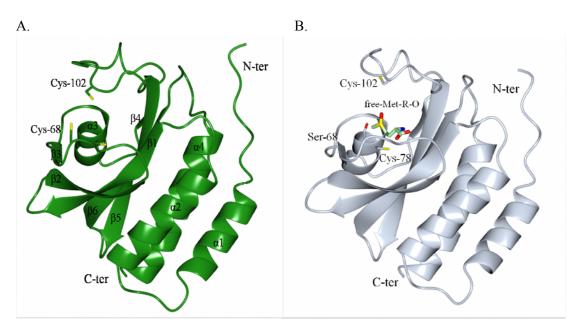
## **Supplementary Figures**

Figure S1

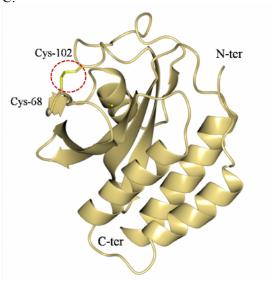
				α1		α2		
			202			000000000000000000000000000000000000000		
		ļ	10		20 30	40		
S.aureus		MITINPI	YTL	LKKQAAS	LIEDEHHMIAIL	SNMSALLNDNLL	42	
E.coli	MSLLILIGW	QIQVRQPSI	YIMNKTER	YADLNRDFNA	LMAGETSFLATL	ANTSALLYERLT	60	
Saccharomyces	MGSSTGF	HADHVNYS	SNLNKEEI	LEQLLLSYEG	LSDGQVNWVCNL	SNASSLIWHAYR	58	
		β1	β2	<b>B</b> 3	α3	<b>B4</b>		
		→	· <u> </u>	+ ∸i	000000000	→		
		50	60	7 <b>0</b>	80	90		
S.aureus	QINWVO	FYLLE	QNELILGP	FQGHPACVHI	PIGKGVCGTAVSE	RRIQVVADVHQ	95	
E.coli	DINWAG	FYLLE	DDTLVLGP	FQGKIACVRI	PVGRGVCGTAVAR	NQVQRIEDVHV	113	
Saccharomyces	SLAVDINWAG	FYVIQASE	ENTLILGP	FQGKVACQMI	QFGKGVCGTAASI	KEIQIVPDVNK	118	
		85	β5 <u>β6</u>			al		
		p			00000000	00000000000		
	100	110	L20	130	140	150		
S.aureus	FKGHIACDAL	SKSEIVVE	IFKDD-KI	IGVLDIDAPI	TORFDDNDKEHLE	AIVKIIEKQLA	154	
E.coli	FDGHIACDA	SNSEIVLE	LVVKN-QI	IGVLDIDSTV	FGRFTDEDEQGLE	QLVAQLEKVLA	172	
Saccharomyces	YPGHIACDG	TKSEIVVE	IISNDGKT	LGVIDIDCLD	YEGFDHVDKEFLE	KLAKLINKSCV	178	
S.aureus								
E.coli	TTDYKKFF7	SVAGEGGS	189					
Saccharomyces	FK		180					

**Figure S1**. Multiple sequence alignment of fRMsrs. Sequences of *E. coli*, *S. cerevisiae* and *S. aureus* fRMsrs were aligned with BioEdit (http://www.mbio.ncsu.edu/BioEdit/bioedit.html). Catalytic Cys-102 is highlighted in red, resolving Cys-68 in blue and conserved Cys-78 in green. Secondary  $\alpha$ -helices and  $\beta$ -strands determined from *S. aureus* fRMsr are indicated.



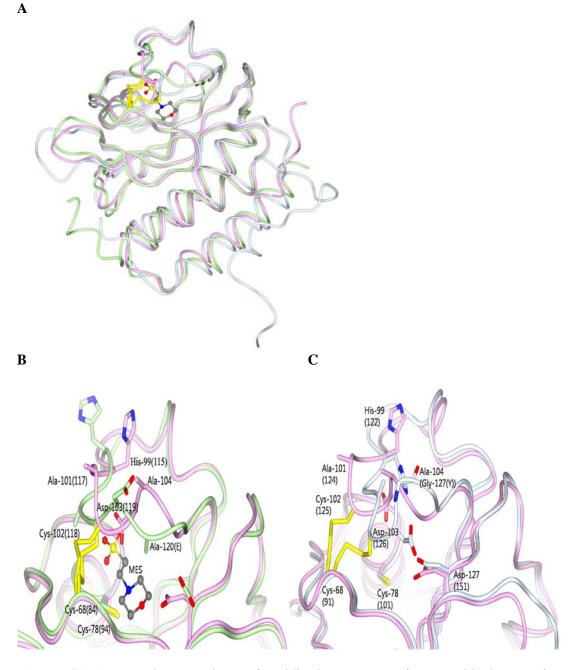


С.



**Figure S2**. Structures of *S. aureus* fRMsrs. (A) Reduced form (fRMsr<sub>red</sub>). The overall structure of fRMsr<sub>red</sub> is composed of six antiparallel  $\beta$ -strands ( $\beta$ 1- $\beta$ 6) and four  $\alpha$ -helices ( $\alpha$ 1- $\alpha$ 4). (B) Substratebound form (fRMsr<sub>sub</sub>). The substrate free Met-R-O in C68S fRMsr is indicated by a green stick model. (C) Oxidized form (fRMsr<sub>ox</sub>). A disulfide bond formed by Cys-68 and Cys-102 is shown in red dotted circle.





**Figure S3.** Structural comparison of oxidized *S. aureus* fRMsr with known fRMsrs. (A) Comparison of overall structures. The backbone models for *S. aureus, E. coli*, and *S. cerevisiae* are shown in light purple, light green and light cyan, respectively. Disulfide bonds between Cys-68 and Cys-102 are represented by yellow sticks. MES in *E. coli* fRMsr is shown by a stick model. (B) Comparison of active sites between *S. aureus* (light purple) and *E. coli* (light green) fRMsrs. Disulfide bonds are represented by yellow sticks and MES in *E. coli* fRMsr is shown by a stick model. Numbers in parenthesis represents the corresponding amino acid number of *E. coli* fRMsr. Ala-120 is from *E. coli*. (C) Comparison of active sites between *S. aureus* (light purple) and *S. cerevisiae* (light cyan) fRMsrs. Disulfide bonds are represented by yellow sticks. Number of *E. coli* fRMsr. Ala-120 is from *E. coli*. (C) Comparison of active sites between *S. aureus* (light purple) and *S. cerevisiae* (light cyan) fRMsrs. Disulfide bonds are represented by yellow sticks. Number in parenthesis represents the corresponding amino acid number of *S. cerevisiae* fRMsr. Gly-127 is from *S. cerevisiae*.