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Supporting information for article:

**Monothiol and dithiol glutaredoxin-1 from *Clostridium oremlandii*:
identification of domain-swapped structures by NMR, X-ray
crystallography and HDX mass spectrometry**

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Woo, Sung-Joon Lee and Kwang Yeon Hwang**

Table S1 Melting temperature of d-cGrx1 and m-cGrx1 based on the CD absorbance at 222nm.

| | T _m (°C) | T _m error (+/−) | ΔH (kcal/mol) |
|-----------------|---------------------|----------------------------|---------------|
| Dithiol cGrx1 | 69.12 | 0.055 | 47.35 |
| Monothiol cGrx1 | 53.42 | 0.102 | 50.34 |

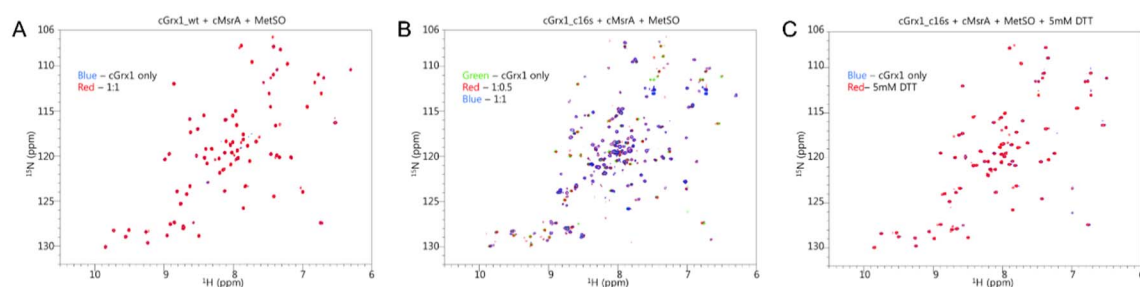


Figure S1 Comparison of 2D ^1H , ^{15}N -HSQC spectra. (a) d-cGrx1 with cMsrA and 5mM Met-O. d-cGrx1 in alone is shown as *blue* and in presence of cMsrA and 5mM Met-O is shown as *red* peaks. (b) m-cGrx1 with cMsrA and 5mM Met-O. m-cGrx1 in alone is shown as *green*, in molar ratio of 1:0.5 with cMsrA is shown as *red* and in molar ratio of 1:1 with cMsrA is shown as *blue* peaks. (c) m-cGrx1 with 5mM DTT after incubating with cMsrA and 5mM Met-O. m-cGrx1 in alone is shown as *blue*, and with 5mM DTT after incubating with cMsrA and 5mM Met-O is shown as *red* peaks.

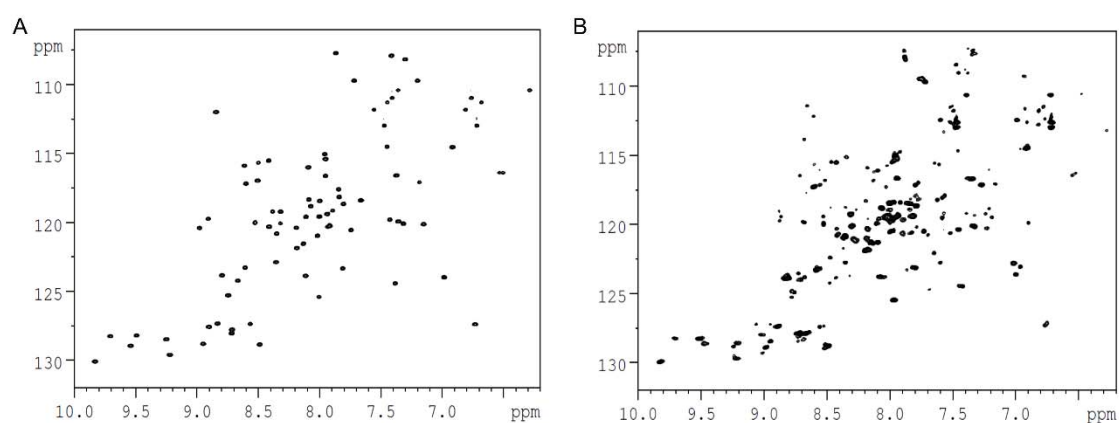


Figure S2 2D $[^1\text{H}, ^{15}\text{N}]$ -HSQC spectra of m-cGrx1 and d-cGrx1 with 5mM oxidized Glutathione (GSSG). (a) 2D $[^1\text{H}, ^{15}\text{N}]$ -HSQC spectra of d-cGrx1 with 5mM GSSG. (b) 2D $[^1\text{H}, ^{15}\text{N}]$ -HSQC spectra of m-cGrx1 with 5mM GSSG.

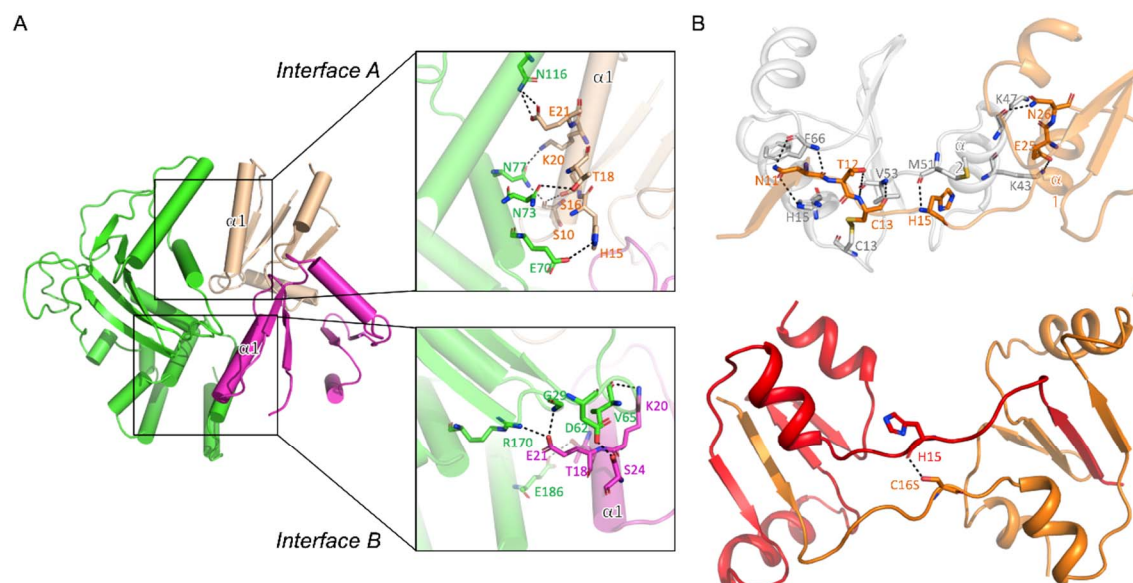
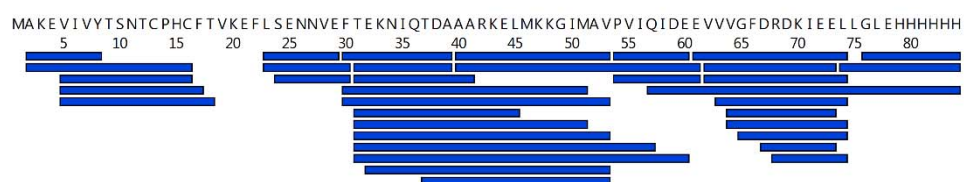


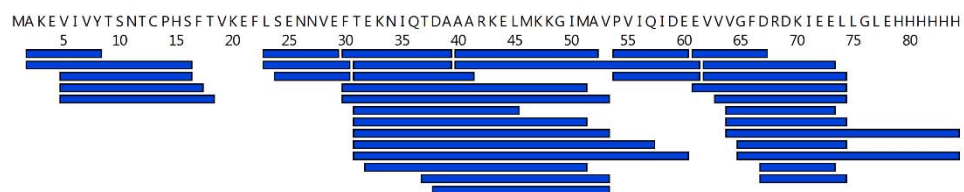
Figure S3 (a) Close view of interfaces between m-cGrx1 and cMsrA. *Interface A* and *Interface B* indicate the interface between disulfide dimeric m-cGrx1 and cMsrA, domain-swapping m-cGrx1 and cMsrA, respectively. The hydrogen bonds are shown as dash line. (b) Interactions of subunits of β 1-swap. Interactions between disulfide dimeric m-cGrx1 (grey) and hinge loop of domain-swapping m-cGrx1 (orange). Interaction between each hinge loop of domain-swapped dimer. The hydrogen bonds are shown as dash line.

d-cGrx1



Total: 36 Peptides, 94.0% Coverage, 6.44 Redundancy

m-cGrx1(C16S)



Total: 37 Peptides, 94.0% Coverage, 6.62 Redundancy

Figure S4 Sequence coverage of cGrx1. The peptides of cGrx1 obtained via peptide digestion and LC-IMS/MS analysis was shown as blue bars along the sequence.

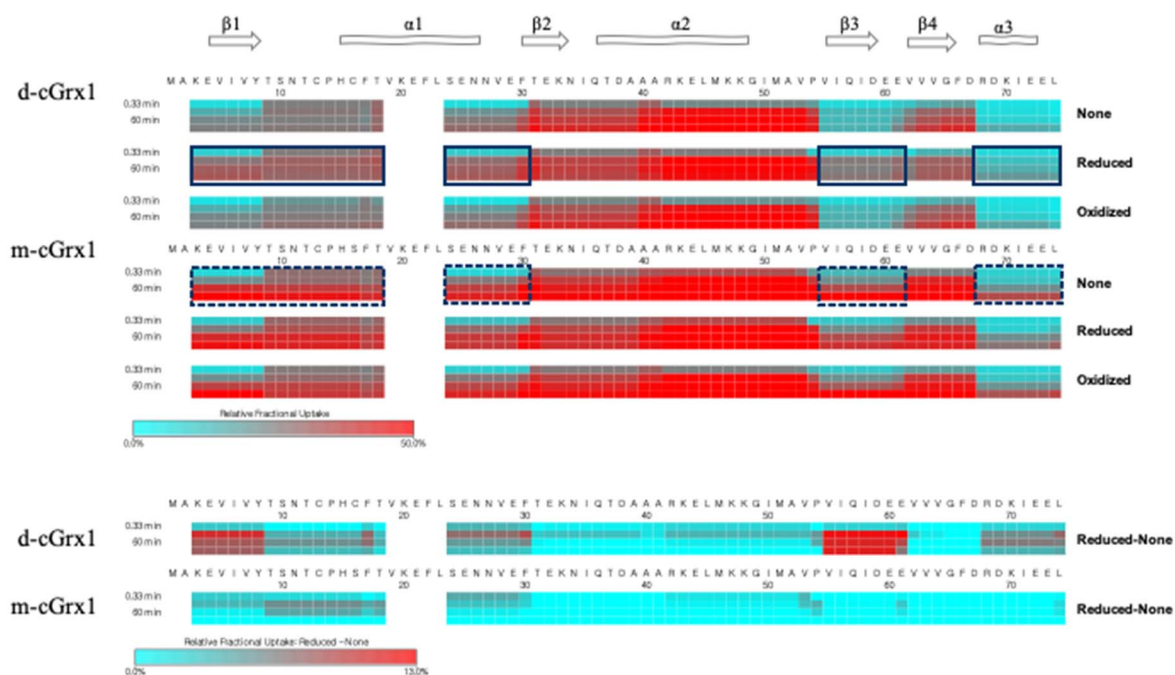


Figure S5 Heat maps of differential deuterium uptake for d- and m-cGrx1. The differential deuterium uptake, observed in the presence of TCEP of d-cGrx, is shown as bold box. The differential deuterium uptake between d-cGrx and m-cGrx1 is shown as dashed box.

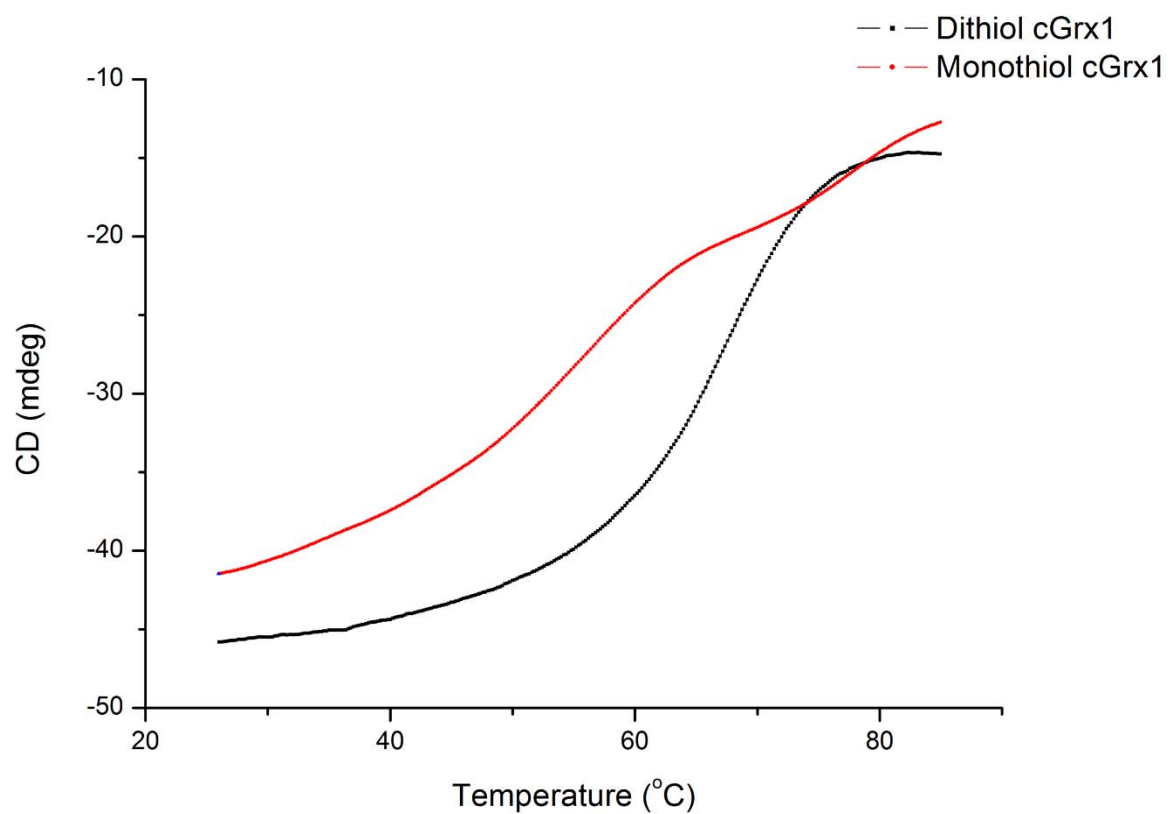


Figure S6 Thermal stability of cGrx1s monitored by CD spectroscopy. Thermal stability of d-cGrx1 (black) and m-cGrx1(red).