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Article

Yeast-Mediated Stereoselective Reduction of α-Acetylbutyrolactone

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S1 Preparation of (3*R*, 1′*S*)-α'-1'-hydroxyethyl-γ-butyrolactone 2

Pure (3*R*, 1′*S*)-α'-1'-hydroxyethyl-γ-butyrolactone **2** was prepared as follow:

The culture of *Rhodotorula marina* AM77 (50 mL, 12.0 g/L) was centrifuged at 5000 rpm for 3 min The culture was re-suspended in two flasks with 100 mL of sterile medium with addition of 5% glycerol. In next step, α-acetylbutyrolactone **1** (summarily 0.12 g, 9.4 mM) was added. After two hours, the medium, which contained product and mycelium was extracted three times with ethyl acetate (100 mL). The organic fraction was dried over anhydrous magnesium sulphate, the solvent was evaporated *in vacuo* and analysed by GC (chiral column). Product of biotransformation was purified by means of column chromatography (Kieselgel 60, 230–400 mesh; hexane: diethyl ether 1:1; 67 mg, 56% R_t = 0.1). Next, the optical rotation was determined. The obtained value of optical rotation ($[a]_{20}^{D}$ = +18.4 (c = 0.7; $CHCl_3$) was compared with literature data [17]. The configuration of biotransformation product was determined as (3*R*, 1′*S*).

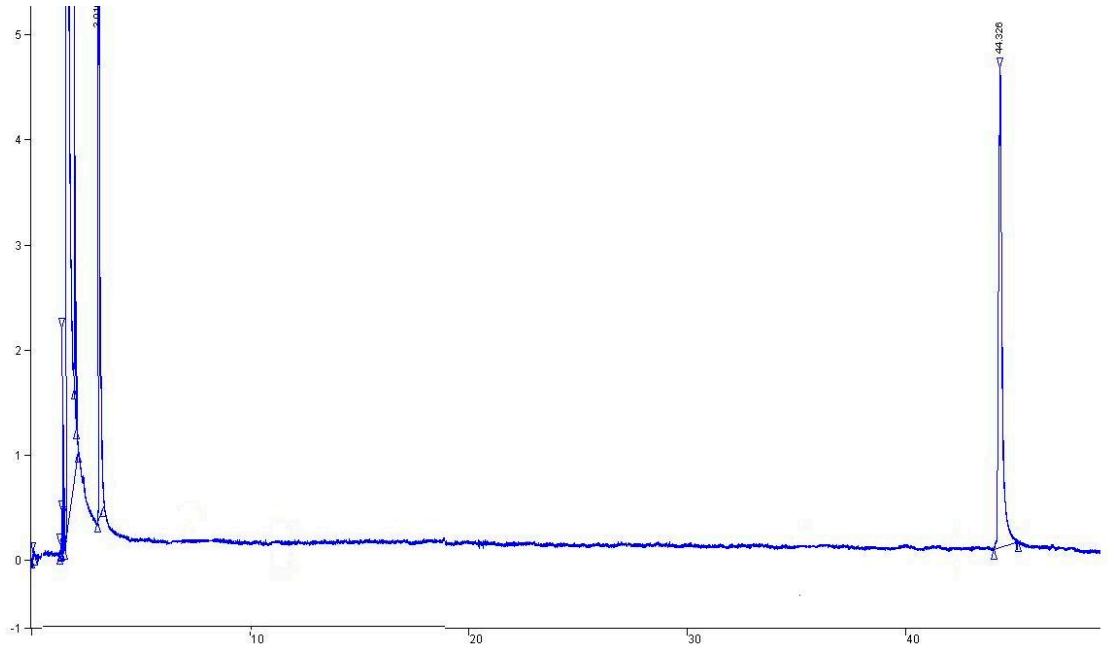

Figure S1. GC chromatogram of biotransformation of α-acetylbutyrolactone **1** by *Rhodotorula marina* AM77, ((3*R*, 1′*S*)-α'-1'-hydroxyethyl-γ-butyrolactone **2d** R_t = 44.3 min).

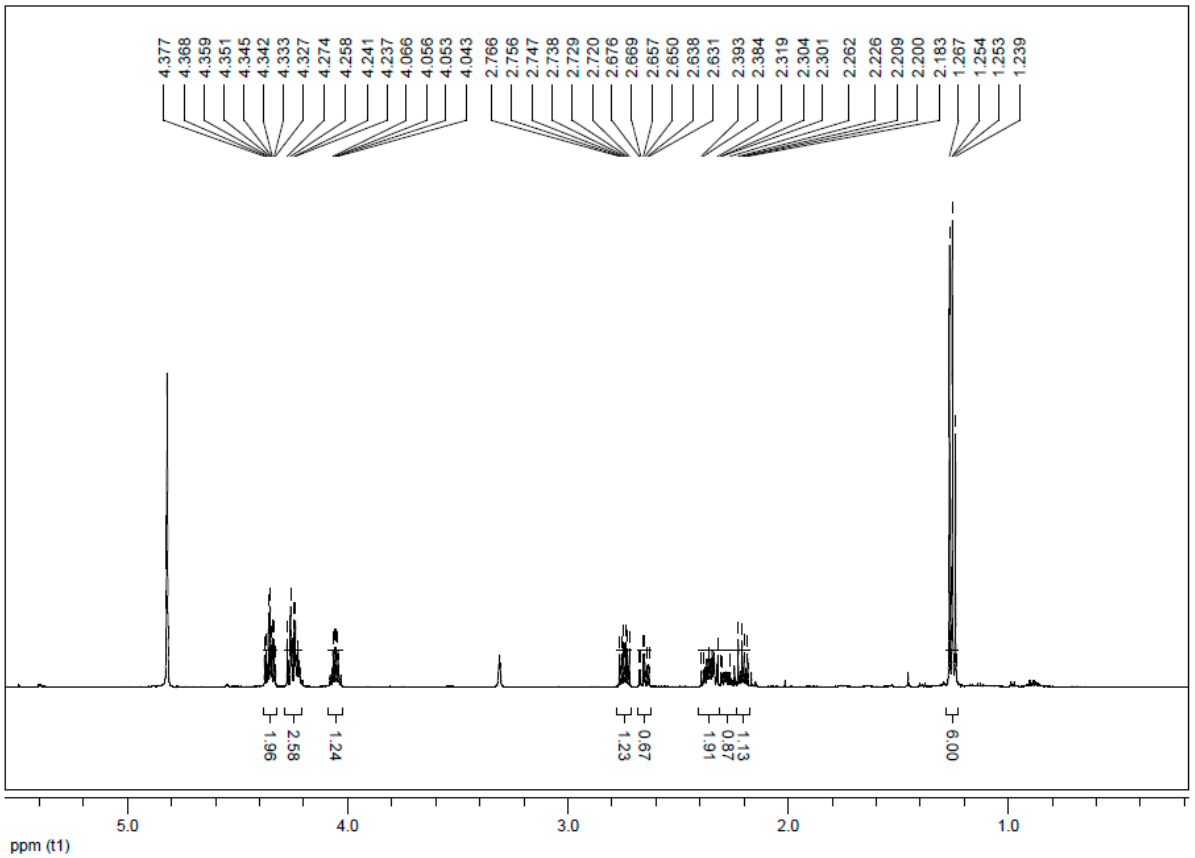

Figure S2. ^{1}H NMR (500 MHz, CD3OD) spectrum of α'-1'-hydroxyethyl-γ-butyrolactone **2**.

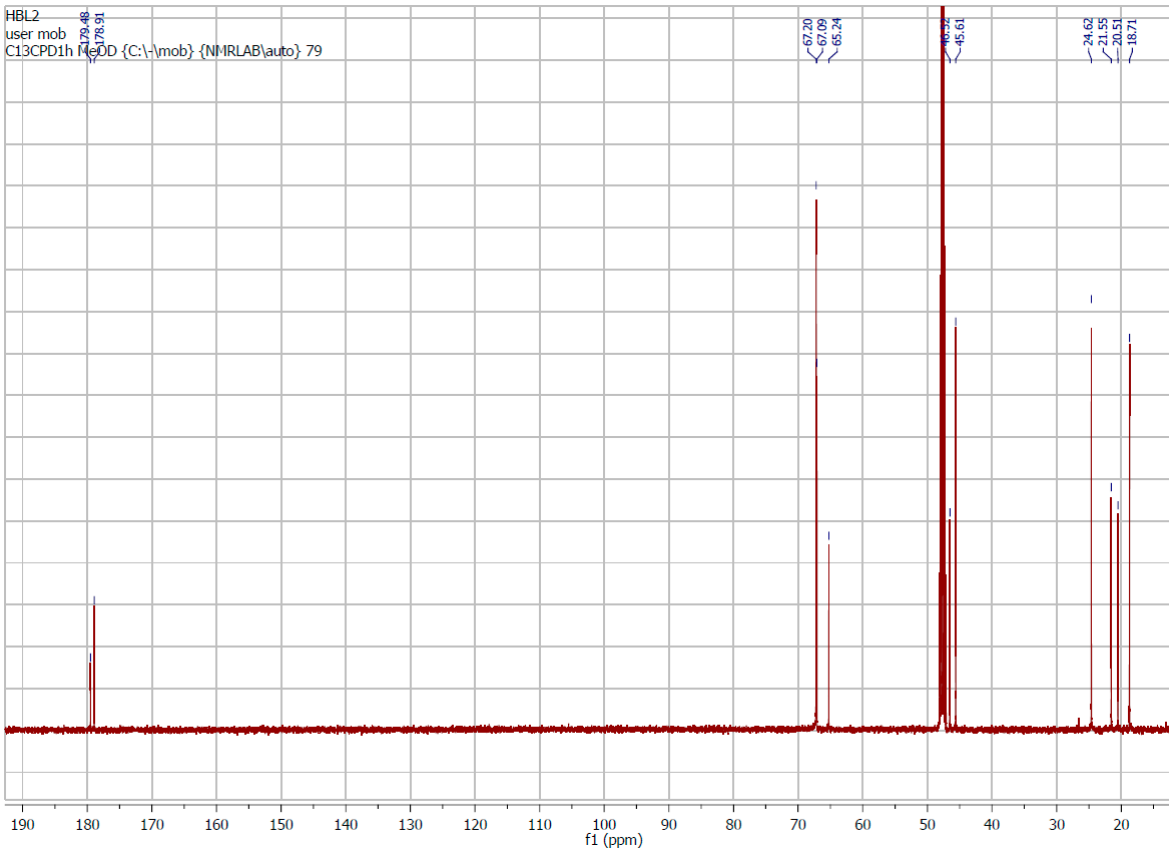

Figure S3. ^{13}C NMR (500 MHz, CD3OD) spectrum of α'-1'-hydroxyethyl-γ-butyrolactone **2**.

The chemical standard was analyzed also using a gas chromatograph (GC-MS), Saturn 2000 Varian Chrompack (Varian, Palo Alto, CA, USA), with a column ZB-1 (Phenomenex, CA, USA; (30 m × 0.25 mm ID × 0.25 μm film). The mass spectrometer with an ion-trap analyzer was set at 1508 for all analyses with an electron multiplier voltage of 1350 V. Scanning was performed from *m*/*z* 40 to 200 in 70 eV EI (electronic impact) at 1 scan/s. Helium, at a flow rate of 1.0 mL/min, was the carrier gas used in the analyses; the selected split ratio was 1:100 and the oven program was: 75 °C (hold 3 min), 75–80 °C (rate 2 °C/min), 80–150 °C (rate 17 °C/min), 150–280 (rate 30 °C/min), 280 °C (hold 1 min) The injector was held at 250 °C.

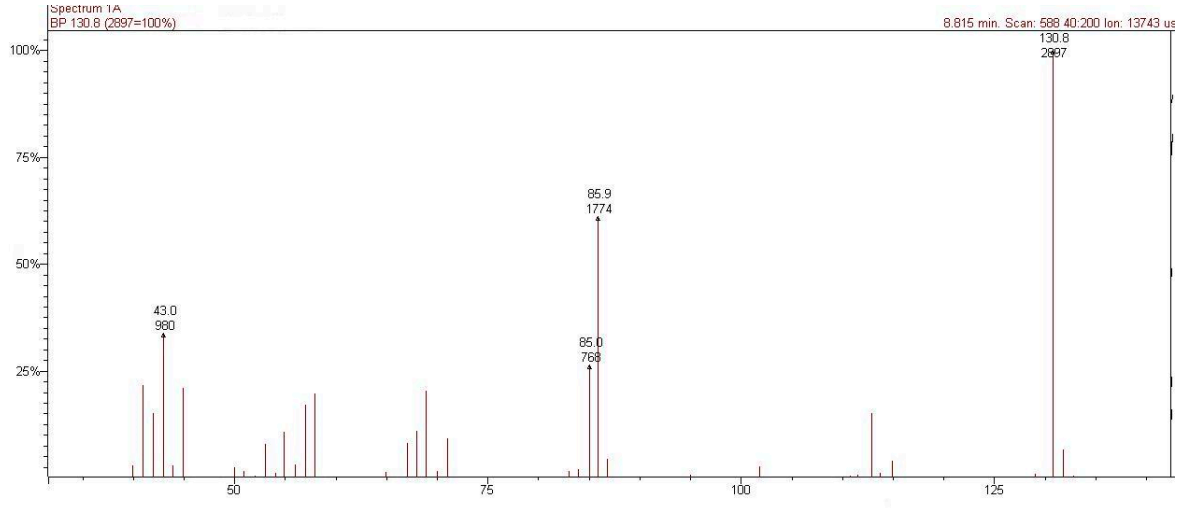

Figure S4. Mass spectrum of *anti* stereoisomer of α'-1'-hydroxyethyl-γ-butyrolactone **2**.

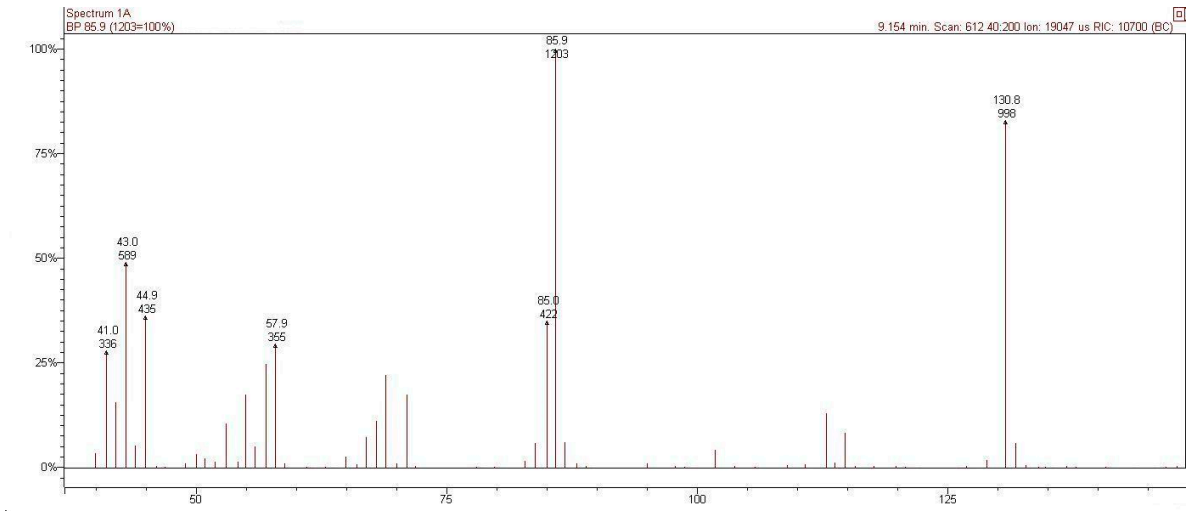

Figure S5. Mass spectrum of *syn* stereoisomer of α′-1′-hydroxyethyl-γ-butyrolactone **2**.

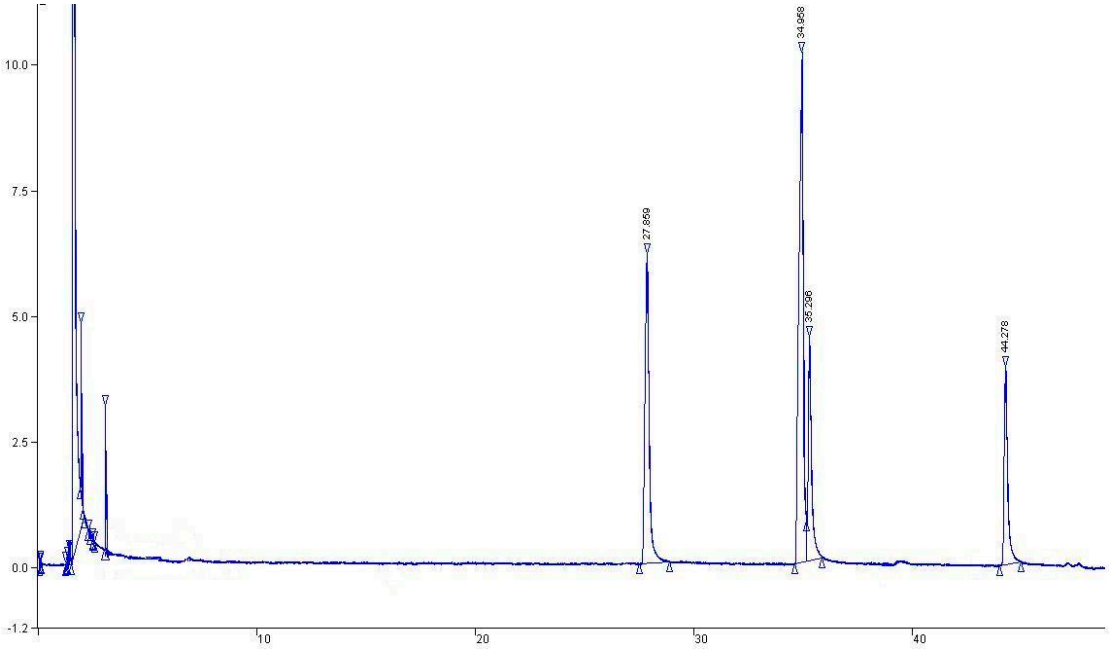

Figure S6. GC chromatogram of biotransformation of α-acetylbutyrolactone **1** by *Candida viswanathi* AM120 (Substrate **1** R_t = 27.9 min; ((3*S*,1′*S*)-**2a** R_t = 34.9 min; (3*R*,1′*R*)-**2b** R_t = 35.5 min; (3*R*,1′*S*)-**2d** R_t = 44.3 min).

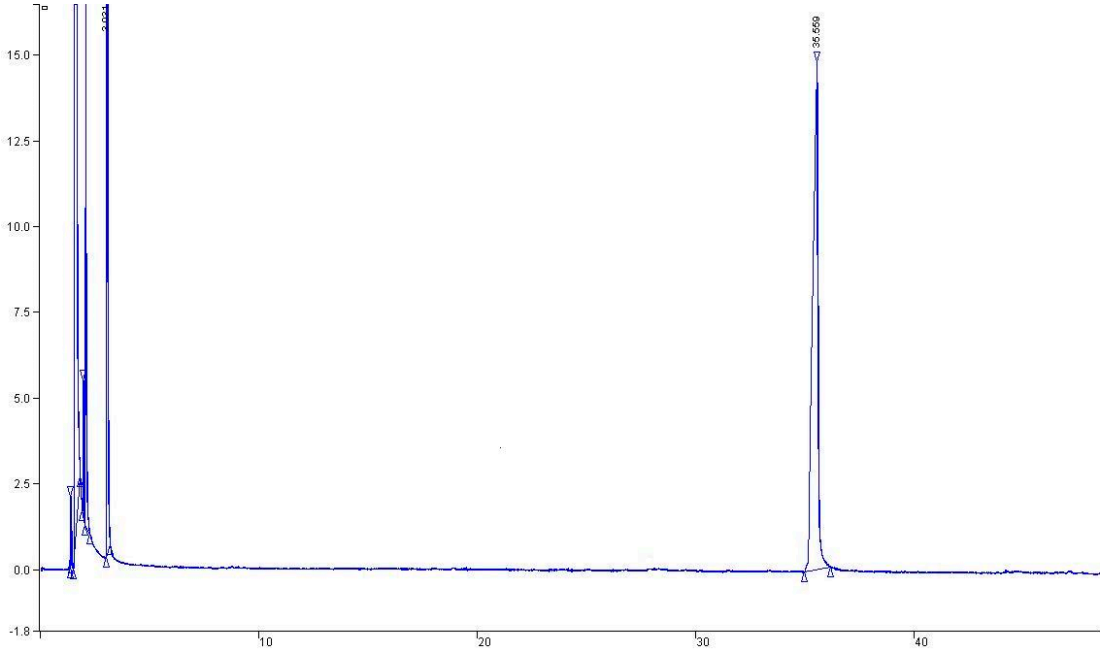

Figure S7. GC chromatogram of biotransformation of α-acetylbutyrolactone **1** by *Yarrowia lipolytica* P26A ((3*R*,1′*R*)-α'-1'-hydroxyethyl-γ-butyrolactone **2b** R_t = 35.5 min).