Supporting Information for

Construction and Optimization of a Biocatalytic Route for Menthone Amination

Hui-Jue Zhu, Jiang Pan, Chun-Xiu Li, Fei-Fei Chen* and Jian-He Xu*

Laboratory of Biocatalysis and Synthetic Biotechnology, State Key Laboratory of Bioreactor Engineering, Shanghai Collaborative Innovation Centre for Biomanufacturing, College of Biotechnology, East China University of Science and Technology, Shanghai 200237, People's Republic of China.

* Corresponding authors: Dr. Fei-Fei Chen and Prof. Jian-He Xu. E-mail: feifeichen@mail.ecust.edu.cn; jianhexu@ecust.edu.cn

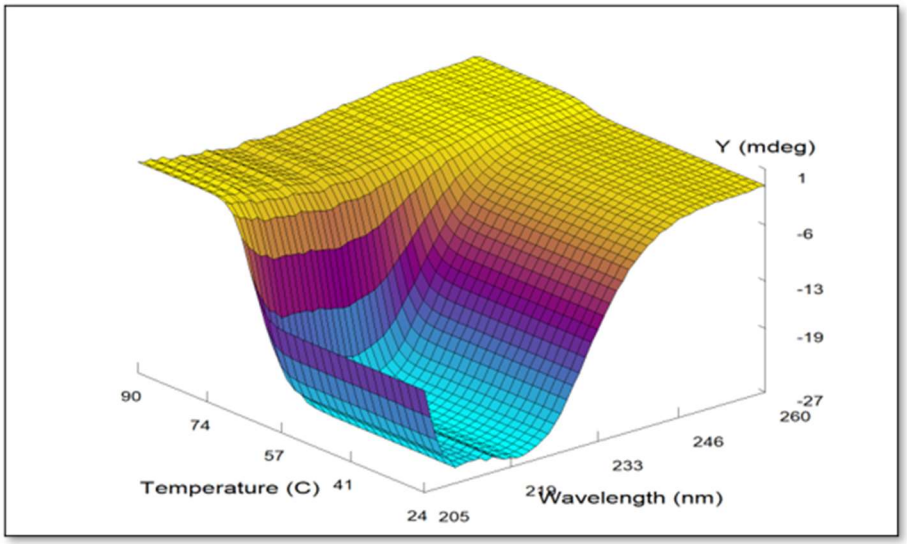

Figure. S1. Melting temperatures of the *Vf*TA.

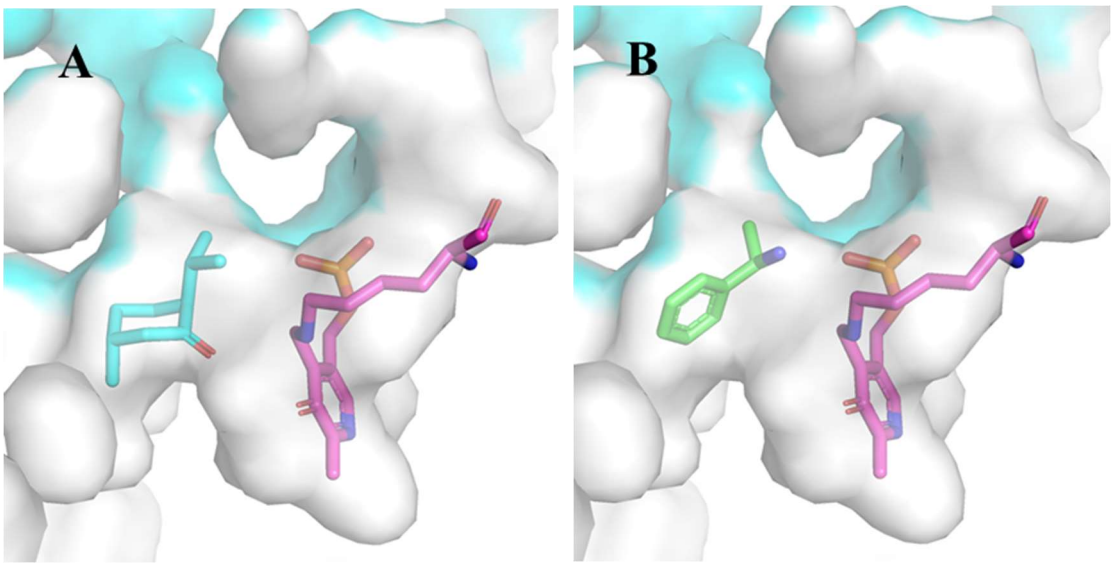

Figure. S2. Docking results of (−)-menthone (bule) and *S*-MBA (green) with *Vf*TA. Structure of *Vf*TA with monomers A and B, is shown in white and palecyan, respectively. The catalytic K285-PLP covalent complex is highlighted in red.

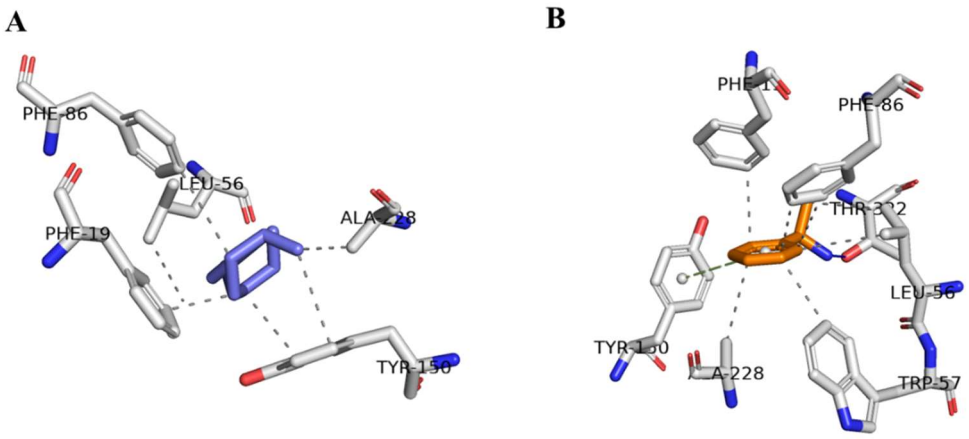

Figure.S3. Interactions between residues (white) around the (−)-menthone (bule) and *S*-MBA (orange).

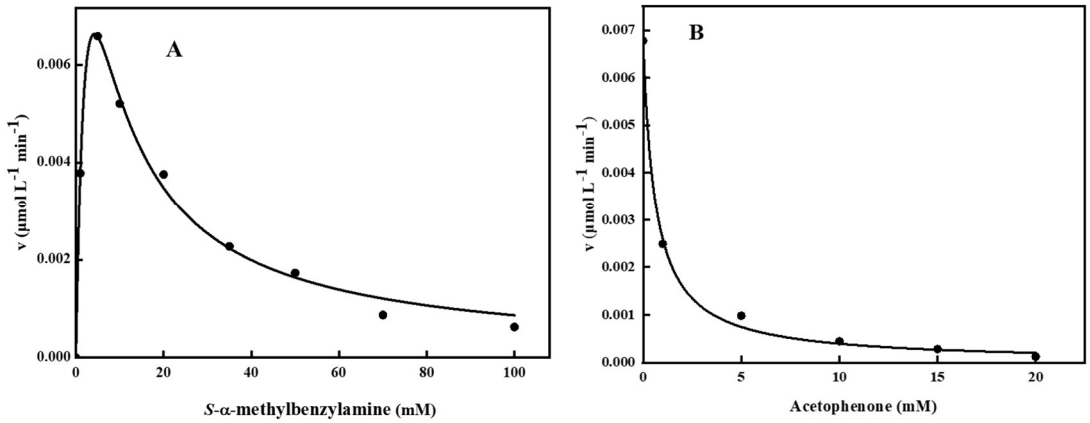

Figure. S4. Kinetic curves of inhibition of *Vf*TA towards *S*-MBA and acetophenone. (A) Kinetic curve for *Vf*TA towards substrate *S*-MBA; (B) Kinetic curve for *Vf*TA towards acetophenone.

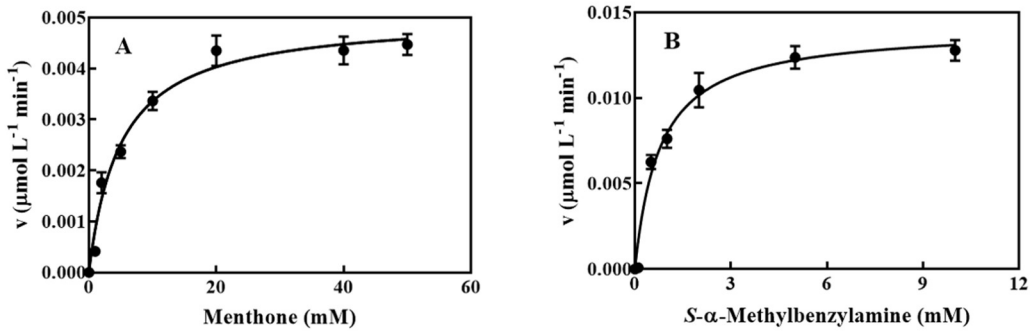

Figure. S5. Kinetic curves of *Vf*TA towards substrate and amino donor.
(A) Kinetic curve of *Vf*TA towards substrate (−)-menthone; (B) Kinetic curve of *Vf*TA towards amino donor *S*-MBA.

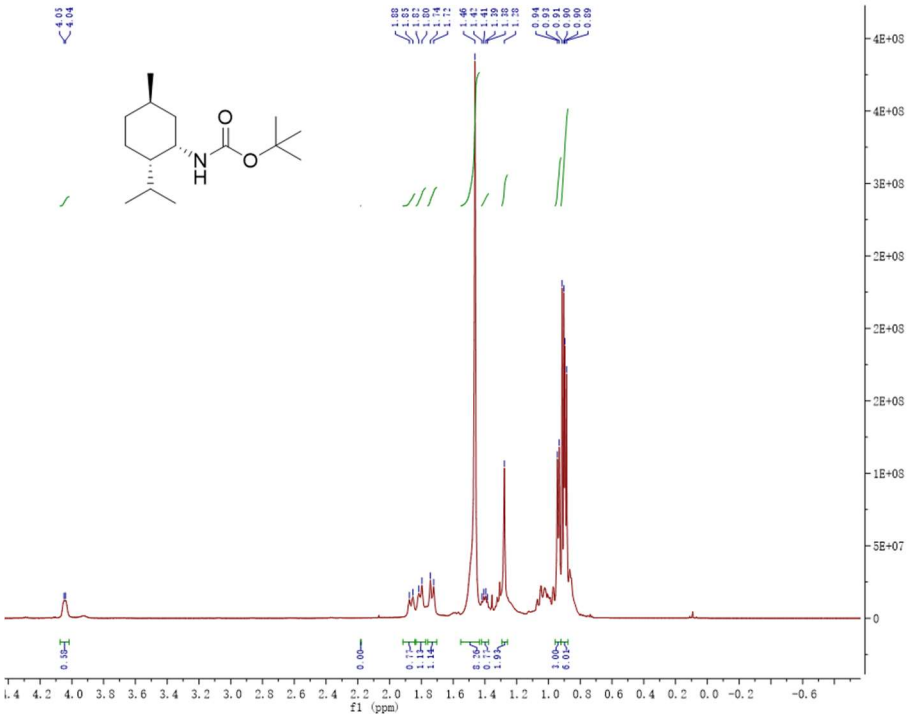

Figure. S6. ^{1}H NMR of the (+)-N-Boc-neomenthylamine.