Supplementary material:

Optimization of the lipase-catalyzed selective amidation of phenylglycinol

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FIGURE CAPTIONS

FIGURE S1. Production assay of the ^{1}H NMR.
^{1}HNMR:(400 MHZ, $CDCl_3$), δ7.28-7.38（m, 5H）, 6.08(br s, 1H), 5.05-5.10(m, 1H), 3.93(ddd, J = 11.0, 6.0, 4.0 HZ 2H), 2.61(brs, 1H), 2.25 (t,J=7.5HZ, 2H), 1.60-1.70 (m, 2H), 1.20-1.35 (m, 12H), 0.88(t, J=7.0HZ, 3H).
FIGURE S2. Assay of the FT-IR spectra.
IR (KBr), v/cm^{-1}:3304, 2926, 1648 (-CH=O), 1540, 1460, 1197, 1039, 700 cm^{-1}.

FIGURE S3. Gas chromatography of compound a.
FIGURE S4. Gas chromatography of compound b.
FIGURE S5. Gas chromatography of compound c.
FIGURE S6. Gas chromatography of compound d.
FIGURE S7. Gas chromatography of compound e.
FIGURE S8. Gas chromatography of compound f

FIGURE S9. Mass spectrometry of amide of compound a.
FIGURE S10. Mass spectrometry of ester of compound a.
FIGURE S11. Mass spectrometry of dimer of compound a.
FIGURE S12. Mass spectrometry of amide of compound b.
FIGURE S13. Mass spectrometry of ester of compound b.
FIGURE S14. Mass spectrometry of dimer of compound b.
FIGURE S15. Mass spectrometry of amide of compound c.
FIGURE S16. Mass spectrometry of ester of compound c.
FIGURE S17. Mass spectrometry of amide of compound d.
FIGURE S18. Mass spectrometry of ester of compound d.
FIGURE S19. Mass spectrometry of dimer of compound d.
FIGURE S20. Mass spectrometry of amide of compound e.
FIGURE S21. Mass spectrometry of ester of compound e.
FIGURE S22. Mass spectrometry of dimer of compound e.
FIGURE S23. Mass spectrometry of amide of compound f.

FIGURE S24. Protein sequence alignment of four kinds of lipases

FIGURE S25. Structure alignment of four kinds of lipase

FIGURE S26. Selection of enzyme amount in organic solvent and solvent-free system

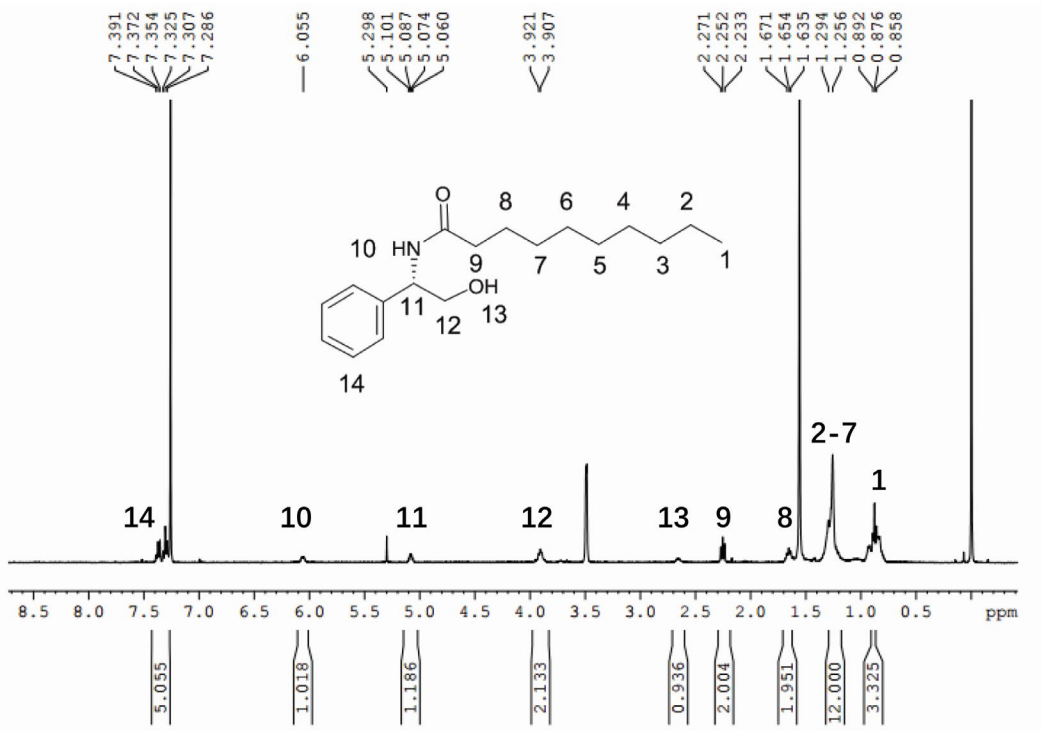

FIGURE S1. Production assay of the ^{1}H NMR.

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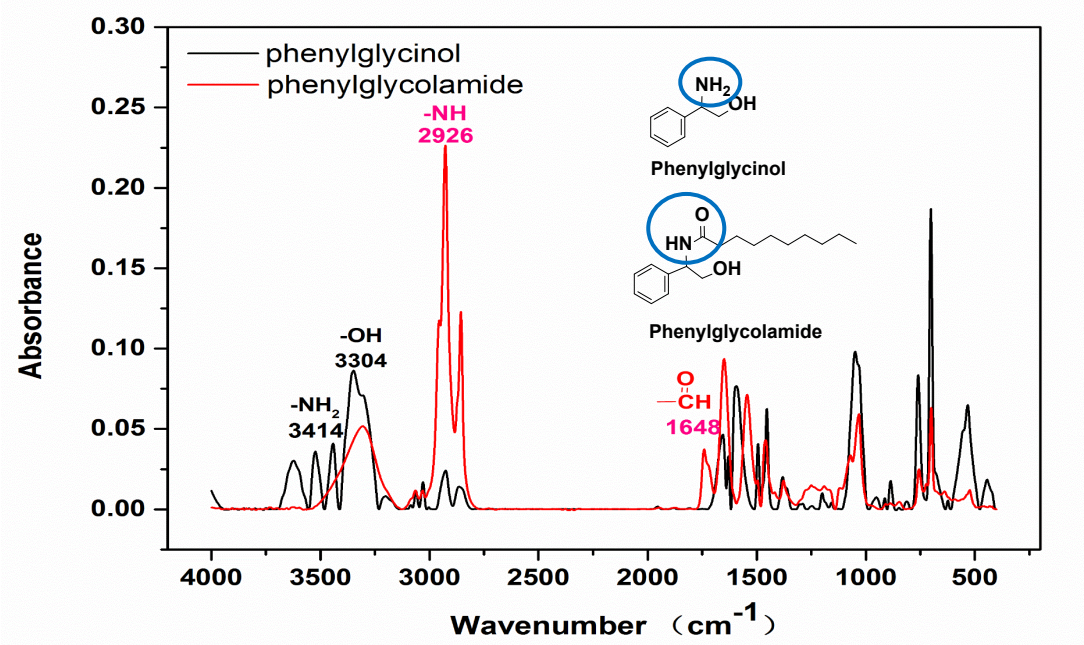


FIGURE S2. Assay of the FT-IR spectra.

IR (KBr), v/cm^{-1}:3304, 2926, 16489（-CH=O）, 1540, 1460, 1197, 1039, 700 cm^{-1}.

a. Ethanolamine

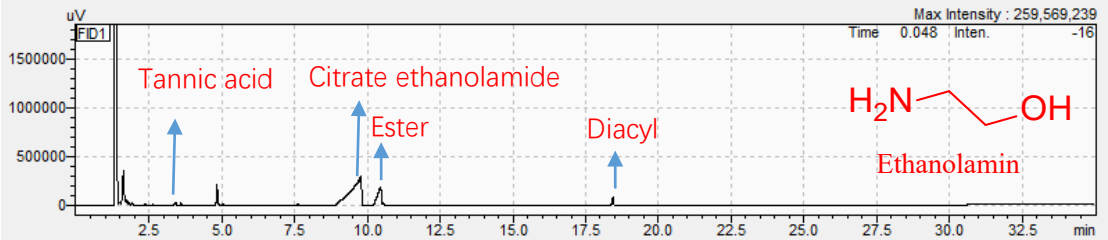


FIGURE S3. Gas chromatography of compound a.

b.2-amino-1-butanol

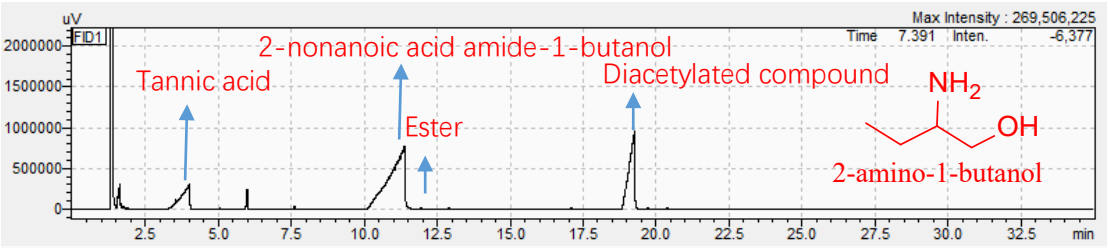


FIGURE S4. Gas chromatography of compound b.

c.Phenylalanine

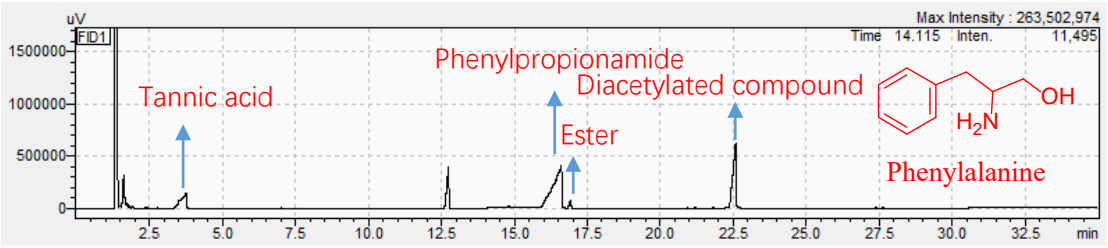


FIGURE S5. Gas chromatography of compound c.

d.Phenylglycinol

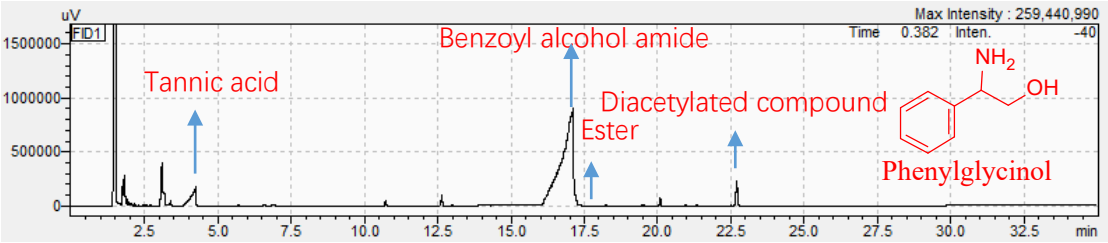


FIGURE S6. Gas chromatography of compound d.

e.Isopropanolamine

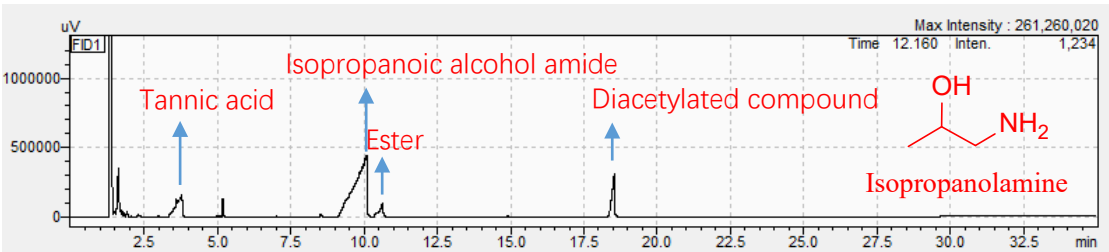


FIGURE S7. Gas chromatography of compound e.

f.3-amino-3-phenyl-1-propanol

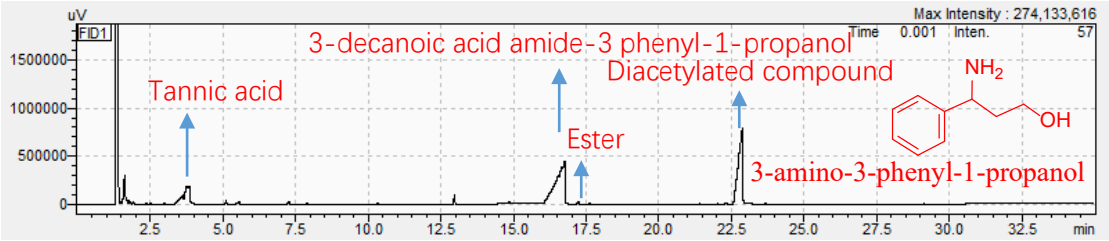


FIGURE S8. Gas chromatography of compound f

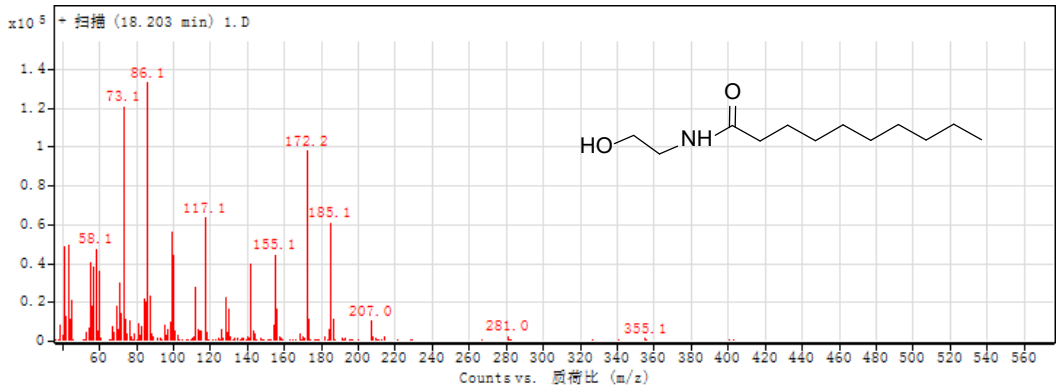


FIGURE S9. Mass spectrometry of amide of compound a.

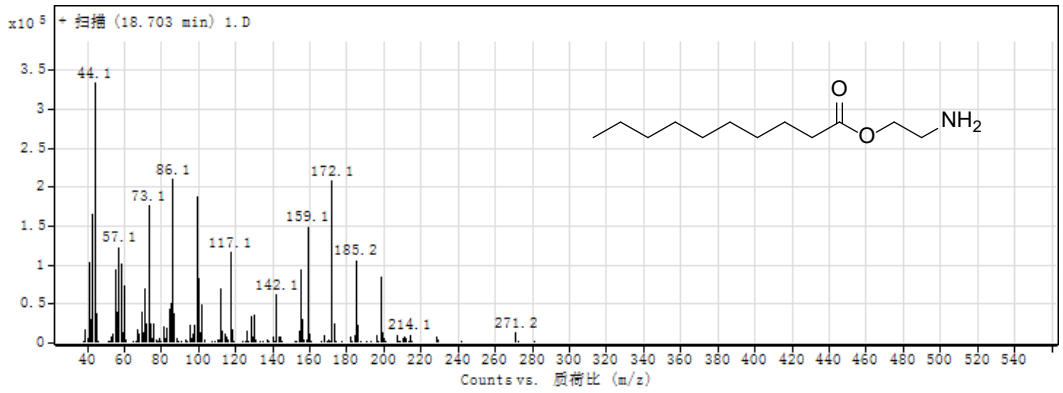


FIGURE S10. Mass spectrometry of ester of compound a.

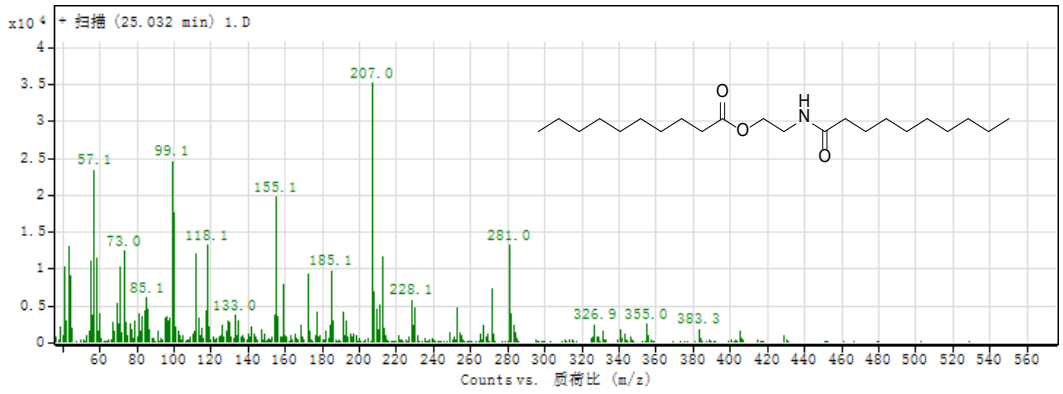


FIGURE S11. Mass spectrometry of dimer of compound a.

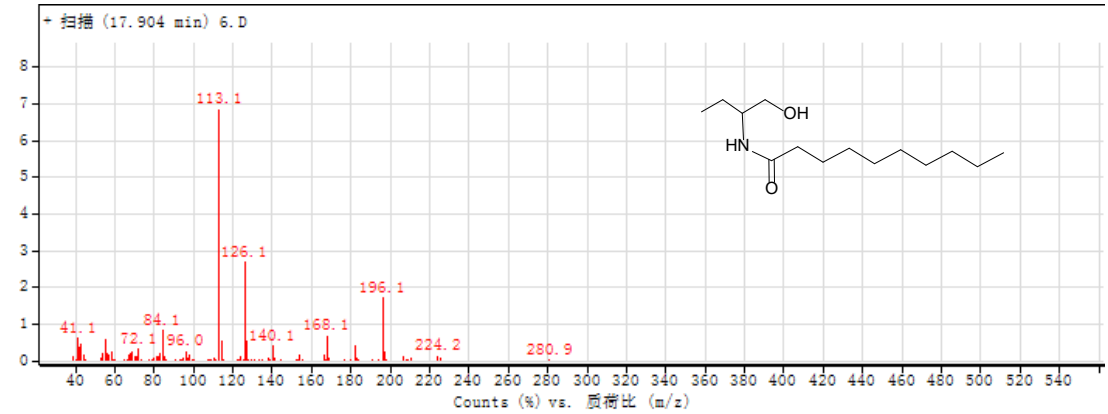


FIGURE S12. Mass spectrometry of amide of compound b.

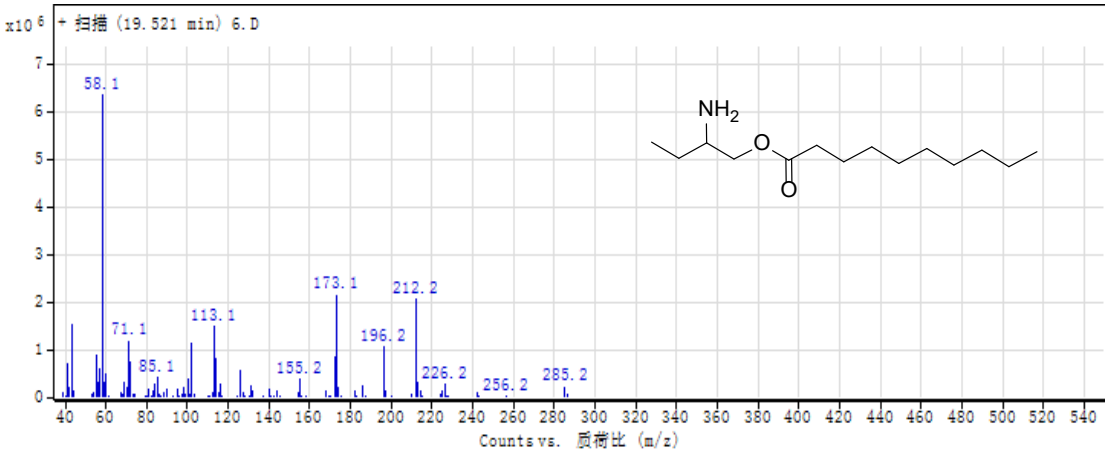


FIGURE S13. Mass spectrometry of ester of compound b.

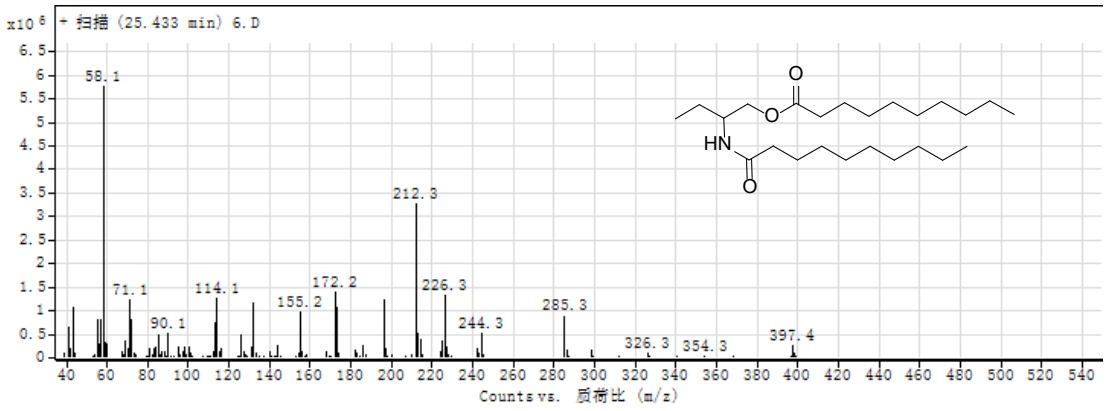


FIGURE S14. Mass spectrometry of dimer of compound b.

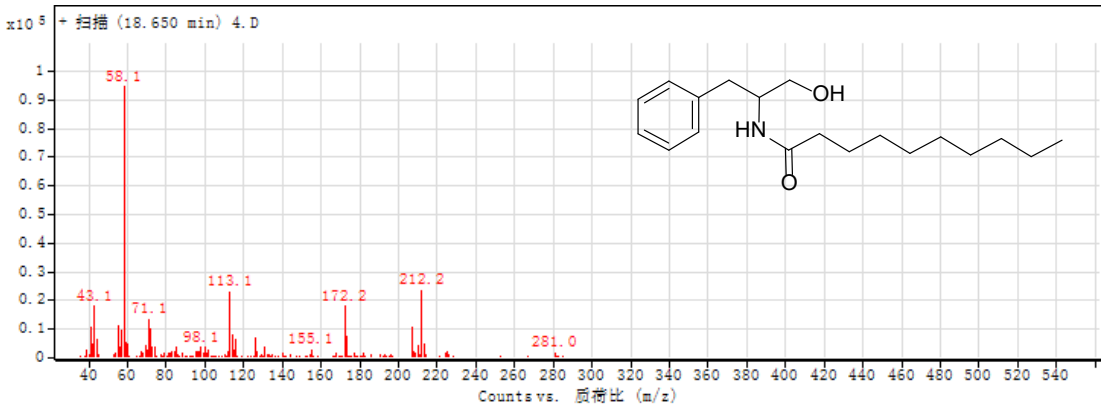


FIGURE S15. Mass spectrometry of amide of compound c.

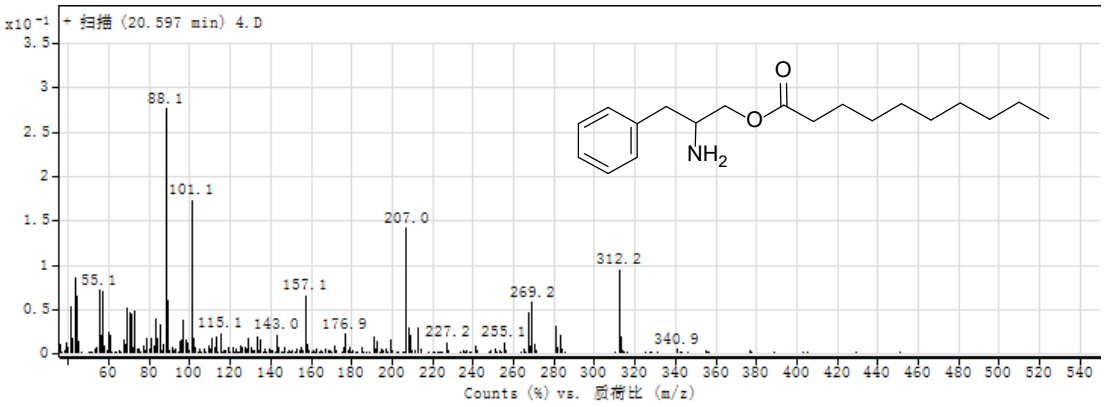


FIGURE S16. Mass spectrometry of ester of compound c.

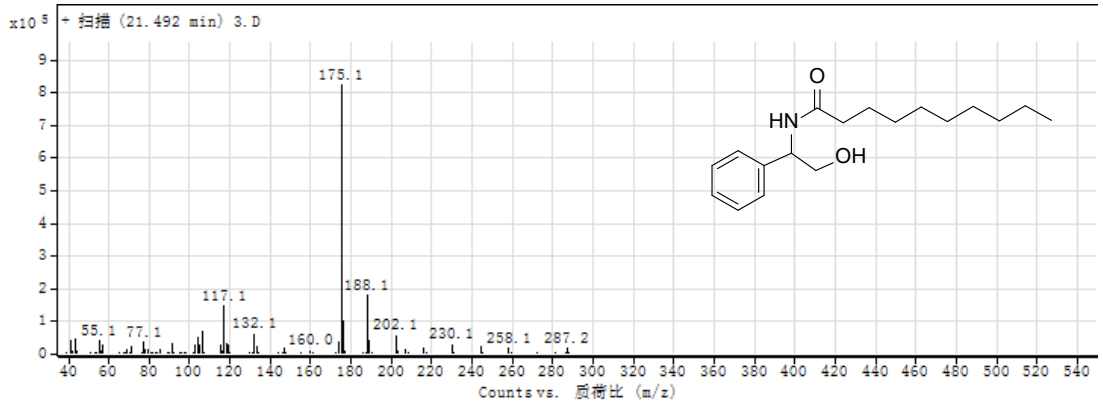


FIGURE S17. Mass spectrometry of amide of compound d.

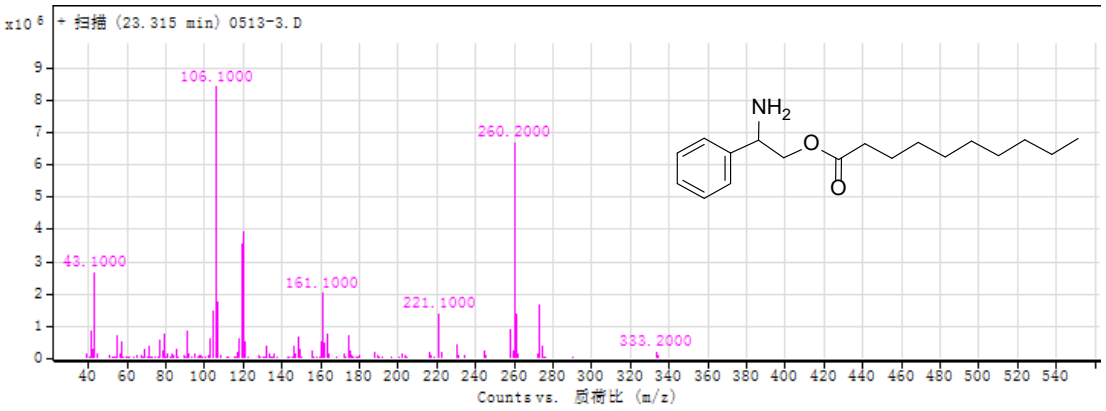


FIGURE S18. Mass spectrometry of ester of compound d.

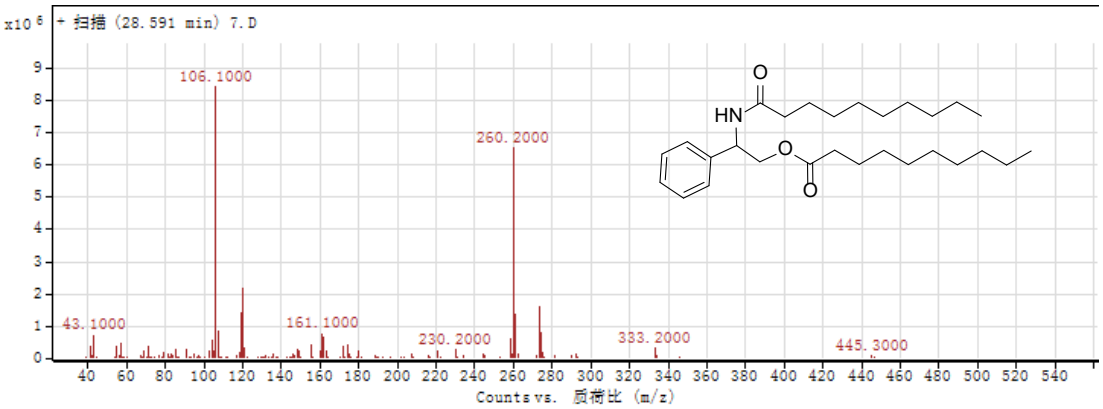


FIGURE S19. Mass spectrometry of dimer of compound d.

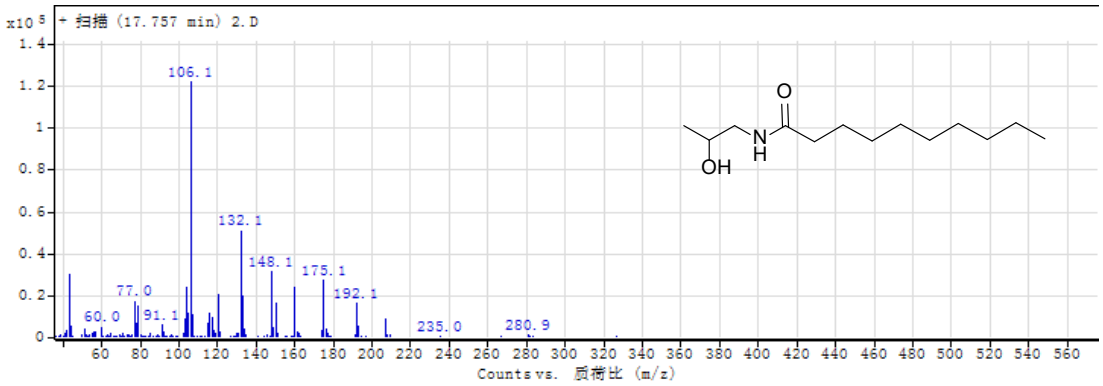


FIGURE S20. Mass spectrometry of amide of compound e.

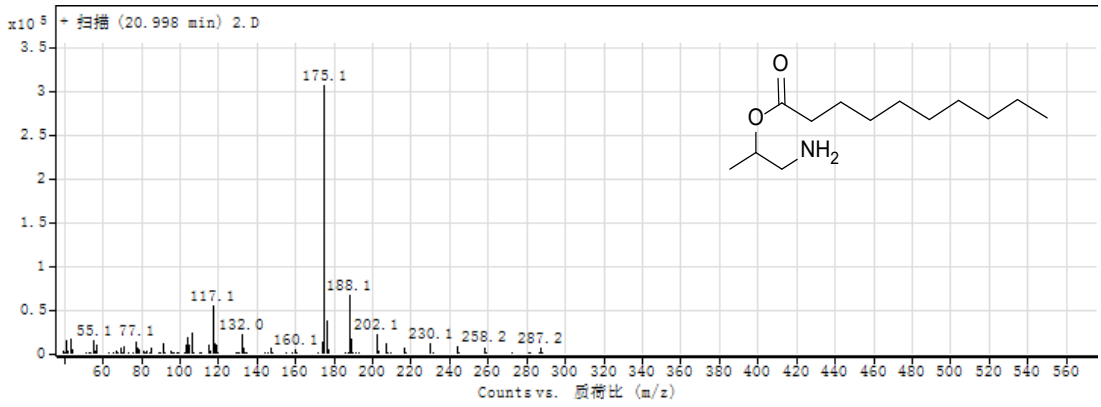


FIGURE S21. Mass spectrometry of ester of compound e.

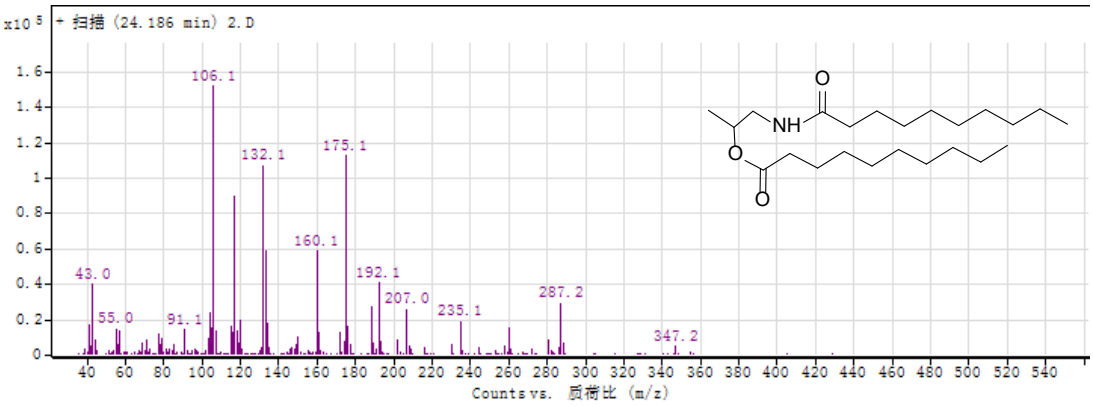


FIGURE S22. Mass spectrometry of dimer of compound e.

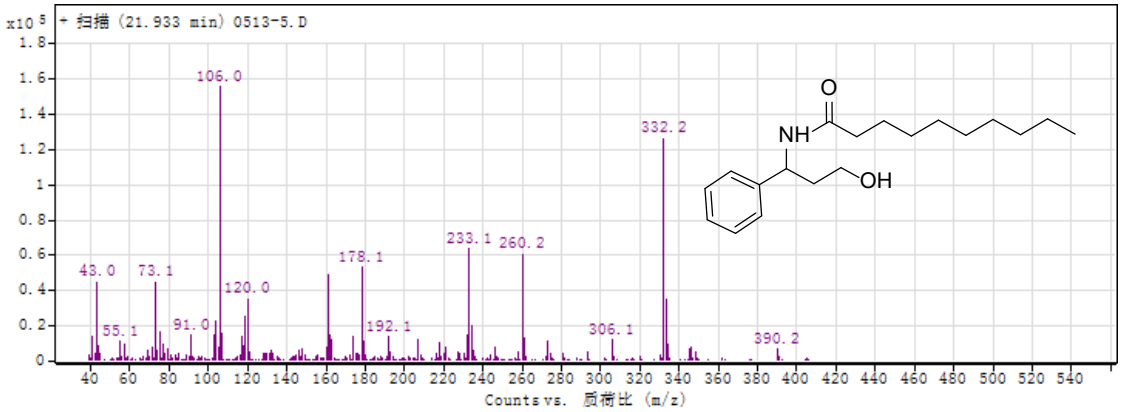


FIGURE S23. Mass spectrometry of amide of compound f.

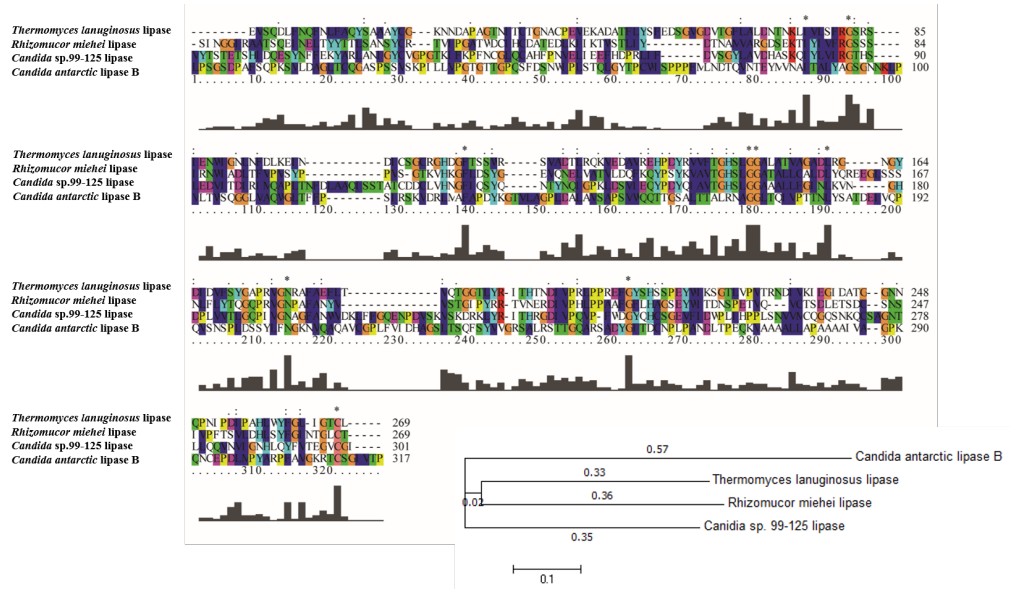
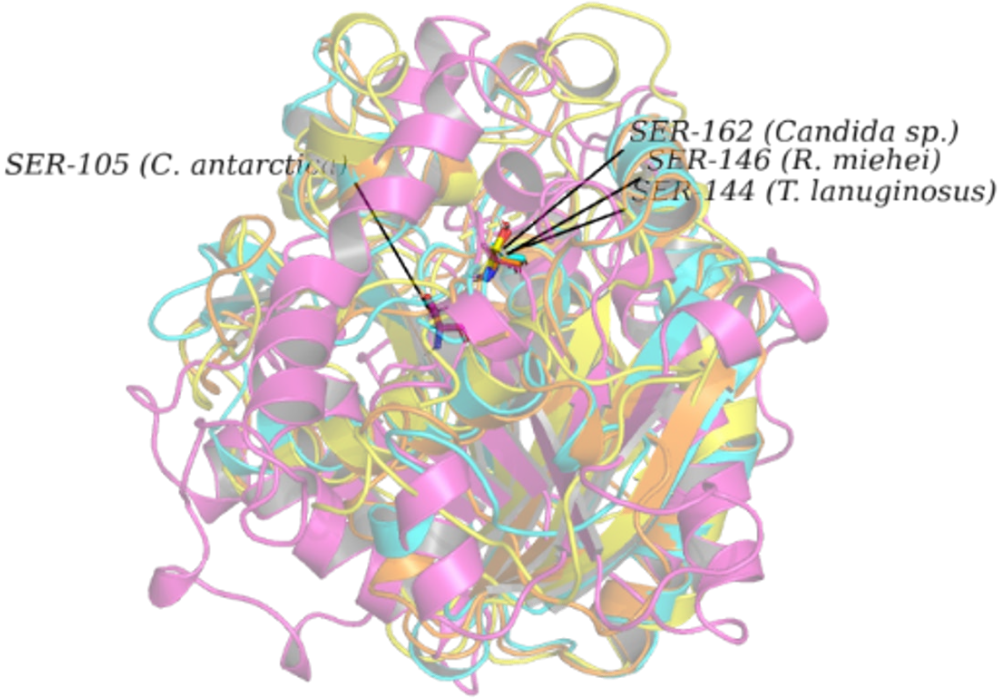


Figure S24 Protein sequence alignment of four kinds of lipases



Thermomyces lanuginosus **lipase, color in cyan;** ***Rhizomucor miehei*** **lipase, color in orange;** ***Candida*** **sp.99-125 lipase, color in yellow;** ***Candida antarctic*** **lipase B; color in purple**

Figure S25 Structure alignment of four kinds of lipase

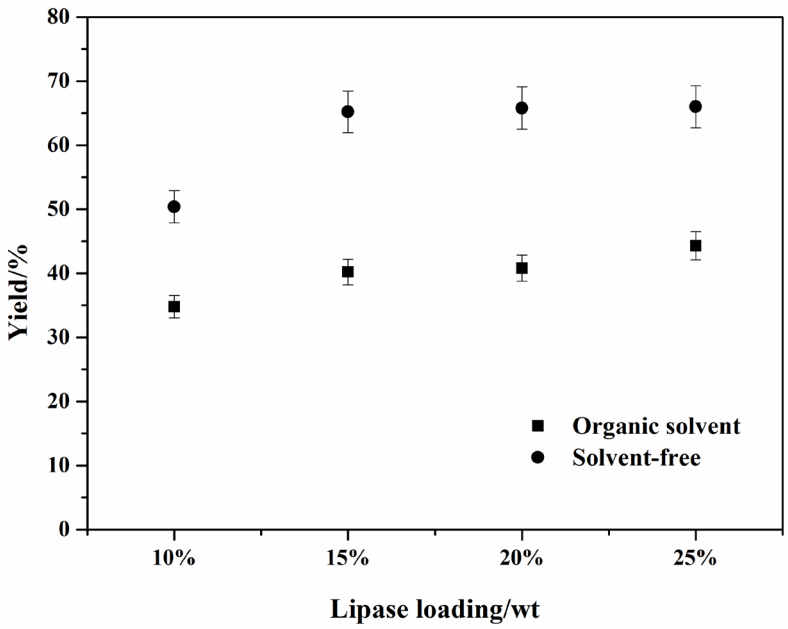


Figure S26 Effect of Novozym 435 amounts on the amidation reaction in organic solvent and solvent-free system.

Figure S26 caption : Effect of Novozym 435 amounts on the amidation reaction in organic solvent and solvent-free system. Enzymatic reaction conditions: molar ratio of phenylglycinol and capric acid at 1:1, and Novozym 435 loadings varied from 10 wt% to 25 wt%. The reaction was carried out at 40 °C for 24 h, separately in organic solvents and solvent-free systems.