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Supplemental information

Oxygenolytic sulfoquinovose degradation by an iron-dependent alkanesulfonate dioxygenase

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Supporting information

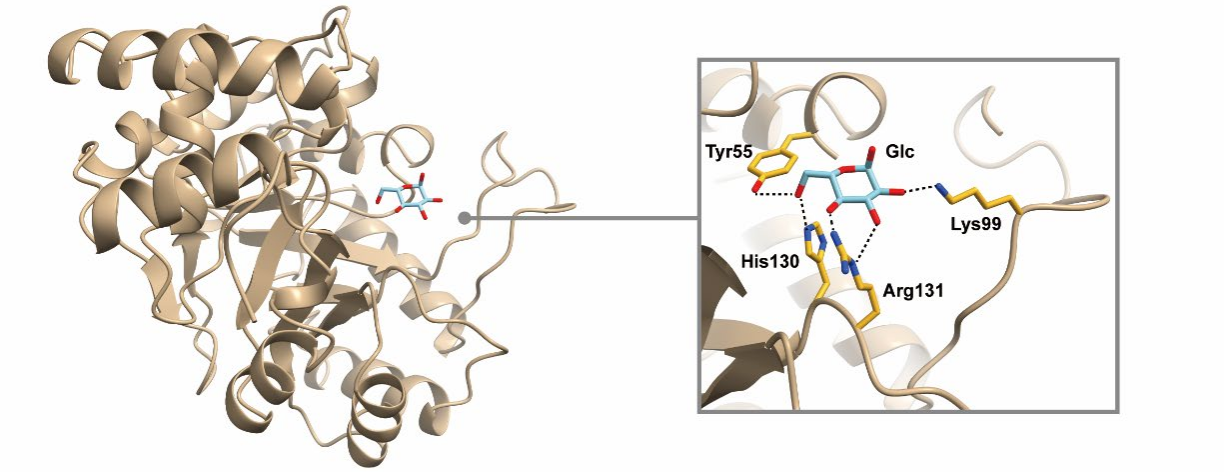

Figure S1. Related to Figure 4.

AlphaFold model of the active site of SquF (UniProt A0A1A9EZ66). The position of the substrate glucose was estimated by overlaying with the crystal structure of *Agrobacterium tumefaciens* glucose-6-dehydrogenase (PDB 7BC1)**.**

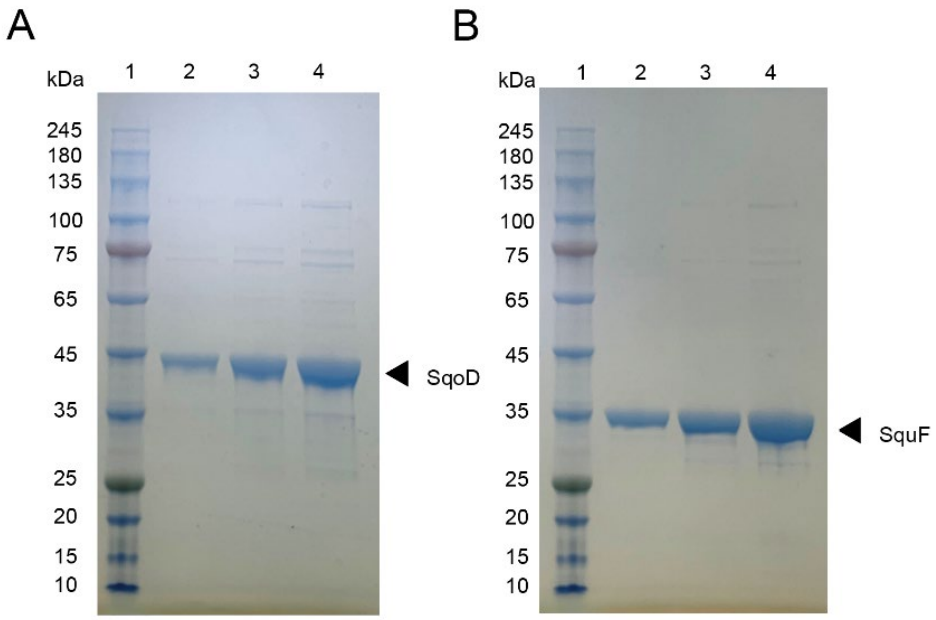

Figure S2. Related to Figure 1.

SDS-PAGE gels. (A) SDS polyacrylamide gradient gel (8-16%) with: lane 1, protein molecular weight marker (Genstar, Shenzhen); and lane 2-4: 1, 2, 4 μg of the purified protein *Ma*SqoD. (B) SDS polyacrylamide gradient gel (8-16%) with: lane 1, protein molecular weight marker; and lane 2-4: 1, 2, 4 μg of the purified protein *Ma*SquF.

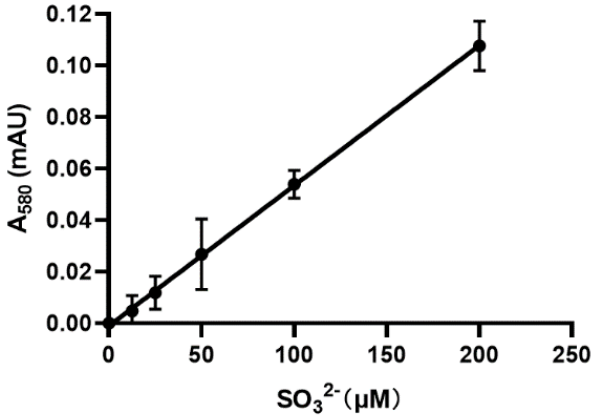

Figure S3. Related to Figure 2 and Figure 5.

Standard curve of sulfite. Serial dilutions of sodium sulfite (200, 100, 50, 25, 12.5, 0 μM) were used to establish a standard curve as a reference. Data are represented as mean +/- SD.

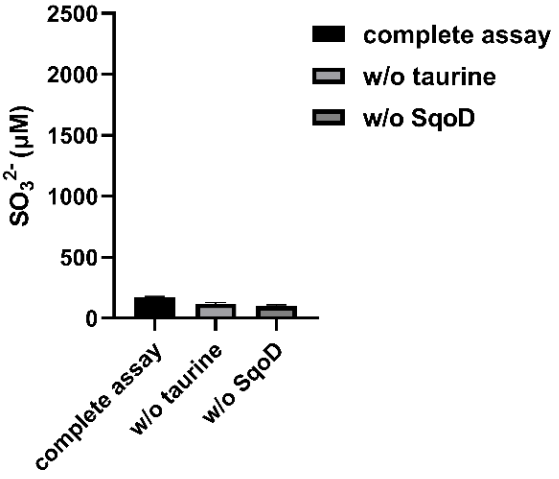

Figure S4. Related to Figure 2.

Detection of sulfite formation in the *Ma*SqoD-catalyzed taurine cleavage by a colorimetric Fuchsin assay. No sulfite release was detected when SQ was replaced with taurine as the sulfonate substrate. Data are represented as mean +/- SD.

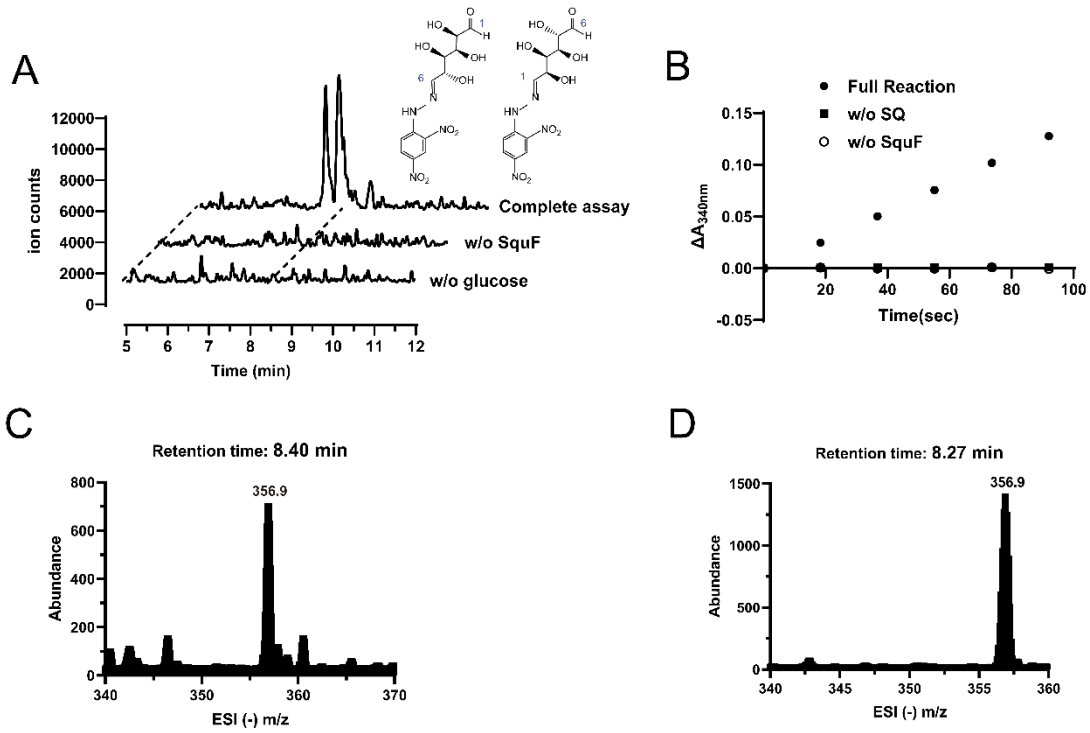

Figure S5. Related to Figure 3.

Glucose-6-dehydrogenase assays of purified *Ma*SquF. (A) Extracted ion chromatograms (m/z (-) 356.9, the predicted mass of DNPH-6-dehydroglucose monoanion) of the DNPH derivatized products of the *Ma*SquF reaction. (B) Spectrophotometric activity assay monitoring NADPH formation accompanying glucose oxidation by *Ma*SquF. (C-D) ESI (−) m/z spectrum of the DNPH-6-dehydroglucose peaks in (A).

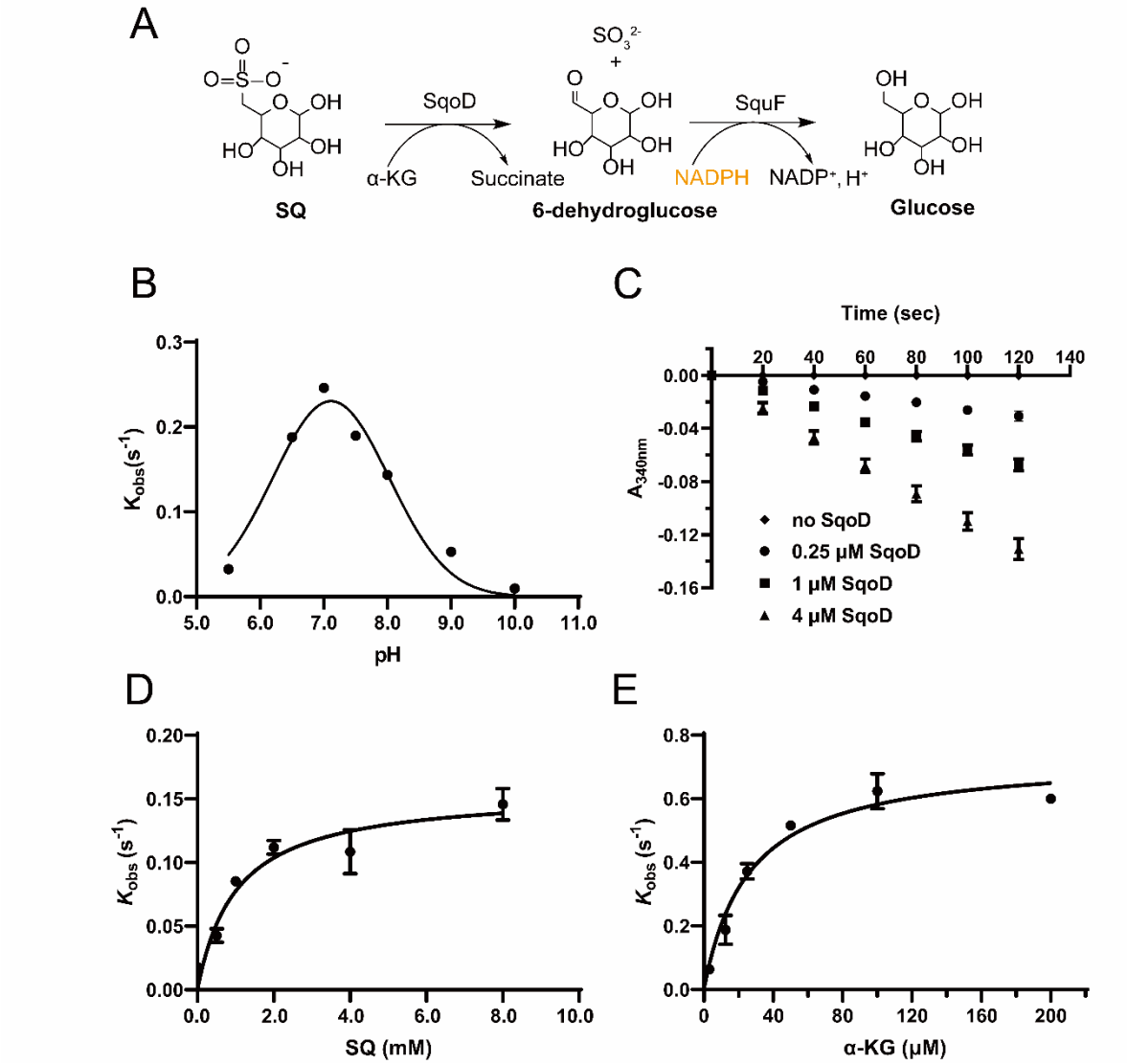

Figure S6. Related to Figure 1.

SquF-coupled enzyme activity assays for SqoD. (A) The mechanism for SquF-coupled enzyme activity assay. (B) pH-dependence of the SqoD-catalyzed reaction. (C) SqoD dose-dependent assays. (D-E) Michaelis-Menten plot for SQ or αKG as the substrate. The error bars represent the standard deviation of three individual experiments. Data are represented as mean +/- SD.

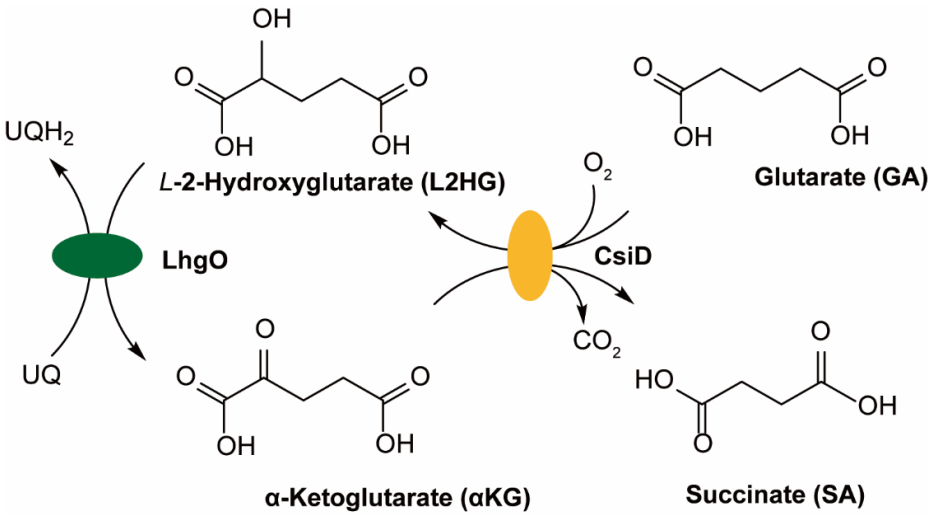

Figure S7. Related to Figure 1.

The Fe/αKG-dependent dioxygenase (CsiD) in *E. coli* lysine degradation

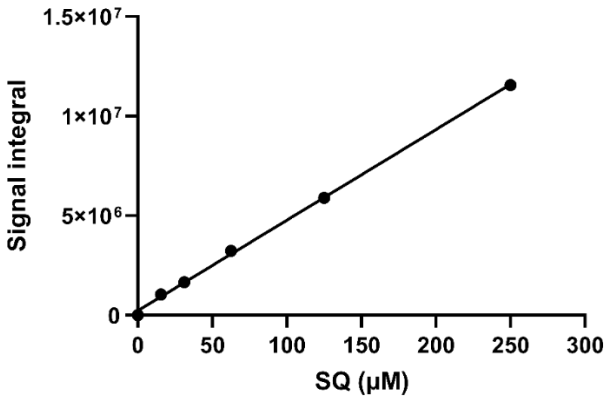

Figure S8. Related to Figure 5.

The standard curve of SQ by LC-MS. Serial dilutions of SQ (250, 125, 62.5, 31.2, 15.6, 0 μM) were used to establish a standard curve as a reference. The standard curve was established by integrals of the EIC peaks.

Table S1. Related to Figure 1.

The Pfam codes and information for the relevant genes in the text.

Pfam code	Protein	Organism	Locus tag	UniProt	PDB
PF00296	SquD/SmoC	*Agrobacterium tumefaciens*	Atu3279	A9CEY7	/
PF00248	SquF/SmoB	*Agrobacterium tumefaciens*	Atu3278	A9CEY6	7BC1
		Marinobacterium aestuarii	A8C75_10870	A0A1A9EZ66	/
PF02668	TauD	*Escherichia coli*	JW0360	P37610	1OS7
	SqoD	*Marinobacterium aestuarii*	A8C75_10885	A0A1A9EZ58	/

Table S2. Related to Figure 5.

Primers used for qPCR experiments.

Primer name	Primer sequence 5'-3'
F-Mu-TauD	GTTTTATTCCGCGGATTCCCTG
R-Mu-TauD	GTCACTTGTGTTCTTGGTGCTG
F-Mu-SquF	GCGCTTGTTGCAATCTCACA
R-Mu-SquF	AATCCGTCTAGCTGTATCGCTG
F-16S rRNA	CAATGGCGTATACAAAGGGCTG
R-16S rRNA	CCACGATTACTAGCGATTCCGA