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SUPPLEMENTARY MATERIAL TO

Application of the redox system of *Nocardia corallina* B-276 in the enantioselective biotransformation of ketones and alcohols

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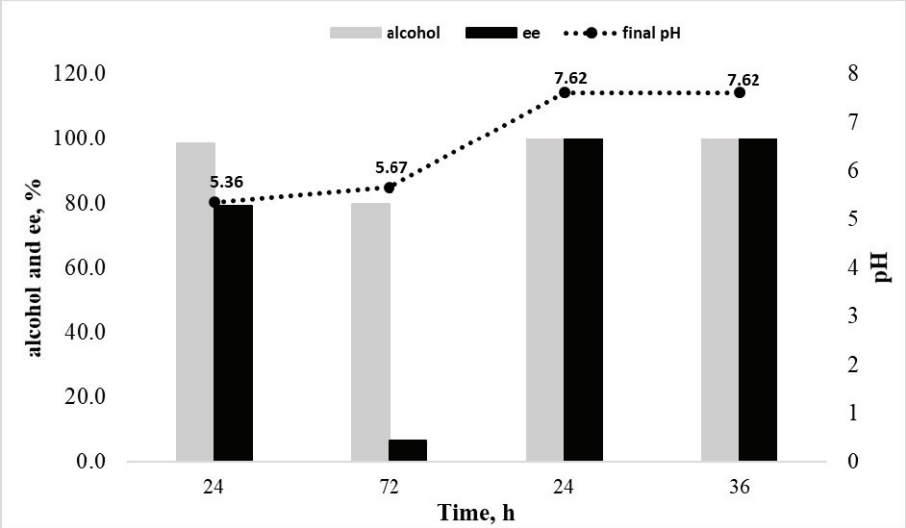

Fig. S-1. Reduction of ketone **1a** with *N. corallina* biomass, obtained at the final pH of the culture medium (5.36, 5.67 and 7.62).

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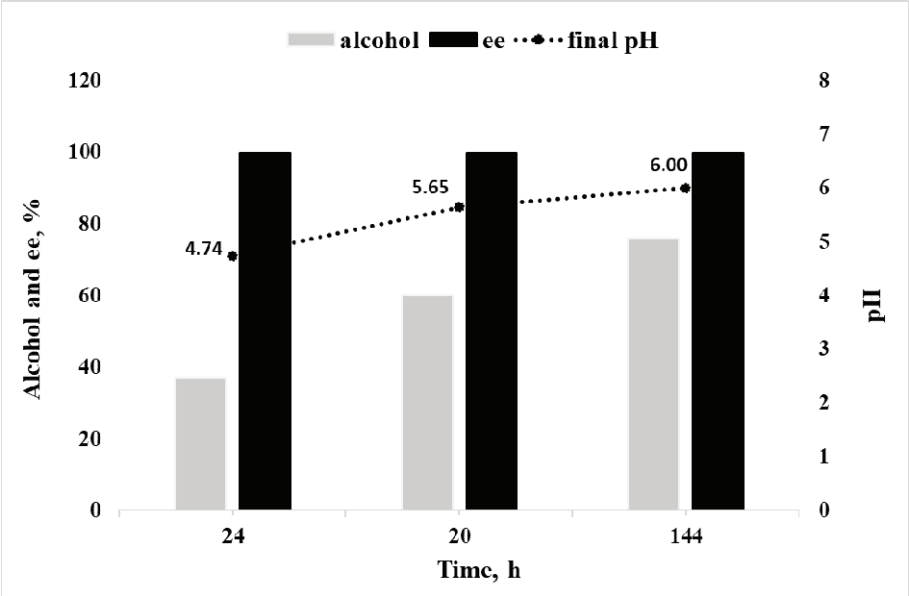

Fig. S-2. Biotransformation of **2a** with *N. corallina* biomass, obtained at the uncontrolled pH of the culture medium (4.74, 5.65 and 6.00).

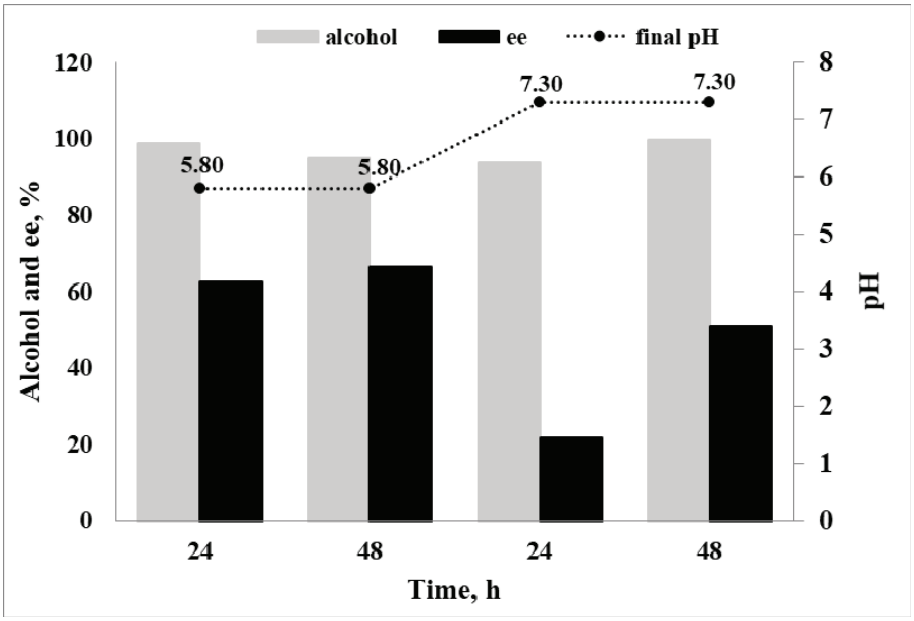

Fig. S-3. Biotransformation of **3a** with *N. corallina* biomass obtained at the uncontrolled pH of the culture medium (5.80 and 7.30).

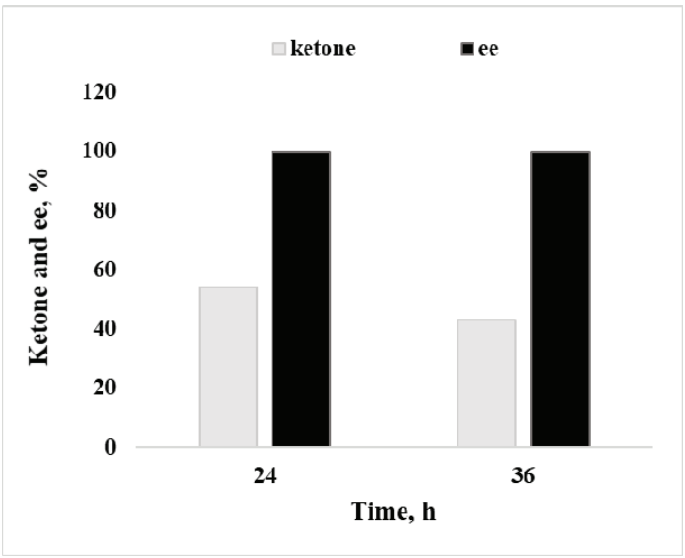

Fig. S-4. Biotransformation of **1b** with *N. corallina* biomass, final pH 7.62.

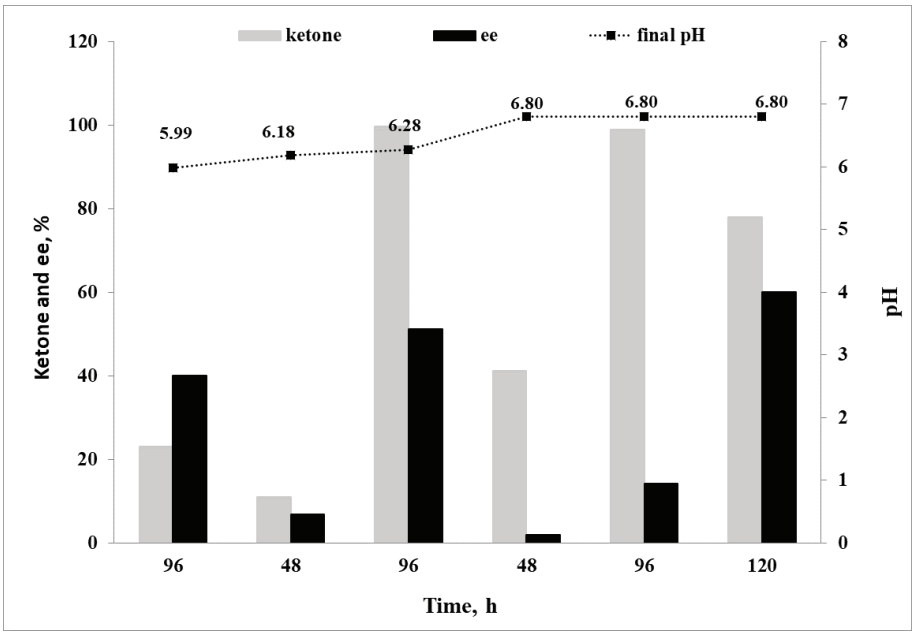

Fig. S5. Biotransformation of **2b** with *N. corallina* biomass obtained at the uncontrolled pH of the culture medium (5.99, 6.18, 6.28 and 6.80).

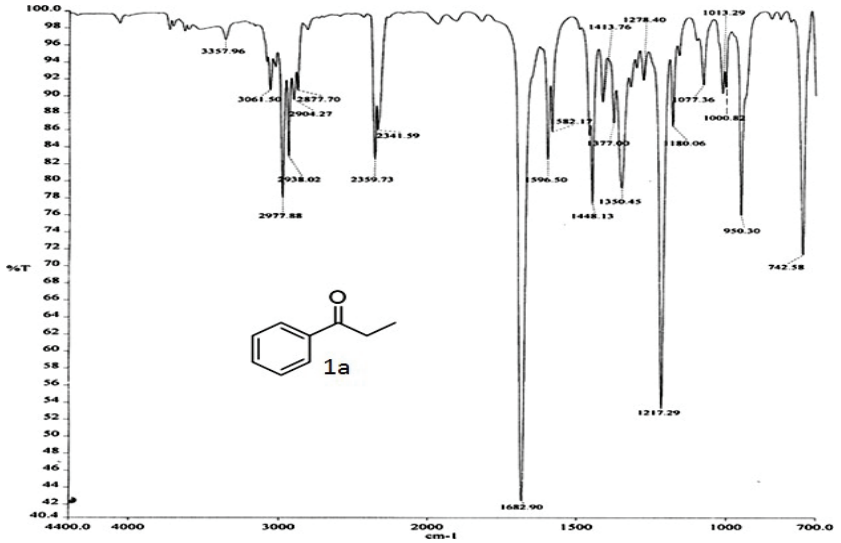

Fig. S-6. IR spectrum of 1-phenyl-1-propanone (**1a**).

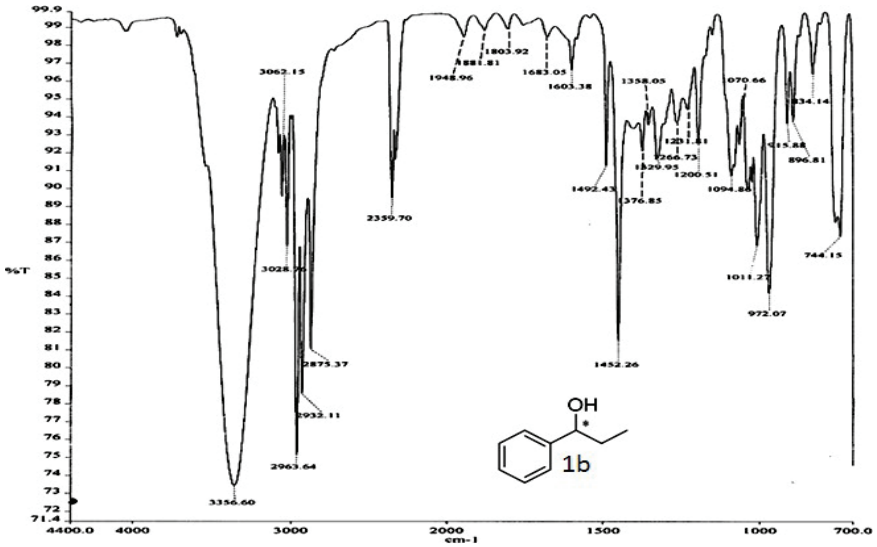

Fig. S-7. IR spectrum of 1-phenylpropan-1-ol (**1b**).

*The ^{1}H- and ^{13}C-NMR spectra of 1-phenyl-1-propanone (**1a**)*

^{1}H-NMR (600 MHz, $CDCl_3$, δ / ppm): 1.20 (3H, *t*, *J* = 7.3 Hz, CH_3), 2.96 (2H, *q*, *J* = 7.2 Hz, CH_2), 7.42 (2H, *t*, *J* = 7.7 Hz, CH), 7.51 (1H, *t*, *J* = 7.4 Hz, CH), 7.94 (2H, *dd*, *J* = 8.4 & 1.3 Hz, CH).

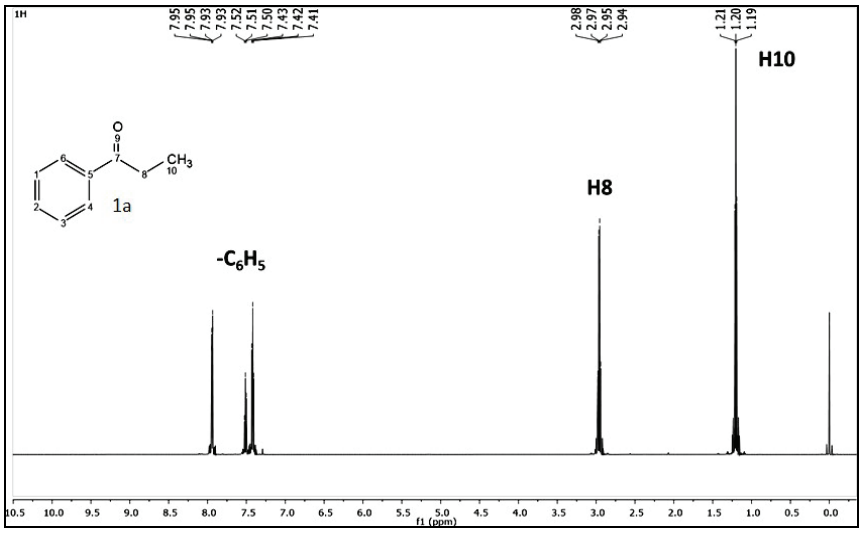

Figure S-8. ^{1}H-NMR spectrum of 1-phenyl-1-propanone (**1a**), in $CDCl_3$.

^{13}C-NMR (100 MHz, $CDCl_3$, δ/ ppm): 8.4 (C10), 31.7 (C8), 127.9/128.5 (C4, 3, 6 & 1), 132.9 (C2), 136.9 (C5), 200.7 (C7).

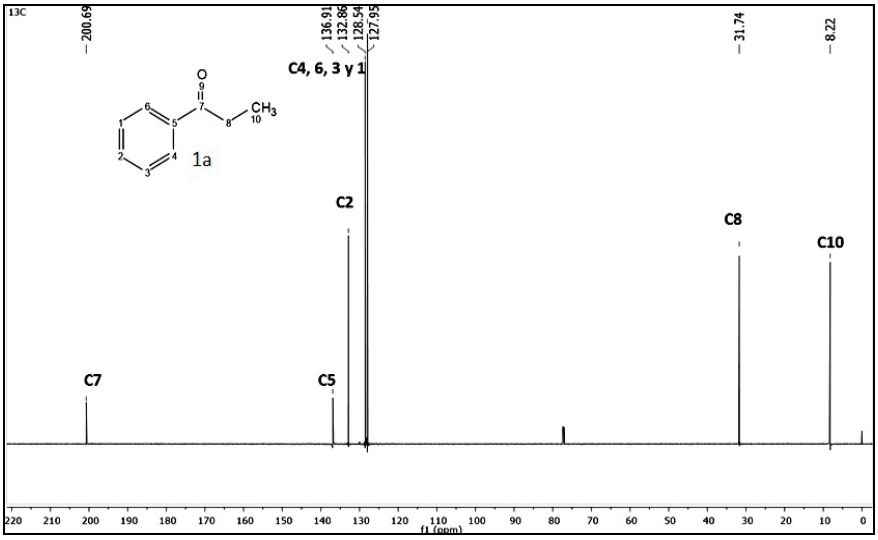

Fig. S-9. ^{13}C-NMR spectrum of 1-phenyl-1-propanone (**1a**), in $CDCl_3$.

*The ^{1}H- and ^{13}C-NMR spectra of 1-phenylpropan-1-ol (**1b**)*

^{1}H-NMR (600 MHz, $CDCl_3$, δ / ppm): 0.77 (3H, *t*, J = 7.5 Hz, CH_3), 1.61 (2H, *ddt*, J = 2.1, 13.6 & 6.9 Hz, CH_2), 3.99 (1H, *s*, OH), 4.41 (1H, *t*, J = 6.7 Hz, CH), 7.13–7.19 (5H, *dt*, J = 12.8 & 6.9 Hz, CH).

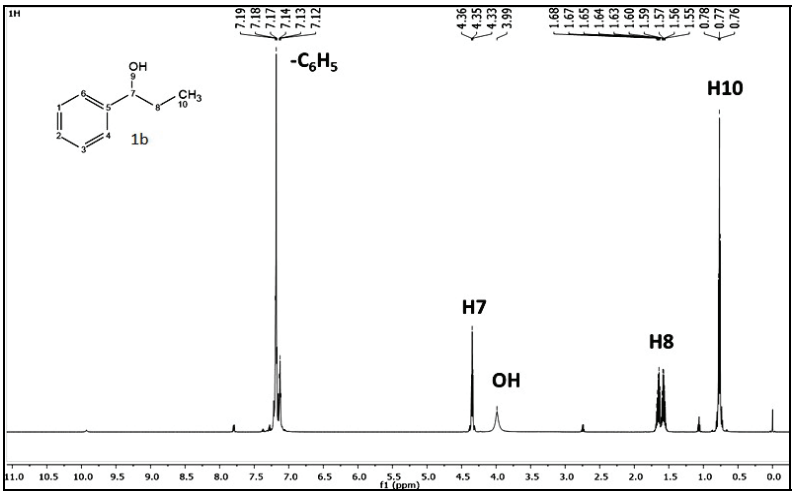

Fig. S-10. ^{1}H-NMR spectrum of 1-phenylpropan-1-ol (**1b**), in $CDCl_3$.

^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): δ 10.2 (C10), 31.9 (C8), 75.7 (C7), 126.2 (C2), 127.3 (C6 & C4), 128.3 (C1 & C3) and 144.9 (C5) ppm.

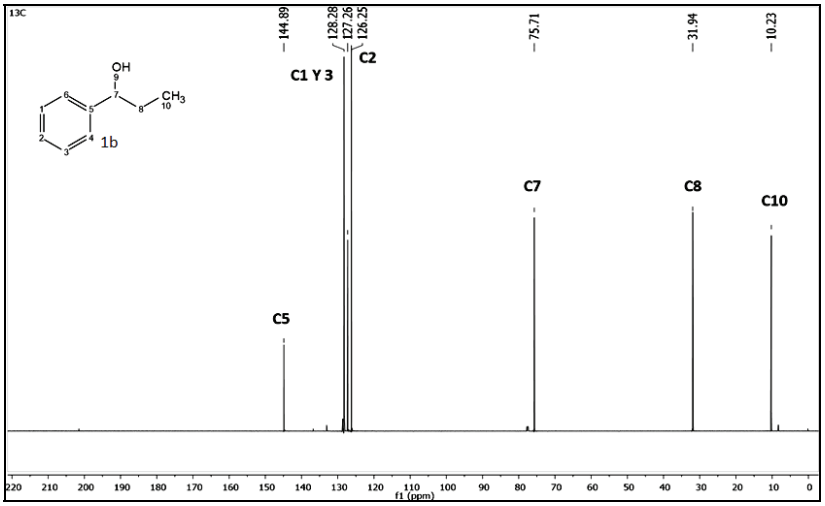

Fig. S-11. ^{13}C-NMR spectrum of 1-phenylpropan-1-ol (**1b**), in $CDCl_3$.

The GC chromatograms of **1a** and **1b** with retention times of 4.39 and 5.63 min, respectively under conditions reported in the Experimental Section.

Fig. S-12. GC chromatograms of 1-phenyl-1-propanone (**1a**) and 1-phenylpropan-1-ol (**1b**).

The HPLC chromatogram of a mixture of **1a** & ***rac*-(1b)**, separately **1a** and (*S*)-**1b** & (*R*)-**1b** with retention times of: (20.4, 11.4 and 9.6 min, respectively, column OB-H and 7.7, 14.9 and 12.7 min, respectively, column OD) with conditions reported in the Experimental Section.

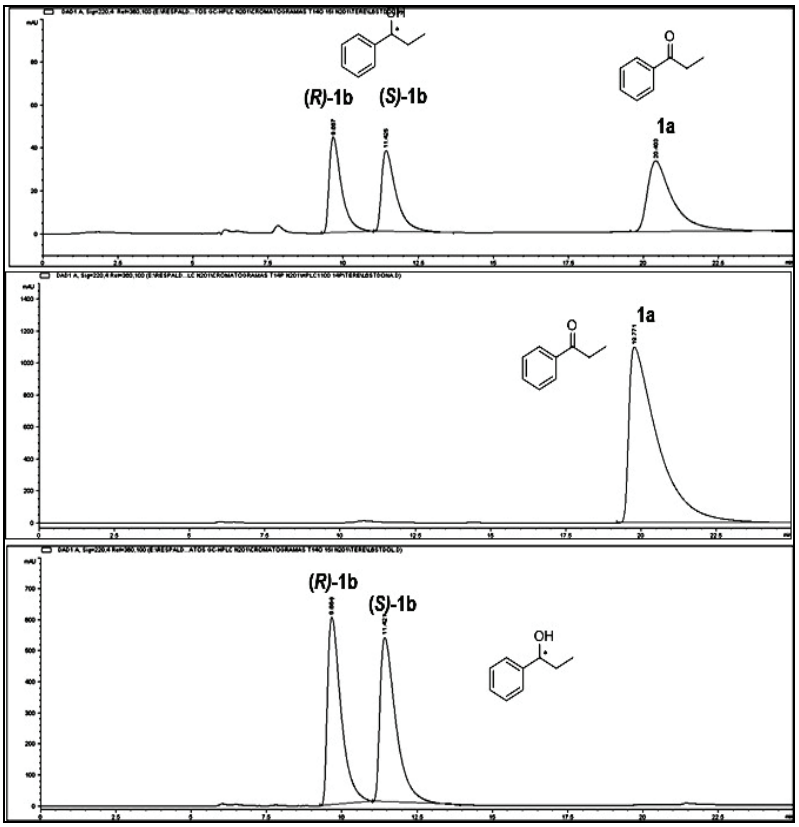

Fig. S-13. HPLC chromatogram (OB-H column) of mixture of 1-phenyl-1-propanone (**1a**) & *rac*-1-phenylpropan-1-ol (**1b**), separately **1a** and (*S*)-**1b** *&* (*R*)-**1b.**

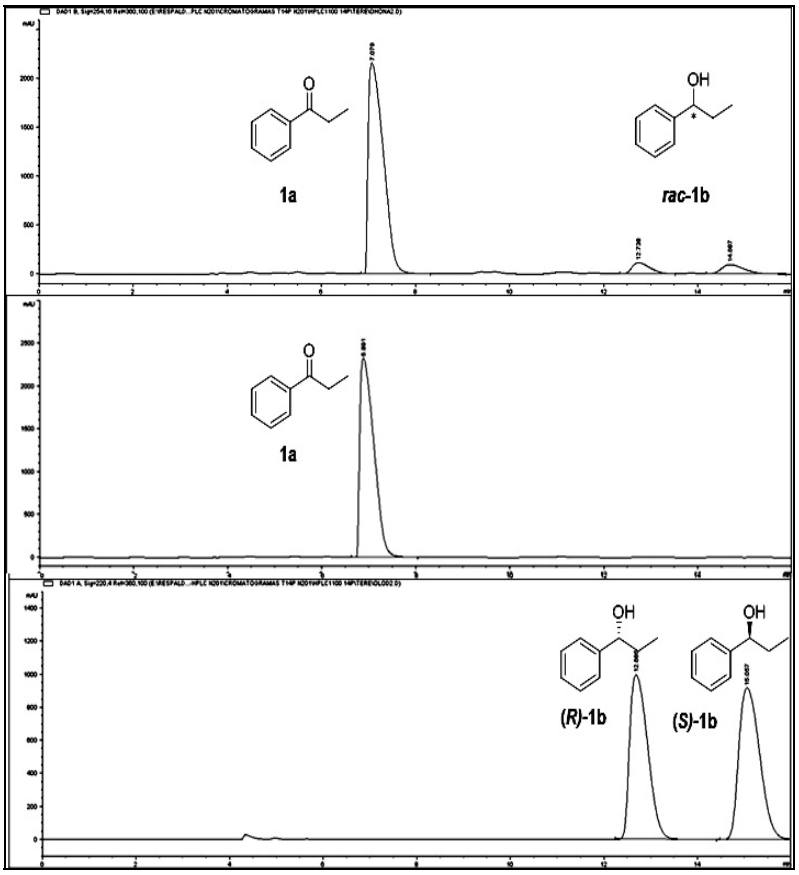

Fig. S-14. HPLC chromatogram (OD column) of a mixture of 1-phenyl-1-propanone (**1a**) & *rac*-1-phenylpropan-1-ol (**1b**), separately **1a** and (*S*)-**1b** **&** (*R*)-**1b**.

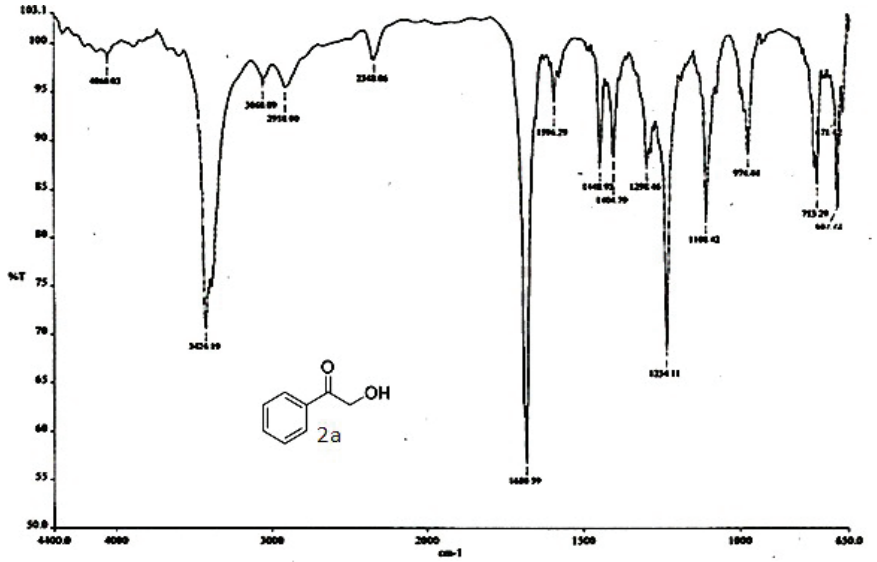

Fig. S-15. IR spectrum of 2-hydroxy-1-phenylethanone (**2a**).

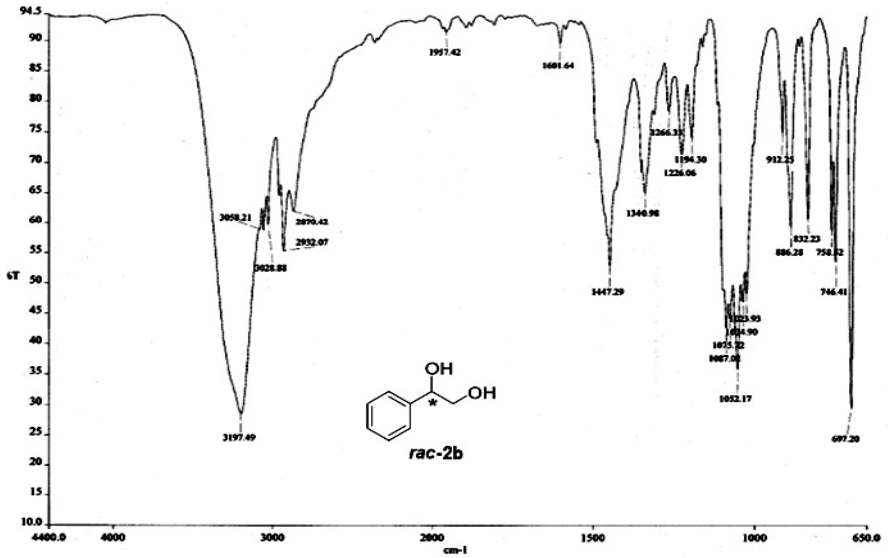

Fig. S-16. IR spectrum of 1-phenyl-1,2-ethanediol (**2b**).

*The ^{1}H- and ^{13}C-NMR spectra of 2-hydroxy-1-phenylethanone (**2a**)*

^{1}H-NMR (600 MHz, $CDCl_3$, δ / ppm): 4.9 (2H, *m*, CH_2), 5.4 (1H, *s*, OH), 7.5 (2H, *dd*, J = 11.9 & 3.9 Hz, CH), 7.63 (1H, *t*, J = 7.7 Hz, CH), 7.93 (2H, *dd*, J = 8.3 & 1.1 Hz, CH).

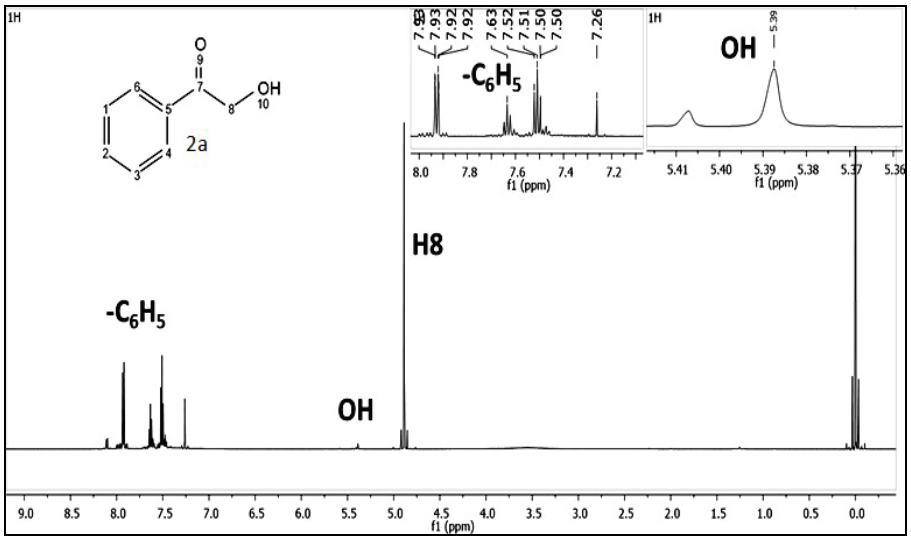

Fig. S-17. ^{1}H-NMR spectrum of 2-hydroxy-1-phenylethanone (**2a**) in $CDCl_3$.

^{13}C-NMR (100 MHz, CDCl3, δ / ppm): 65.5 (C8), 127.7/128.4 (C4 & C1), 128.9/129.5 (C6 & C1), 133.6 (C2), 198.4 (C7).

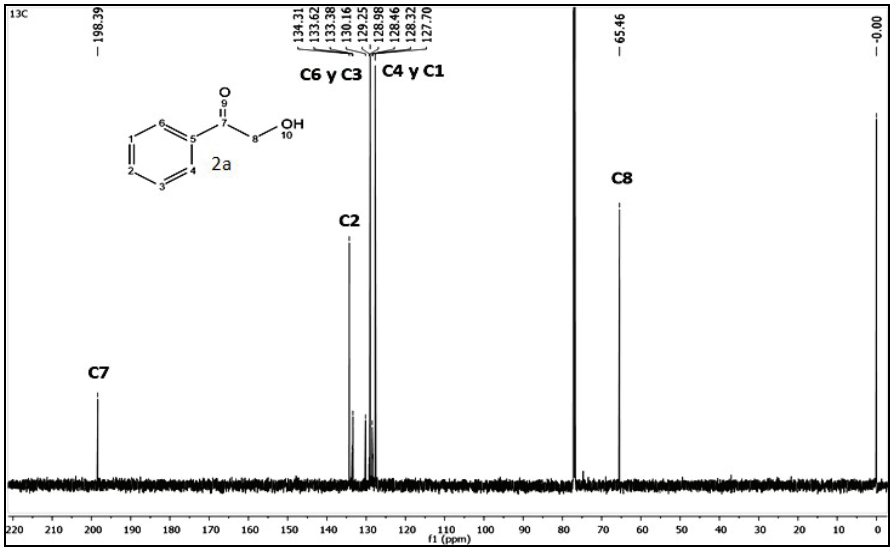

Fig. S-18. ^{13}C-NMR spectrum of 2-hydroxy-1-phenylethanone (**2a**), in $CDCl_3$.

*The ^{1}H- and ^{13}C-NMR spectra of 1-phenyl-1,2-ethanediol (**2b**)*

^{1}H-NMR (600 MHz, $CDCl_3$, δ / ppm): 2.3 (1H, *s*, OH), 3.2 (1H, *s*, OH), 3.49–3.78 (2H, *m*, CH_2) 4.8 (1H, *dd*, J = 8.4 & 3.3 Hz, CH), 7.09–7.48 (5H, *m*, CH).

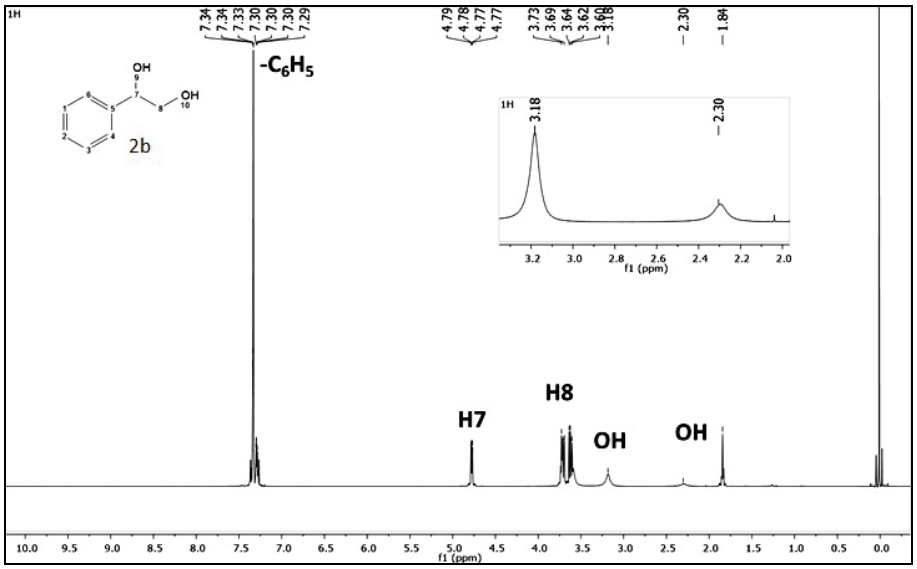

Fig. S-19. ^{1}H-NMR spectrum of 1-phenyl-1,2-ethanediol (**2b**) in $CDCl_3$.

^{13}C-NMR (100 MHz, $CDCl_3$ δ / ppm,): 67.95/68.04 (C8), 74.7 (C7), 126.07 (C4 & C6), 127.9 & 128.5 (C1, 2 & C3), 140.5 (C5).

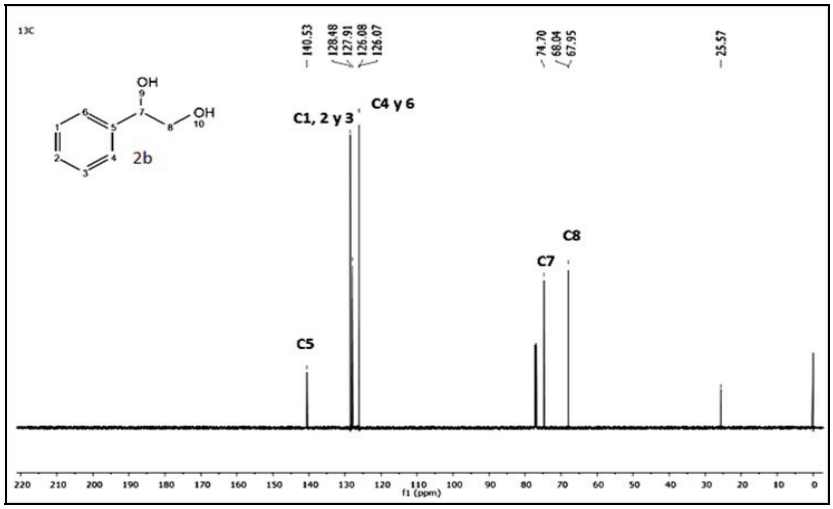

Fig. S-20. ^{13}C-NMR spectrum of 1-phenyl-1,2-ethanediol (**2b**), in $CDCl_3$.

The GC chromatograms of **2a** and **2b** with retention times of 4.90 and 5.79 min, respectively, with conditions reported in the Experimental Section.

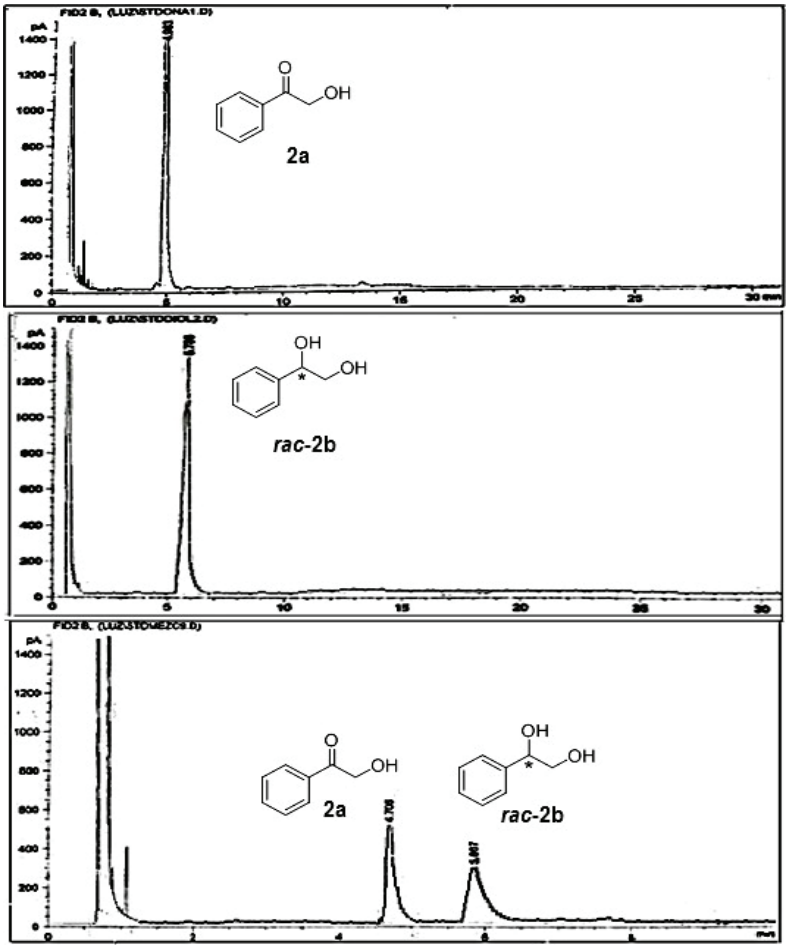

Fig. S-21. GC chromatograms of 2-hydroxy-1-phenylethanone (**2a**) and 1-phenyl-1,2-ethanediol (**2b**) and a mixture of **2a** and *rac*-**2b**.

The HPLC chromatograms of mixtures of **2a**, (*S*)-**2b** and (*R*)-**2b** with retention times of 17.12, 11.38 and 9.04 min, respectively, with conditions reported in the Experimental Section.

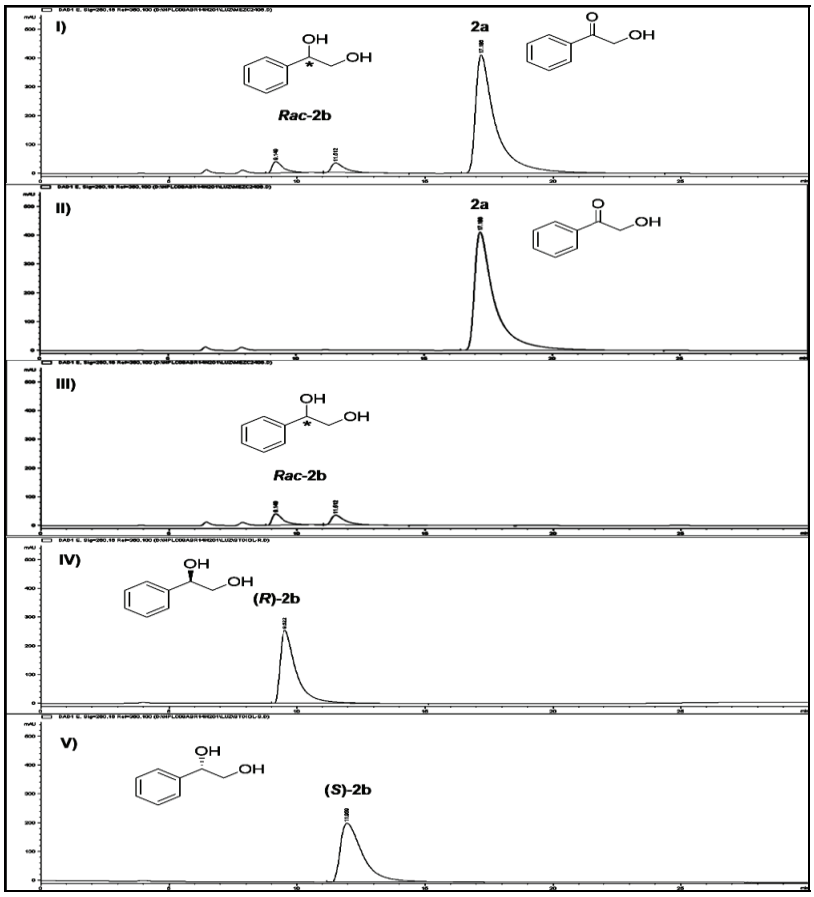

Fig. S-22. HPLC chromatogram of: I) mixture of 2-hydroxy-1-phenylethanone (**2a**) and *rac*-1-phenyl-1,2-ethanediol (*rac*-**2b**); II) 2-hydroxy-1-phenylethanone (**2a**); III) r*ac*-1- phenyl-1,2-ethanediol (*rac*-**2b**); IV) (*R*)-1-phenyl-1,2-ethanediol (*R*-**2b**); V) (*S*)-1-phenyl-1,2-ethanediol (*S***2b**)

The HPLC chromatograms of mixtures of **2a**, (*S*)-**2b** and (*R*)-**2b** with retention times of 28.9, 18.9 and 15.1 min, respectively, under the conditions reported in the Experimental Section.

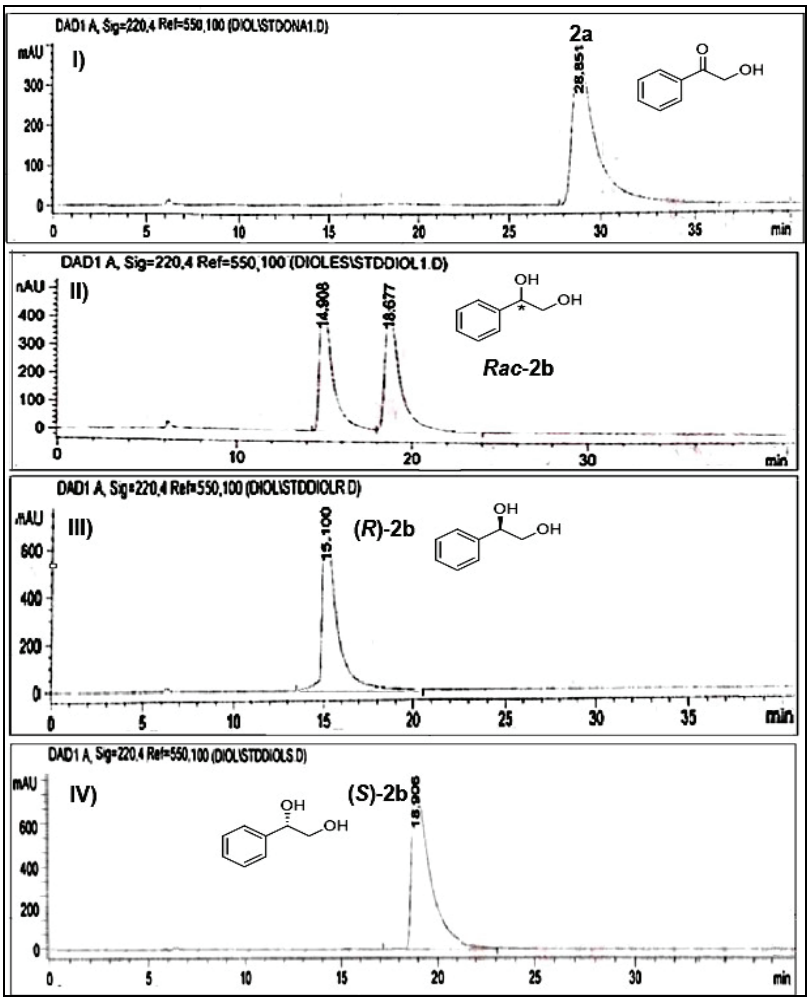

Fig. S-23. HPLC chromatogram of: I) 2-hydroxy-1-phenylethanone (**2a**); II) *rac*-1-phenyl-1,2-ethanediol (*rac*-**2b**); III) (*R*)-1-phenyl-1,2-ethanediol (*R*-**2b**); IV) (*S*)-1-phenyl-1,2-ethanediol ((*S*)-**2b**).

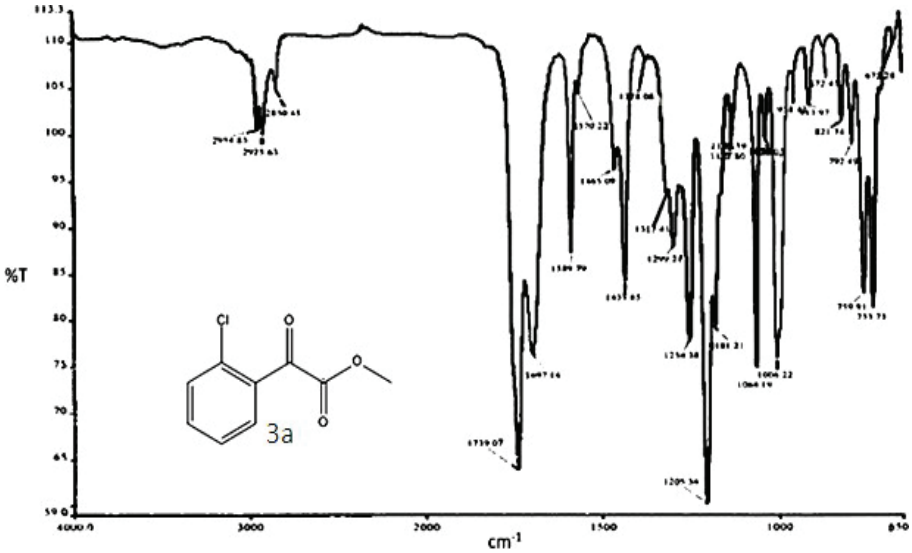

Fig. S-24. IR spectrum of methyl (2-chlorophenyl)(oxo)acetate (**3a**).

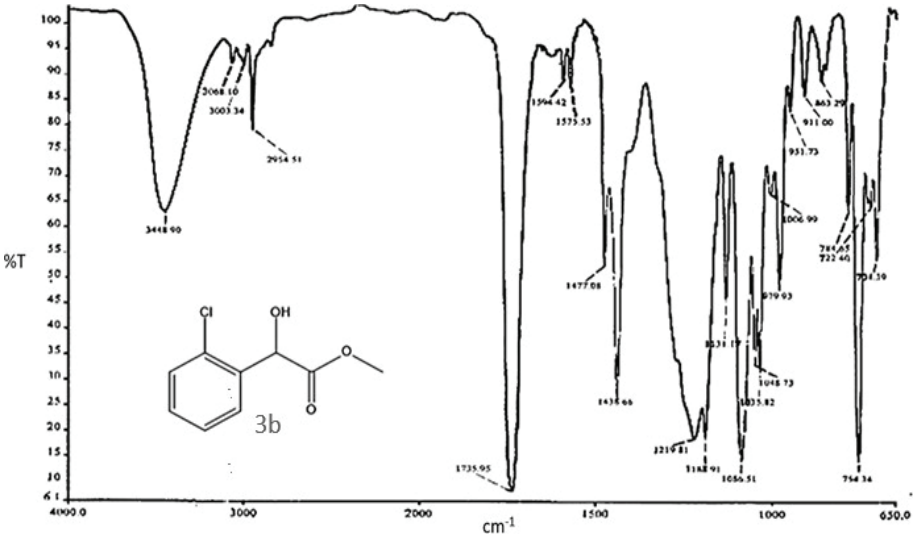

Fig. S-25. IR spectrum of methyl (2-chlorophenyl)(hydroxy)acetate (**3b**).

*The ^{1}H- and ^{13}C-NMR spectra of methyl (2-chlorophenyl)(oxo)acetate (**3a**)*

^{1}H-NMR (600 MHz, $CDCl_3$, δ / ppm): 3.96 (3H, *s*), 7.43 (2H, *m*), 7.53 (1H, *ddd*, *J* =8.0, 7.4 & 1.7 Hz), 7.77 (1H, *dd*, *J* =7.7 & 1.7 Hz).

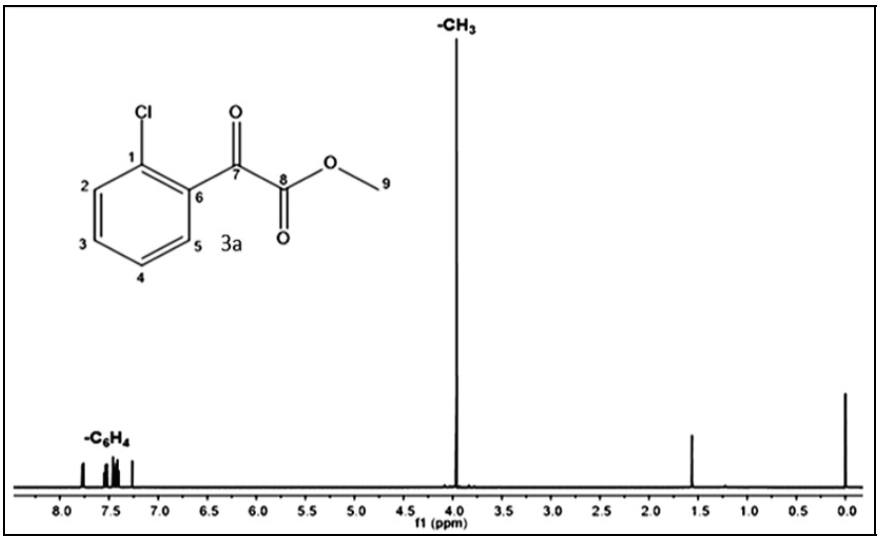

Fig. S-26. ^{1}H-NMR spectrum of methyl (2-chlorophenyl)(oxo)acetate (**3a**), in $CDCl_3$

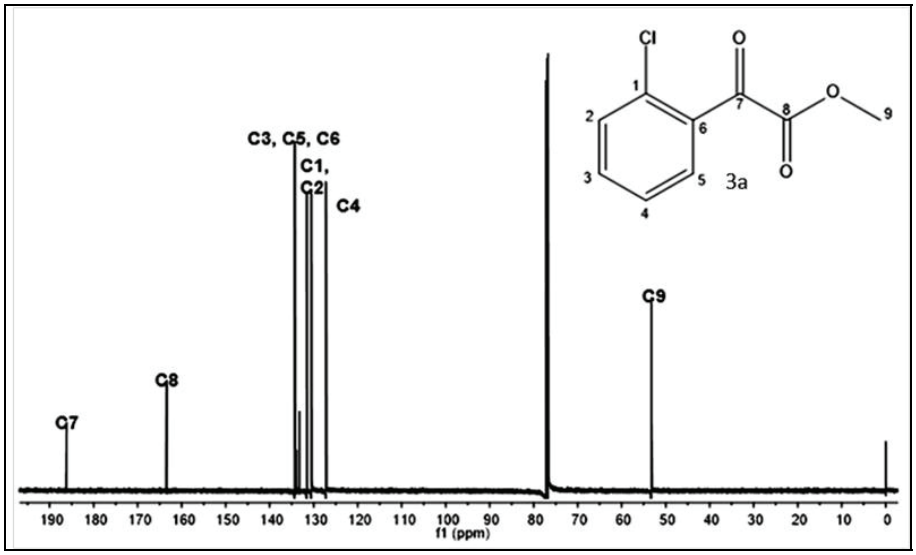

Fig. S-27. ^{13}C-NMR spectrum of methyl (2-chlorophenyl)(oxo)acetate (**3a**), in $CDCl_3$.

^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 53.2 (C9), 127.2 (C4), 130.5 (C2), 131.6 (C5), 133.2 (C6), 133.9 (C1), 134.3 (C3), 163.4 (C8), 186.2 (C7).

*The ^{1}H- and ^{13}C-NMR spectra of methyl (2-chlorophenyl)(hydroxy)acetate (**3b**)*

^{1}H-NMR (600 MHz, $CDCl_3$, δ / ppm): 3.6 (1H, *d*, J = 5.1 Hz, OH), 3.8 (3H, *s*, CH_3), 5.6 (1H, *d*, J = 5.1 Hz, CH) 7.3 (2H, *m*), 7.4 (2H, *m*).

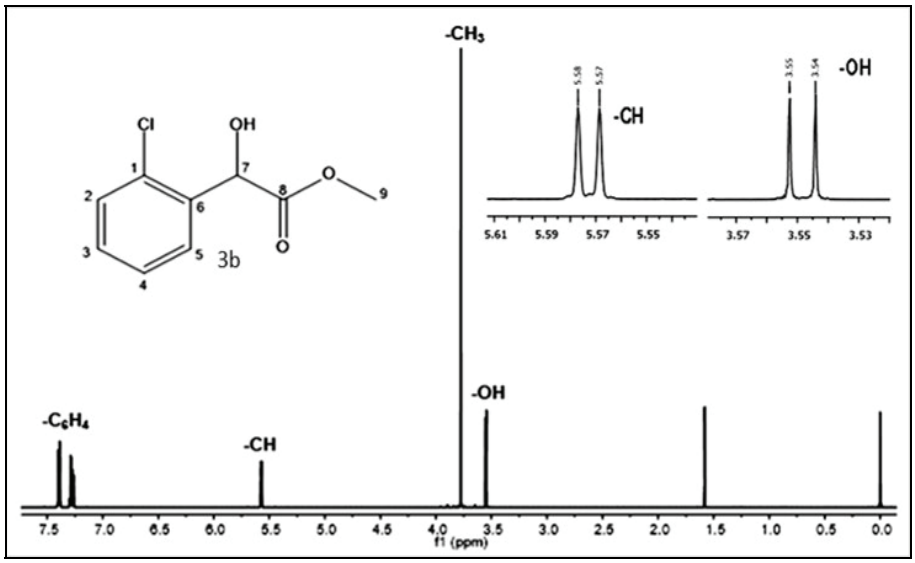

Fig. S-28. 1H-NMR spectrum of methyl (2-chlorophenyl)(hydroxy)acetate (**3b**), in $CDCl_3$.

^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 53.2 (C9), 70.3 (C7), 127.1 (C4), 128.8 (C2), 129.7(C5), 129.9 (C3), 133.41 (C1), 135.9 (C6), 173.7 (C8).

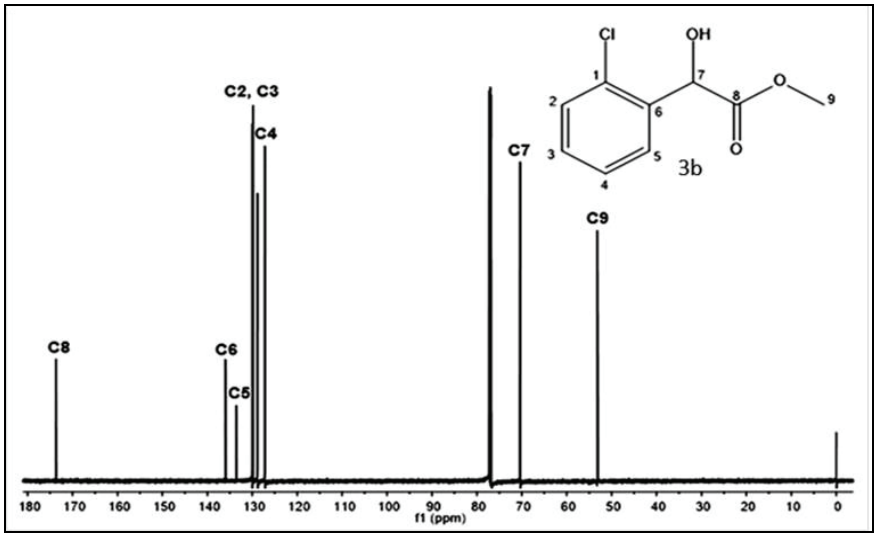

Fig. S-29. ^{13}C-NMR spectrum of methyl (2-chlorophenyl)(hydroxy)acetate (**3b**), in $CDCl_3$.

The GC chromatograms of **3a** and **3b** with retention times of 4.6 and 6.1 min, respectively, under conditions reported in the Experimental Section.

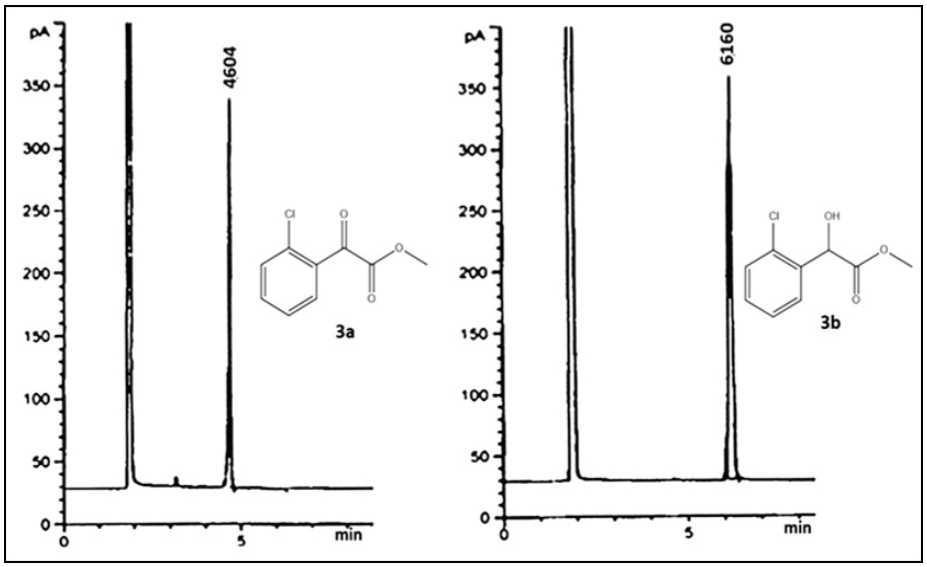

Fig. S-30. GC chromatograms of methyl (2-chlorophenyl)(oxo)acetate (**3a**) and methyl (2-chlorophenyl)(hydroxy)acetate (**3b**).

The HPLC chromatogram of the mixture of **3a,** (*S*)-**3b** and (*R*)-**3b** with retention times of 7.0, 8.9 and 10.2 min, respectively, under conditions reported in the Experimental Section.

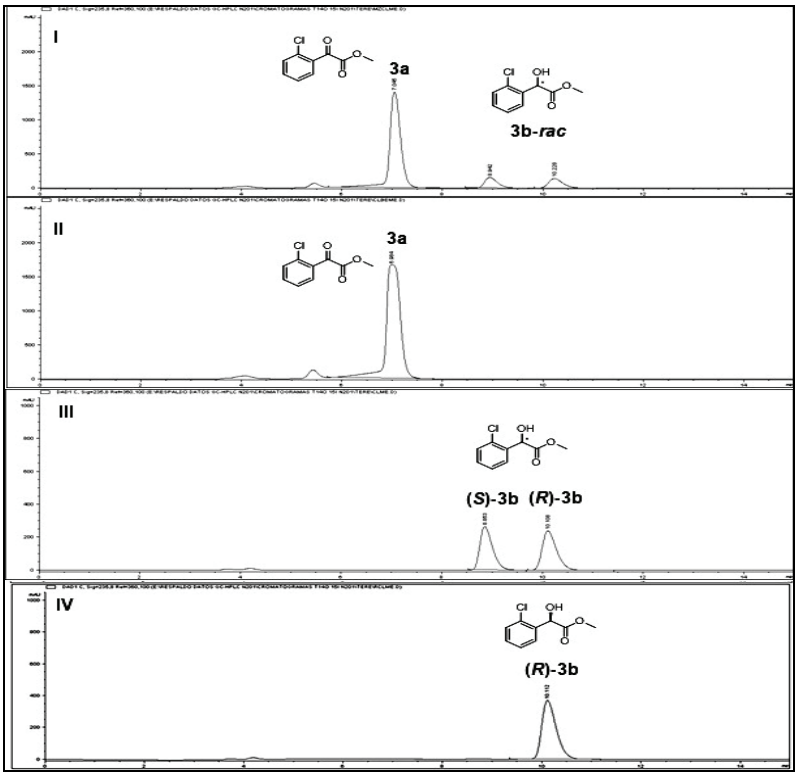

Fig. S-31. HPLC chromatogram of: I) mixture of methyl (2-chlorophenyl)(oxo)acetate (**3a**) and *rac*-methyl (2-chlorophenyl)(hydroxy)acetate (*rac*-**3b**); II) methyl (2-chlorophenyl)(oxo)-acetate (**3a**); III) *rac*-methyl (2-chlorophenyl)(hydroxy)acetate (*rac*-**3b**) and IV (*R*)-methyl (2-chlorophenyl)(hydroxy)acetate (*R*-**3b**).

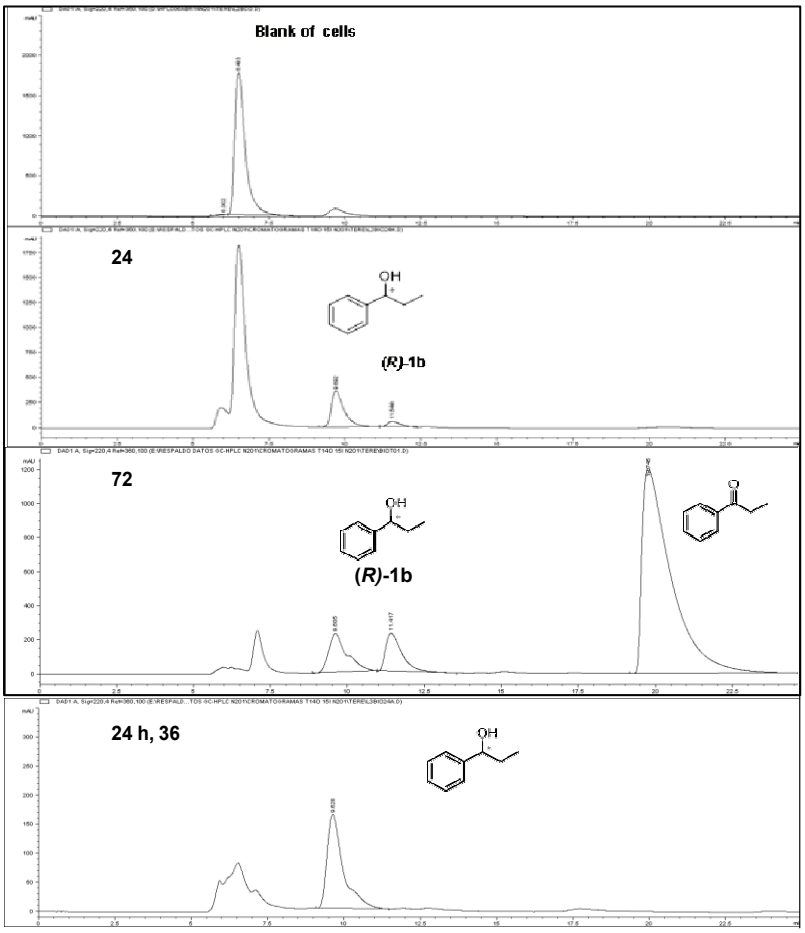

Fig. S-32. HPLC chromatogram of Fig. 2. Reduction of ketones **1a** with *N. corallina* biomass, final pH (5.36, 5.67 and 7.62).

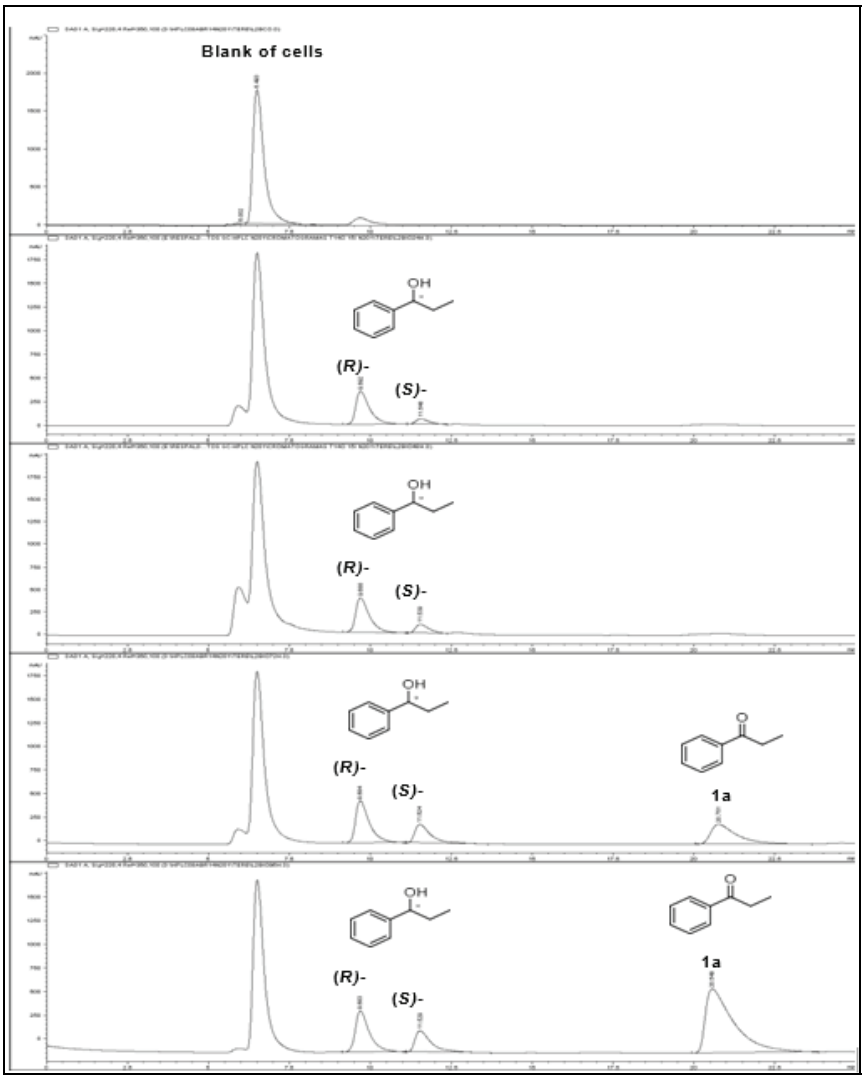

Fig. S-33. HPLC chromatogram of Fig. 3. Biotransformation of **1a** with *N. corallina* biomass, final pH 5.36.

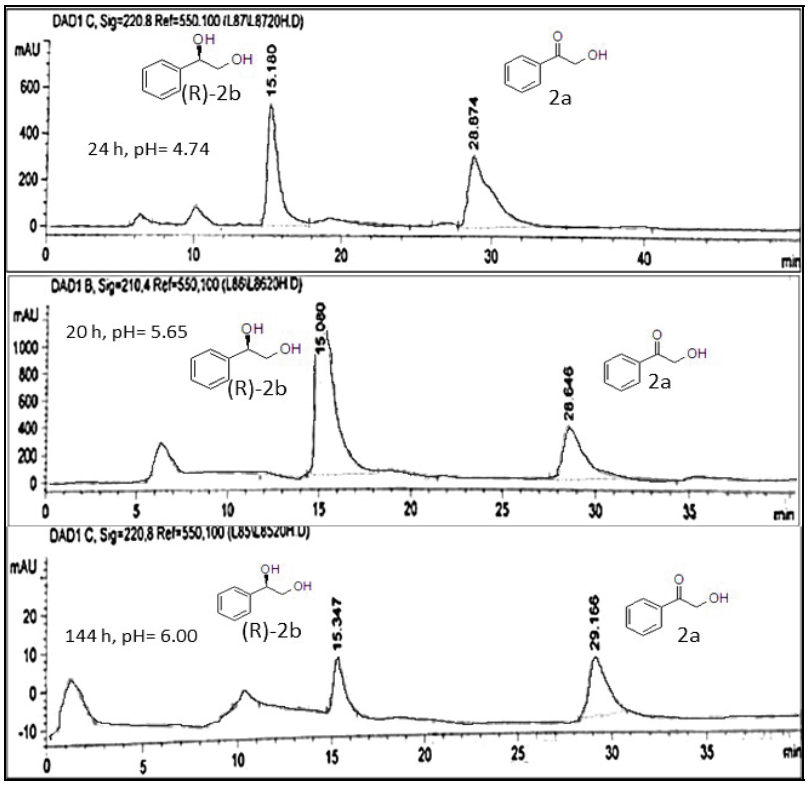

Fig. S-34. HPLC chromatogram of Fig. 4. Biotransformation of **2a** with *N. corallina* biomass, for different final pH values and times.

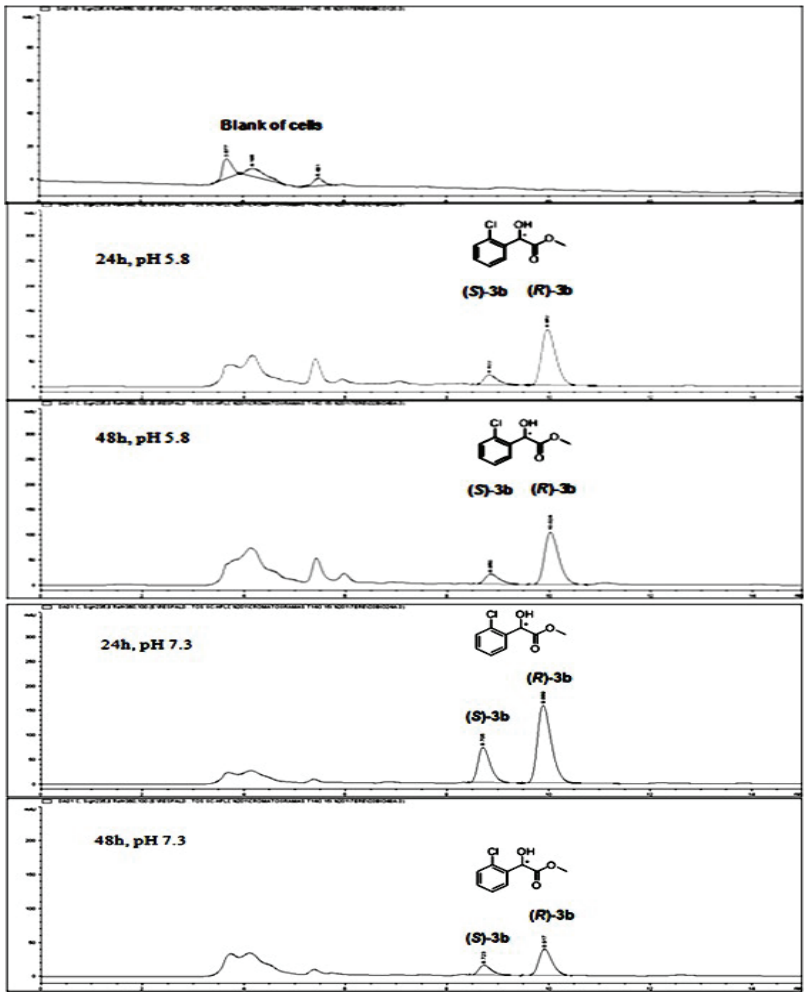

Fig. S-35. HPLC chromatogram of Fig. 5. Biotransformation of **3a** with *N. corallina* biomass, final pH 5.8 and 7.3.

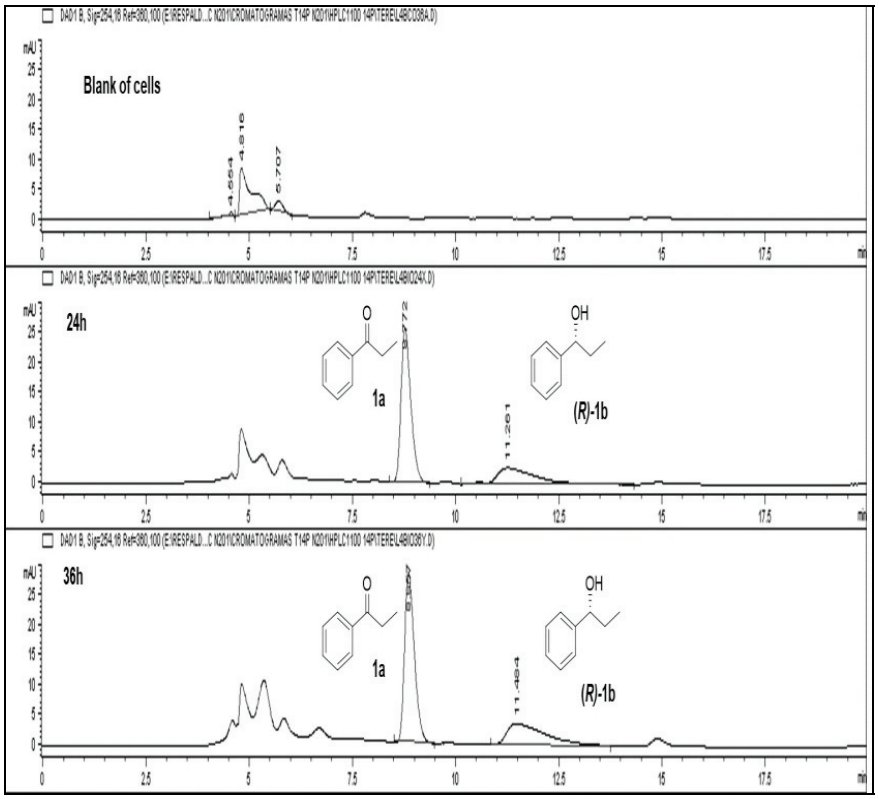

Fig. S-36. HPLC chromatogram of Fig. 6. Biotransformation of **1b** with *N. corallina* biomass, final pH 7.62.

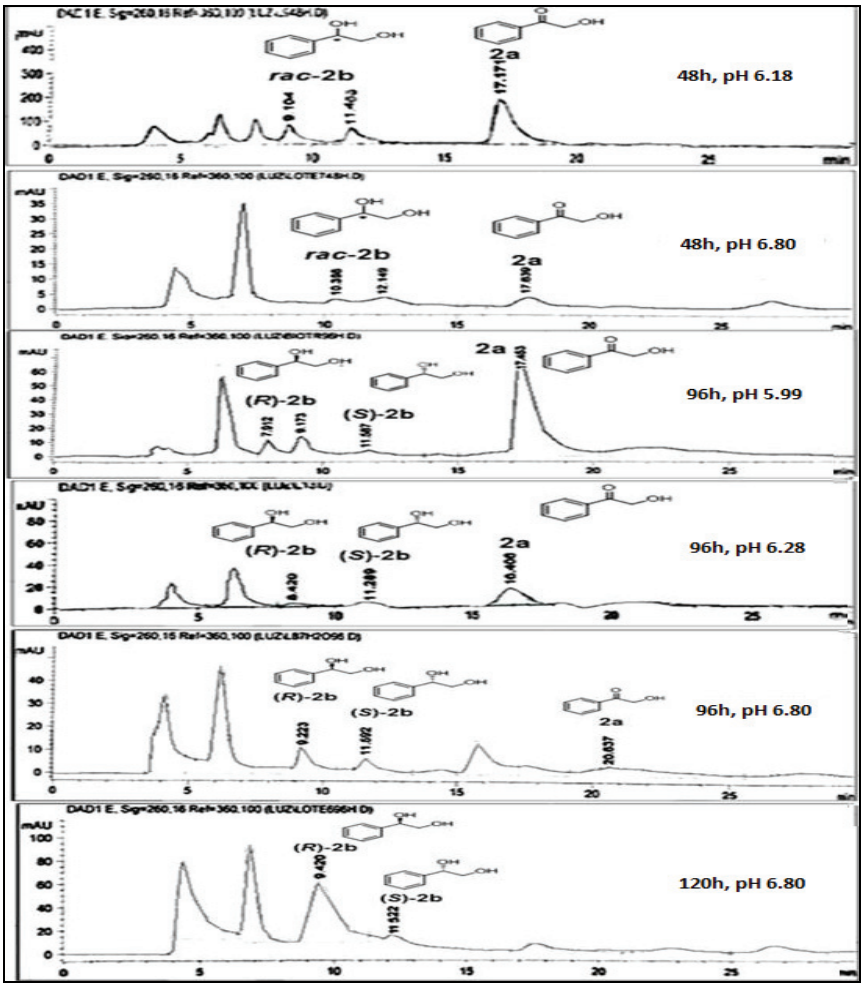

Fig. S-37. HPLC chromatogram of Fig. 7. Biotransformation of **2b** with *N. corallina* biomass, at different final pH values and times.

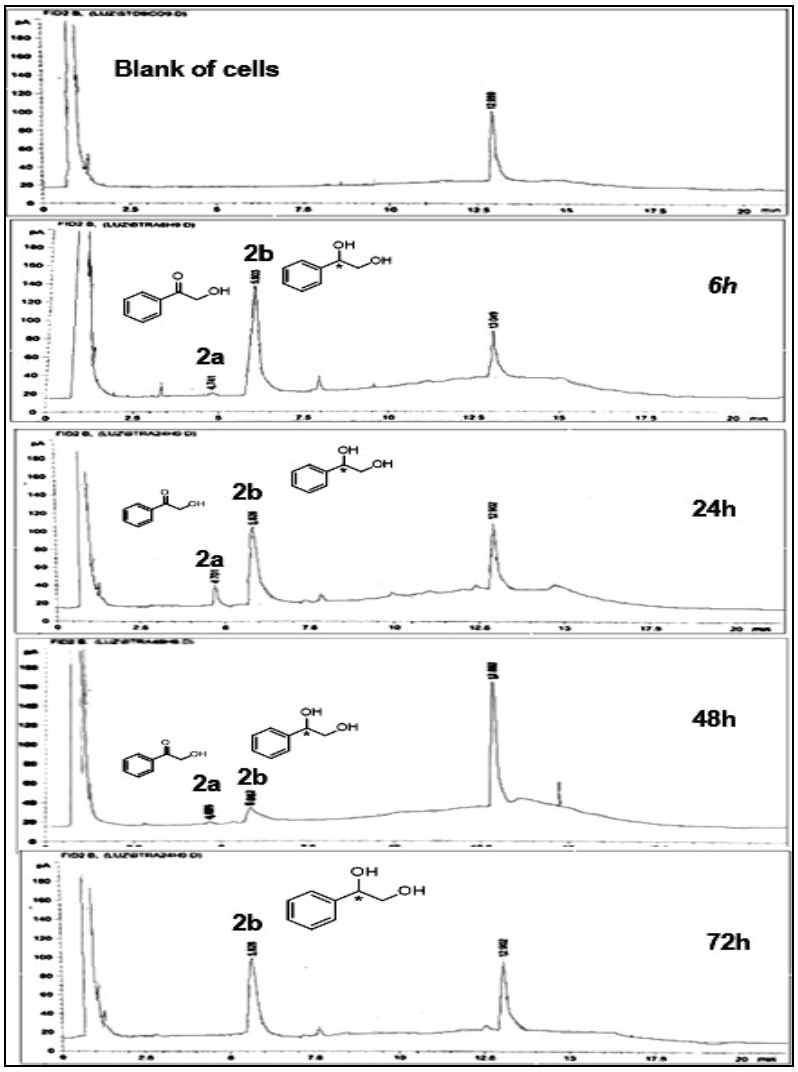

Fig. S-38. CG chromatogram of Fig. 8. Biotransformation of **2b** with *N. corallina* biomass, final pH 5.9.

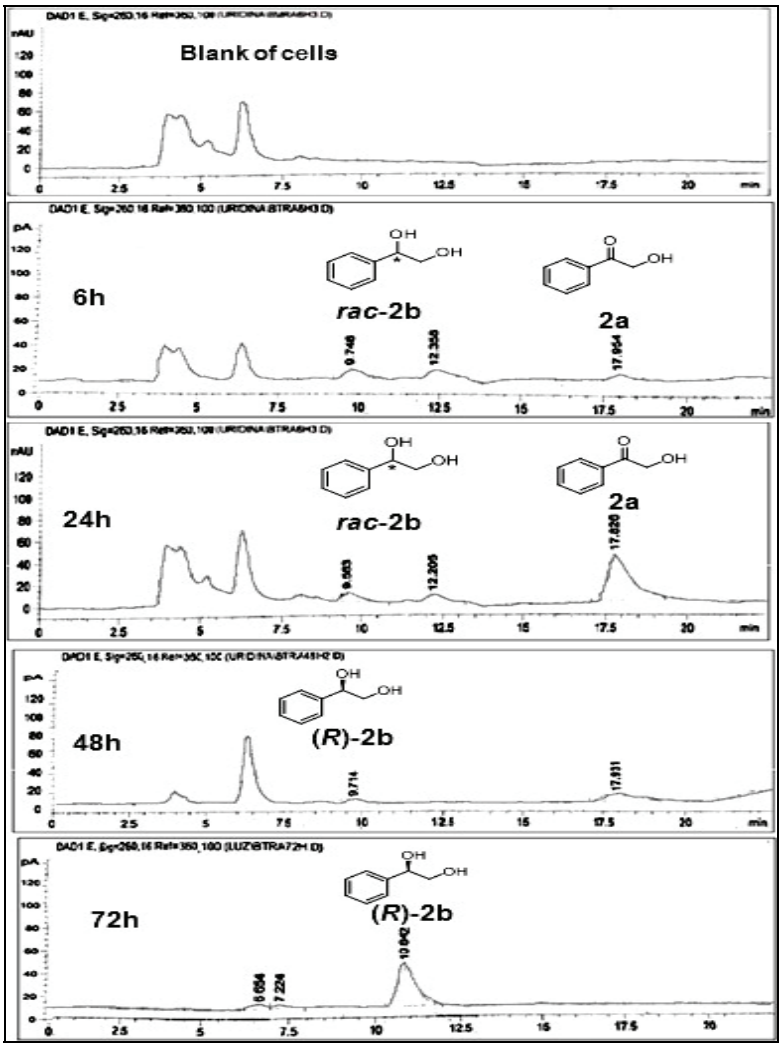

Fig. S-39. HPLC chromatogram of Fig. 8. Biotransformation of **2b** with *N. corallina* biomass, final pH 5.9.

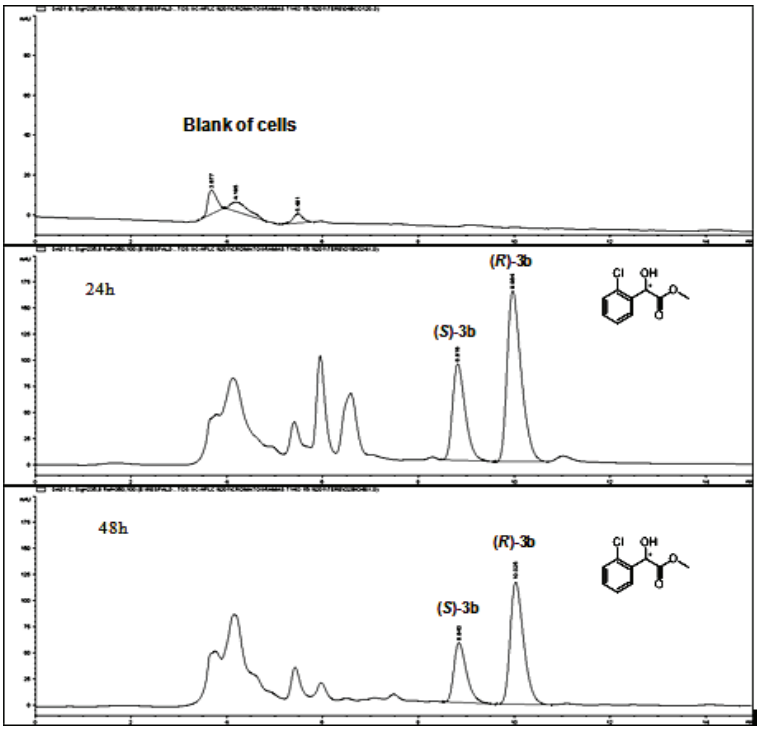

Fig. S-40. HPLC chromatogram of Fig. 9. Biotransformation of **3b** with *N. corallina* biomass, final pH 5.9.

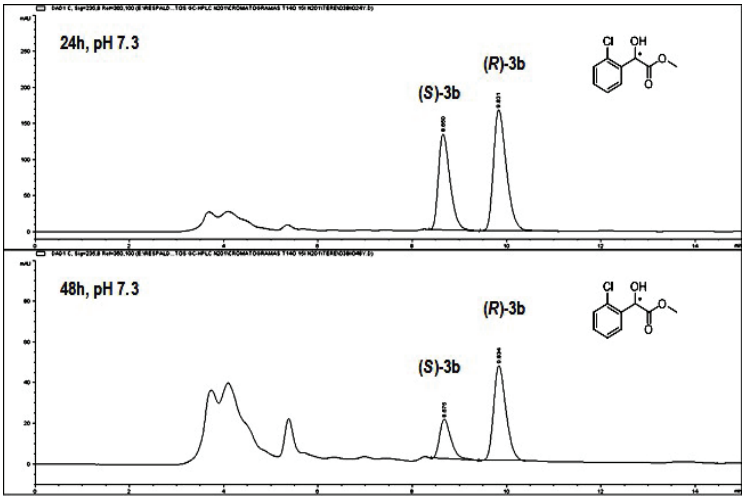

Fig. S-41. HPLC chromatogram of Fig. 9. Biotransformation of **3b** with *N. corallina* biomass, final pH 7.3.