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Bioreduction of the Chalcones by Fungus *Scedosporium apiospermum* EJCP13

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Supplementary Information

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Spectroscopic NMR and MS data to compounds 1 – 6

(2*E*)-1-(4-hydroxy-phenyl)-3-(2-methoxy-phenyl)-prop-2-en-1-one (1)

LRESIMS: *m/z* 255 $[M+H]^+$; ^{1}H NMR (400 MHz; $CDCl_3$) δ 8.10 (d, 1H, *J* 15.6, H-3), 7.99 (d, 2H, *J* 8.7, H-2'/H-6'), 7.61 (d, 1H, *J* 15.6, H-2), 7.60 (dd,1H, *J* 8.4, 1.5, H-9), 7.37 (ddd, 1H, *J* 8.4, 8.1, 2.1, H-7), 6.99 (dd, 1H, *J* 8.4, 8.1, H-8), 6.93 (t, 1H, *J* 8.4, H-6), 6.92 (d, 2H, *J* 8.7, H-3'/H-5'), 3.92 (s, 3H, OMe); ^{13}C NMR (400 MHz; $CDCl_3$) δ 189.5, 158.6, 139.7, 138.4, 131.6, 131.1, 128.7, 126.2, 122.5, 124.0, 120.8, 115.4, 111.2, 55.6.

(2*E*)-1-(4-hydroxy-phenyl)-3-(4- methoxy-phenyl)-prop-2-en-1-one (2)

LRESIMS: *m/z* 253 $[M-H]^-$; ^{1}H NMR (400 MHz; $CDCl_3$) δ 8.00 (d, 2H, *J* 8.8, H-2'/H-6'), 7.79 (d, 1H, *J* 15.8, H-3), 7.60 (d, 2H, *J* 8.8, H-5/H-9), 7.43 (d, H-2, *J* 15.8, H-2), 6.95(d, 2H, *J* 8.8, H-6/H-8), 6.94 (d, 2H, *J* 8.8, H-3'/H-5'), 3.87 (s, 3H, OMe); ^{13}C NMR (400 MHz; $CDCl_3$) δ 189.0, 161.6, 159.8, 144.1, 131.0, 130.1, 129.1, 127.8, 119.5, 115.4, 114.4, 55.4.

(2*E*)-1-(4-hydroxy-phenyl)-3-phenyl-prop-2-en-1-one (3)

LRESIMS: *m/z* 223 $[M-H]^-$; ^{1}H NMR (400 MHz; $CDCl_3$) δ 8.02 (d, 2H, *J* 8.7, H-2'/H-6'), 7.84 (d, 1H, *J* 15.6, H-2), 7.63-7.6 (m, 2H, H-5/H-9), 7.55 (d, 1H, *J* 15.8, H-3), 7.40-7.43 (m, 3H, H-6/H-7/H-8), 6.96 (d, 2H, *J* 8.7, H-3'/H-5'); ^{13}C NMR (400 MHz; $CDCl_3$) δ 115.5, 121.8, 128.4, 128.9, 130.4, 131.1, 131.2, 135.0, 144.3, 160.1, 189.0.

1-(4-hydroxy-phenyl)-3-(2-methoxy-phenyl)-propan-1-one (4)

LRESIMS: *m/z* 257 $[M+H]^-$; ^{1}H NMR (400 MHz; $CDCl_3$) δ 7.92 (d, 2H, *J* 8.7, H-2'/H-6'), 7.20 (d, 1H, *J* 7.7, H-9), 7.21 (dd, 1H, *J* 7.7, 2.1, H-8), 6.89 (d, 2H, *J* 8.7, H-3'/H-5'), 6.88 (dd, 1H, *J* 8.2, 7.7, H-7), 6.86 (d, 1H, *J* 8.2, H-6), 3.83 (s, 3H, OMe), 3.22 (t, 2H, *J* 7.7, H-2), 3.04 (t, 2H, *J* 7.7, H-3); ^{13}C NMR (400 MHz; $CDCl_3$) δ 199.6, 160.6, 157.7, 131.0, 130.3, 130.1, 129.7, 127.7, 120.7, 115.5, 110.4, 55.4, 38.9, 26.4.

1-(4-hydroxy-phenyl)-3-(4-methoxy-phenyl)-propan-1-one (5)

LRESIMS: *m/z* 255 $[M-H]^-$; ^{1}H NMR (400 MHz; $CDCl_3$) δ 7.89 (d, 2H, *J* 8.6, H-2'/H-6'), 7.16 (d, 2H, *J* 8.4, H-5/H-9), 6.90 (d, 2H, *J* 8.4, H-6/H-8), 6.84 (d, 2H, *J* 8.4, H-3'/H-5'), 3.79 (s, 3H, OMe), 3.23 (t, 2H, *J* 7.7, H-2), 3.00 (t, 2H, *J* 7.7, H-3); ^{13}C NMR (400 MHz; $CDCl_3$) δ 199.5, 161.1, 158.1, 133.4, 131.0, 129.6, 129.5, 115.7, 114.1, 55.5, 40.5, 29.8.

1-(4-hydroxy-phenyl)-3-phenyl-propan-1-one (6)

LRESIMS: *m/z* 225 $[M-H]^-$; ^{1}H NMR (400 MHz; $CDCl_3$) δ 7.91 (d, 2H, *J* 8.7, H-2'/H-6'), 7.20-7.33 (m, 5H, H-5/H-6/H-7/H-8/H-9), 6.92 (d, 2H, *J* 8.7, H-3'/H-5'), 3.28 (t, 2H, *J* 7.7, 2H, H-2), 3.07 (t, 2H, *J* 7.7, H-3); ^{13}C NMR (400 MHz; $CDCl_3$) δ 199.3, 161.1, 141.4, 131.0, 128.7, 128.6, 126.3, 122.0, 115.7, 40.3, 30.7.

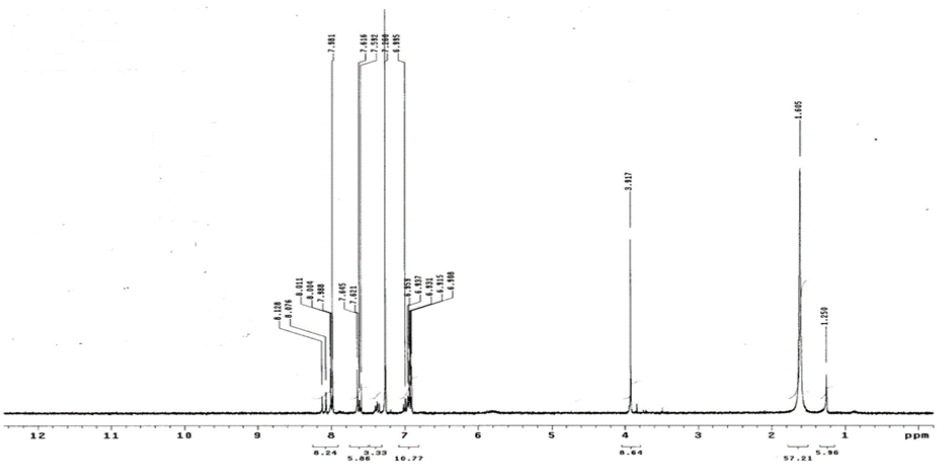

Fig. S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **1**.

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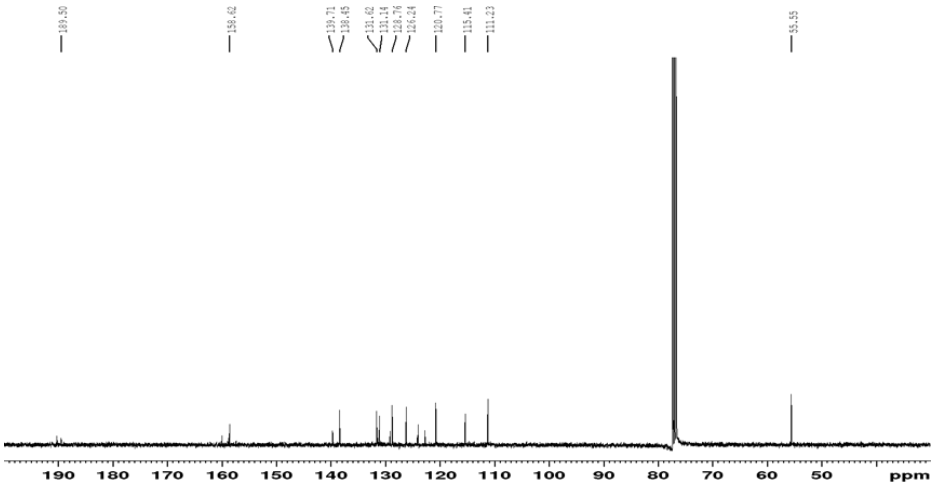

Fig. S2. ^{13}C NMR spectrum (400 MHz, $CDCl_3$) of compound **1**.

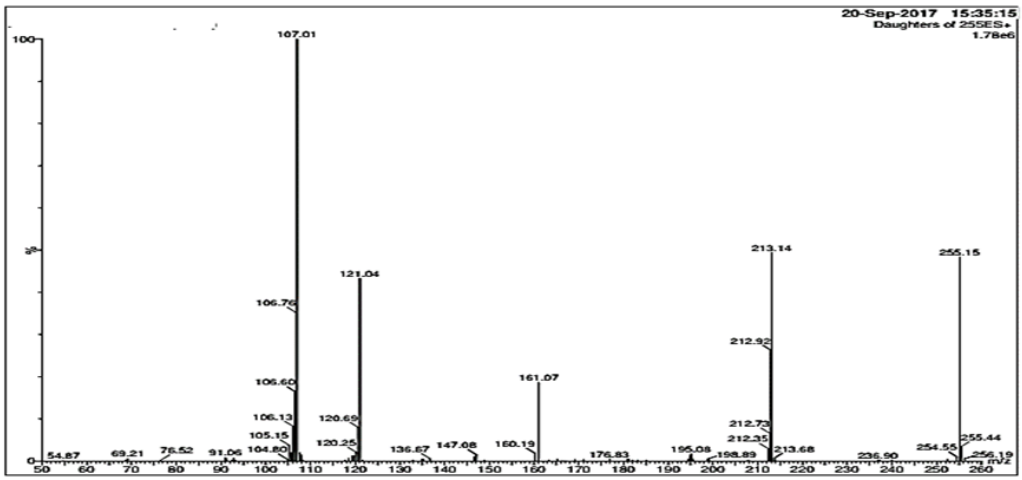

Fig. S3. Mass spectrum MS/MS ESI(+) of compound **1**.

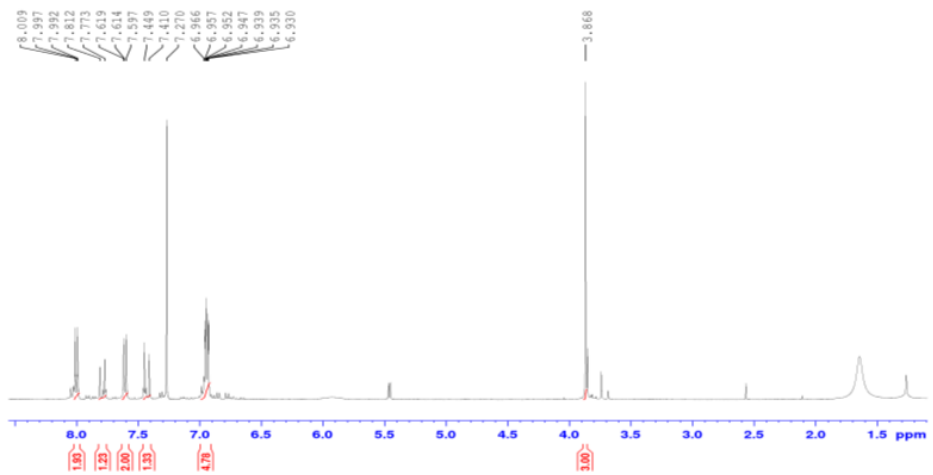

Fig. S4. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **2**.

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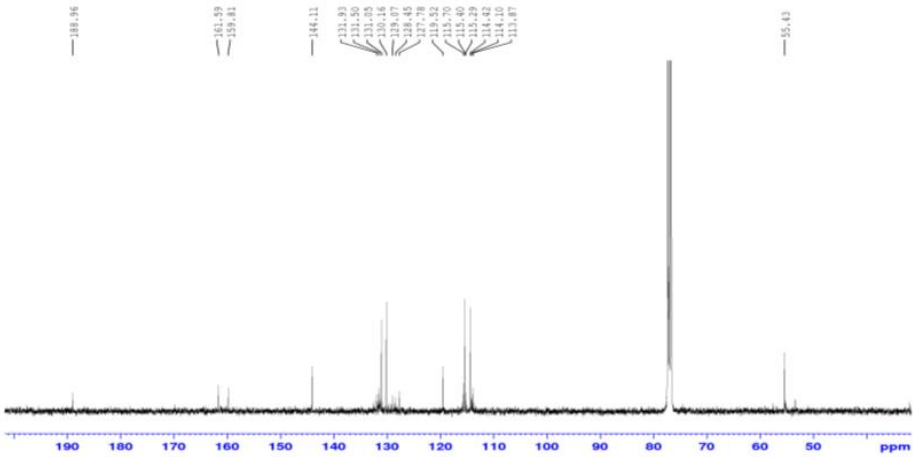

Fig. S5. ^{13}C NMR spectrum (400 MHz, $CDCl_3$) of compound **2**.

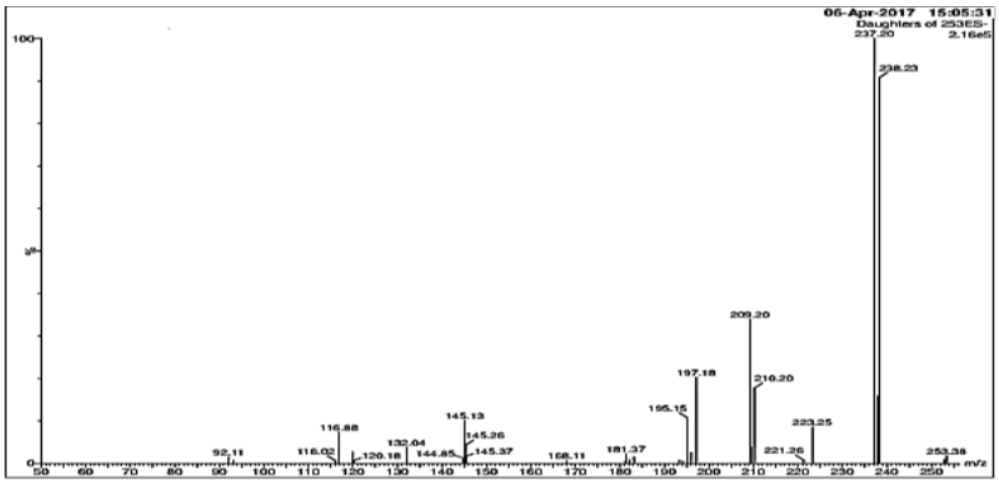

Fig. S6. Mass spectrum MS/MS ESI(-) of compound **2**.

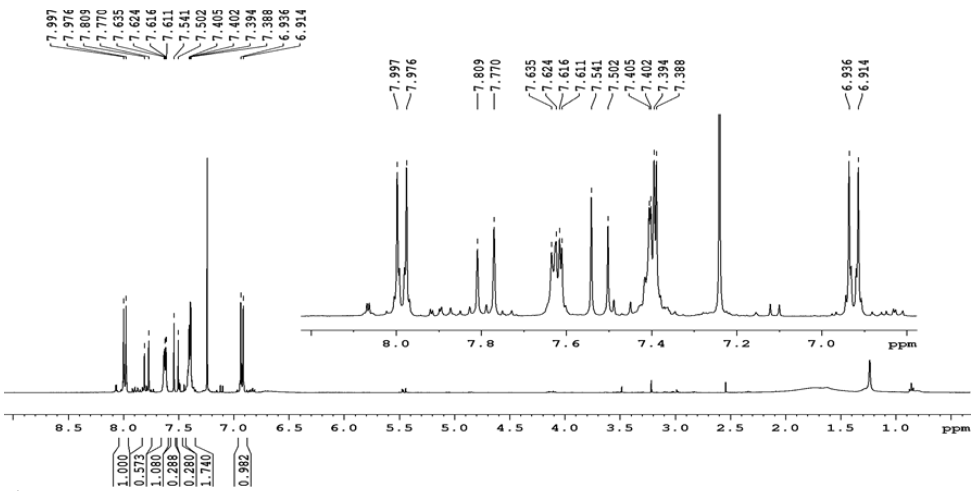

Fig. S7. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **3**.

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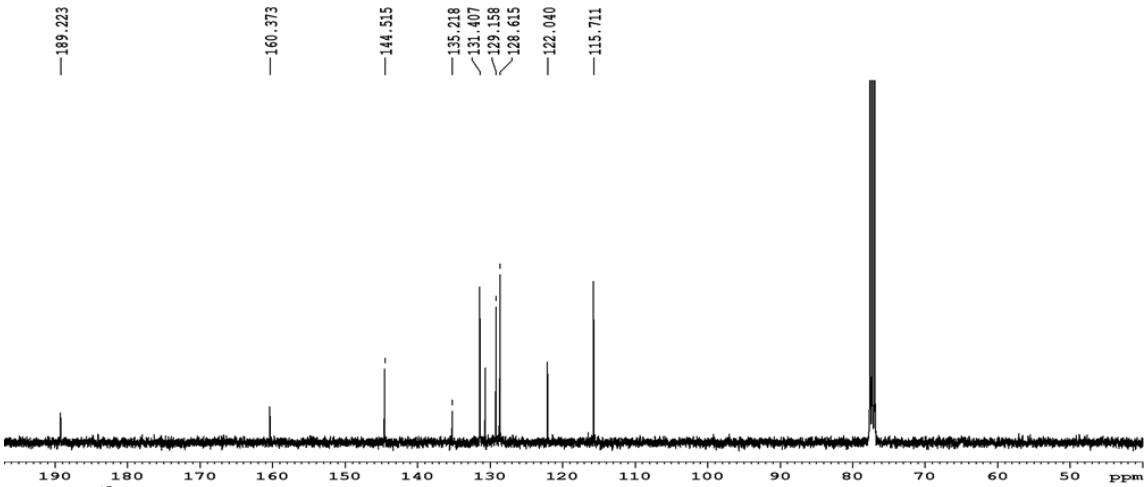

Fig. S8. ^{13}C NMR spectrum (400 MHz, $CDCl_3$) of compound **3**.

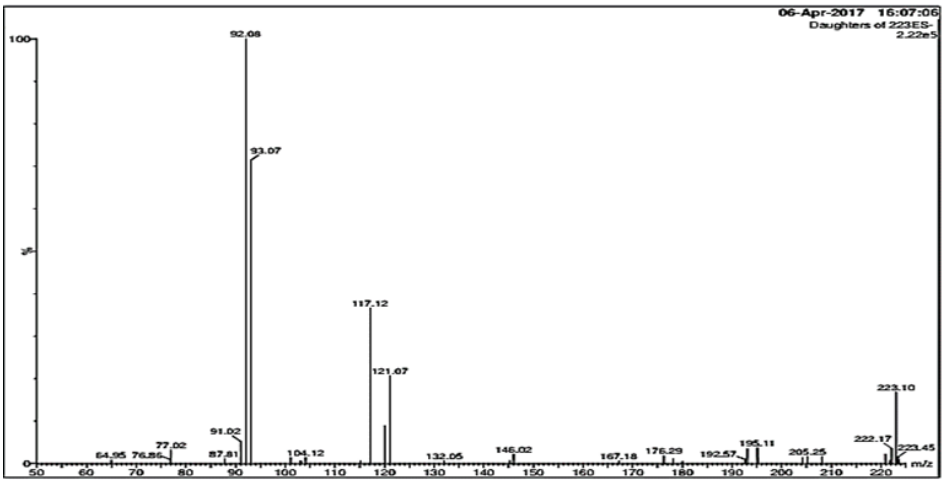

Fig. S9. Mass spectrum MS/MS ESI(-) of compound **3**.

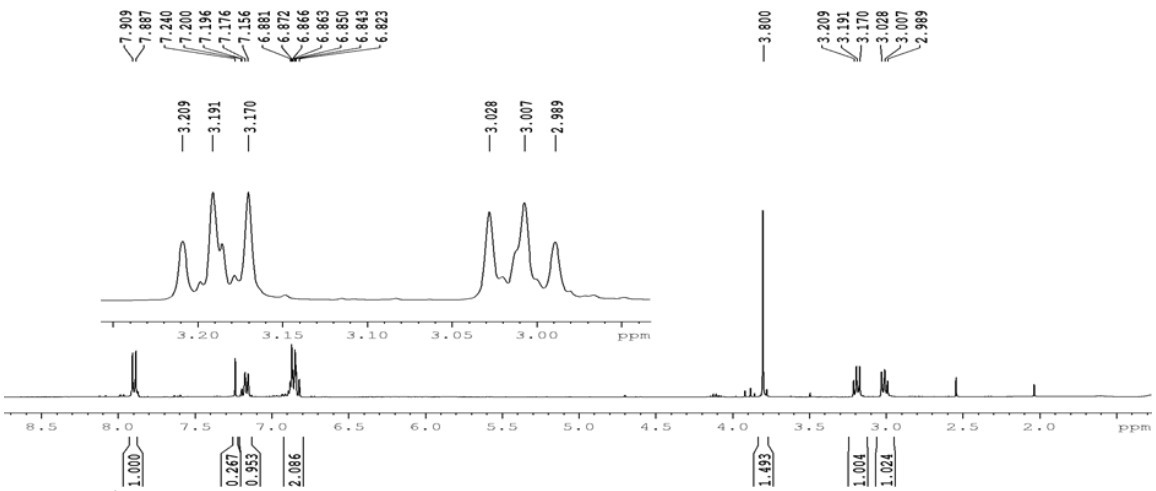

Fig. S10. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **4**.

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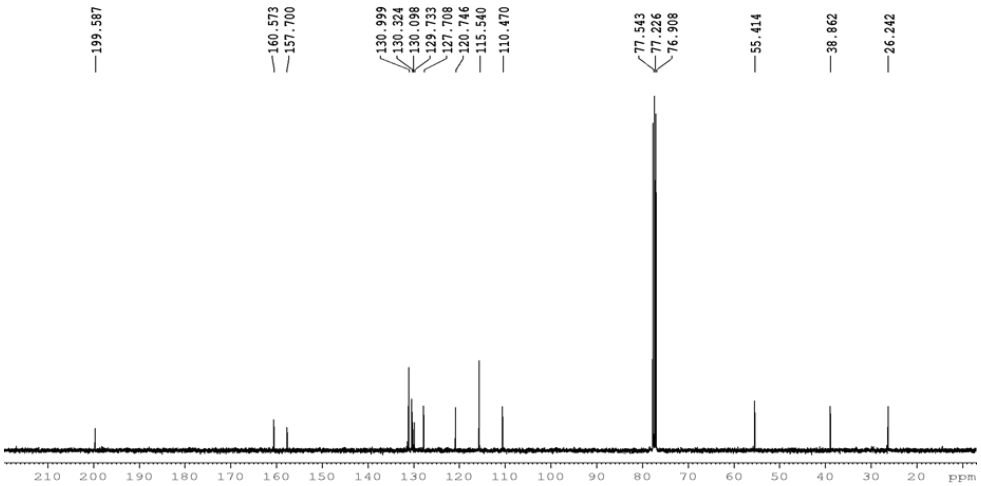

Fig. S11. ^{13}C NMR spectrum (400 MHz, $CDCl_3$) of compound **4**.

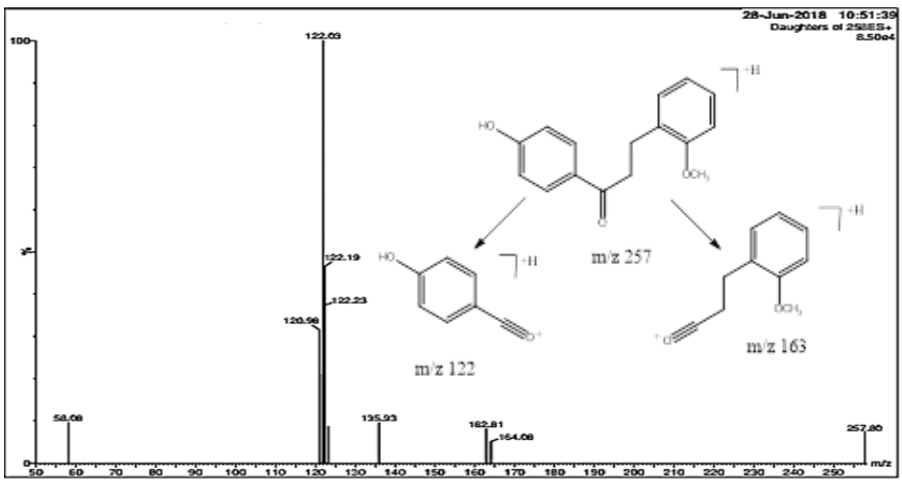

Fig. S12. Mass spectrum MS/MS ESI(+) of compound **4**.

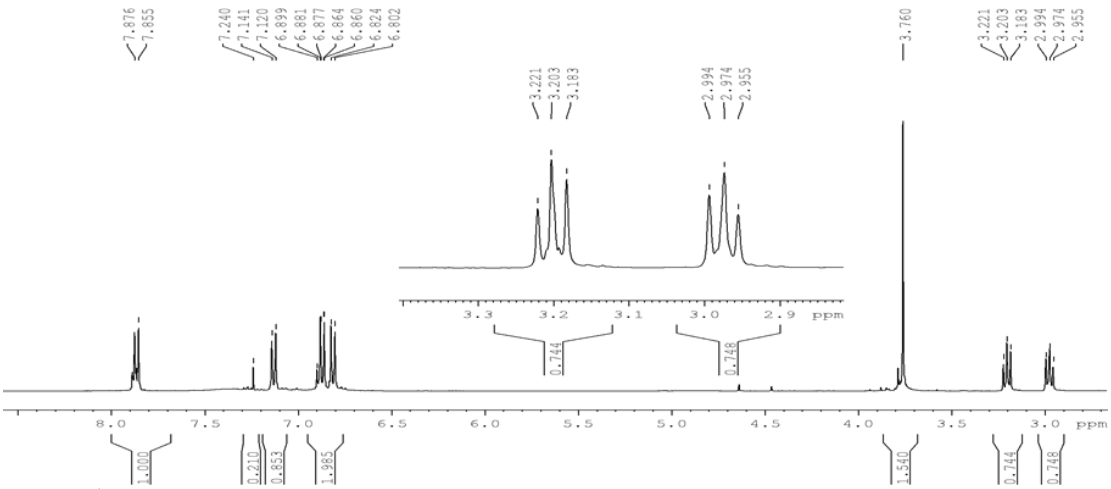

Fig. S13. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **5**.

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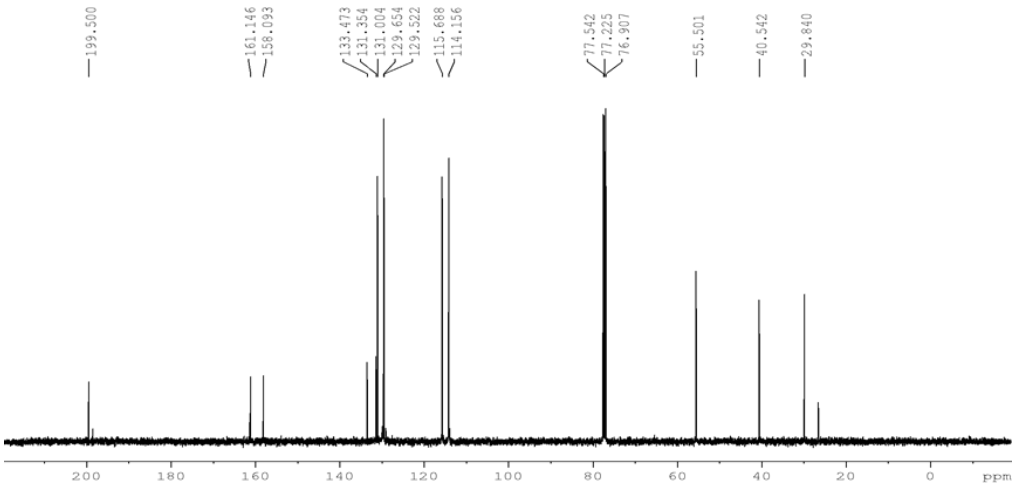

Fig. S14. ^{13}C NMR spectrum (400 MHz, $CDCl_3$) of compound **5**.

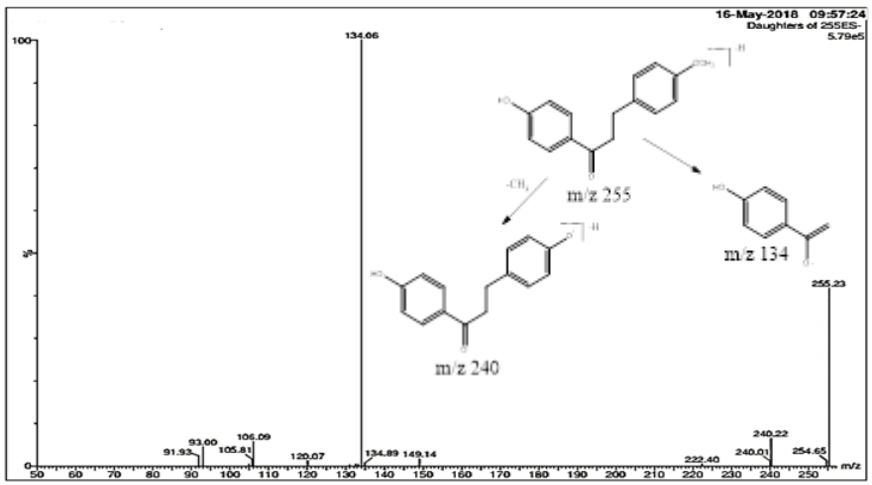

Fig. S15. Mass spectrum MS/MS ESI(-) of compound **5**.

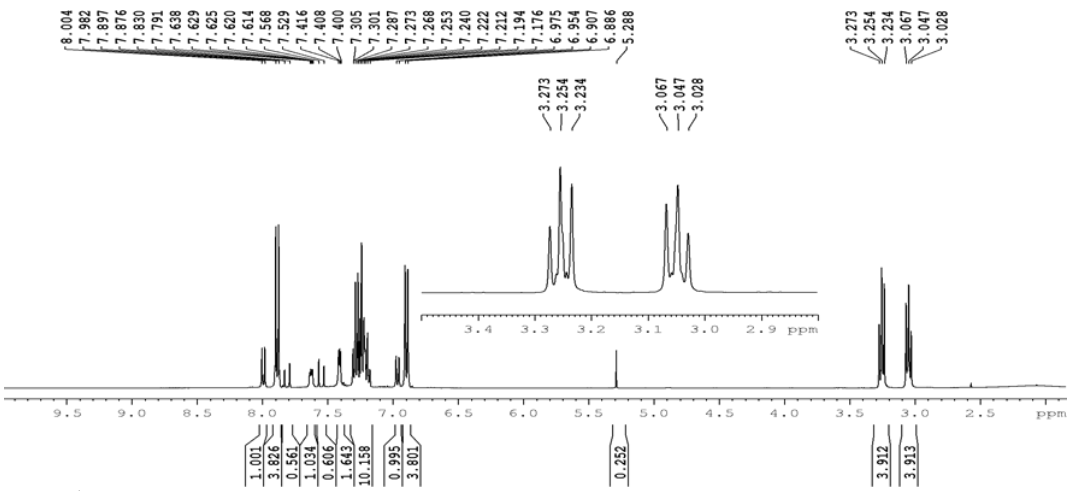

Fig. S16. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **6**.

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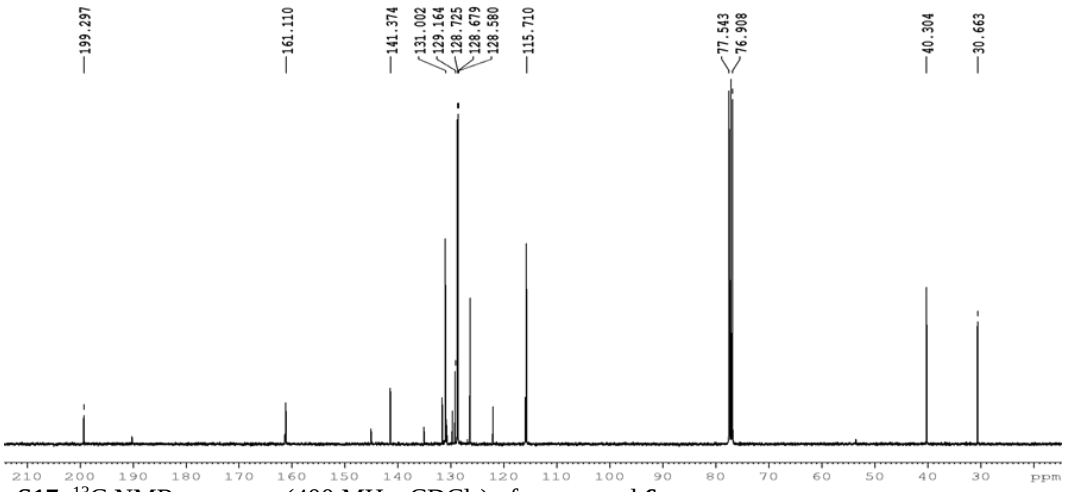


Fig. S17. ^{13}C NMR spectrum (400 MHz, $CDCl_3$) of compound **6**.

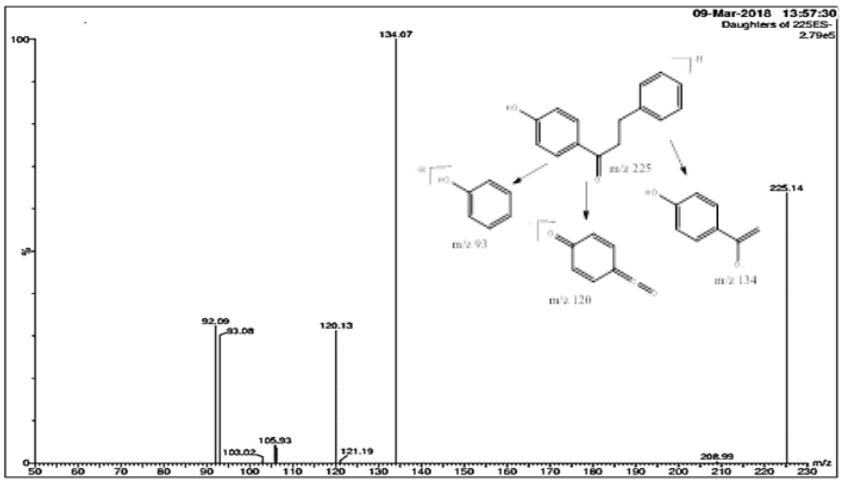
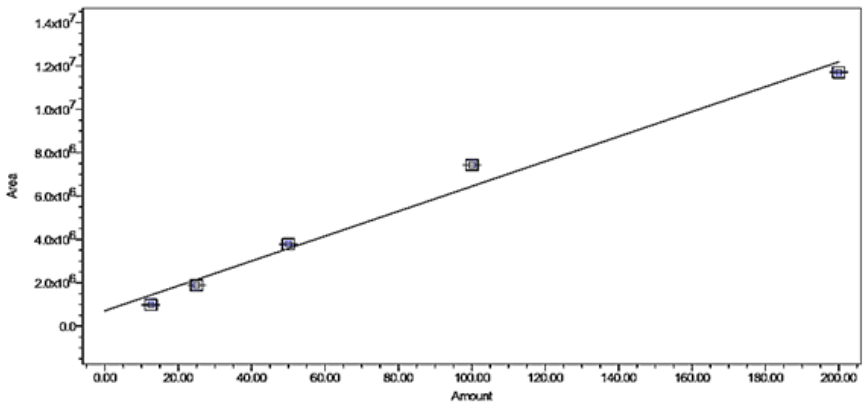


Fig. S18. Mass spectrum MS/MS ESI(-) of compound **6**.



Peak Name: Peak1 280.0nm; RT: 5.767; Fit Type: Linear (1st Order); Cal Curve Id: 4730; R: 0.998189; R^2: 0.996381; Weighting: None; Equation: Y = 5.61e+004 X + 5.51e+005; Normalized Intercept/Slope: 0.092432; RSD(E): 7.845065

Fig. S19. Calibration curve of biotransformation product compound **4** (12.5 - 200.0 µg/mL).

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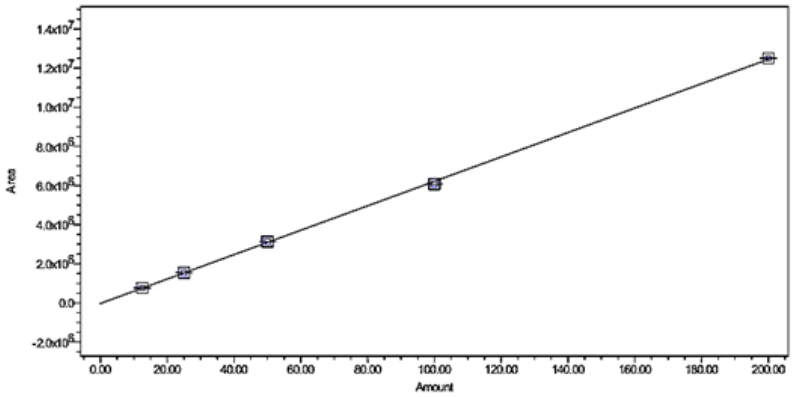

Fig. S20. Calibration curve of biotransformation product compound **5** (12.5 - 200.0 µg/mL).

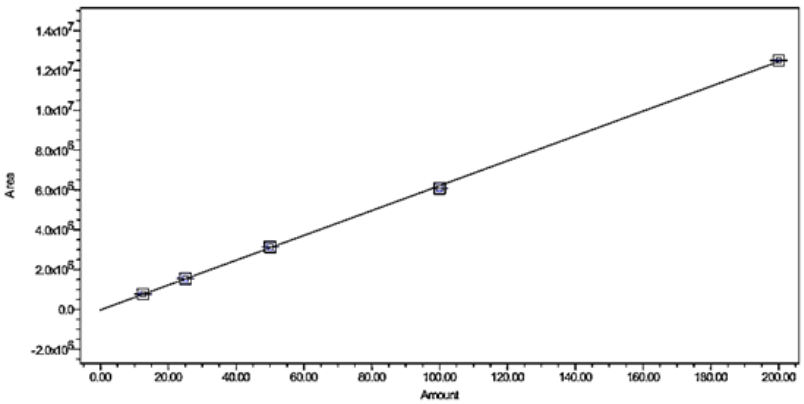

Fig. S21. Calibration curve of biotransformation product compound **6** (12.5 - 200.0 µg/mL).

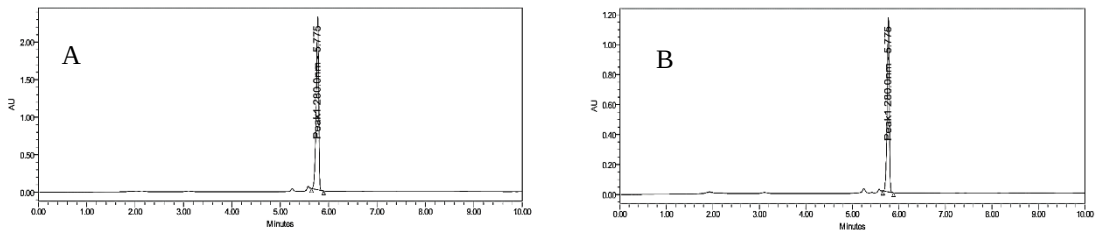

Fig. S22: Comparison by HPLC analyze of compound **4** obtained via synthesis (**A**) and bioreduction (**B**). HPLC-DAD (210 nm to 600 nm), Sunfire C18 reverse phase column (150 mm x 4.6 mm; 5 µm; Waters), C18 guard column (20 mm x 4.6; 5 µm, Waters), injection volume of 20 µL, column temperature 40 °C; linear exploratory gradient elution of H_2O/MeOH 50:50 to 0: 100, 10 min.

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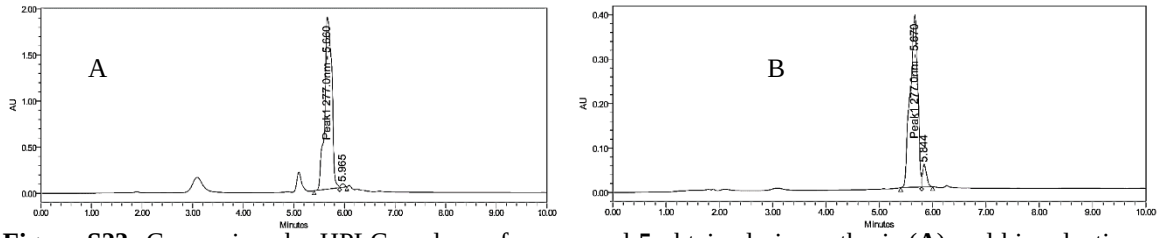

Figure S23: Comparison by HPLC analyze of compound **5** obtained via synthesis (**A**) and bioreduction (**B**). HPLC-DAD (210 nm to 600 nm), Sunfire C18 reverse phase column (150 mm x 4.6 mm; 5 µm; Waters), C18 guard column (20 mm x 4.6; 5 µm, Waters), injection volume of 20 µL, column temperature 40 °C; linear exploratory gradient elution of H_2O/MeOH 50:50 to 0: 100, 10 min.

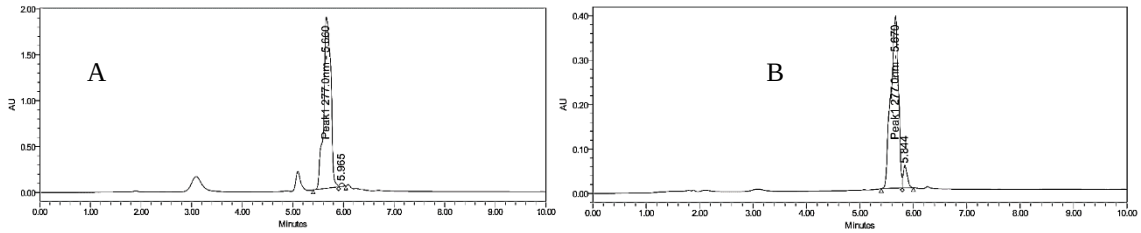

Fig. S23: Comparison by HPLC analyze of compound **5** obtained via synthesis (**A**) and bioreduction (**B**). HPLC-DAD (210 nm to 600 nm), Sunfire C18 reverse phase column (150 mm x 4.6 mm; 5 µm; Waters), C18 guard column (20 mm x 4.6; 5 µm, Waters), injection volume of 20 µL, column temperature 40 °C; linear exploratory gradient elution of H_2O/MeOH 50:50 to 0: 100, 10 min.

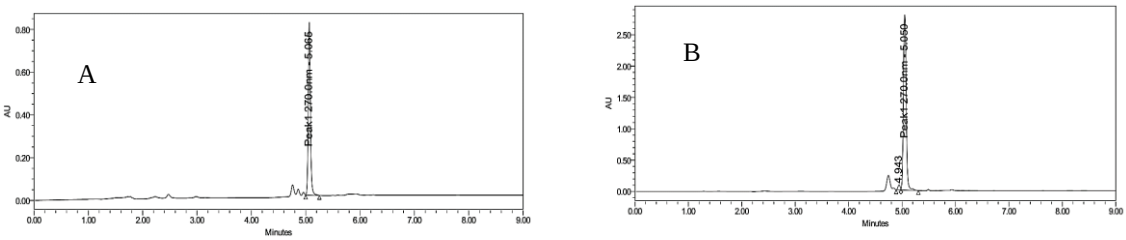

Figure S24: Comparison by HPLC analyze of compound **6** obtained via synthesis (**A**) and bioreduction (**B**). HPLC-DAD (210 nm to 600 nm), Sunfire C18 reverse phase column (150 mm x 4.6 mm; 5 µm; Waters), C18 guard column (20 mm x 4.6; 5 µm, Waters), injection volume of 20 µL, column temperature 40 °C; linear exploratory gradient elution of H_2O/MeOH 50:50 to 0: 100, 10 min.