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CHEMICAL CONSTITUENTS FROM THE AERIAL PARTS OF *Sophora mollis*

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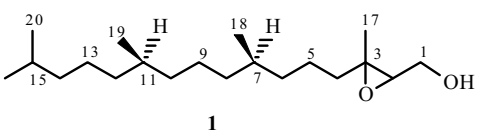
Sophora mollis (Royle) Baker is a perennial shrub and is widely distributed in southwestern China, Pakistan, India, Iran, Afghanistan, and Nepal [1]. In previous studies, quinolizidine alkaloids and flavonoids have been isolated from this plant [2–4]. In our investigation into the chemical constituents of *S. mollis*, eight compounds were isolated and identified from the aerial parts of *S. mollis* for the first time.

The aerial parts of *S. mollis* were collected during July 2006 from Chitral in the north of Pakistan. Taxonomic identification was done by Naveed Ahmad, Department of Botany, University of Peshawar, Pakistan. A voucher specimen (JA-08-C) was deposited in the herbarium at the Department of Botany, University of Peshawar, Peshawar, Pakistan.

Air dried, powdered aerial parts (2.9 kg) were extracted with n-hexane for 8 days using a Soxhlet extractor. The *n*-hexane extract was separated from the plant residue by decantation and filtration. The filtered *n*-hexane extract was left overnight. A pale yellow solid precipitated (MRK-2, 13 g) and was filtered out. The filtrate was concentrated under vacuum to obtain a residue (MRK-1, 51.9 g). The plant residue was further extracted with acetone using a Soxhlet extractor for one week. The acetonic extract was concentrated under reduced pressure by a vacuum rotary evaporator, which afforded a residue (MRK-3, 65 g). The MRK-3 fraction was subjected to column chromatography on silica gel eluted with petroleum ether–acetone (30:1, 15:1, 8:1, 4:1, 2:1, 1:1, 0:1) to give seven subfractions, A-G. Fraction B was then chromatographed on silica gel using petroleum ether with increasing amounts of EtOAc as eluent to give compounds **1**, **2**, **5**, and **6**. Fraction C was rechromatographed on a silica gel column using a $CHCl_3$–EtOAc gradient solvent system to afford compound **7**. Fraction D was chromatographed on silica gel using $CHCl_3$ with increasing amounts of acetone as eluent to give compound **3**. Fraction E was chromatographed on a silica gel column using a $CHCl_3$–acetone gradient solvent system to afford compound **4**. Similarly, fraction F was chromatographed on silica gel using $CHCl_3$ with increasing amounts of acetone as eluent to give compound **8**.

The structures of all compounds were determined by spectroscopic evidence, including EI-MS, 1D NMR, and 2D NMR. The spectroscopic data of all compounds were in good agreement with the literature data.

(*E*)-Phytyl Epoxide (1). $C_{20}H_{40}O_2$, colorless oil. EI-MS *m/z* (%): 312 $[M]^+$ (1), 284 (1), 269 (1), 256 (1), 250 (1), 157 (1), 43 (100). ^1H NMR (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 3.85 (1H, dd, J = 12.0, 4.3, H-1a), 3.68 (1H, dd, J = 12.0, 6.6, H-1b), 2.99 (1H, dd, J = 6.6, 4.3, H-2), 1.29 (3H, s, H-17), 0.86 (6H, d, J = 6.8, H-18, H-19), 0.87 (6H, d, J = 6.8, H-16, H-20). ^{13}C NMR (100 MHz, $CDCl_3$, δ, ppm): 61.3 (C-1), 63.1 (C-2), 61.7 (C-3), 39.3 (C-4), 24.7 (C-5), 36.9 (C-6), 32.7 (C-7), 37.4 (C-8), 22.5 (C-9), 37.2 (C-10), 32.7 (C-11), 37.2 (C-12), 24.4 (C-13), 38.8 (C-14), 24.7 (C-15), 22.7 (C-16), 16.7 (C-17), 19.6 (C-18), 19.7 (C-19), 22.6 (C-20) [5].



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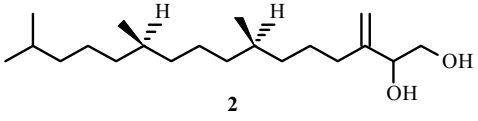

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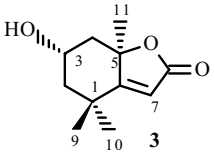

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7,11,15-Trimethyl-3-methylenehexadecane-1,2-diol (2). $C_{20}H_{40}O_2$, colorless oil. EI-MS *m/z* (%): 312 $[M]^+$ (1), 282 (1), 281 (2), 263 (1), 149 (2), 137 (4), 123 (6), 109 (12), 97 (18), 95 (18), 83 (29), 81 (18), 71 (49), 69 (32), 57 (51), 43 (100). ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 5.11 (1H, br.s, H-17a), 4.94 (1H, br.s, H-17b), 4.19 (1H, dd, J = 7.2, 3.2, H-2), 3.76 (1H, dd, J = 10.4, 3.2, H-1a), 3.51 (1H, dd, J = 10.4, 7.2, H-1b), 1.99 (2H, m, H-4), 1.00–1.60 (19H, m), 0.87 (6H, d, J = 7.2, H-16, H-20), 0.85 (6H, d, J = 7.2, H-18, H-19). ^{13}C NMR (100 MHz, $CDCl_3$, δ, ppm): 65.7 (C-1), 75.1 (C-2), 148.5 (C-3), 33.0 (C-4), 25.4 (C-5), 36.8 (C-6), 32.7 (C-7), 37.4 (C-8), 24.4 (C-9), 37.4 (C-10), 32.8 (C-11), 37.3 (C-12), 24.7 (C-13), 39.3 (C-14), 27.9 (C-15), 22.6 (C-16), 110.4 (C-17), 19.7 (C-18), 19.6 (C-19), 22.7 (C-20) [6].

Loliolide (3). $C_{11}H_{16}O_3$, colorless needles. EI-MS *m/z* (%): 196 $[M]^+$ (7), 181 (2), 163 (9), 153 (6), 140 (19), 111 (46), 95 (13), 57 (22), 43 (100). ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 5.70 (1H, s, H-7), 4.34 (1H, m, H-3), 2.47 (1H, dd, J = 14.4, 3.6, H-4a), 1.99 (1H, dd, J = 14.4, 3.6, H-2a), 1.79 (3H, s, H-11), 1.70 (1H, dd, J = 14.4, 3.6, H-4b), 1.54 (1H, dd, J = 14.4, 3.6, H-2b), 1.47 (3H, s, H-10), 1.28 (3H, s, H-9). ^{13}C NMR (100 MHz, $CDCl_3$, δ, ppm): 35.9 (C-1), 47.3 (C-2), 66.8 (C-3), 45.7 (C-4), 86.7 (C-5), 182.4 (C-6), 112.9 (C-7), 171.9 (C-8), 30.6 (C-9), 26.5 (C-10), 27.0 (C-11) [7].

Scopoletin (4). $C_{10}H_8O_4$, colorless needles. EI-MS *m/z* (%): 192 $[M]^+$ (90), 177 (61), 164 (28), 149 (65), 121 (43), 79 (43), 69 (100), 51 (63). ^{1}H NMR (400 MHz, $(CD_3)_2CO$, δ, ppm, J/Hz): 8.81 (1H, s, 7-OH), 7.85 (1H, d, J = 9.6, H-4), 7.20 (1H, s, H-5), 6.79 (1H, s, H-8), 6.18 (1H, d, J = 9.6, H-3), 3.90 (3H, s, 6-OCH_3). ^{13}C NMR (100 MHz, $(CD_3)_2CO$, δ, ppm): 160.5 (C-2), 112.6 (C-3), 145.4 (C-4), 109.3 (C-5), 145.7 (C-6), 151.1 (C-7), 103.0 (C-8), 150.3 (C-9), 111.4 (C-10), 56.0 (6-OCH_3) [8].

Hexacosanol (5). $C_{26}H_{54}O$, white lamellar. EI-MS *m/z* (%): 364 $[M–H_2O]^+$ (1). ^{1}H NMR [9].

Octacosanol (6). $C_{28}H_{58}O$, white lamellar. EI-MS *m/z* (%): 392 $[M–H_2O]^+$ (1). ^{1}H NMR [10].

***β*-Sitosterol (7).** $C_{29}H_{50}O$, colorless crystals. EI-MS *m/z* (%): 414 $[M]^+$ (12). ^{1}H NMR [11].

Daucosterol (8). $C_{35}H_{60}O_6$, white amorphous powder. EI-MS *m/z* (%): 575 $[M–H]^+$ (15). ^{1}H NMR [12].

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