Candida tropicalis CE017: A New Brazilian Enzymatic Source for the Bioreduction of Aromatic Prochiral Ketones

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(S)-1-Phenylethanol, 1b



¹H NMR (CDCl₃, 300.13 MHz): δ 1.39 (d, *J* 6.5 Hz, 3H, H₂), 2.03 (s, 1H, OH), 4.77 (q, *J* 6.5 Hz, 1H, H₁), 7.25 (m, 5H, H₂, + H₃, + H₄, + H₅, + H₆). (Figure S1)

¹³C NMR (CDCl₃, 75.5 MHz): δ 25.3 (C₂), 70.5 (C₁), 125.5 (C₂,+C₆), 127.6 (C₄), 128.6 (C₃,+C₅), 146.0 (C₁). (Figure S2)

Conditions for determination of the conversion by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ (1a) 5.5 in and $t_{\rm R}$ (1b) 8.5 min. Column Spherisorb. (Figure S3)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ 10.2 (*S*) and $t_{\rm R}$ 15.4 (*R*) min. Column OB-H. $[\alpha]_{\rm D}^{25} = -47.0$, c 1.1, CHCl₃, for 97% *ee* of (*S*)-enantiomer. lit.: $[\alpha]_{\rm D}^{22} = -62.8$ (*c* 1.0, CHCl₃), 98.5% *ee*. (Figures S4 and S5)



Figure S1. ¹H NMR spectrum of 1b (CDCl₃, 300.13 MHz).

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Figure S5. Chromatogram of the product by C. tropicalis (1b).

(S)-1-(2-Nitrophenyl)ethanol, **2b**



¹H NMR (CDCl₃, 300.13 MHz): δ 1.55 (3H, d, *J* 6.3 Hz, H₂), 5.40 (1H, q, *J* 6.3 Hz, H₁), 7.41 (1H, dt, *J* 8.1 and 1.2 Hz, H₄), 7.63 (1H, dt, *J* 8.1 and 1.5 Hz, H₅), 7.82 (1H, dd, *J* 8.1 and 1.2 Hz, H₆), 7.88 (1H, dd, *J* 8.1 and 1.5 Hz, H₃). (Figure S6)

¹³C NMR (CDCl₃, 75.5 MHz): δ 24.2 (C₂), 65.4 (C₁), 124.2 (C₃), 127.5 (C₆), 128.0 (C₄), 133.5 (C₅), 140.9 (C₁ + C₂). (Figure S7)

Conditions for determination of the conversion by GC: Injector 225 °C, Detector 250 °C, 80 °C (5 °C min⁻¹) 180 °C (0 min), $t_{\rm R}$ (**2a**) 8.4 min and $t_{\rm R}$ (**2b**) 9.2 min. Column HP-1. (Figure S8)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹, hexane:IPA (97:3), 20 °C, t_R 22.1 min (*R*) and t_R 23.9 (*S*) min. Column AS. $[\alpha]_D^{25} = +29.8$, c 0.4, CHCl₃, for 99% *ee* of (*S*)-enantiomer. (Figures S9 and S10)



Figure S6. ¹H NMR spectrum of 2b (CDCl₃, 300.13 MHz).



Figure S7. ¹³C NMR spectrum of **2b** (CDCl₃, 75.5 MHz).



Figure S8. Chromatogram of the separation: $t_{\rm R}$ (2a) 8.4 min and $t_{\rm R}$ (2b) 9.2 min.



Figure S9. Chromatogram of the racemic mixture of **2b**: t_{R} 22.1 min (*R*) and t_{R} 23.9 (*S*) min.



Figure S10. Chromatogram of the product by C. tropicalis (2b).

(S)-1-(3-Nitrophenyl)ethanol, **3b**



¹H NMR (CDCl₃, 300.13 MHz): δ 1.47 (3H, d, *J* 6.6 Hz, H₂), 4.96 (1H, q, *J* 6.6 Hz, H₁), 7.47 (1H, t, *J* 7.8 Hz, H₅), 7.67 (1H, d, *J* 7.8 Hz, H₆), 8.04 (1H, ddd, *J* 8.3, 2.1

and 0.9 Hz, H₄.), 8.18 (1H, t, *J* 1.8 Hz, H₂.). (Figure S11) ¹³C NMR (CDCl₃, 75.5 MHz): δ 25.2 (C₂), 69.1 (C₁), 120.2 (C₄.), 122.1 (C₂.), 129.3 (C₅.), 131.6 (C₆.), 147.8 (C₁.), 148.1 (C₃.). (Figure S12)

Conditions for determination of the conversion by GC: Injector 225 °C, Detector 250 °C, 80 °C (5 °C min⁻¹) 180 °C (0 min), $t_{\rm R}$ (**3a**) 9.5 min and $t_{\rm R}$ (**3b**) 11.4 min. Column HP-1. (Figure S13)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹, hexane:IPA (90:10), 20 °C, $t_{\rm R}$ 12.8 min (*S*) and $t_{\rm R}$ 14.2 (*R*) min. Column OB-H. [α]_D²⁵ = -34.9, c 0.5 CH₂Cl₂, for 99% *ee* of (*S*)-enantiomer. (Figures S14 and S15)



Figure S11. ¹H NMR spectrum of 3b (CDCl₃, 300.13 MHz).



Figure S12. ¹³C NMR spectrum of 3b (CDCl₃, 75.5 MHz).





Figure S15. Chromatogram of the product by C. tropicalis (3b).





¹H NMR (CDCl₃, 300.13 MHz): δ 1.50 (3H, d, *J* 6.6 Hz, H₂), 5.01 (1H, q, *J* 6.6 Hz, H₁), 7.53 (2H, d, *J* 8.7 Hz, H₂, + H₆), 8.17 (2H, d, *J* 8.7 Hz, H₃, + H₅). (Figure S16)

¹³C NMR (CDCl₃, 75.5 MHz): δ 25.3 (C₂), 69.5 (C₁), 123.6 (C₂, + C₆), 126.0 (C₃, + C₅), 147.0 (C₁), 153.1 (C₄). (Figure S17)

Conditions for determination of the conversion by GC: Injector 225 °C, Detector 250 °C, 80 °C (5 °C min⁻¹) 180 °C (0 min), $t_{\rm R}$ (4a) 9.6 min and $t_{\rm R}$ (4b) 11.8 min. Column HP-1. (Figure S18)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ 11.7 min (*R*) and $t_{\rm R}$ 13.6 (*S*) min. Column AS. $[\alpha]_{\rm D}^{25} = -24.6$, c 0.5, CHCl₃, for 96% *ee* of (*S*)-enantiomer. (Figures S19 and S20)



Figure S16. ¹H NMR spectrum of 4b (CDCl₃, 300.13 MHz).



Figure S17. ¹³C NMR spectrum of 4b (CDCl₃, 75.5 MHz).



Figure S18. Chromatogram of the separation: $t_{\rm R}$ (4a) 9.6 min and $t_{\rm R}$ (4b) 11.8 min.



Figure S19. Chromatogram of the racemic mixture of 4b: $t_{\rm R}$ 11.7 min (*R*) and $t_{\rm R}$ 13.6 (*S*). min.



Figure S20. Chromatogram of the product by C. tropicalis (4b).

(S)-1-(2-Methoxyphenyl)ethanol, 5b



¹H NMR (CDCl₃, 300.13 MHz): δ 1.52 (3H, d, *J* 6.6 Hz, H₂), 3.88 (3H, s, OCH₃), 5.11 (1H, q, *J* 6.6 Hz, H₁), 6.90 (1H, dd, *J* 7.5 and 1.5 Hz, H₃), 6.98 (1H, dt, *J* 8.5 and 1.5

Hz, H₅.), 7.29 (1H, dt, *J* 8.5 and 1.5 Hz, H₆.), 7.36 (1H, dd, *J* 7.5 and 1.5 Hz, H₄.). (Figure S21)

¹³C NMR (CDCl₃, 75.5 MHz): δ 22.8 (C₂), 55.2 (OCH₃), 66.3 (C₁), 110.3 (C₃.), 120.7 (C₅.), 126.0 (C₆.), 128.2 (C₄.), 133.4 (C₁.), 156.4 (C₂.). (Figure S22)

Conditions for determination of the conversion by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ (**5a**) 6.3 min and $t_{\rm R}$ (**5b**) 7.1 min. Column Spherisorb. (Figure S23)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ 10.3 (*S*) and $t_{\rm R}$ 16.8 (*R*) min. Column OB-H. $[\alpha]_{\rm D}^{25} = -4.5$, c 0.4, CH₂Cl₂, for 56% *ee* of (*S*)-enantiomer. (Figures S24 and S25)



Figure S21. ¹H NMR spectrum of 5b (CDCl₃, 300.13 MHz).



Figure S22. ¹³C NMR spectrum of 5b (CDCl₃, 75.5 MHz).



Figure S23. Chromatogram of the separation: $t_{\rm R}$ (**5a**) 6.3 min and $t_{\rm R}$ (**5b**).



Figure S24. Chromatogram of the racemic mixture of 5b: t_{R} 10.3 (S) and t_{R} 16.8 (R) min.



Figure S25. Chromatogram of the product by C. tropicalis (5b).

(S)-1-(3-Methoxyphenyl)ethanol, **6b**



¹H NMR (CDCl₃, 300.13 MHz): δ 1.47 (3H, d, J 6.6 Hz, H₂), 3.81 (3H, s, OCH₃), 4.83 (1H, q, J 6.6 Hz, H₁), 6.81 (1H, dd, J 8.5 and 1.2 Hz, H₆), 6.93 (2H, m, H₂, + H₄),

7.26 (1H, t, *J* 8.5 Hz, H₅.). (Figure S26) ¹³C NMR (CDCl₃, 75.5 MHz): δ 25.0 (C₂), 55.1 (OCH₃), 70.0 (C₁), 110.8 (C₂.), 112.7 (C₄.), 117.6 (C₆.), 129.3 (C₅.), 147.6 (C₁.), 159.6 (C₃.). (Figure S27)

Conditions for determination of the conversion by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ (**6a**) 5.1 min and $t_{\rm R}$ (**6b**) 5.9 min. Column Spherisorb. (Figure S28)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, t_R 20.1 min (*S*) and t_R 29.6 min (*R*). Column OB-H. $[\alpha]_D^{25} = -21.6$, c 0.34, MeOH, for 80% *ee* of (*S*)-enantiomer. (Figures S29 and S30)



Figure S26. ¹H NMR spectrum of 6b (CDCl₃, 300.13 MHz).



Figure S27. ¹³C NMR spectrum of 6b (CDCl₃, 75.5 MHz).



Figure S28. Chromatogram of the separation: $t_{\rm R}$ (6a) 5.1 min and $t_{\rm R}$ (6b) 5.9 min.



Figure S29. Chromatogram of the racemic mixture of 6b: $t_R = 20.1 \min(S)$ and $t_R = 29.6 \min(R)$.



Figure S30. Chromatogram of the product by C. tropicalis (6b).

(S)-1-(4-Methoxyphenyl)ethanol, 7b



¹H NMR (CDCl₃, 300.13 MHz): δ 1.48 (3H, d, *J* 6.3 Hz, H₂), 3.82 (3H, s, OCH₃), 4.84 (1H, q, *J* 6.3 Hz, H₁), 6.88 (2H, d, *J* 8.7 Hz, H₃, + H₅), 7.30 (2H, d, *J* 8.7 Hz, H₂, and H₆). (Figure S31)

¹³C NMR (CDCl₃, 75.5 MHz): δ 24.3 (C₂), 55.2 (OMe), 69.8 (C₁), 126.6 (C₂, + C₆), 113.8 (C₃, + C₅), 137.9 (C₁), 158.9 (C₄). (Figure S32)

Conditions for determination of the conversion by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ (7a) 7.3 min and $t_{\rm R}$ (7b) 8.5 min. Column Spherisorb. (Figure S33)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹; hexane:IPA (95:5); 20 °C, $t_{\rm R}$ 13.4 min (*S*) and $t_{\rm R}$ 18.7 (*R*) min. Column OB-H. $[\alpha]_{\rm D}^{25} = -2.2$, c 0.5, CH₂Cl₂, for 9% *ee* of (*S*)-enantiomer. (Figures S34 and S35)



Figure S31. ¹H NMR spectrum of 7b (CDCl₃, 300.13 MHz).



Figure S32. ¹³C NMR spectrum of 7b (CDCl₃, 75.5 MHz).



Figure S33. Chromatogram of the separation: $t_{\rm R}$ (7a) 7.3 min and $t_{\rm R}$ (7b) 8.5 min.



Figure S34. Chromatogram of the racemic mixture of 7b: $t_{\rm R}$ 13.4 min (S) and $t_{\rm R}$ 18.7 (R) min.



Figure S35. Chromatogram of the product by C. tropicalis (7b).

(S)-1-(4-Chlorophenyl)ethanol, **8b**



¹H NMR (CDCl₃, 300.13 MHz): δ 1.46 (3H, d, *J* 6.5 Hz, H₁), 4.85 (1H, q, *J* 6.5 Hz, H₂), 7.30 (4H, m, H₂.+ H₃.+ H₅.+ H₆.). (Figure S36)

¹³C NMR (CDCl₃, 75.5 MHz): δ 25.1 (C₂), 69.6 (C₁), 126.7 (C₂), 128.5 (C₃), 132.9 (C₄), 144.1 (C₁). (Figure S37) Conditions for determination of the conversion by GC:

Injector 225 °C, Detector 250 °C, 90 °C (3 °C min⁻¹) 105 °C (5 °C min⁻¹) 120 °C (20 °C min⁻¹) 200 °C (0 min), $t_{\rm R}$ (8a) 5.0 min and $t_{\rm R}$ (8b) 5.6 min. Column HP-1. (Figure S38)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ 7.5 min (*S*) and $t_{\rm R}$ 8.5 min (*R*). Column OB-H. $[\alpha]_{\rm D}^{25} = -32.4$, CH₂Cl₂, c 0.5, for 62% *ee* of (*S*)-enantiomer. (Figures S39 and S40)



Figure S36. ¹H NMR spectrum of 8b (CDCl₃, 300.13 MHz).



Figure S37. ¹³C NMR spectrum of 8b (CDCl₃, 75.5 MHz).



Figure S38. Chromatogram of the separation: $t_{\rm R}$ (8a) 5.0 min and $t_{\rm R}$ (8b) 5.6 min.



Figure S39. Chromatogram of the racemic mixture of **8b**: $t_{\rm R}$ 7.5 min (*S*) and $t_{\rm R}$ 8.5 min (*R*).



Figure S40. Chromatogram of the product by C. tropicalis (8b).





¹H NMR (CDCl₃, 300.13 MHz): δ 3.56 (1H, dd, *J* 11.4 and 3.3 Hz, H₂), 3.66 (1H, dd, *J* 11.4 and 8.7 Hz, H₂), 4.81 (1H, dd, *J* 8.7 and 3.6 Hz, H₁), 7.30 (5H, m, H₂ + H₃ + H₄ + H₅, +H₆). (Figure S41)

¹³C NMR (CDCl₃, 75.5 MHz): δ 50.8 (C₂), 74.0 (C₁), 126.0 (C₂, + C₆), 128.4 and 128.6 (C₃, + C₅), 139.9 (C₁). (Figure S42)

Conditions for determination of the conversion by GC: Injector 225 °C, Detector 250 °C, 90 °C (3 °C min⁻¹) 105 °C (5 °C min⁻¹) 120 (20 °C min⁻¹) 200 °C (0 min), $t_{\rm R}$ (**9a**) 4.1 min and $t_{\rm R}$ (**9b**) 4.3 min. Column HP-1. (Figure S43)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ 13.2 (*R*) and $t_{\rm R}$ 17.6 (*S*) min. Column OB-H. $[\alpha]_{\rm D}^{25} = -18.8$, c 0.26, CH₂Cl₂, for 89% *ee* of (*R*)-enantiomer. (Figures S44 and S45)



Figure S41. ¹H NMR spectrum of 9b (CDCl₃, 300.13 MHz).



Figure S42. ¹³C NMR spectrum of 9b (CDCl₃, 75.5 MHz).



Figure S43. Chromatogram of the separation: $t_{\rm R}$ (9a) 4.1 min and $t_{\rm R}$ (9b) 4.3 min.



Figure S44. Chromatogram of the racemic mixture of 9b: t_{R} 13.2 (*R*) and t_{R} 17.6 (*S*) min.



Figure S45. Chromatogram of the product by C. tropicalis (9b).

(R)-2-Chloro-1-(3,4-dichlorophenyl)ethan-1-ol, 10b



¹H NMR (CDCl₃, 300.13 MHz): δ 3.59 (1H, dd, *J* 11.4 and 8.7 Hz, H₂), 3.72 (1H, dd, *J* 11.4 and 3.6 Hz, H₂), 4.87 (1H, dd, *J* 8.7 and 3.6 Hz, H₁), 7.21 (1H, dd, *J* 8.4 and

1.8 Hz, H₆.), 7.43 (1H, d, *J* 8.4 Hz, H₅.), 7.51 (1H, d, *J* 1.8 Hz, H₂.). (Figure S46)

¹³C NMR (CDCl₃, 75.5 MHz): δ 50.4 (C₂), 72.8 (C₁), 125.4 (C₆), 128.1 (C₂), 130.6 (C₅), 132.4 (C₄), 132.8 (C₃), 140.0 (C₁). (Figure S47)

Conditions for determination of the conversion by GC: Injector 225 °C, Detector 250 °C, 80 °C (5 °C min⁻¹) 180 °C (0 min); $t_{\rm R}$ (**10a**) 13.6 and $t_{\rm R}$ (**10b**) 14.8 min. Column HP-1. (Figure S48)

Conditions for determination of the *ee* by HPLC: 0.8 mL min⁻¹, hexane:IPA (95:5), 20 °C, $t_{\rm R}$ 13.0 min (*S*) and $t_{\rm R}$ 14.9 (*R*) min. Column IA. $[\alpha]_{\rm D}^{25} = -13.3$, c 0.5, CHCl₃, for 90% *ee* of (*R*)-enantiomer. (Figures S49 and S50)



Figure S46. ¹H NMR spectrum of 10b (CDCl₃, 300.13 MHz).



Figure S47. ¹³C NMR spectrum of 10b (CDCl₃, 75.5 MHz).







Figure S50. Chromatogram of the product by *C. tropicalis* (10b).