SUPPLEMENTARY INFORMATION

Suppression of fecal phenol production by oral supplementation of sesamol: Inhibition of tyrosine phenol-lyase by sesamol

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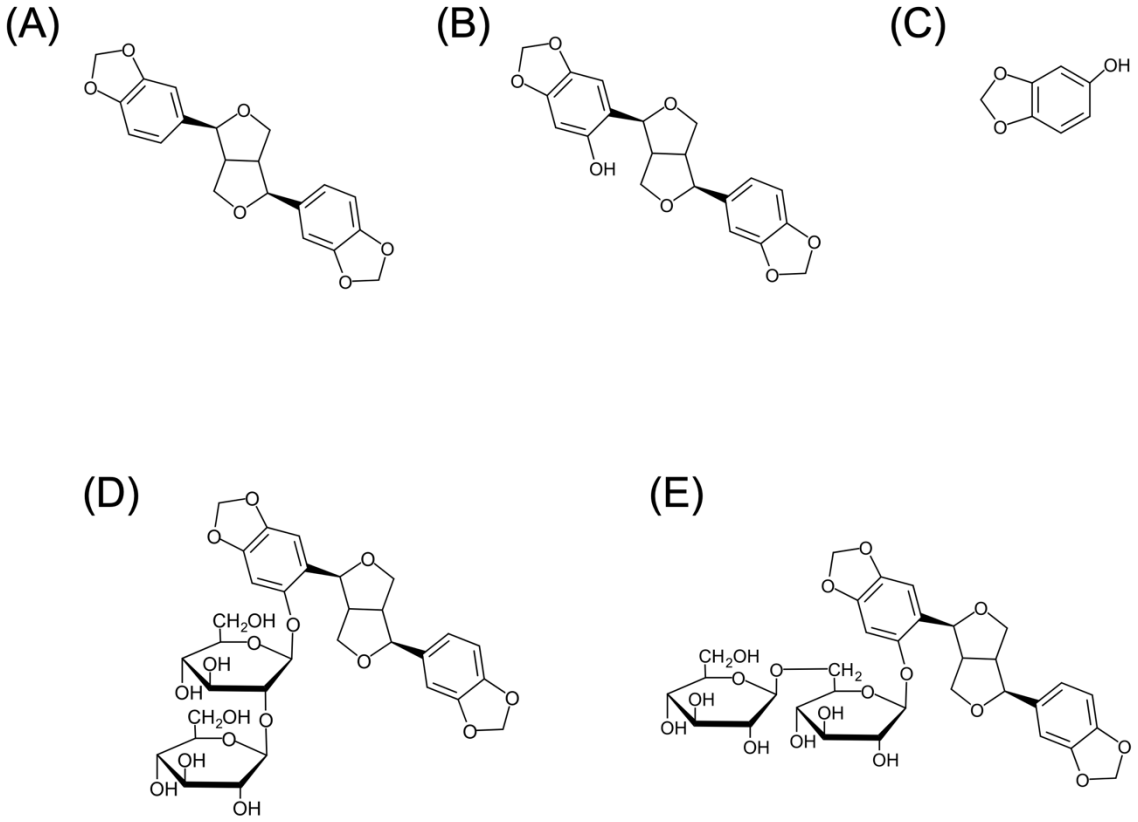
Abbreviations

PLP, pyridoxal 5′-phosphate; TPL, tyrosine phenol-lyase

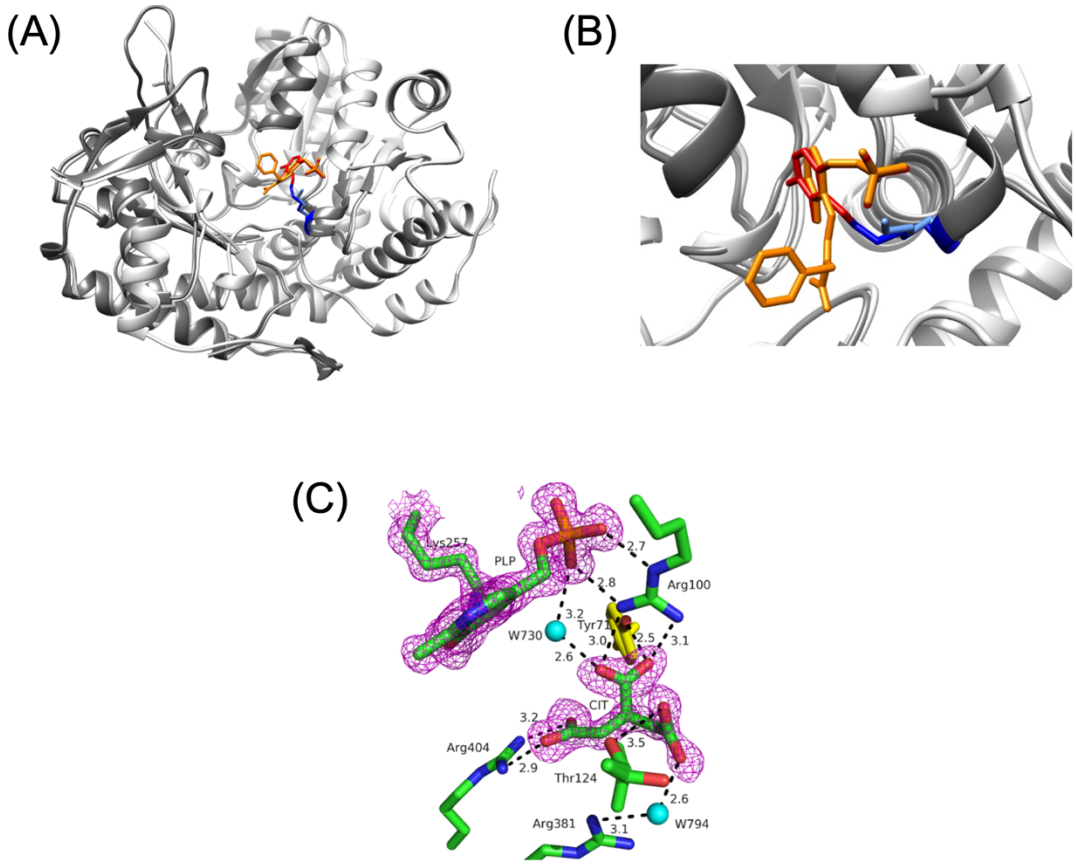
Supplementary Table S1. Bacterial species used in this study[a]

Family	Species	TPL homologue (Accession No.)
Clostridiaceae	*Clostridium cochlearium*	WP_095178356
Enterobacteriaceae	*Citrobacter freundii*	WP_136397520
Enterobacteriaceae	*Citrobacter koseri*	WP_200074673
Enterobacteriaceae	*Kluyvera intermedia*	HAU8266257
Lachnospiraceae	*Lacrimispora sphenoides*	SEU04514
Morganellaceae	*Morganella morganii*	WP_108656538

[a] Type strains used in this study are as follows: *C. cochlearium* JCM 1396^T, *C. freundii* JCM 1657^T, *C. koseri* JCM 1658^T, *K. intermedia* JCM 1238^T, *L. sphenoides* JCM 1415^T, *M. morganii* JCM 1672^T.



Supplementary Fig. S1. Structures of sesame-related compounds used in this study. (A) (+)-sesamin, (B) sesaminol, (C) sesamol, (D) SDG(β1-2), and (E) SDG(β1-6).



Supplementary Fig. S2. Comparison of the crystal structures of *Pa*TPL and *Cf*TPL. Superimposition of the monomer structures (A) and the active site structures (B) of *Pa*TPL (PDB code, 7FJK; main chain, dim gray; side chain in Lys257, blue; binding cofactor PLP, red) and *Citrobacter freundii* TPL (*Cf*TPL; PDB code, 6DUR; main chain, light gray; side chain in Lys257, sky blue; binding L-phenylalanine quinonoid complex, orange) are shown. Similar to *Cf*TPL (Phillips & Craig, 2018), *Pa*TPL forms a tetramer with two catalytic dimers intertwined at their *N*-termini, in which one catalytic dimer comprises two catalytic pockets with the same architecture at the interface of two subunits (see **Fig. 6A** of the main article for details). In (A) and (B), PLP (red stick) is bound to Lys257 (blue stick) of each of the subunits to form the internal aldimine, a catalytically competent form of PLP-dependent enzymes. (C) Hydrogen bond network around the catalytic residues of *Pa*TPL identified in one of the four catalytic pockets. The electron density maps of citric acid (a component of the reservoir solution) and the internal aldimine formed between PLP and Lys257 are shown. Hydrogen bonds are indicated by a dashed line. CIT, citric acid; W, water. All of the three carboxyl groups of the bound citric acid are hydrogen-bonded with the protein directly or via water molecules, for which Tyr71, Arg100, Thr124, Arg381, and Arg404 are responsible. Tyr71 is a residue from the neighboring subunit in the catalytic dimer, and its hydroxyl group is proposed to serve as a proton donor to enable the β-elimination of phenol from the substrate L-tyrosine (Katayama & Kumagai, 2010). In addition, Thr124 and Arg381 reportedly play important roles in the release of phenol (Katayama & Kumagai, 2010). No electron density map corresponding to citric acid was observed in the remaining three catalytic sites.

References

Katayama, T. & Kumagai, H. (2010). Tyrosine phenol-lyase. In M. C. Flickinger (Ed.), Encyclopedia of Industrial Biotechnology (pp. 4752–4757). U.S.A.: John Wiley & Sons.

Phillips, R. S. & Craig, S. (2018). Crystal structures of wild-Type and F448A mutant *Citrobacter freundii* tyrosine phenol-lyase complexed with a substrate and inhibitors: implications for the reaction mechanism. *Biochemistry*, **57**, 6166–6179.