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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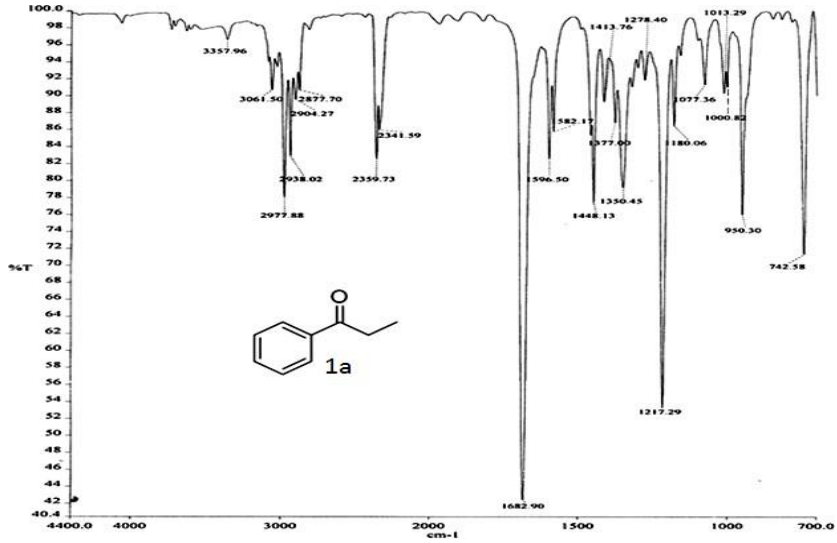

Figure S-1. IR spectrum of 1-phenyl-1-propanone (**1a**).

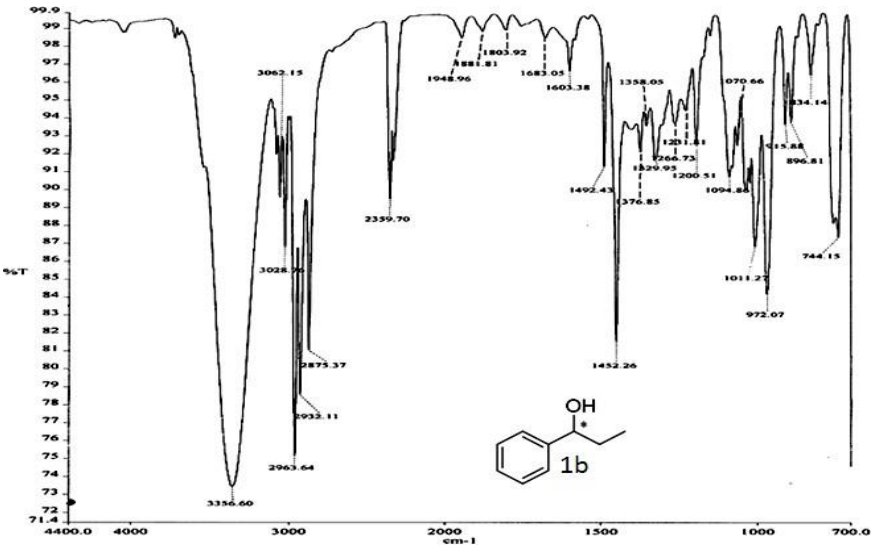

Figure S-2. IR spectrum of 1-phenylpropan-1-ol (**1b**).

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

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

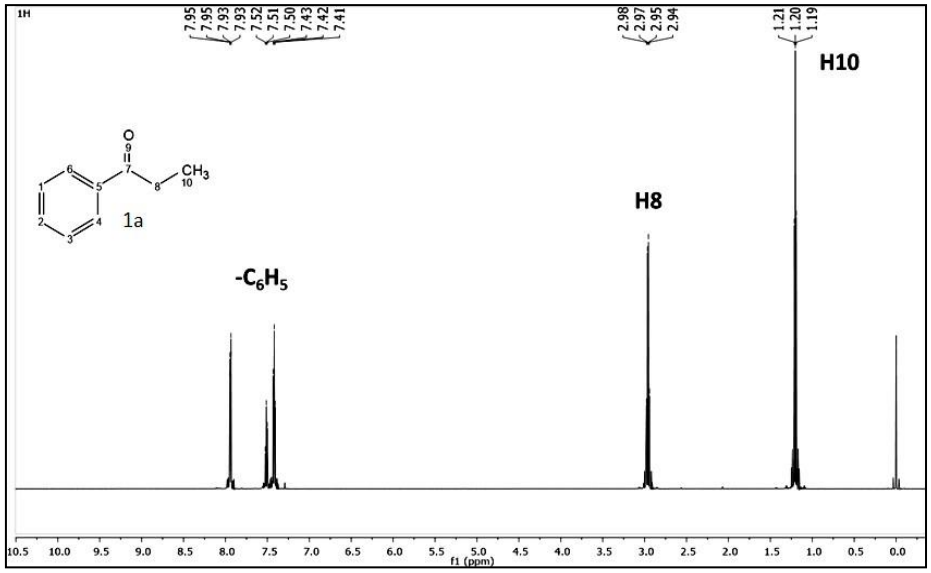

Figure S-3. NMR of ^{1}H spectrum of 1-phenyl-1-propanone (**1a**), in $CDCl_3$.

^{13}C NMR (100 MHz, $CDCl_3$): δ 8.4 (C10), 31.7 (C8), 127.9/128.5 (C4, 3, 6 y C1), 132.9 (C2), 136.9 (C5) and 200.7 (C7) ppm.

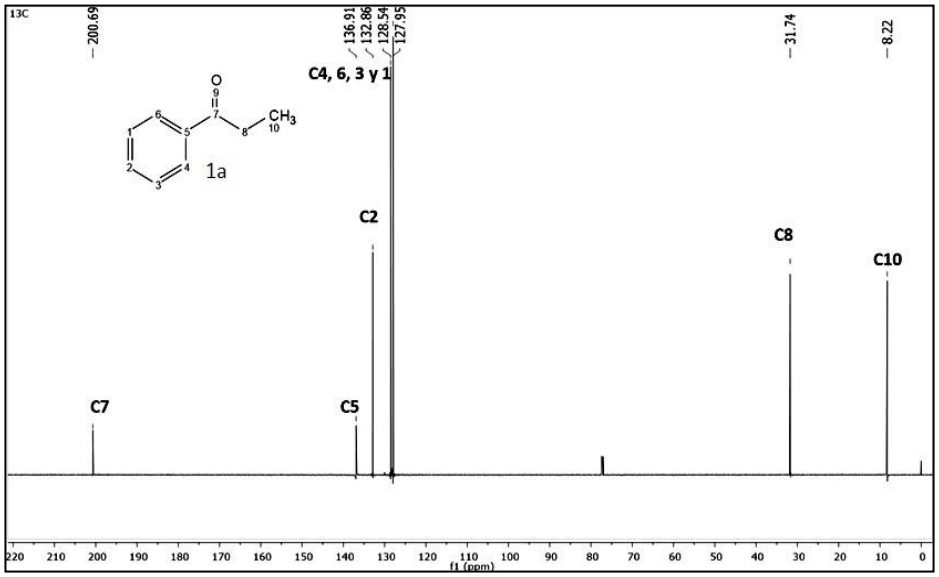

Figure S-4. NMR of ^{13}C spectrum of 1-phenyl-1-propanone (**1a**), in $CDCl_3$.

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

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

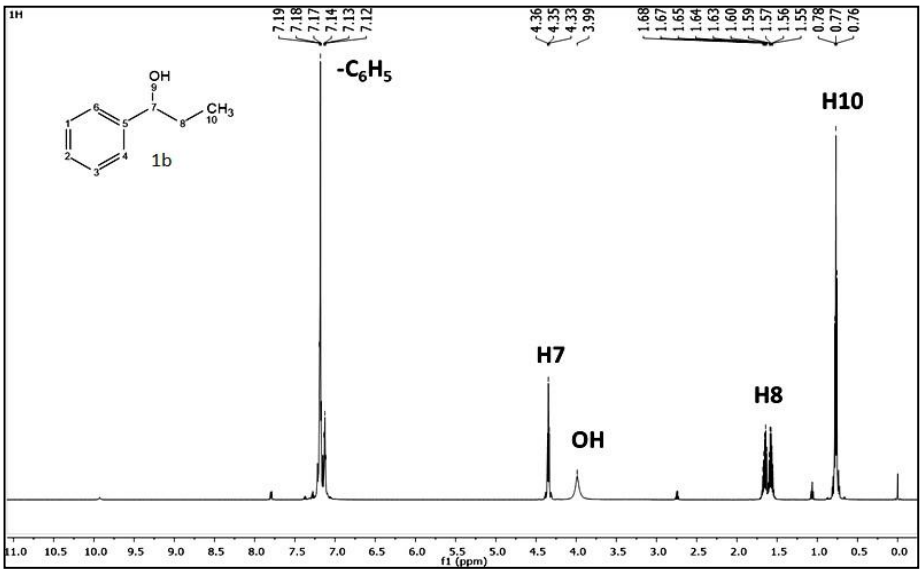

Figure S-5. NMR of ^{1}H spectrum of 1-phenylpropan-1-ol (**1b**), in $CDCl_3$.

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

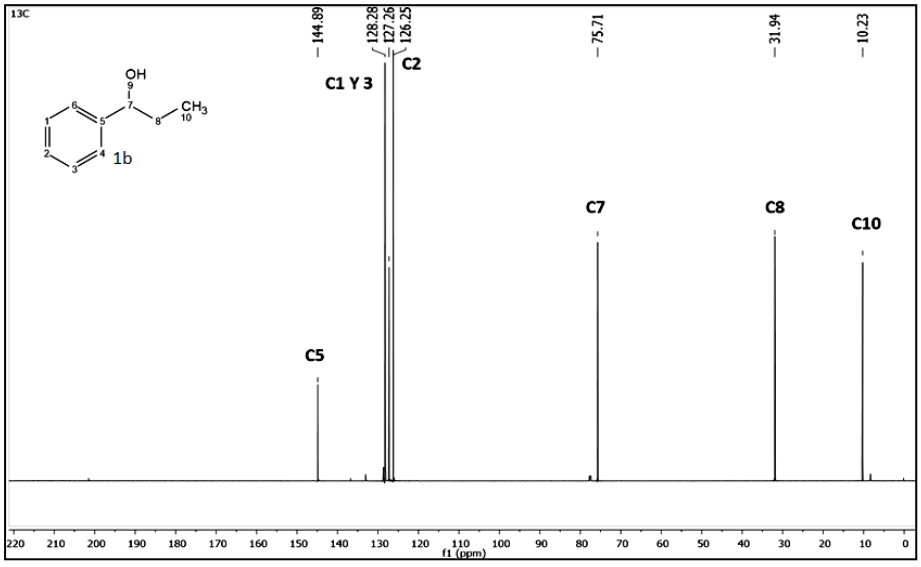

Figure S-6. NMR of ^{13}C spectrum of 1-phenylpropan-1-ol (**1b**), in $CDCl_3$.

The GC chromatograms of **1a** and **1b** with retention times of 4.39 and 5.63 minutes respectively with conditions reported on the Experimental Section.

Figure S-7. GC chromatograms of 1-phenyl-1-propanone (**1a**) and 1-phenylpropan-1-ol (**1b**).

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

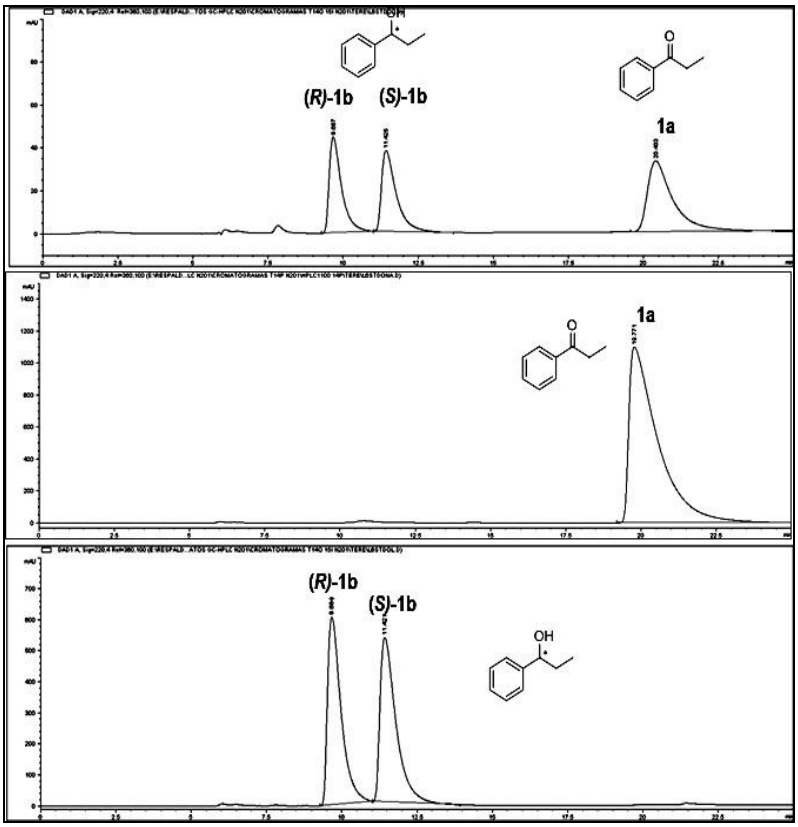

Figure S-8. HPLC chromatogram (OB-H column) of mixture of 1-phenyl-1-propanone (**1a**) and *rac*-1-phenylpropan-1-ol (**1b**), separately **1a** and (*S*)-**1b,** (*R*)-**1b**.

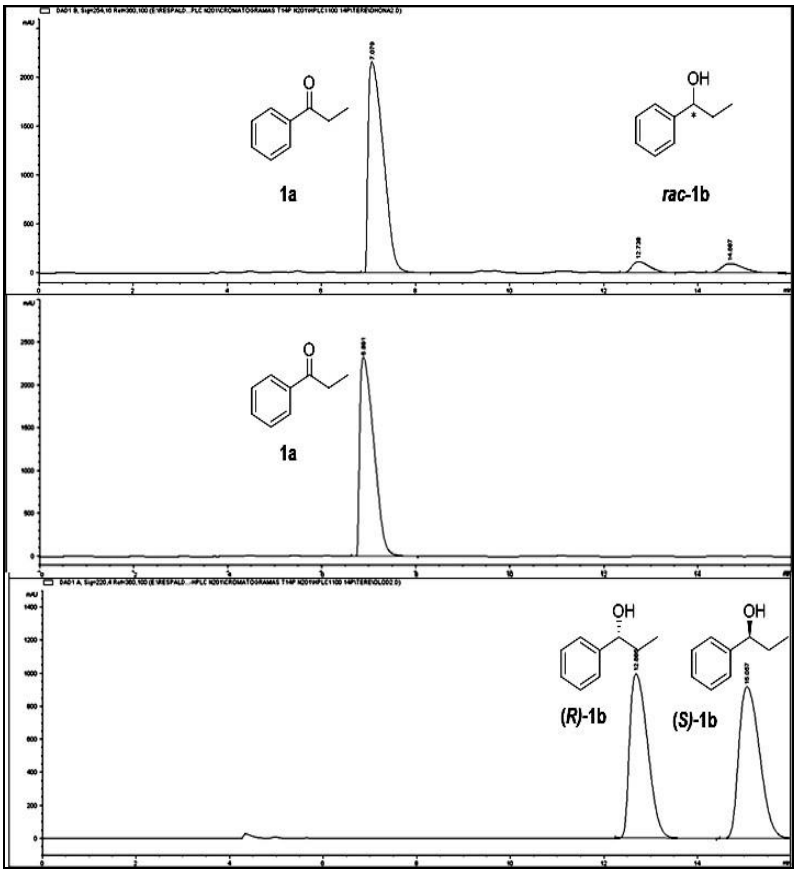

Figure S-9. HPLC chromatogram (OD column) of mixture of 1-phenyl-1-propanone (**1a**) and *rac*-1-phenylpropan-1-ol (**1b**), separately **1a** and (*S*)-**1b,** (*R*)-**1b**.

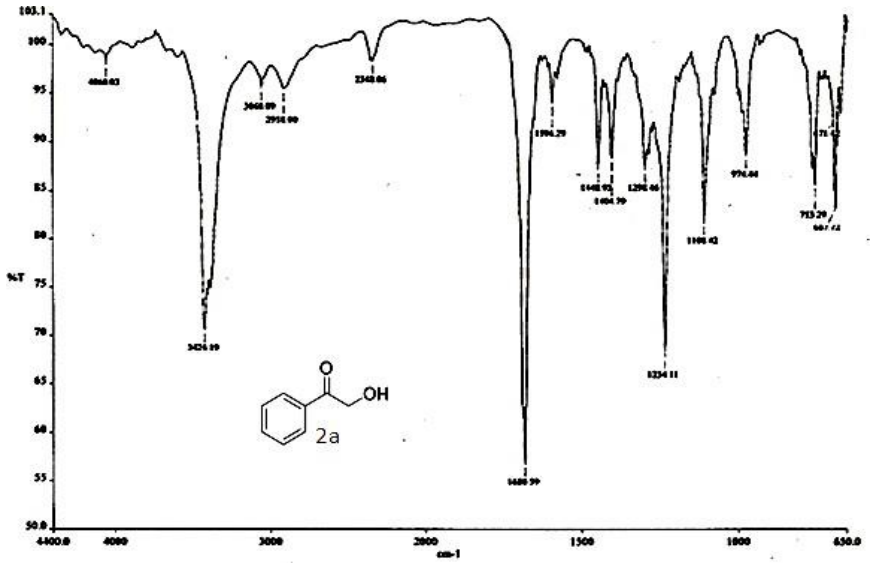

Figure S-10. IR spectrum of 2-hydroxy-1-phenylethanone (**2a**).

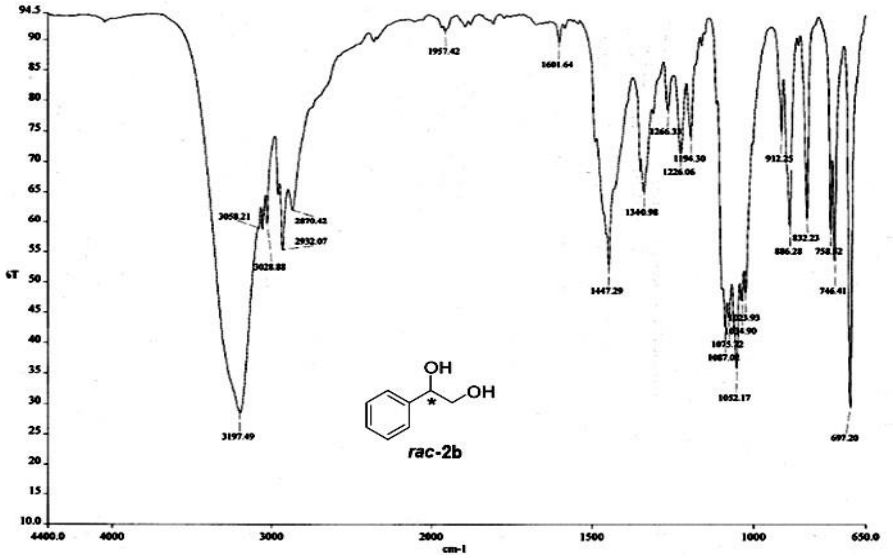

Figure S-11. IR spectrum of 1-phenyl-1,2-ethanediol (**2b**).

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

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

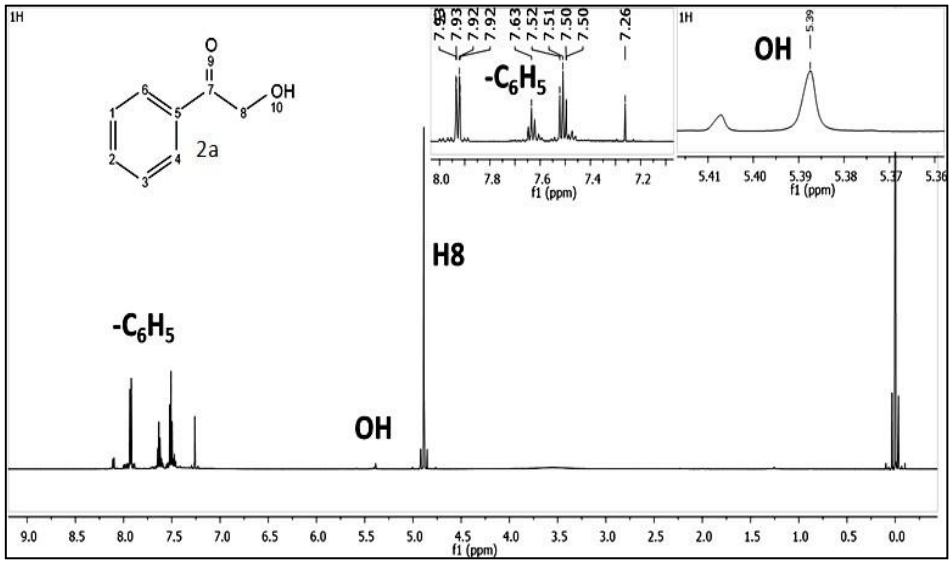

Figure S-12. NMR of ^{1}H spectrum of 2-hydroxy-1-phenylethanone (**2a**) in $CDCl_3$.

^{13}C NMR (100 MHz, $CDCl_3$): δ 65.5 (C8), 127.7/128.4 (C4 y C1), 128.9/129.5 (C6 y C1), 133.6 (C2), 198.4 (C7) ppm.

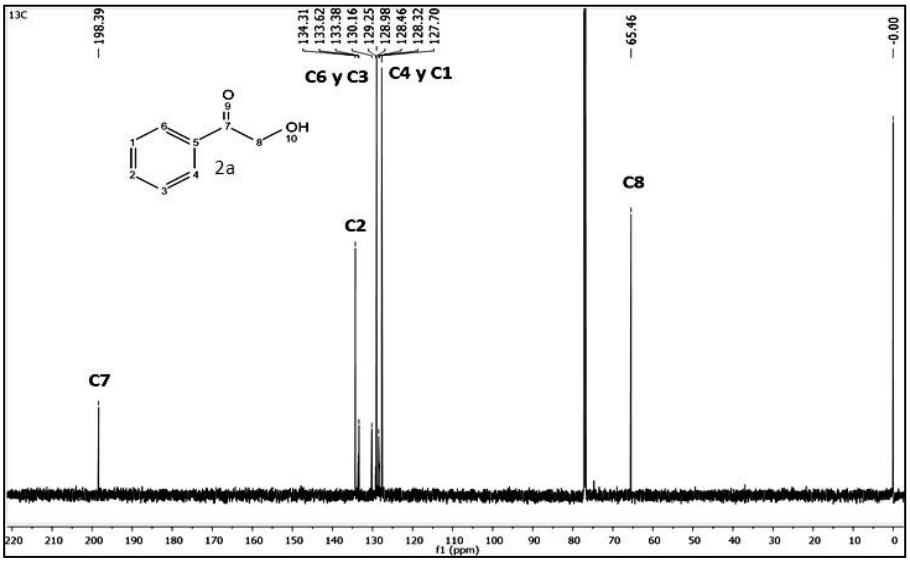

Figure S-13. NMR of ^{13}C spectrum of 2-hydroxy-1-phenylethanone (**2a**), in $CDCl_3$.

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

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

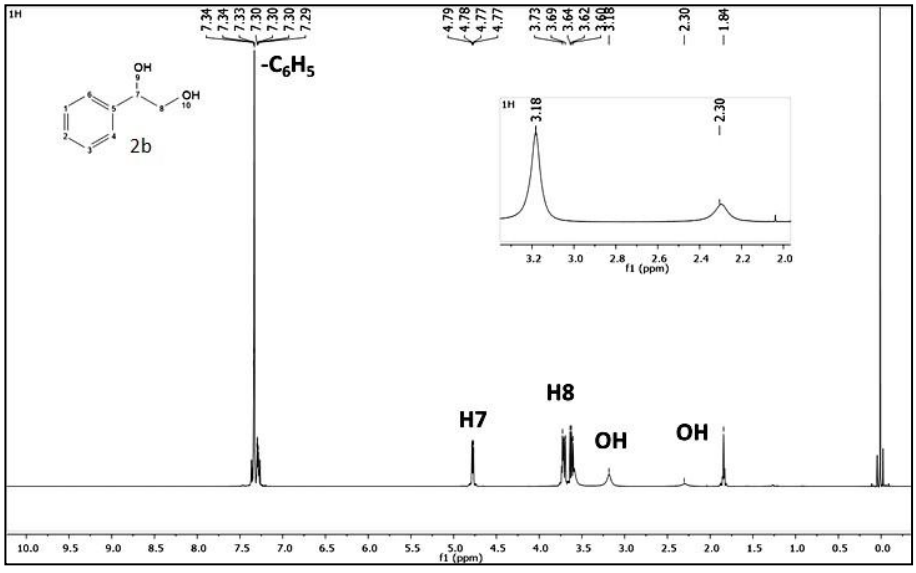

Figure S-14. NMR of ^{1}H spectrum of 1-phenyl-1,2-ethanediol (**2b**) in $CDCl_3$.

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

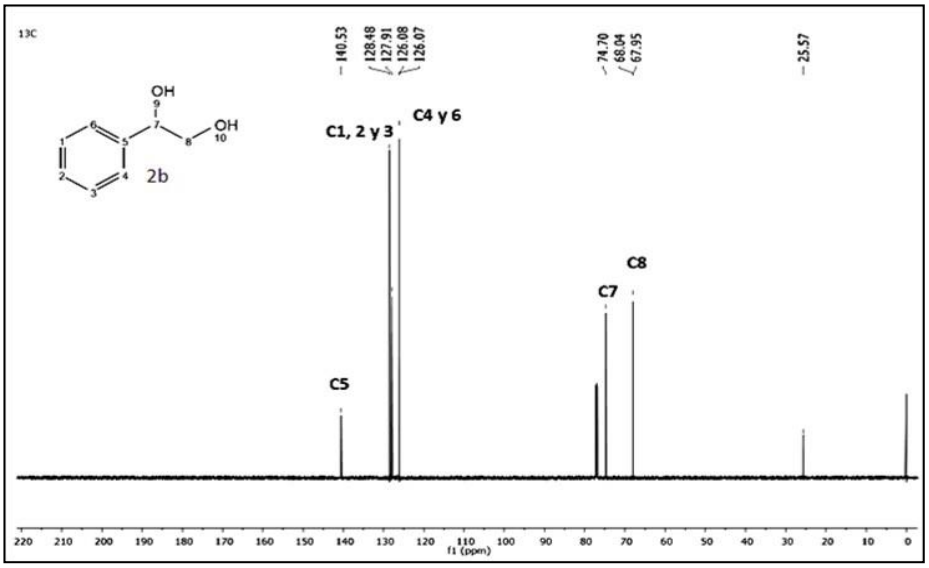

Figure S-15. NMR of ^{13}C spectrum of 1-phenyl-1,2-ethanediol (**2b**), in $CDCl_3$.

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

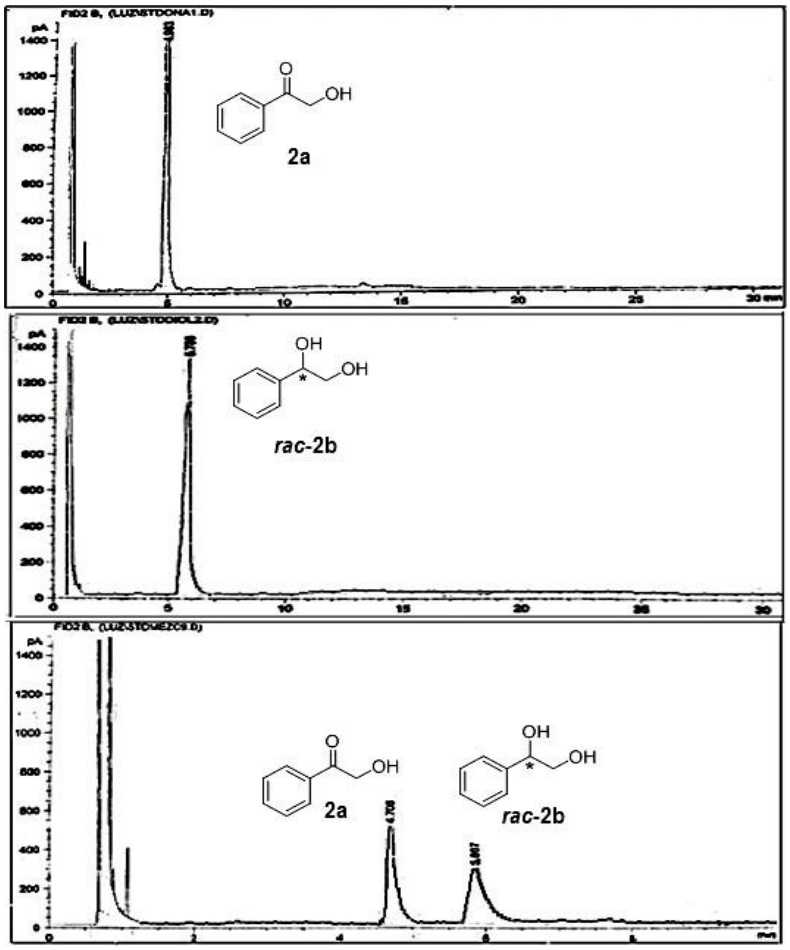

Figure S-16. GC chromatograms of 2-hydroxy-1-phenylethanone (**2a**) and 1-phenyl-1,2-ethanediol (**2b**) and mixture of **2a** and *rac*-**2b**.

The HPLC chromatogram of the mixture of **2a,** (*S*)-**2b** and (*R*)-**2b** with retention times of 17.12, 11.38 and 9.04 minutes respectively with conditions reported on the Experimental Section.

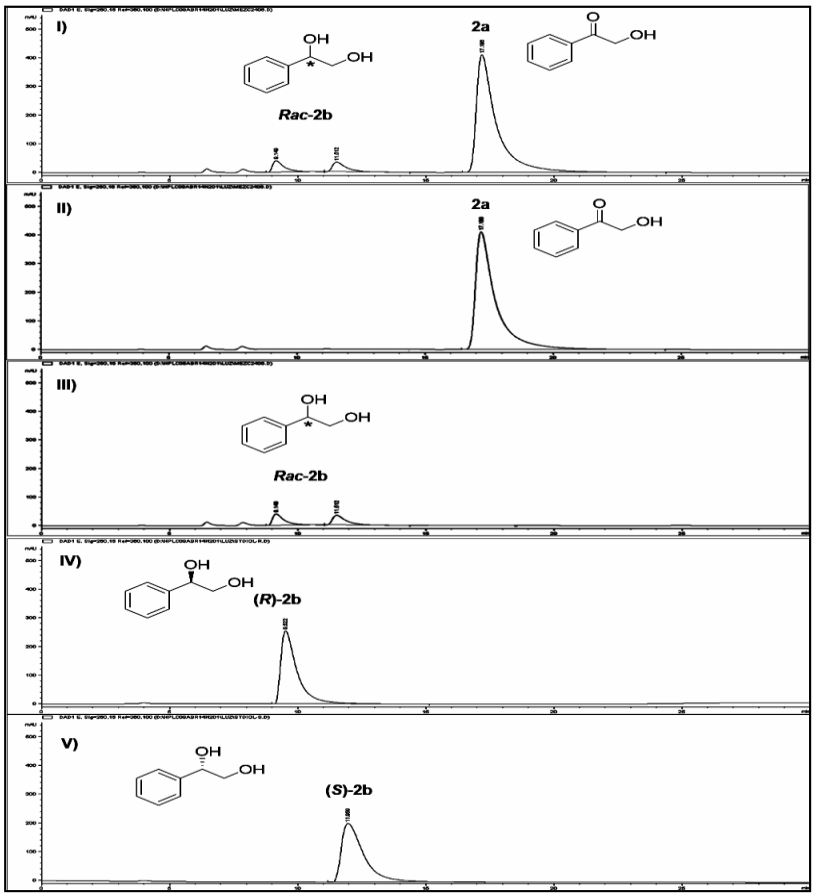

Figure S-17. HPLC chromatogram of: I) mixture of 2-hydroxy-1-phenylethanone (**2a**) and *rac*-1-phenyl-1,2-ethanediol (*rac*-**2b**); II) 2-hydroxy-1-phenylethanone (**2a**); III) r*ac*-1-phenyl-1,2-ethanediol (*rac*-**2b**); IV) (*R*)-1-phenyl-1,2-ethanediol (*R*-**2b**); V) (*S*)-1-phenyl-1,2-ethanediol (*S*-**2b**).

The HPLC chromatogram of the mixture of **2a,** (*S*)-**2b** and (*R*)-**2b** with retention times of 28.9, 18.9 and 15.1 minutes respectively with conditions reported on the Experimental Section.

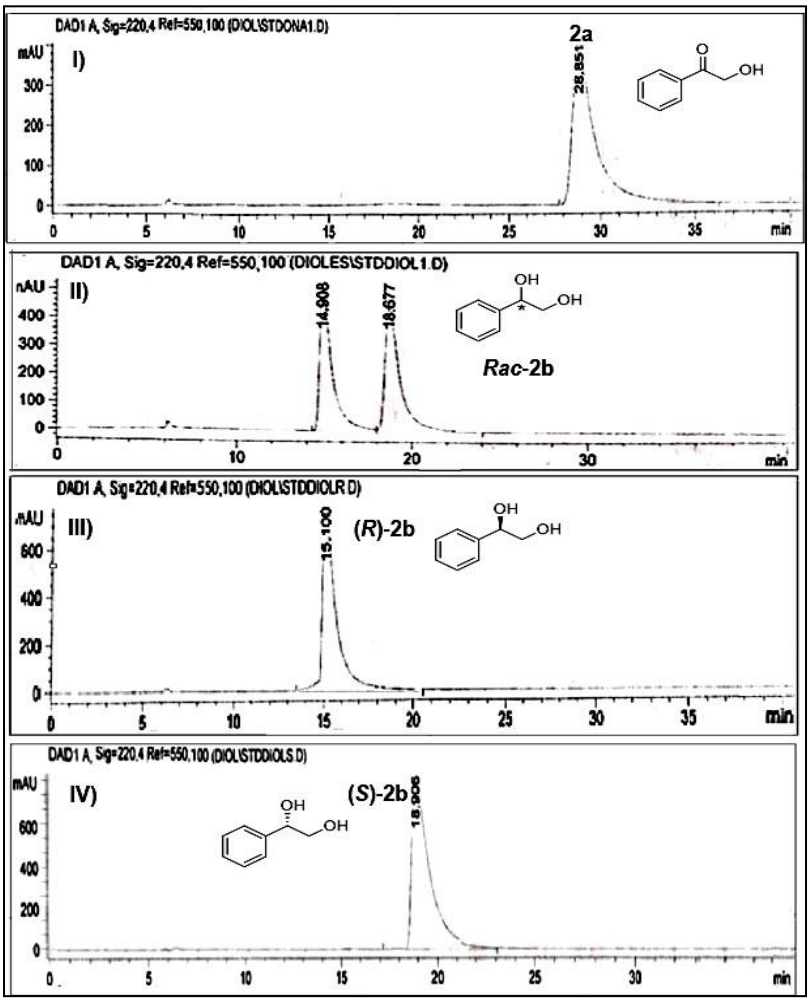

Figure S-18. HPLC chromatogram of: I) 2-hydroxy-1-phenylethanone (**2a**); II) r*ac*-1-phenyl-1,2-ethanediol (*rac*-**2b**); III) (*R*)-1-phenyl-1,2-ethanediol (*R*-**2b**); IV) (*S*)-1-phenyl-1,2-ethanediol (*S*-**2b**).

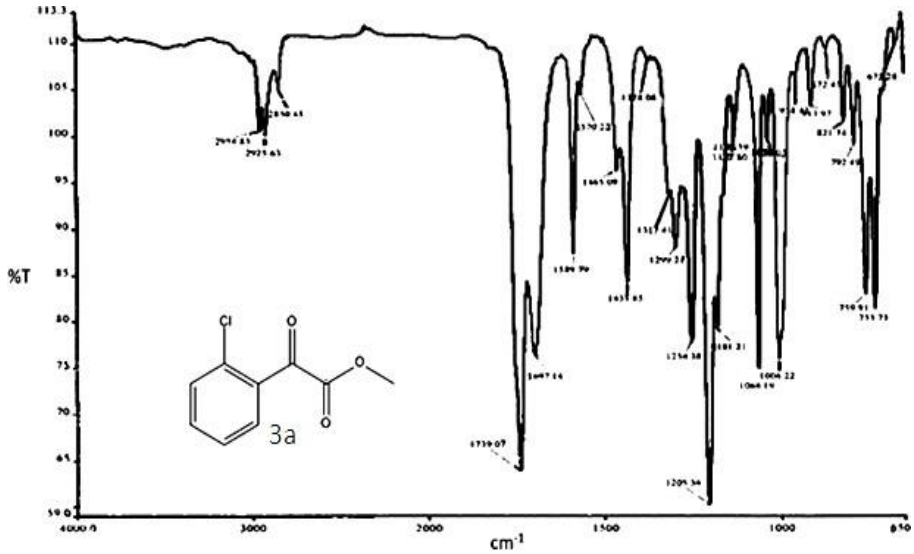

Figure S-19. IR spectrum of methyl (2-chlorophenyl)(oxo)acetate (**3a**).

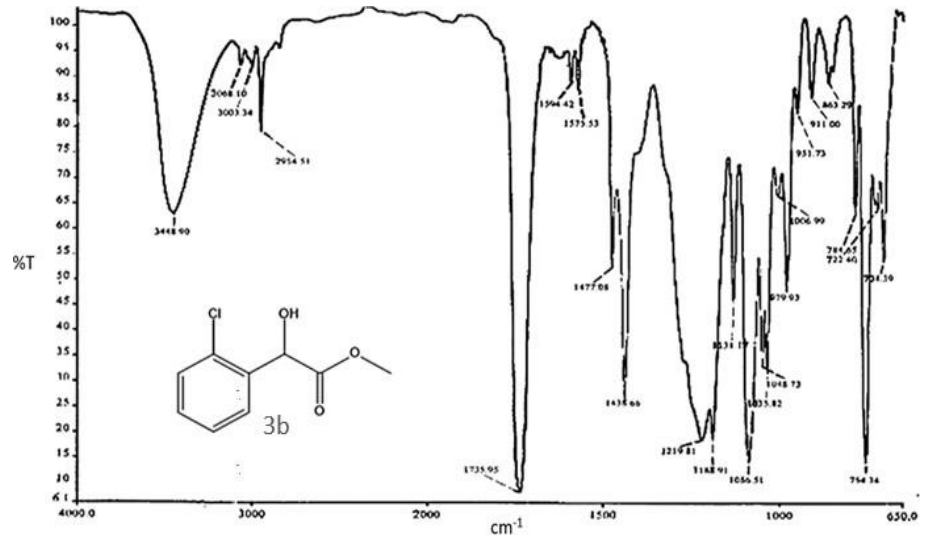

Figura S-20. IR spectrum of methyl (2-chlorophenyl)(hydroxy)acetate (**3b**).

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

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

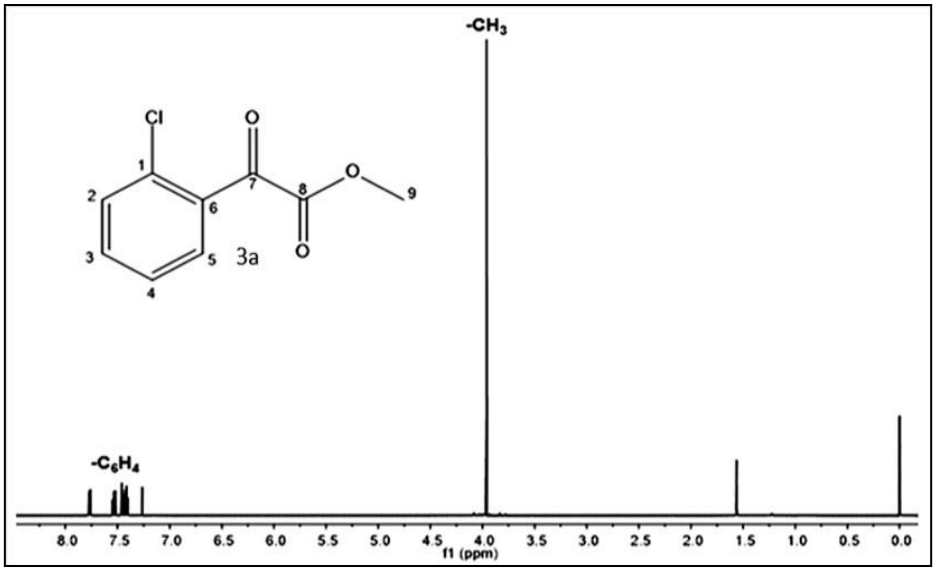

Figure S-21. NMR of ^{1}H spectrum of methyl (2-chlorophenyl)(oxo)acetate (**3a**), in $CDCl_3$.

^{13}C NMR (100 MHz, $CDCl_3$): δ 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) ppm.

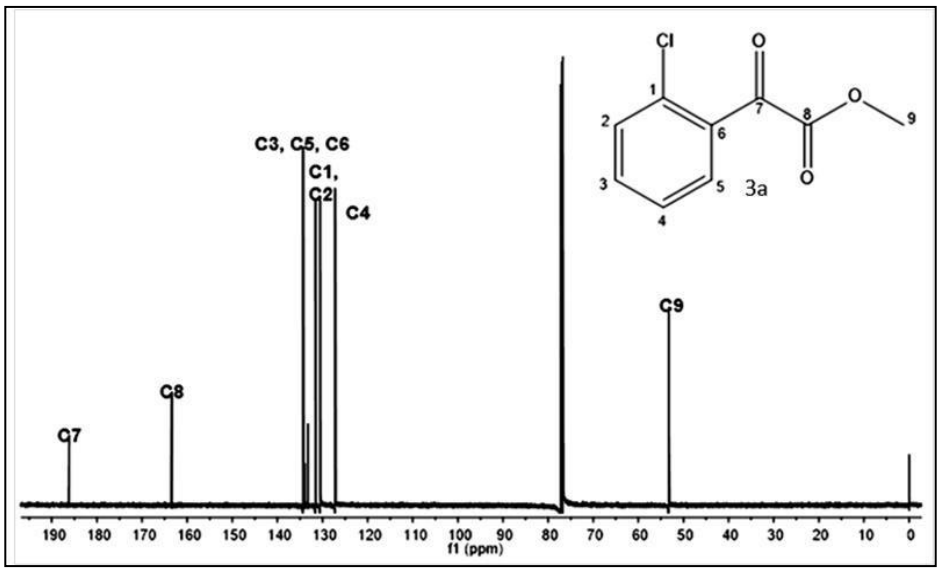

Figure S-22. NMR of ^{13}C spectrum of methyl (2-chlorophenyl)(oxo)acetate (**3a**), in $CDCl_3$.

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

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

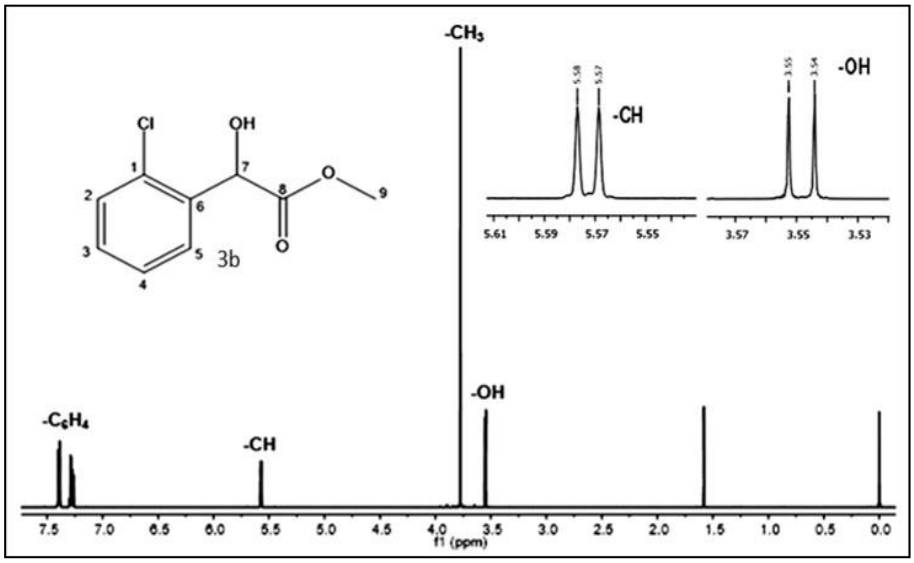

Figure S-23. NMR of ^{1}H spectrum of methyl (2-chlorophenyl)(hydroxy)acetate (**3b**), in $CDCl_3$.

^{13}C NMR (100 MHz, $CDCl_3$): δ 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) ppm.

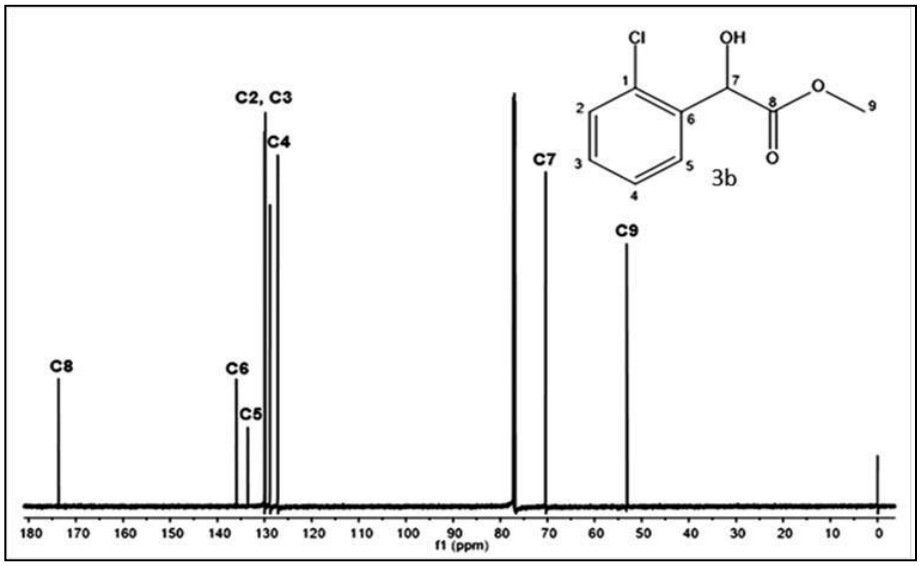

Figure S-24. NMR of ^{13}C spectrum of methyl (2-chlorophenyl)(hydroxy)acetate (**3b)**, in $CDCl_3$.

The GC chromatograms of **3a** and **3b** with retention times of 4.6 and 6.1 minutes respectively with conditions reported on the Experimental Section.

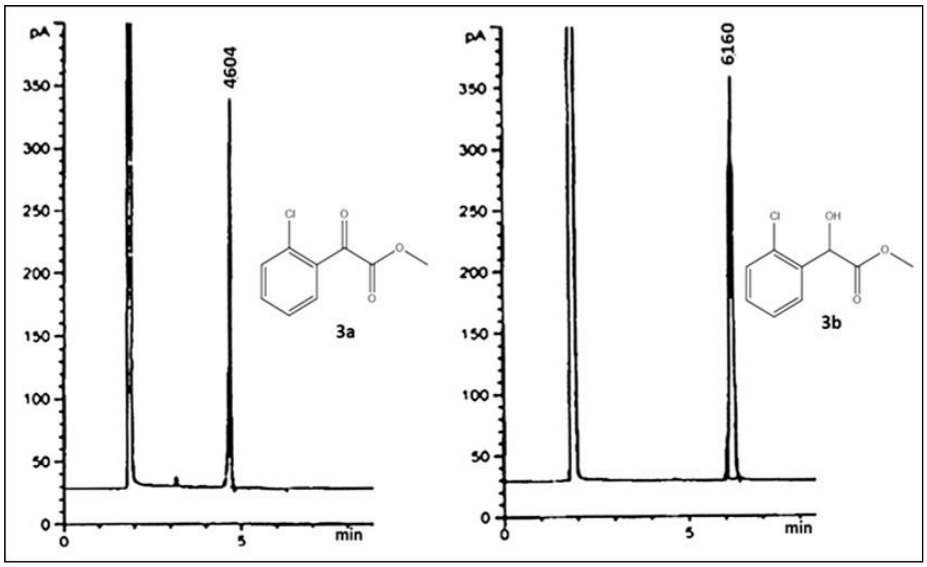

Figure S-25. GC chromatograms of methyl (2-chlorophenyl)(oxo)acetate (**3a**) and methyl (2-chlorophenyl)(hydroxy)acetate (**3b**).

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

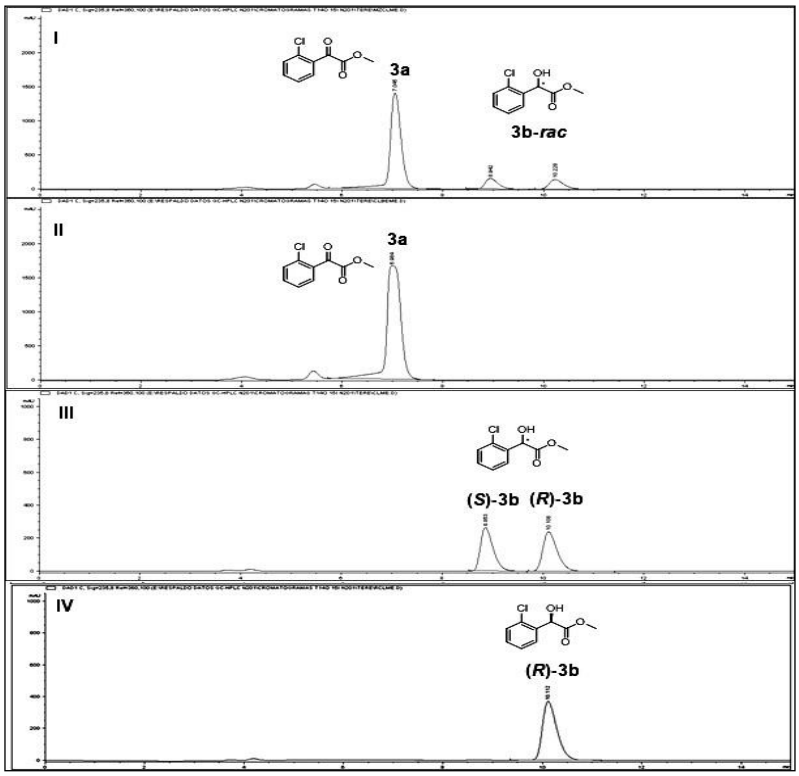

Figure S-26. HPLC chromatogram of: I) mixture of methyl (2-chlorophenyl)(oxo)acetate (**3a**) and *rac*-methyl (2-chlorophenyl)(hydroxy)acetate (*rac*-**3b**); II) methyl (2-chlorophenyl)(oxo)acetate (**3a**); III) *rac*-methyl (2-chlorophenyl)(hydroxy)acetate (*rac*-**3b**) and IV (*R*)-methyl (2-chlorophenyl)(hydroxy)acetate (*R*-**3b**).

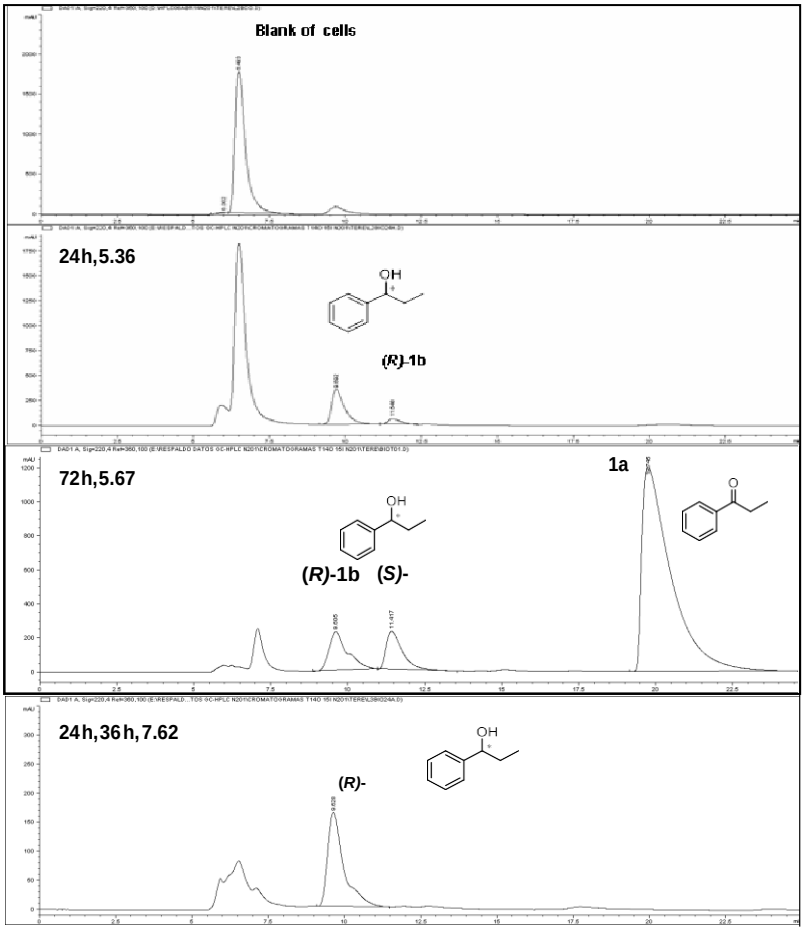

Figure S-27. HPLC chromatogram of Figure 2. Reduction of ketones **1a** with *N. corallina* biomass, final pH (5.36, 5.67 and 7.62).

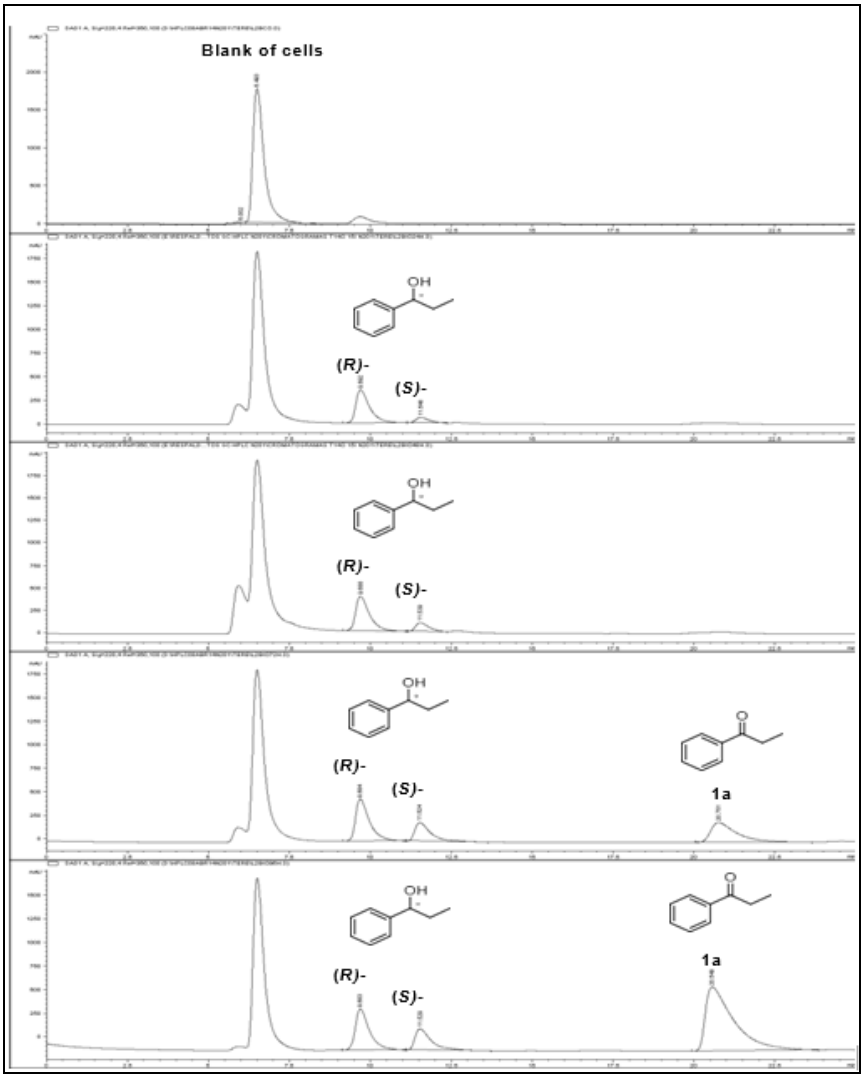

Figure S-28. HPLC chromatogram of Figure 3. Biotransformation of **1a** with *N. corallina* biomass, final pH 5.36.

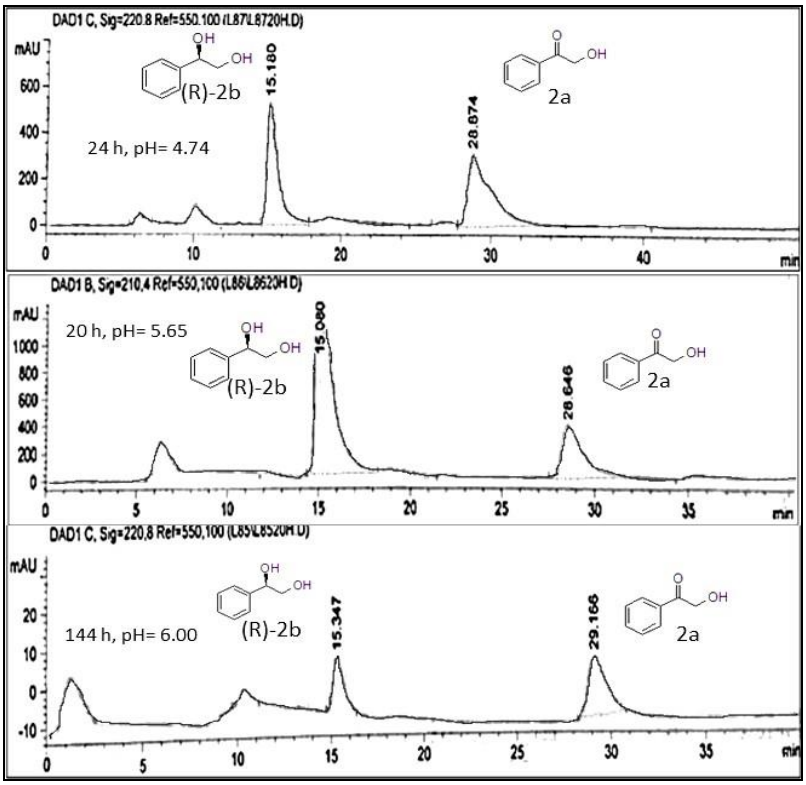

Figure S-29. HPLC chromatogram of Figure 4. Biotransformation of **2a** with *N. corallina* biomass, different final pH and time.

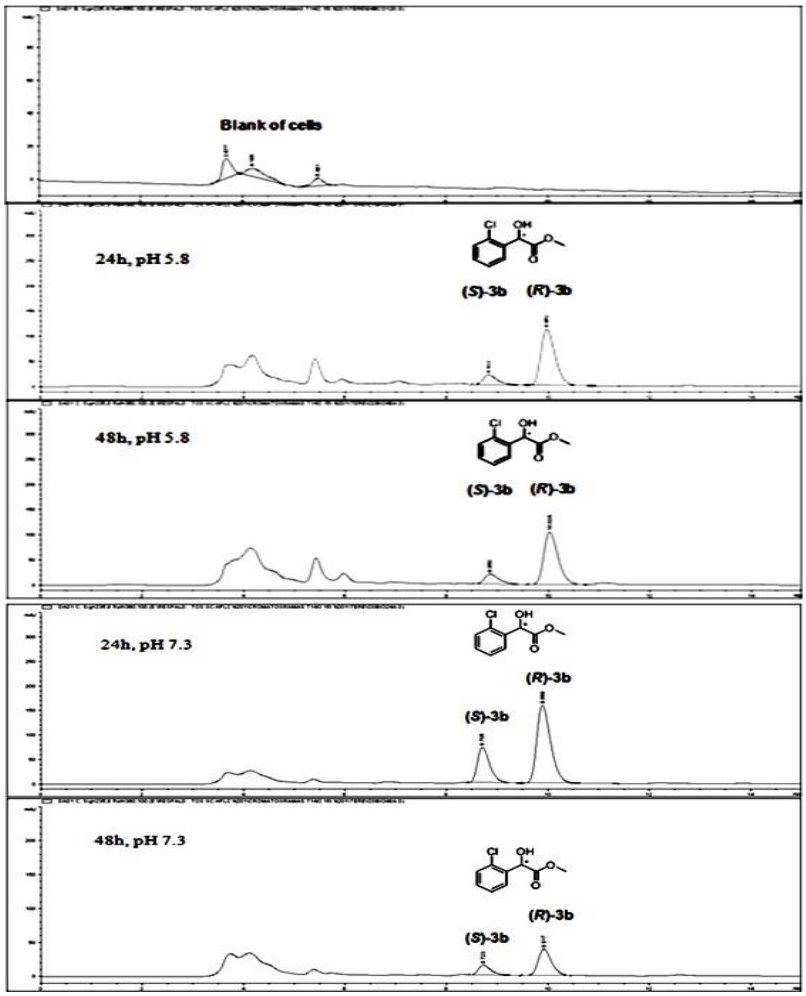

Figure S-30. HPLC chromatogram of Figure 5. Biotransformation of **3a** with *N. corallina* biomass, final pH 5.8 and 7.3.

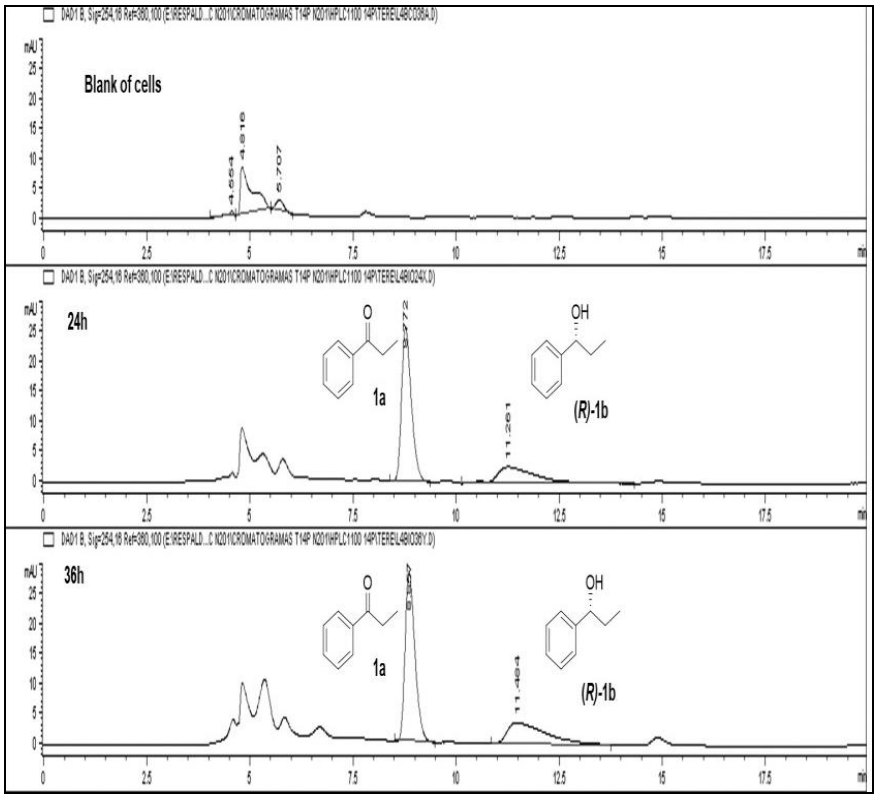

Figure S-31. HPLC chromatogram of Figure 6. Biotransformation of **1b** with *N. corallina* biomass, final pH 7.62.

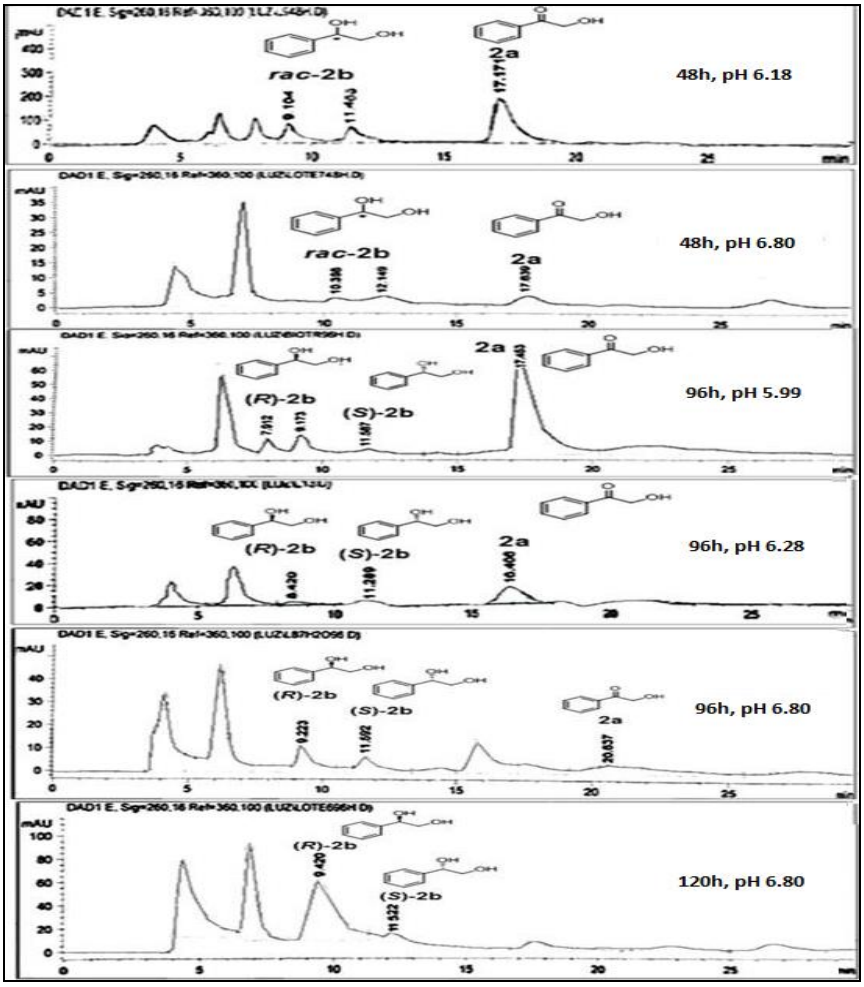

Figure S-32. HPLC chromatogram of Figure 7. Biotransformation of **2b** with *N. corallina* biomass, different final pH and time.

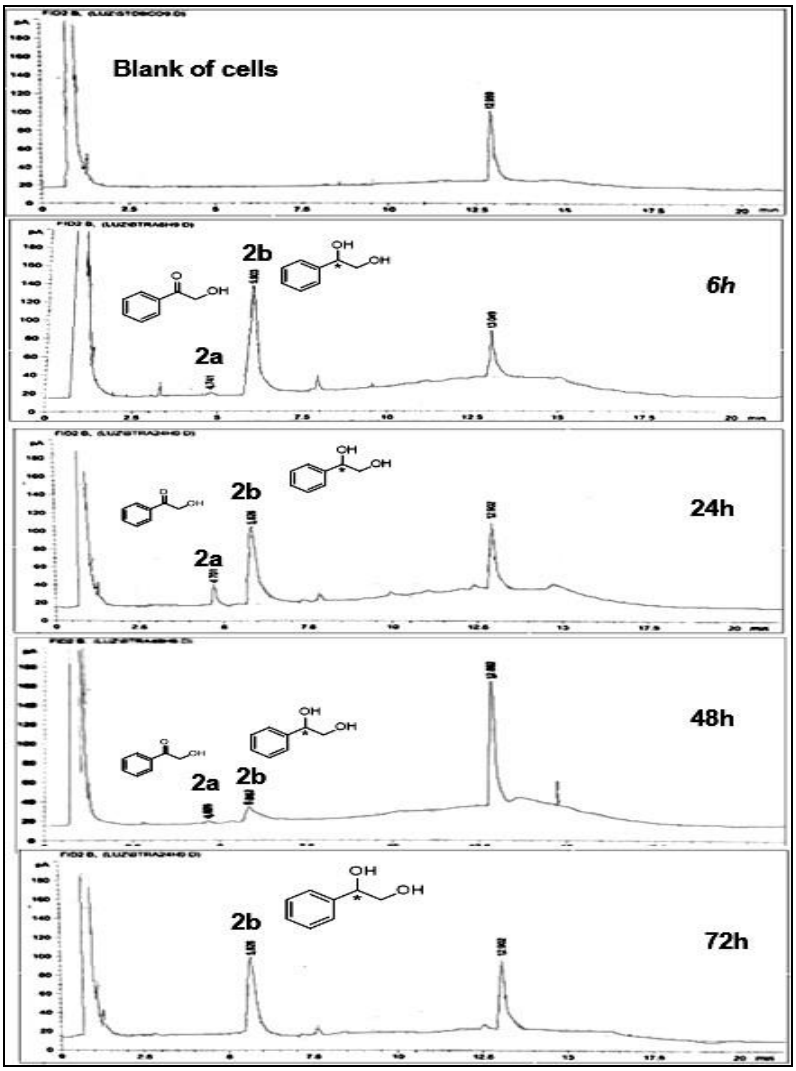

Figure S-33. CG chromatogram of Figure 8. Biotransformation of **2b** with *N. corallina* biomass, final pH 5.9.

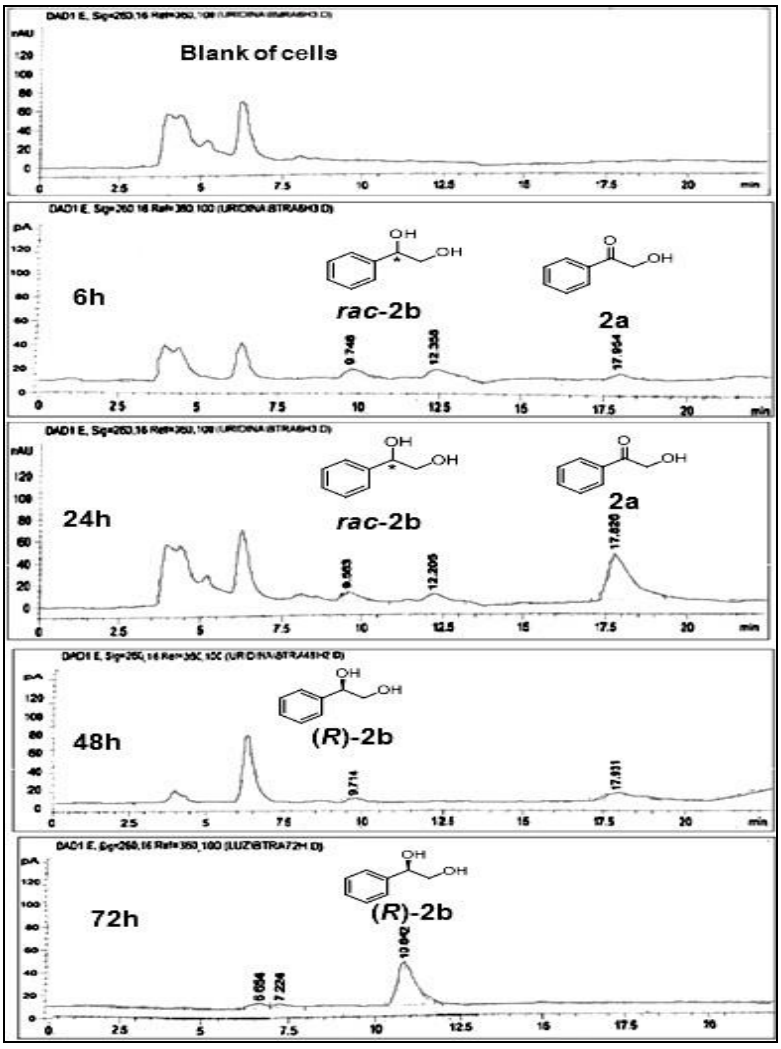

Figure S-34. HPLC chromatogram of Figure 8. Biotransformation of **2b** with *N. corallina* biomass, final pH 5.9.

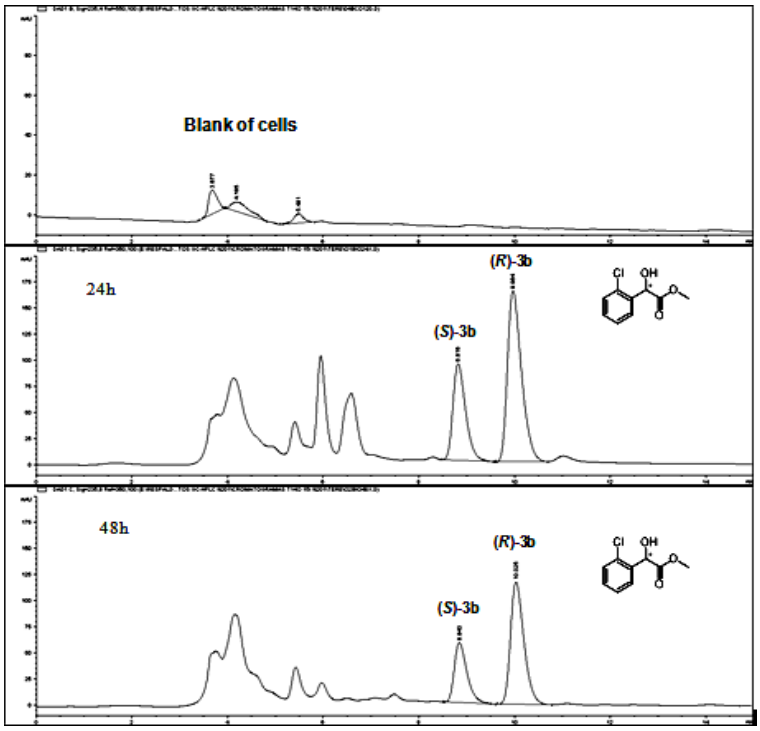

Figure S-35. HPLC chromatogram of Figure 9. Biotransformation of **3b** with *N. corallina* biomass, final pH 5.9.

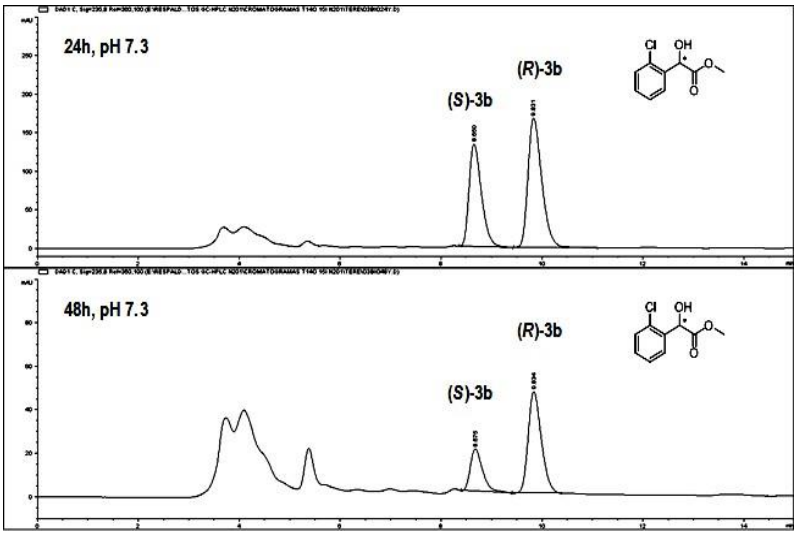

Figure S-36. HPLC chromatogram of Figure 9. Biotransformation of **3b** with *N. corallina* biomass, final pH 7.3.