

Supporting Information:

Three Active Phytotoxic Compounds from the Leaves of *Albizia richardiana* (Voigt.) King and Prain for the Development of Bioherbicides to Control Weeds

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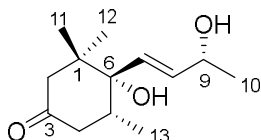
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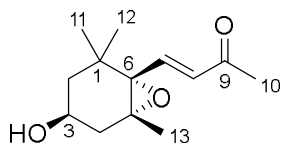
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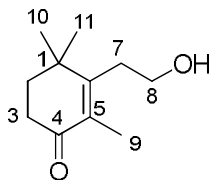
4,5-dihydrovomifoliol: colorless oil; ^1H NMR (500 MHz, CD_3OD) 5.84 (1H, dd, $J = 15.7, 5.8$ Hz, H-8), 5.66 (1H, dd, $J = 15.7, 1.2$ Hz, H-7), 4.34, (1H, q, H-9), 2.87 (1H, d, $J = 13.6$ Hz, H-2 ax), 2.45 (1H, dd, $J = 14.1, 12.1$ Hz, H-4 ax), 2.31-2.22 (1H, m, H-5), 2.12 (1H, ddd, $J = 14.1, 4.6, 2.3$ Hz, H-4 eq), 1.82 (1H, dd, $J = 13.6, 2.3$, H-2 eq), 1.27 (3H, d, $J = 6.4$ Hz, H₃-13), 0.98 (3H, s, H₃-11), 0.92 (3H, s, H₃-12), 0.90 (3H, d, $J = 6.7$ Hz, H₃-13); HRESIMS m/z 249.1463 (calcd for $\text{C}_{13}\text{H}_{22}\text{O}_3\text{Na}$, 249.1467).



3-Hydroxy-5 α ,6 α -epoxy- β -ionone; colorless oil; ^1H NMR (500 MHz, CD_3OD) 7.17 (1H, d, $J = 15.8$ Hz, H-7), 6.18 (1H, d, $J = 15.8$ Hz, H-8), 3.76 (1H, m, H-3), 2.30 (1H, ddd, $J = 14.3, 5.1, 1.7$ Hz, H-4), 2.29 (3H, s, H-10), 1.66 (1H, dd, $J = 14.3, 9.2$ Hz, H-4), 1.58 (1H, ddd, $J = 12.9, 3.4, 1.7$ Hz, H-2), 1.27 (1H, dd, $J = 12.9, 10.8$ Hz, H-2), 1.19 (3H, s, H-13), 1.18 (3H, s, H-12), 0.96 (3H, s, H-11); HRESIMS m/z 247.1306 (calcd for $\text{C}_{13}\text{H}_{20}\text{O}_3\text{Na}$ 247.1310).



3-(2-Hydroxyethyl)-2,4,4-trimethyl-2cyclohexen-1-one; colorless oil; ^1H NMR (500 MHz, CDCl_3) 3.73 (2H, t, $J = 8.0$ Hz, 8-H), 2.58 (2H, t, $J = 8.0$ Hz, 7-H), 2.47 (2H, t, $J = 6.6$ Hz, 3-H), 1.81 (3H, s, 9-H), 1.81 (2H, t, $J = 6.6$ Hz, 2-H), 1.17 (6H, s, 11-H and 10-H); ^{13}C NMR (125 MHz, CDCl_3) 199.3, 160.0, 141.5, 132.5, 61.4, 37.4, 36.3, 34.4, 27.0, 12.0; HRESIMS m/z 183.1385 (calcd for $\text{C}_{11}\text{H}_{19}\text{O}_2$ 183.1385).



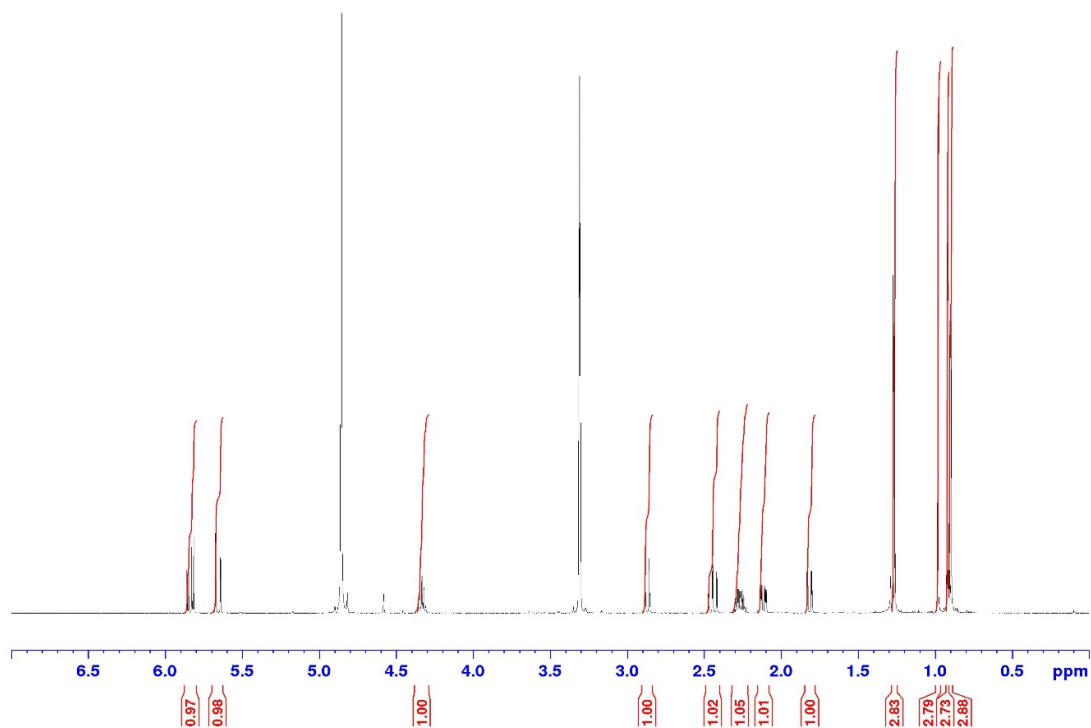


Figure S1. ^1H NMR spectrum of compound 1 (4,5-dihydrovomifoliol) in CD_3OD (500 MHz).

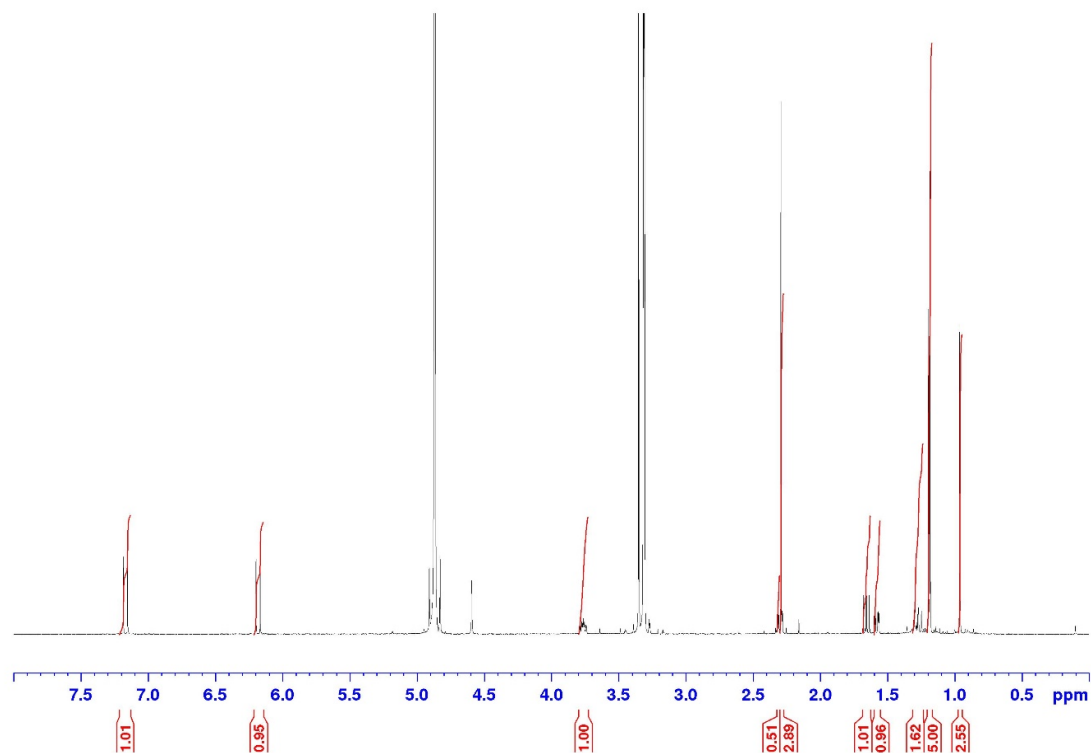


Figure S2. ^1H NMR spectrum of compound 2 (3-Hydroxy-5 α ,6 α -epoxy- β -ionone) in CD_3OD (500 MHz).

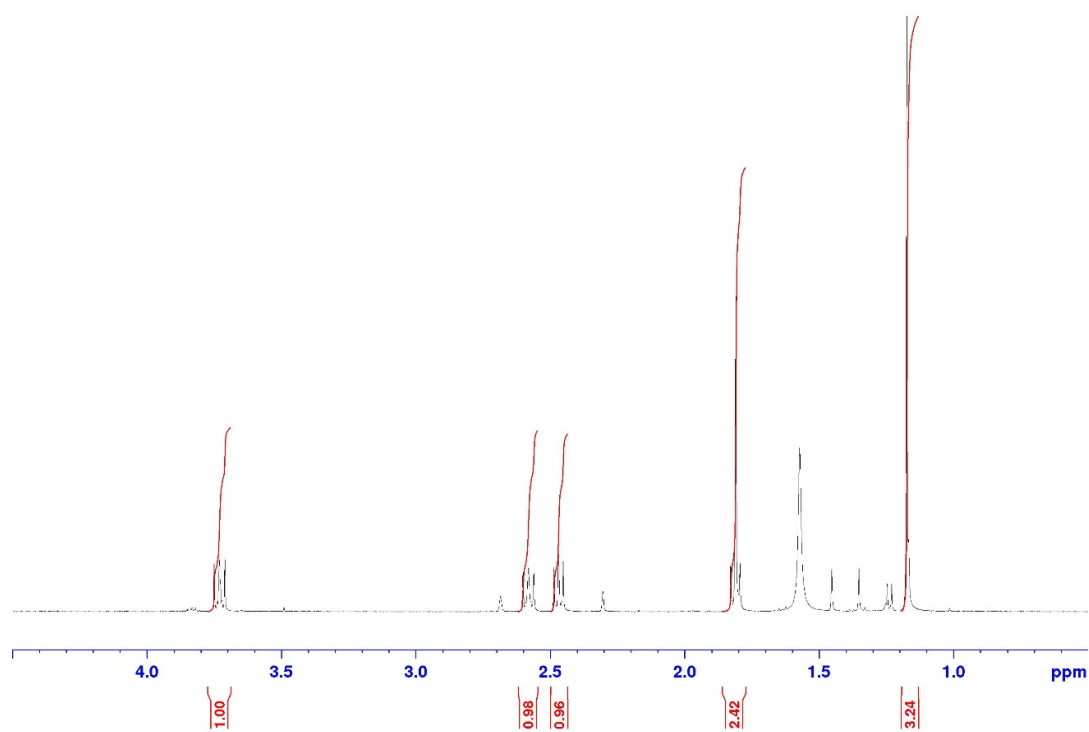


Figure S3. ¹H NMR spectrum of compound 3 (3-(2-Hydroxyethyl)-2,4,4-trimethyl-2cyclohexen-1-one) in CDCl₃ (500 MHz).

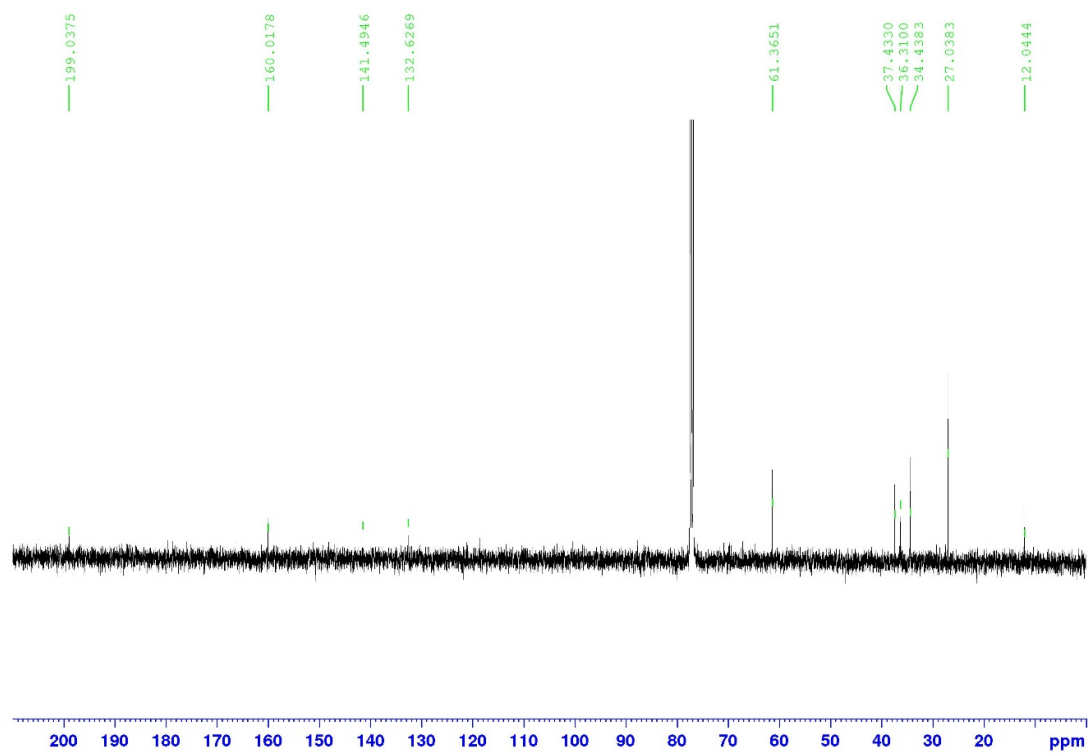


Figure S4. ^{13}C NMR spectrum of compound 3 (3-(2-Hydroxyethyl)-2,4,4-trimethyl-2cyclohexen-1-one) in CDCl_3 (125 MHz).

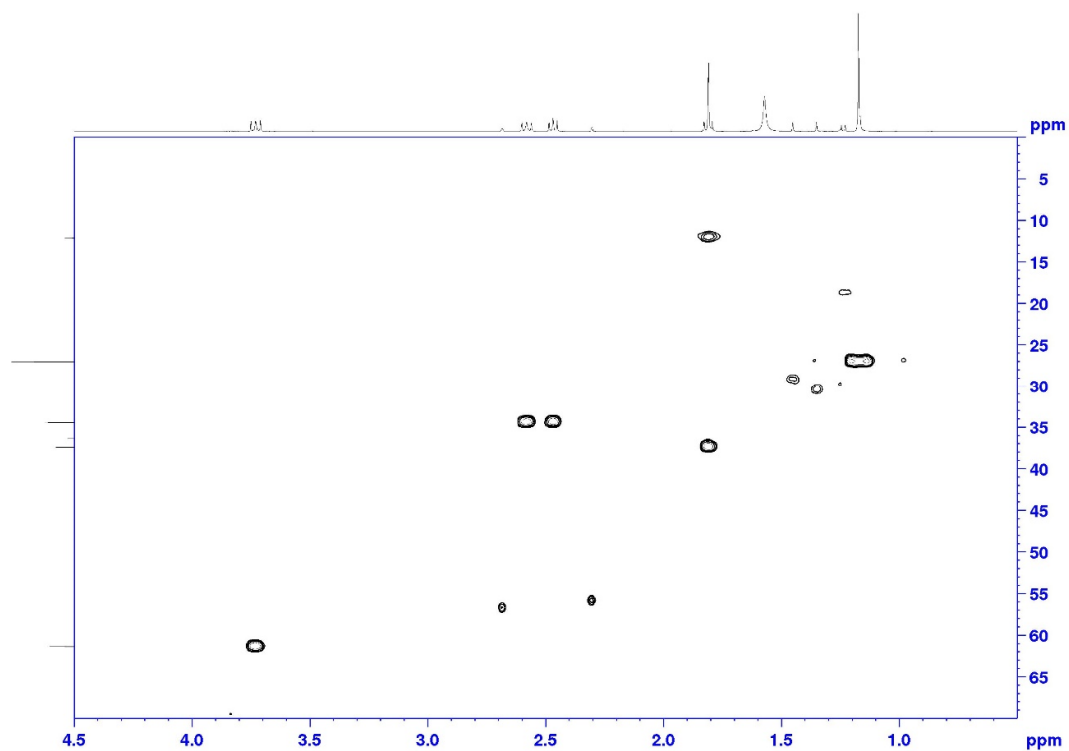


Figure S5. HSQC spectrum of compound 3 (3-(2-Hydroxyethyl)-2,4,4-trimethyl-2cyclohexen-1-one) in CDCl_3 (500 MHz).

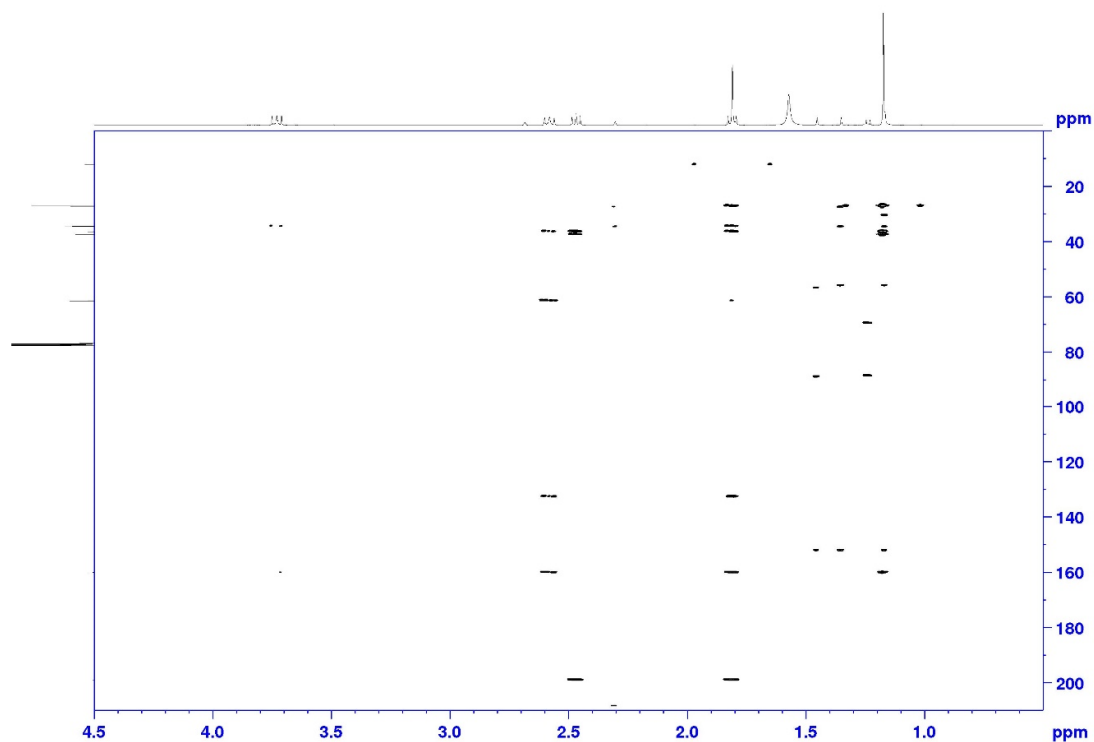


Figure S6. HMBC spectrum of compound 3 (3-(2-Hydroxyethyl)-2,4,4-trimethyl-2cyclohexen-1-one) in CDCl_3 (500 MHz).

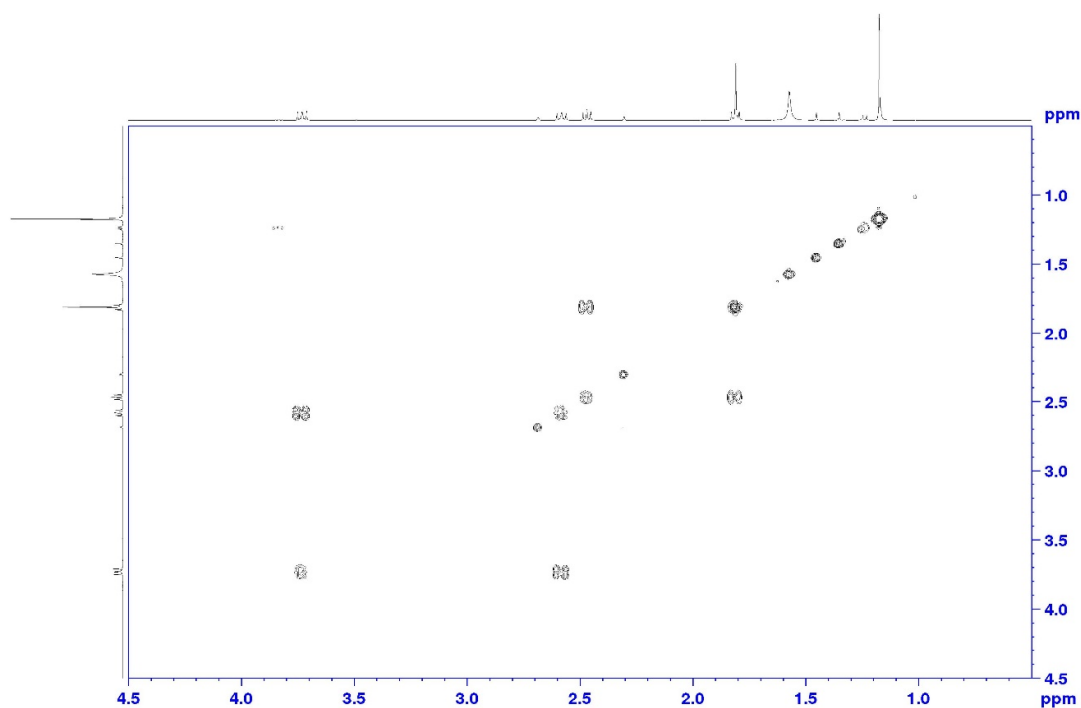


Figure S7. COSY spectrum of compound 3 (3-(2-Hydroxyethyl)-2,4,4-trimethyl-2cyclohexen-1-one) in CDCl_3 (500 MHz).

OK-14-60-2
210305_teruya10 37 (0.232)

1: TOF MS ES+
1.26e+003

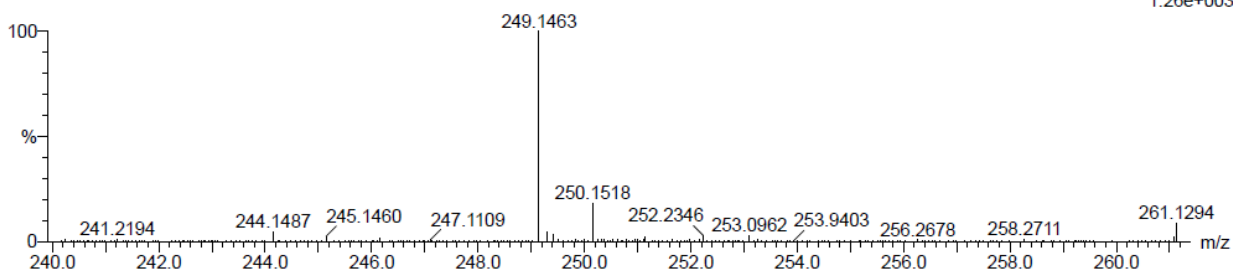


Figure S8. HRESIMS spectrum of compound 1 (4,5-dihydrovomifoliol).

OK-14-60-3
210305_teruya11 30 (0.195)

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2.17e+003

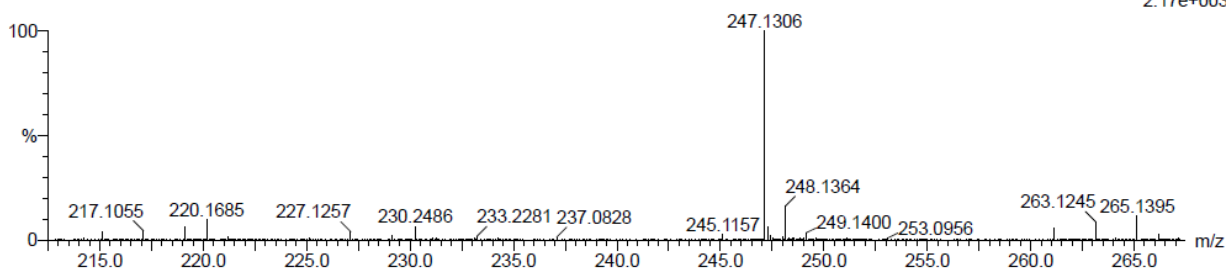


Figure S9. HRESIMS spectrum of compound 2 (3-Hydroxy-5 α ,6 α -epoxy- β -ionone).

OK-14-68-2
210305_teruya12 42 (0.258)

1: TOF MS ES+
4.73e+002

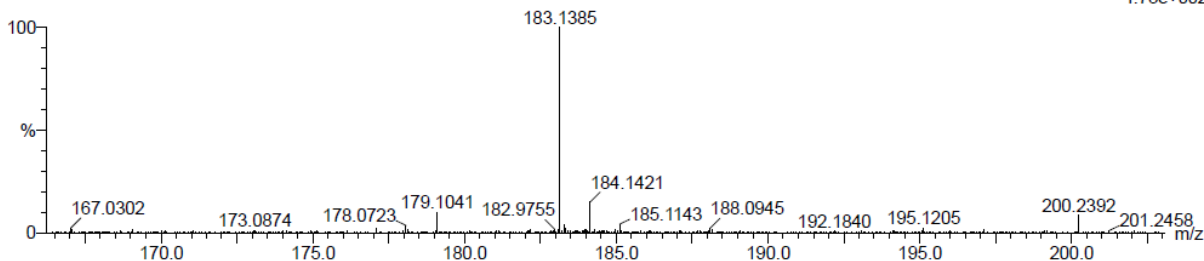


Figure S10. HRESIMS spectrum of compound 3 (3-(2-Hydroxyethyl)-2,4,4-trimethyl-2-cyclohexen-1-one).