

Additional file 2

Spectroscopic data of the individual converted products.

S-1 HREI-MS: calculated for $C_{15}H_{24}O$ (M^+), 220.1827; found 220.1825. 1H -NMR ($CDCl_3$) δ : 1.05 (d, $J=6.8$ Hz, H-12), 1.15 (s, 3H, H-14), 1.17 (s, 3H, H-15), 1.25 (m, 1H, H-4b), 1.32 (m, 1H, H-4a), 1.45 (s, 3H, H-13), 1.63-1.68 (2H, H-3), 1.88-1.92 (2H, H-5), 2.06 (d, $J=8.0$ Hz, 2H, H-8), 2.56 (m, 1H, H-2), 5.09 (dd, $J=8.0, 8.0$ Hz, 1H, H-7), 6.05 (d, $J=16.2$ Hz, 1H, H-11), 6.24 (d, $J=16.2$ Hz, H-1, H-10). ^{13}C -NMR ($CDCl_3$) δ : 14.0 (C-12), 16.5 (C-13), 21.9 (C-4), 25.9 (C-14), 26.3 (C-15), 32.4 (C-3), 40.4 (C-5), 41.6 (C-8), 39.6 (C-9), 47.3 (C-2), 122.2 (C-7), 126.6 (C-11), 137.4 (C-6), 151.9 (C-10), 205.3 (C-1).

S-2 HREI-MS: calculated for $C_{15}H_{24}O_2$ (M^+), 236.1776; found 236.1778. 1H -NMR ($CDCl_3$) δ : 1.03 (d, $J=6.8$ Hz, 3H, H-12), 1.15 (s, 3H, H-14), 1.17 (s, 3H, H-15), 1.18 (m, 1H, H-4b), 1.31 (m, 1H, H-4a), 1.63-1.68 (2H, H-3), 1.91 (m, 1H, H-5b), 2.06 (m, 1H, H-5a), 2.13-2.17 (2H, H-8), 2.56 (m, 1H, H-2), 3.92 (d, $J=12.2$ Hz, 1H, H-13b), 4.02 (d, $J=12.2$ Hz, 1H, H-13a), 5.20 (dd, $J=8.5, 8.5$ Hz, 1H, H-7), 6.04 (d, $J=16.2$ Hz, H-11), 6.12 (d, $J=16.2$ Hz, H-10). ^{13}C -NMR ($CDCl_3$) δ : 13.8 (C-12), 22.4 (C-4), 25.7 (C-14), 26.4 (C-15), 31.9 (C-3), 35.0 (C-5), 40.9 (C-8), 41.1 (C-9), 47.1 (C-2), 59.5 (C-13), 126.0 (C-7), 126.9 (C-11), 140.1 (C-6), 152.3 (C-10), 205.2 (C-1).

S-3 HREI-MS: calculated for $C_{15}H_{24}O_2$ (M^+), 236.1776; found 236.1779. 1H -NMR ($CDCl_3$) δ : 1.00 (d, $J=7.0$ Hz, 3H, H-12), 1.12 (s, 3H, H-14), 1.20-1.28 (2H, H-4), 1.26 (s, 3H, H-15), 1.50 (s, 3H, H-13), 1.63-1.68 (2H, H-3), 1.90-2.05 (2H, H-5), 2.67 (m, 1H, H-2), 4.24 (d, $J=9.8$ Hz, 1H, H-8), 5.09 (d, $J=9.8$ Hz, 1H, H-7), 6.11 (d, $J=16.5$ Hz, 1H, H-11), 6.20 (d, $J=16.5$ Hz, 1H, H-10). ^{13}C -NMR ($CDCl_3$) δ : 12.0 (C-12), 16.5 (C-13), 21.8 (C-4), 25.7 (C-14), 25.9 (C-15), 31.2 (C-3), 39.7 (C-5), 43.2 (C-9), 45.7 (C-2), 75.5 (C-8), 125.3 (C-7), 129.0 (C-11), 139.0 (C-6), 149.2 (C-10), 204.7 (C-1).

A-1 HRAPCI-MS: calculated for $C_{22}H_{17}O_4$ ($M-H^-$), 345.11269; found 345.11245. 1H -NMR ($CDCl_3$) δ : 4.02 (s, 6H, H-9, H-9'), 6.92 (s, 2H, H-2, H-2'), 7.49 (m, 2H, H-7, H-7'), 7.54 (m, 2H, H-6, H-6'), 8.20 (d, $J=7.5$ Hz, 2H, H-8, H-8'), 8.30 (d, $J=7.5$ Hz, 2H, H-5, H-5'). ^{13}C -NMR ($CDCl_3$) δ : 56.3 (C-9, C-9'), 107.9 (C-2, C-2'), 120.4 (C-3, C-3'), 122.7 (C-8, C-8'), 123.5 (C-5, C-5'), 126.2 (C-8a, C-8a'), 126.5 (C-7, C-7'), 127.0 (C-6, C-6'), 128.5 (C-4a, C-4'a), 142.1 (C-4, C-4'), 149.3 (C-1, C-1').

A-2 HRAPCI-MS: calculated for $C_{11}H_9O_2$ ($M-H^-$), 173.18808; found 173.18822. 1H -NMR ($CDCl_3$) δ : 3.99 (s, 3H, H-9), 6.84 (d, $J=7.8$ Hz, H-2), 6.84 (d, $J=7.8$ Hz, H-6), 7.30 (dd, $J=7.8, 8.4$ Hz, H-7), 7.39 (dd, $J=7.8, 8.6$ Hz, H-3), 7.74 (d, $J=8.6$ Hz, H-4), 7.85 (d, $J=8.4$ Hz, H-8). ^{13}C -NMR ($CDCl_3$) δ : 55.6 (C-9), 104.5 (C-2), 109.5 (C-6), 113.6 (C-4), 114.7 (C-8), 125.1 (C-7), 125.3 (C-4a), 125.3 (C-3), 126.9 (C-8a), 151.2 (C-5), 155.4 (C-1).

A-3 HRAPCI-MS: calculated for $C_{11}H_9O_2$ ($M-H^-$), 173.18808; found 173.18831. 1H -NMR ($CDCl_3$) δ : 3.98

(s, 3H, H-9), 5.77 (s, 1H, OH-2), 7.23 (d, $J=8.5$ Hz, 1H, H-3), 7.36 (dd, $J=8.0, 8.4$ Hz, 1H, H-6), 7.49 (dd, $J=8.0, 8.2$ Hz, 1H, H-7), 7.57 (d, $J=8.5$ Hz, 1H, H-4), 7.79 (d, $J=8.0$ Hz, 1H, H-5), 7.94 (d, $J=8.2$ Hz, 1H, H-8). ^{13}C -NMR (CDCl_3) δ : 61.6 (C-9), 117.4 (C-3), 120.3 (C-8), 123.5 (C-6), 125.3 (C-4), 126.3 (C-7), 128.0 (C-8a), 128.3 (C-5), 139.2 (C-4a), 144.3 (C-1), 145.4 (C-2).

A-4 HRAPCI-MS: calculated for $\text{C}_{12}\text{H}_{11}\text{O}_2$ (M-H) $^-$, 187.07591; found 187.07565. ^1H -NMR (CDCl_3) δ : 1.52 (t, $J=7.0$ Hz, 3H, H-10), 4.16 (q, $J=7.0$ Hz, 2H, H-9), 7.23 (d, $J=8.7$ Hz, 1H, H-3), 7.33 (dd, $J=7.9, 8.1$ Hz, 1H, H-6), 7.47 (dd, $J=8.1, 8.6$ Hz, 1H, H-7), 7.55 (d, $J=8.7$ Hz, 1H, H-2), 7.78 (d, $J=7.9$ Hz, 1H, H-5), 7.92 (d, $J=8.6$ Hz, 1H, H-8). ^{13}C -NMR (CDCl_3) δ : 15.9 (C-10), 70.1 (C-9), 117.3 (C-3), 120.5 (C-8), 123.5 (C-6), 125.1 (C-2), 126.2 (C-7), 128.3 (C-5), 128.3 (C-8a), 129.6 (C-4a), 138.5 (C-1), 145.8 (C-4).

A-5 HRAPCI-MS: calculated for $\text{C}_{12}\text{H}_{11}\text{O}_2$ (M-H) $^-$, 187.07591; found 187.07588. ^1H -NMR (CDCl_3) δ : 1.54 (t, $J=7.0$ Hz, 3H, H-10), 4.20 (q, $J=7.0$ Hz, 2H, H-9), 6.83 (d, $J=7.0$ Hz, 1H, H-2), 6.85 (d, $J=6.4$ Hz, 1H, H-6), 7.29 (dd, $J=6.4, 8.6$ Hz, 1H, H-7), 7.37 (dd, $J=7.0, 8.5$ Hz, 1H, H-3), 7.71 (d, $J=8.5$ Hz, 1H, H-4), 7.89 (d, $J=8.6$ Hz, 1H, H-8). ^{13}C -NMR (CDCl_3) δ : 14.9 (C-10), 63.8 (C-9), 105.3 (C-2), 109.4 (C-6), 113.4 (C-4), 114.9 (C-8), 125.0 (C-7), 125.3 (C-3), 125.4 (C-4a), 127.3 (C-8a), 151.2 (C-5), 154.8 (C-1).

A-6 HRAPCI-MS: calculated for $\text{C}_{11}\text{H}_9\text{O}$ (M-H) $^-$, 157.06534; found 157.06531. ^1H -NMR (CDCl_3) δ : 2.45 (s, 3H, H-9), 6.67 (s, 1H, H-3), 7.22 (s, 1H, H-1), 7.40 (dd, $J=8.0, 8.0$ Hz, 1H, H-6), 7.43 (dd, $J=8.0, 8.6$ Hz, 1H, H-8), 8.10 (d, $J=8.0$ Hz, 1H, H-5). ^{13}C -NMR (CDCl_3) δ : 21.8 (C-9), 110.8 (C-3), 119.8 (C-1), 121.3 (C-5), 122.6 (C-4a), 124.3 (C-7), 126.5 (C-6), 127.0 (C-8), 134.9 (C-8a), 135.8 (C-2), 149.2 (C-4).

A-8 HRAPCI-MS: calculated for $\text{C}_{12}\text{H}_{11}\text{O}$ (M-H) $^-$, 171.08100; found 171.08121. ^1H -NMR (CDCl_3) δ : 2.54 (s, 3H, H-10), 2.58 (s, 3H, H-9), 6.70 (d, $J=7.9$ Hz, 1H, H-3), 7.05 (d, $J=7.9$ Hz, 1H, H-2), 7.37 (d, $J=8.6$ Hz, 1H, H-7), 7.84 (d, $J=8.6$ Hz, 1H, H-8), 7.97 (s, 1H, H-5), ^{13}C -NMR (CDCl_3) δ : 18.8 (C-9), 21.7 (C-10), 108.2 (C-3), 124.1 (C-8), 125.1 (C-2), 126.5 (C-4a), 126.6 (C-1), 128.4 (C-7), 131.7 (C-8a), 134.5 (C-6), 151.0 (C-4).

A-13 HREI-MS: calculated for $\text{C}_{12}\text{H}_{11}\text{NO}$ M $^+$ 185.0841, found 185.0843. ^1H -NMR (CDCl_3) δ : 4.77 (s, 2H, H-7), 7.24 (m, 1H, H-5'), 7.48 (d, $J=8.1$ Hz, 2H, H-3, H-5), 7.99 (d, $J=8.1$ Hz, 2H, H-2, H-6), 7.75 (m, 1H, H-3'), 7.76 (m, 1H, H-4'), 8.70 (d, $J=4.2$ Hz, 1H, H-6'). ^{13}C -NMR (CDCl_3) δ : 65.1 (C-7), 120.6 (C-3'), 122.1 (C-5'), 127.1 (C-6), 127.3 (C-3, C-5), 138.8 (C-1), 138.8 (C-4'), 141.2 (C-4), 157.1 (C-2'), 157.2 (C-6').

A-14 HREI-MS: calculated for $\text{C}_{14}\text{H}_{20}\text{O}_3$ M $^+$, 236.1412; found 236.1422. ^1H -NMR (CD_3Cl) δ : 1.23 (s, 6H, H-12, H-13), 1.50 (d, $J=7.0$ Hz, 3H, H-3), 2.74 (s, 2H, H-10), 3.67 (s, 3H, H-14), 3.72 (q, $J=7.0$ Hz, 1H, H-2), 7.17 (d, $J=8.2$ Hz, 2H, H-6, H-8), 7.24 (d, $J=8.2$ Hz, 2H, H-5, H-9). ^{13}C -NMR (CD_3Cl) δ : 18.6 (C-3), 29.2 (C-12, C-13), 45.1 (C-2), 49.4 (C-10), 52.0 (C-14), 70.7 (C-11), 127.3 (C-5, C-9), 130.8 (C-6, C-8),

136.6 (C-7), 138.8 (C-4), 175.1 (C-1).

A-15 HREI-MS: calculated for $C_{16}H_{15}FO_3$ M+, 274.1005; found 274.1007. 1H -NMR (CD_3Cl) δ : 1.80 (s, 3H, H-3), 3.83 (s, 3H, H-16), 7.37 (m, 1H, H-13), 7.40 (m, 1H, H-5), 7.40 (d, $J=7.3$ Hz, 1H, H-9), 7.43 (m, 2H, H-12, H-14), 7.45 (m, 1H, H-8), 7.54 (d, $J=7.5$ Hz, 2H, H-11, H-15). ^{13}C -NMR (CD_3Cl) δ : 26.9 (C-3), 53.5 (C-16), 74.7 (C-2), 113.0 (C-5), 121.2 (C-9), 126.9 (C-7), 127.8 (C-13), 128.4 (C-12, C-14), 128.9 (C-11, C-15), 130.6 (C-8), 134.6 (C-10), 143.6 (C-4), 158.5 (C-6), 175.3 (C-1).

A-16 HRAPCI-MS: calculated for $C_{16}H_{14}FO_3$ (M-H) $^-$, 273.0927; found 273.0911. 1H -NMR (CD_3Cl) δ : 1.53 (d, $J=7.4$ Hz, 3H, H-3), 3.70 (s, 3H, H-16), 3.75 (q, $J=7.4$ Hz, 1H, H-2), 6.89 (d, $J=8.6$ Hz, 2H, H-12, H-14), 7.09 (dd, $J=1.6, 10.5$ Hz, 1H, H-5), 7.11 (dd, $J=1.5, 7.6$ Hz, 1H, H-9), 7.34 (dd, $J=7.6, 8.8$ Hz, 1H, H-8), 7.41 (dd, $J=1.5, 8.8$ Hz, 2H, H-11, H-15). ^{13}C -NMR (CD_3Cl) δ : 18.4 (C-3), 44.9 (C-2), 52.2 (C-16), 115.3 (C-5), 115.4 (C-12, C-14), 123.5 (C-9), 127.5 (C-7), 128.0 (C-10), 130.3 (C-11, C-15), 130.5 (C-8), 141.2 (C-4), 155.3 (C-13), 159.7 (C-6), 174.6 (C-1).