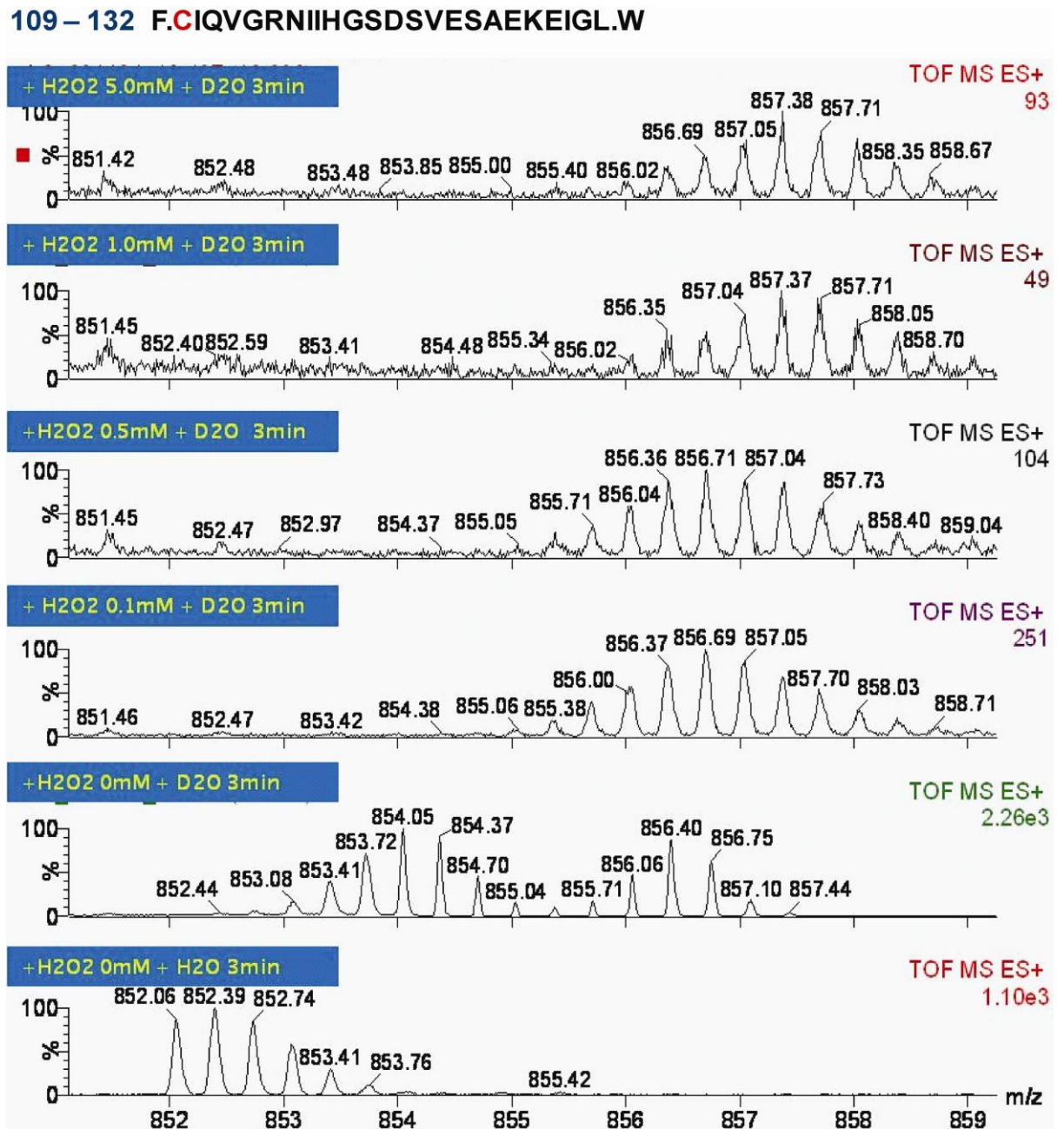
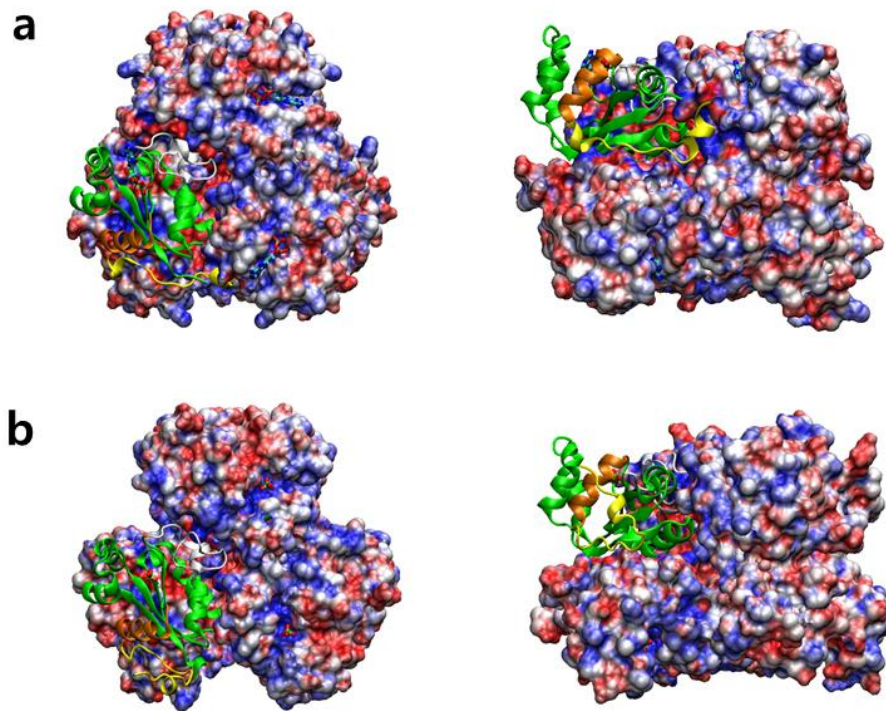


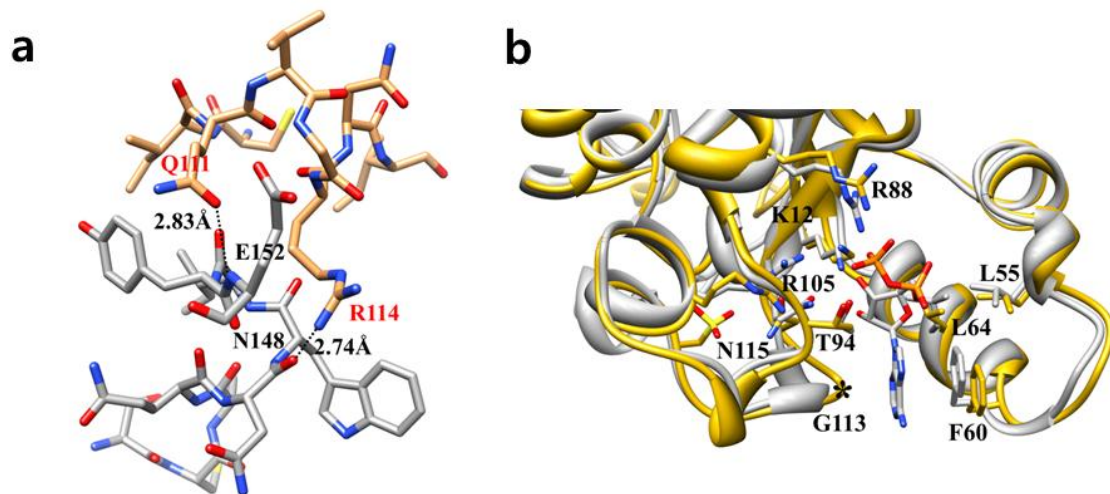
Supplementary Figure S1. HDX ratio of intact Nm23-H1 in response to H₂O₂ monitored by mass spectrometer. Artificial mass increment by protein oxidation was examined D₂O exchange with H₂O as a control.



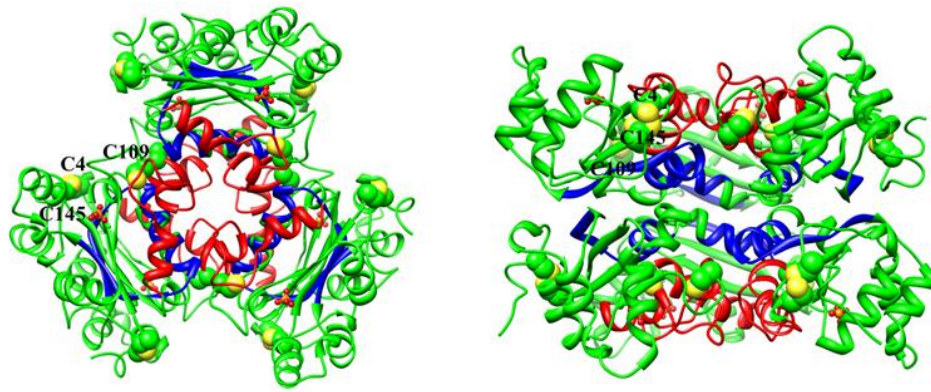
Supplementary Figure S2. HDX ratio on 109-132 residues in native and to 5 mM H₂O₂ treated Nm23-H1 was summarized.



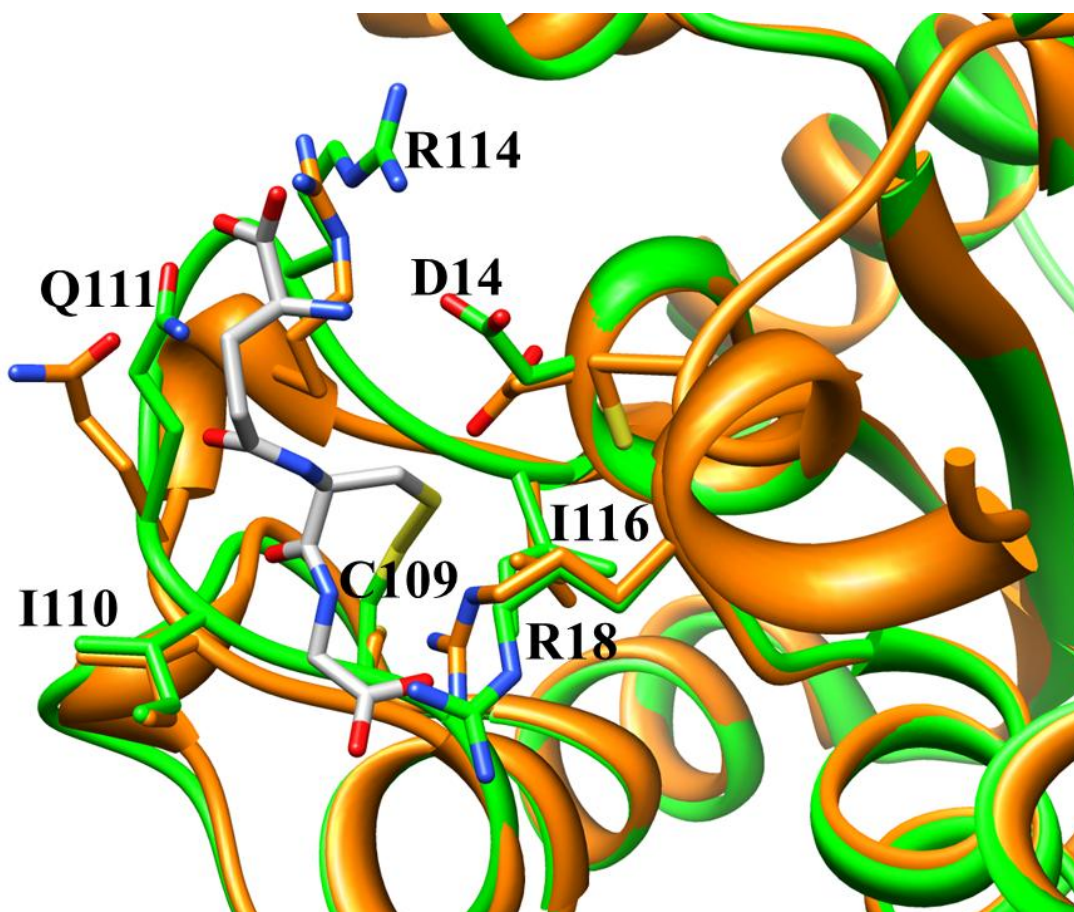
Supplementary Figure S3. Electrostatic surface potentials of Nm23-H1 (a) Oxidized Nm23-H1. Molecular surfaces were created by the VMD molecular graphics software package (Humphrey *et al.*, 1996) after electrostatic calculations using APBS (Baker *et al.*, 2001) (red, negative; blue, positive; white, uncharged). One of subunits is represented with the ribbon model colored by domain. (b) Wild type Nm23-H1. In both (a) and (b), the right figure is obtained by rotating the left through 90° along the X-axis.



Supplementary Figure S4. Diagrams of functionally important regions of Nm23-H1. (a) Interface interaction. Two hydrogen bonds between the K-pn loop region (light gray) and the C-terminal domain (tan) of another subunit in the native form. These hydrogen bonds are broken by oxidative stress. (b) Superposition of active sites. The energy minimized model of the sulfonlated form (yellow) is superposed with the ADP-bound forms (light gray; PDB ID: 2HVE). The residues interacting with ADP are represented and labeled. Gly113 is marked with “*”.



Supplementary Figure S5. Diagrams of Nm23-H1 indicating two interfaces with a large difference in HDX ratio. The blue represents dimeric interfaces and red for the K-pn loop regions. The figure on the right is obtained by rotating the left through 90° along the X-axis.



Supplementary Figure S6. The energy minimized model of glutathionylated Nm23-H1. The residues interacting with glutathione are represented and labeled. Glutathione forms a disulfide bond with Cys109. The average distances of hydrogen bonds of GSH with Arg18 and Arg114 are 2.85 Å and 2.80 Å, respectively.