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EPOXY OCTADECENOIC ESTERS FROM *Vernonia anthelmintica* SEEDS[a]

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Vernonia anthelmintica (L.) Willd., an annual herb plant of Asteraceae, is distributed in Xinjiang of China, sometimes in India and Pakistan. The seeds of *V. anthelmintica* are used for the treatment of many kinds of skin diseases in traditional Uighur medicine in Xinjiang [1, 2]. In previous phytochemical investigations of *V. anthelmintica* seeds, the occurrence of four sesquiterpene lactones has been reported [3–5]. In our sustained investigation of structurally unique and biogenetically interesting epoxy lipids from plants in Xinjiang, three epoxy octadecenoic esters were isolated from the title plant.

The air-dried and powdered seeds of *V. anthelmintica* were extracted three times with *n*-hexane. The solvent was evaporated under vacuum. The *n*-hexane extract was subjected to column chromatography over silica gel in petroleum ether–chloroform solvent systems to afford ethyl vernolate (**1**), 1,3-divernolin (**2**), and 1-vernolin (**3**). Their structures were elucidated by MS and NMR data.

Ethyl vernolate (**1**) was isolated from natural plants for the first time. Meanwhile, we report the NMR data of ethyl vernolate for the first time.

Ethyl Vernolate (1), $C_{20}H_{36}O_3$. Mass spectrum (EI, 75 eV), *m/z* (I_{rel}, %): 324 (M^+, 3), 279 (8), 236 (7), 180 (9), 164 (9), 151 (7), 99 (100). ^{1}H NMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 5.39–5.54 (2H, m, H-9, 10), 4.11 (2H, q, J = 7.2, -CO-O-C<u>H</u>$_2$-), 2.90–2.94 (2H, m, H-12, 13), 2.34–2.40 (1H, m, H-11a), 2.28 (2H, m, H-2), 2.15–2.22 (1H, m, H-11b), 2.02–2.07 (2H, m, H-8), 1.60–1.63 (2H, m, H-3), 1.31–1.58 (16H, m, H-4, 5, 6, 7, 14, 15, 16, 17), 1.25 (3H, t, J = 7.2, -CO-O-CH$_2$-<u>CH</u>$_3$), 0.91 (3H, t, J = 6.8, CH_3-18).

^{13}C NMR spectrum (100 MHz, $CDCl_3$, δ): 173.62 (C-1), 132.41 (C-9), 123.87 (C-10), 59.99 (-CO-O-<u>C</u>H$_2$-), 57.03 (C-13), 56.37 (C-12), 22.41–34.12 (C-2, 3, 4, 5, 6, 7, 8, 11, 14, 15, 16, 17), 14.16, 13.89 (C-Me, C-Me).

1,3-Divernolin (2), $C_{39}H_{68}O_7$. Mass spectrum (ESI), *m/z* 649 $[M + H]^+$. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 5.40–5.54 (4H, m, H-9, 10), 4.13–4.20 (4H, m, -CO-O-C<u>H</u>$_2$-CH(OH)-C<u>H</u>$_2$-O-CO-), 4.08–4.12 (1H, m, -CO-O-CH$_2$-C<u>H</u>(OH)-CH$_2$-O-CO-), 2.92–2.94 (4H, m, H-12, 13), 2.34–2.39 (6H, m, H-11a, 2), 2.16–2.20 (2H, m, H-11b), 2.02–2.06 (4H, m, H-8), 1.61–1.64 (4H, m, H-3), 1.31–1.56 (32H, m, H-4, 5, 6, 7, 14, 15, 16, 17), 0.91 (6H, t, J = 6.8, CH_3-18).

^{13}C NMR spectrum (100 MHz, $CDCl_3$, δ): 173.81 (C-1), 132.53 (C-9), 123.92 (C-10), 68.32 (-CO-O-CH$_2$-<u>C</u>H(OH)-CH$_2$-O-CO-), 65.04 (-CO-O-<u>C</u>H$_2$-CH(OH)-<u>C</u>H$_2$-O-CO-), 57.21 (C-13), 56.54 (C-12), 22.57–34.05 (C-2, 3, 4, 5, 6, 7, 8, 11, 14, 15, 16, 17), 13.97 (C-18).

1-Vernolin (3), $C_{21}H_{38}O_5$. Mass spectrum (ESI), *m/z* 371 $[M + H]^+$. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 5.38–5.55 (2H, m, H-9, 10), 4.12–4.21 (2H, m, -CO-O-C<u>H</u>$_2$-CH(OH)-CH$_2$-OH), 3.90–3.96 (1H, m, -CO-O-CH$_2$-C<u>H</u>(OH)-CH$_2$-OH), 3.57–3.76 (2H, m, -CO-O-CH$_2$-CH(OH)-C<u>H</u>$_2$-OH), 2.92–2.96 (2H, m, H-12, 13), 2.35–2.39 (1H, m, H-11a), 2.33–2.37 (2H, m, H-2), 2.16–2.22 (1H, m, H-11b), 2.02–2.07 (2H, m, H-8), 1.59–1.65 (2H, m, H-3), 1.31–1.59 (16H, m, H-4, 5, 6, 7, 14, 15, 16, 17), 0.91 (3H, t, J = 6.8, CH_3-18).

^{13}C NMR spectrum (100 MHz, $CDCl_3$, δ): 174.28 (C-1), 132.60 (C-9), 123.91 (C-10), 70.24 (-CO-O-CH$_2$-<u>C</u>H(OH)-CH$_2$-OH), 65.15 (-CO-O-<u>C</u>H$_2$-CH(OH)-CH$_2$-OH), 63.35 (-CO-O-CH$_2$-CH(OH)-<u>C</u>H$_2$-OH), 57.35 (C-13), 55.67 (C-12), 22.60–37.10 (C-2, 3, 4, 5, 6, 7, 8, 11, 14, 15, 16, 17), 14.01 (C-18).

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