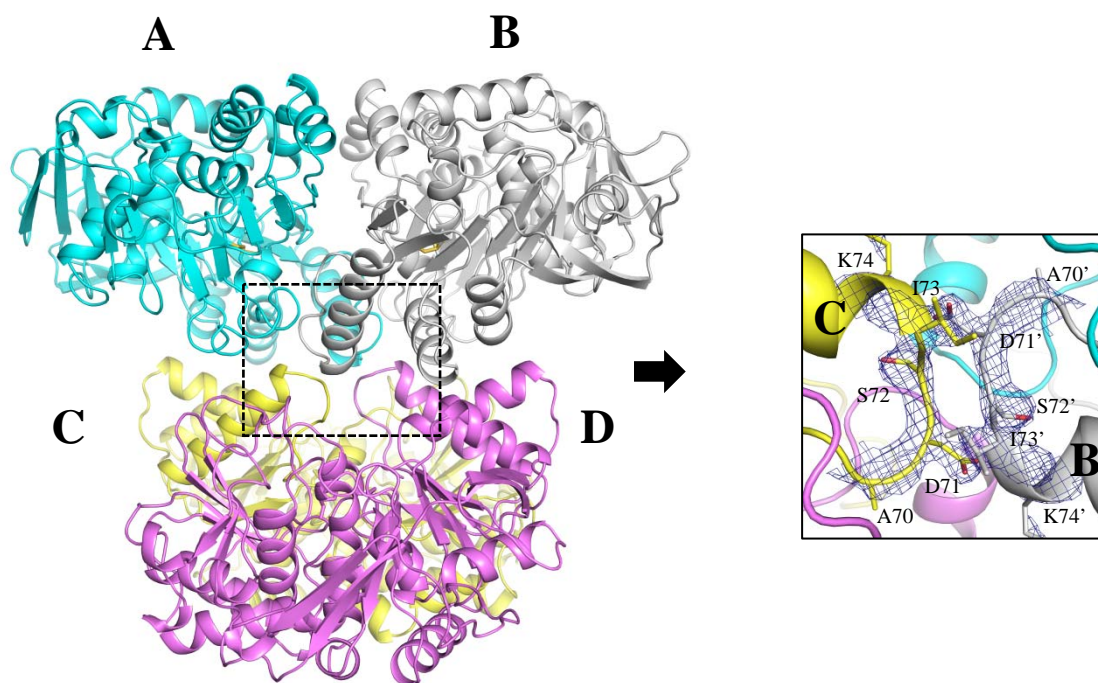
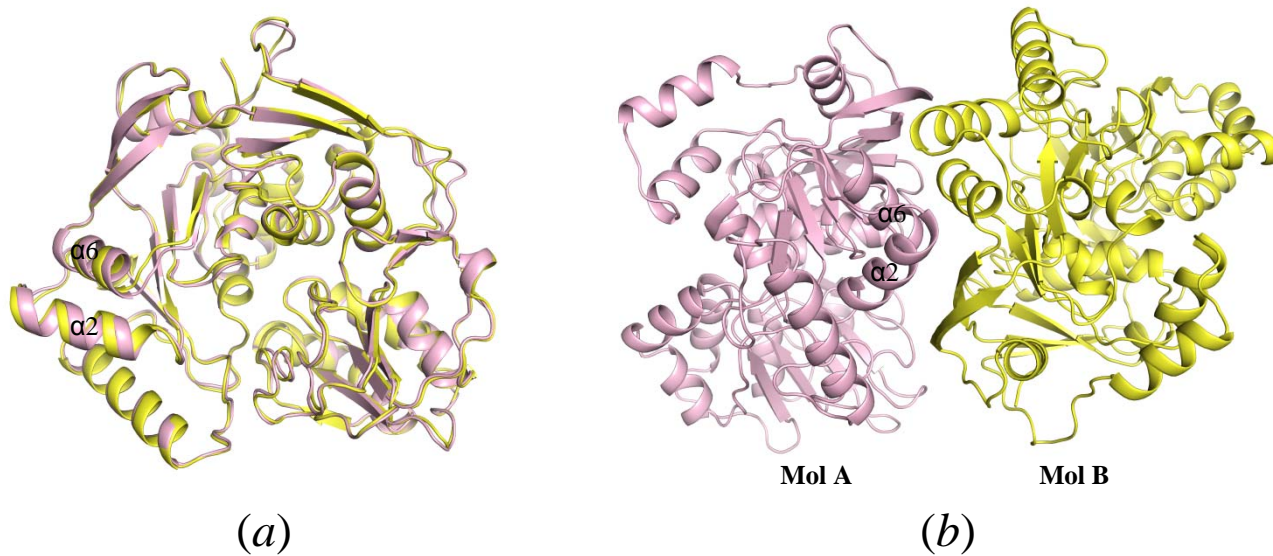


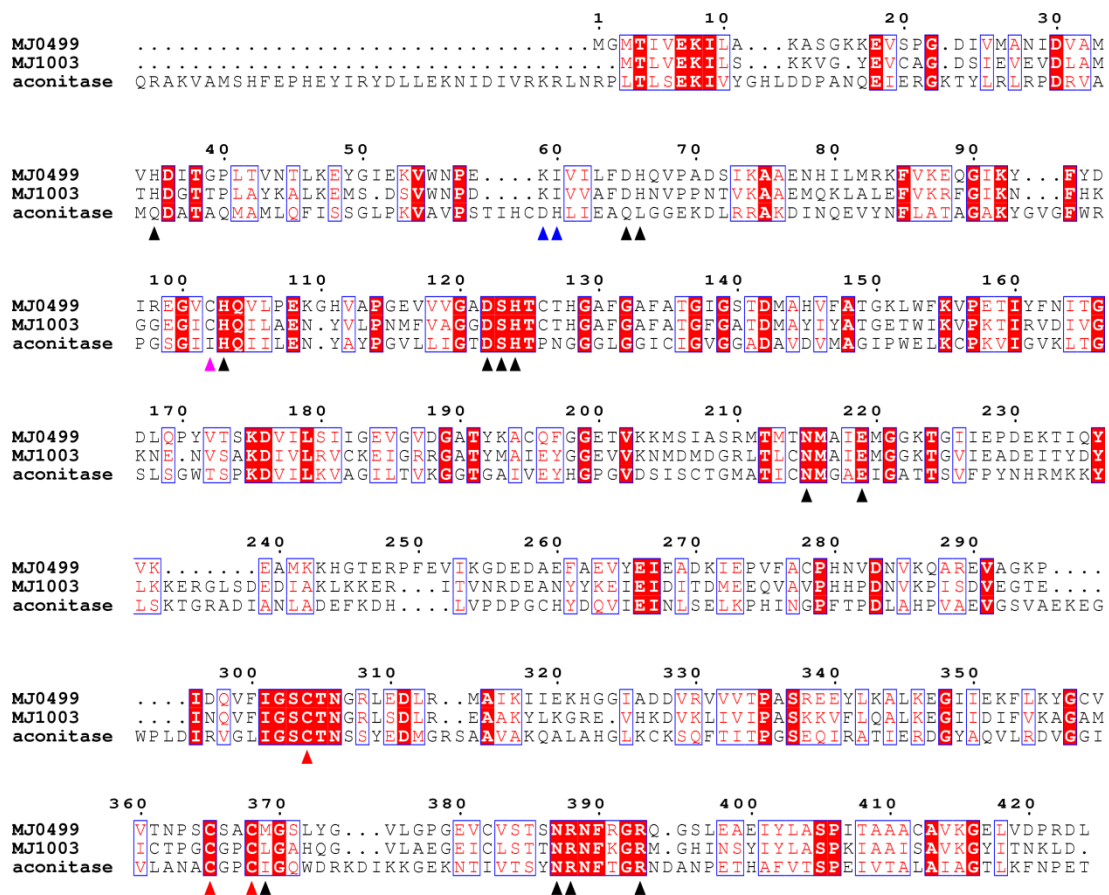
Supporting Figures



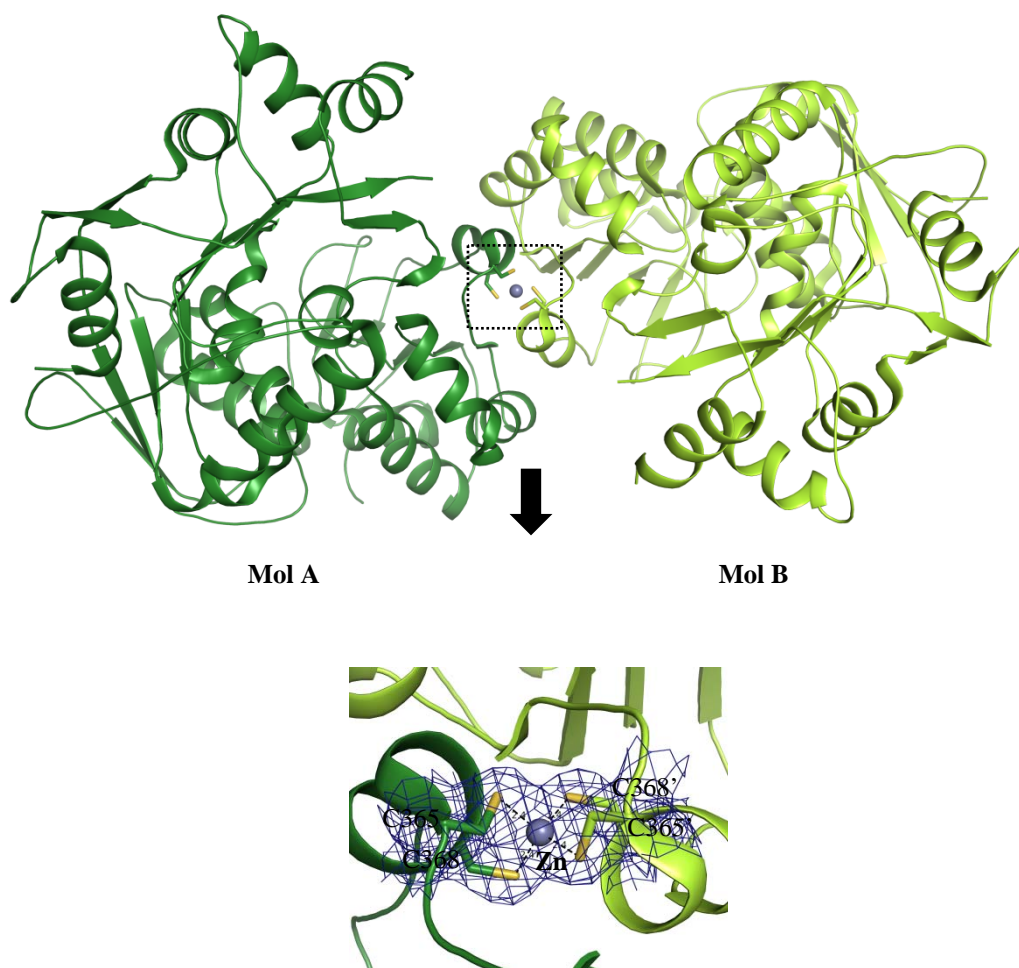
Supporting Figure S1 Crystal packing of ox-MJ0499. The 4 molecules of ox-MJ0499 show close contact in the crystal and form 2 homodimers (AB and CD). The molecules B and C shows close contact, as represented in the box on the right, the 2fo-fc map of A70 to K74 contoured at 1.5 σ . The electron density of D71 side chain is not clearly distinguished from the neighboring I73' residue.



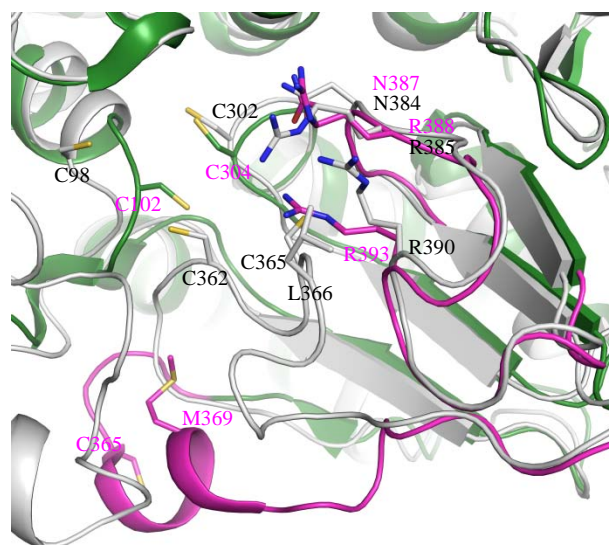
Supporting Figure S2 (a) Asymmetric unit of MJ1003. The 2 molecules of MJ1003 in an asymmetric unit are superposed upon each other. The helices $\alpha 2$ and $\alpha 6$ show structural differences. (b) Crystallographic dimer observed in an asymmetric unit. The 2 chains of MJ1003, MolA and MolB, form a crystallographic dimer and $\alpha 2$ and $\alpha 6$ helices contribute to dimer interaction.



Supporting Figure S3 Multiple sequence alignment of aconitase family proteins. MJ0499 and MJ1003 from *Methanococcus jannaschii*, and mitochondrial aconitase from *Sus scrofa* (PDB entry 5acn). The conserved residues are shaded red and similar residues are displayed in red letters. Residues of active site residues are indicated by black triangles below the aligned sequence and three cysteine residues involved in iron-sulfur cluster binding are indicated by red triangles. The fourth cysteine residue is indicated by a pink triangle. The two residues in aconitase indicated by blue triangles, D100 and H101, align only in the conserved sequences.



Supporting Figure S4 Molecular interaction in the crystal of red-MJ0499. The C365 and C368 residues coordinate an zinc ion (Zn) with the two symmetrical Cys residues from the other molecule. The average distance of zinc ion coordination is 2.4 Å. The interface is shown magnified in the square box and the 2fo-fc map is shown at 1.5 σ cut-off.



Supporting Figure S5 The active site comparison of red-MJ0499 (green) and MJ1003 (gray). The regions showing conformational change upon reduction are indicated in red-MJ0499 in magenta color. The active site residues are represented as stick models and residues are labeled in different colors, magenta for red-MJ0499 and black for MJ1003.

LEUC_YEAST	94	LQVK	TLEN	NV	KQFGV	PYFGMSDAR	QGI	VHTIG	PEE	GFTLP	PGT	TVV	CGDSH
LEUC_SCHPO	93	TQVL	ALENN	IKEFGL	TYYGMNDRR	QGI	VHVI	GPEQG	FFTLP	PGT	TLV	CGDSH	
LEUC_ECOLI	81	IQM	ELIK	NCKEFGV	ELYDLNHPY	QGI	VHVM	GPEQG	VFTLP	PGM	TIV	CGDSH	
LEUC_BACSU	81	RQVT	ALER	NCEEF	GVRLADLHSVD	QGI	VHVG	PELGL	TLP	GKTIV	CGDSH		
LEUC_CORGB	97	LQVS	TLRD	NCEEF	GVRLHMPGDVR	QGI	VHTV	GPEL	GATQ	PGMTIV	CGDSH		
LEUC_MYCTU	88	TQVE	TLRR	NCAEF	GI RLHSMGDIE	QGI	VHVG	PELGL	TQ	PGMTIV	CGDSH		
LEUC_METJA	79	. . HI	LMRK	FVKEQGI	KYF . . YDIRE	GV	CHQVL	PEK	GHVAP	GEVVV	GADSH		

(a)

LYS4_YEAST	108	KKHH	ID . HYP	AGRGI	GHQIMIEE	GYAF	PLN	MTVAS	DSHS	NTY	GG	LGS	LGT
LYS4_CANAL	106	KSQG	ID . FYP	AGRGI	GHQIMIEE	GYAF	PLN	LTVAS	DSHS	NTY	GG	IG	LGT
LYS4_ASHGO	106	AQQGV	D . FYP	ARRGI	GHQIMVEE	GYAF	PLG	LTVAS	DSHS	NTY	GG	VG	LGT
LYS4_SCHPO	148	KQGG	ID . FYP	AGRGI	GHQIMVEE	GYAM	PGS	MAVAS	DSHS	NTY	GG	VG	LGT
LYS4_ASPNC	150	KQHGV	E . FYP	AGRGI	GHQIMVEE	GFAW	PGT	LVVAS	DSHS	NTY	G	AVAS	VG
LYS4_USTMA	125	RKHG	ID . FYP	AGRGI	GHQVLVEE	GYAF	PQT	LAVAS	DSHS	NMY	GG	VG	LGT
HACA_METJA	83	KRFG	IKNFHK	GGEGI	CHQILAEN	. YVL	PNM	FVAGG	DSHT	CTH	GA	FGA	FAT

(b)

Supporting Figure S6 (a) Multiple sequence alignments of IPM isomerases. The partial sequence alignments are represented and the fourth cysteine is indicated by a red triangle. LEUC_YEAST, 3-isopropylmalate dehydratase from *Saccharomyces cerevisiae*; LEUC_SCHPO, 3-isopropylmalate dehydratase from *Schizosaccharomyces pombe*; LEUC_ECOLI, 3-isopropylmalate dehydratase large subunit from *Escherichia coli*; LEUC_BACSU, 3-isopropylmalate dehydratase large subunit from *Bacillus subtilis*; LEUC_CORGB, 3-isopropylmalate dehydratase large subunit from *Corynebacterium glutamicum*; LEUC_MYCTU, 3-isopropylmalate dehydratase large subunit from *Mycobacterium tuberculosis*; LEUC_METJA (MJ0499), Isopropylmalate/citramalate isomerase large subunit from *Methanococcus jannaschii*. (b) Multiple sequence alignments of homoaconitases. The partial sequence alignments are represented and the fourth cysteine is indicated by a red triangle. LYS4_YEAST, homoaconitase from *Saccharomyces cerevisiae*; LYS4_CANAL, homoaconitase from *Candida albicans*; LYS4_ASHGO, homoaconitase from *Ashbya gossypii*; LYS4_SCHPO, homoaconitase from *Schizosaccharomyces pombe*; LYS4_ASPNC, homoaconitase from *Aspergillus niger*; LYS4_USTMA, homoaconitase from *Ustilago maydis*; HACA_METJA (MJ1003), Homoaconitase large subunit from *Methanocaldococcus jannaschii*.