# A new triterpenoid from traditional Chinese medicine *Poria cocos*

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A new triterpenoid, 3,4-secolanosta-4(28),7,9,24Z-tetraen-3,26-dioic acid, along with two known compounds 16-deoxyporicoic acid B and 3-epidehydrotrametenolic acid were isolated from the dried sclerotia of *Poria cocos* Wolf (Polyporaceae). The structures are elucidated by spectroscopic methods and literatures.

**Keywords:** triterpenoid, *Poria cocos* Wolf, Polyporaceae

The sclerotia of *Poria cocos* Wolf (*Polyporaceae*), called Fuling in Chinese is traditionally used in Chinese medicine as a diuretic and sedative.[1,2] Previous phytochemical investigations on the sclerotia of this species showed it contained lanostane-type triterpene acids,[3,4] some of which possessed strong anti-inflammatory effects,[5,6] cytotoxicities against human cancer cell lines,[7] and induced apoptosis in prostate cancer cells[8] and in H-ras-transformed rat2 cells.[9] In addition, some triterpene acids from the epidermis of the sclerotia of *P. cocos* have been reported to possess inhibitory effects on DNA polymerases.[10] In the course of our study, a new triterpenoid was isolated from the dried sclerotia of *P. cocos*. In this paper, we present the isolation and structural elucidation of the new triterpenoid and two known triterpenoids, 16-deoxyporicoic acid B (**2**),[11] and 3-epidehydrotrametenolic acid (**3**),[12] based on the spectroscopic analysis and literature data.

Compound **1** was obtained as a white solid. Its molecular formula was shown to be $C_{30}H_{44}O_4$ based on HR-ESIMS data (*m/z*: 467.3159, calc. for $[M - H]^-$, *m/z*: 467.3161). The $^1H$ NMR spectrum of **1** showed the presence of an isopropenyl group (δ 4.36, 4.82, 1H each, brs, H-28; δ1.73, 3H, s, H-29) and three tertiary methyls (δ 0.67, 1.09, 0.93, 3H each, s, H-18, H-19, H-30) besides an angelic acid unit (δ 6.03, lH, t, $J$ = 6.8 Hz, H-24; δ 2.13, 3H, s, H-27) and a secondary methyl (δ 1.00, 3H, d, $J$ = 6.0 Hz, H-21). These facts indicate that **1** possessed an 3,4-seco-ring A identical to **2**. Further comparison the NMR spectra between **1** and **2** indicated that there were some differences in the side chain. In the HMBC spectrum (Fig. 2), the correlations of $H_3$-21 and C-17, 20 and 22, H-24 and C-25, 26 and 27, showed that the carboxyl group carbons located at C-26 in **1** instead of C-21 in **2**. By further analysis of the HMQC, HMBC and $^1H$-$^1H$ COSY spectra, all the proton and carbon signals have been assigned unambiguously. Therefore, compound **1** is elucidated as 3,4-secolanosta-4(28), 7,9,24Z- tetraen-3,26-dioic acid.

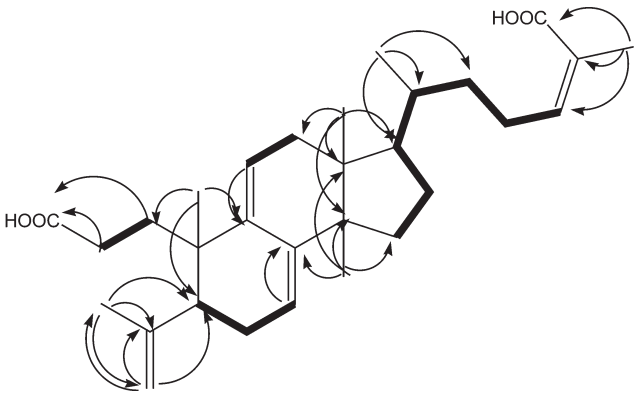


**Fig. 2** The key HMBC (H→C) and COSY (—) correlations of **1**.

## Experimental

IR spectra were recorded as KBr pellets on a Perkin-Elmer 599B spectrophotometer. MS were determined on a Bruker Daltonics Apex III mass spectrometer. NMR spectra were measured on Bruker DRX-400 spectrometers with TMS as the internal standard. and $CDCl_3$ as solvent. Silica gel (200–300 mesh, Qingdao Marine Chemical Co., China) was used for column chromatography and silica gel GF254 for TLC (Qingdao Marine Chemical Co., China). Sephadex LH-20 (GE), reversed-phase C-18 silica gel (60 mesh, Merck). Dionex P680ALPC equipped with an Alltima C-18 column (4.6 × 250 mm) was used for HPLC analysis and a semi-preparative Alltima C-18 column (10 × 250 mm) was used in sample preparation.

*Plant material*

The dried sclerotia of *Poria cocos Wolf* (*Polyporaceae*) were purchased from Wanshoulu Chinese medicine market in Xi'an, P.R. China, in July 2008. A voucher specimen (No. 20080177) is deposited in the laboratory of College of Pharmaceutical Science, Shaanxi University of Chinese Medicine, P.R. China.

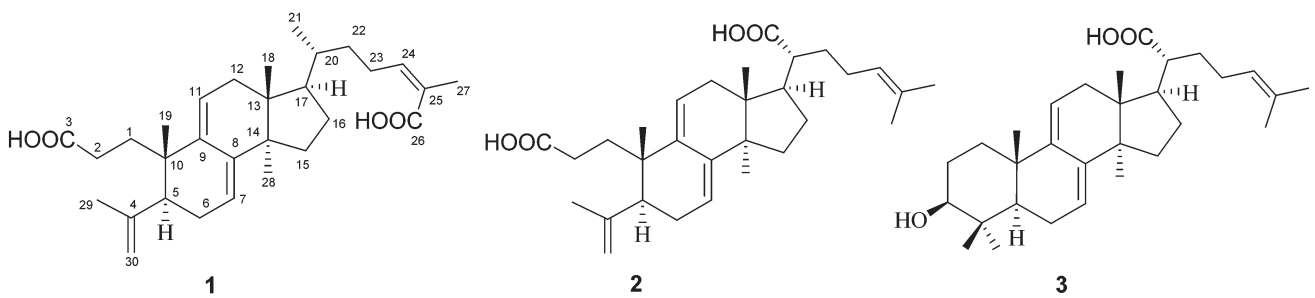


**Fig. 1** Chemical structure of compounds **1–3**.

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**Table 1** $^{1}H$ and $^{13}C$ NMR data (in $CDCl_3$) for compound **1** (δ in ppm, *J* in Hz)

| No. | $\delta_C$ [a] | $\delta_H$ *J* /Hz [b] | No. | $\delta_C$ [a] | $\delta_H$ *J*/Hz [b] |
|---|---|---|---|---|---|
| 1α | 36.3 (t) | 2.10 [c] | 16α | 28.2 (t) | 1.30 [c] |
| 1β | | 1.89 (m) | 16β | | 1. 61 [c] |
| 2α | 30.3 (t) | 2.47 [c] | 17 | 51.3 (d) | 1.13 [c] |
| 2β | | 2.58 [c] | 18 | 16.8 (q) | 0.67 (s) |
| 3 | 176.8 (s) | | 19 | 22.3 (q) | 1.09 (s) |
| 4 | 149.4 (s) | | 20 | 36.5 (d) | 1.49 (m) |
| 5 | 50.9 (d) | 2.32 (brd, 7.1) | 21 | 18.6 (q) | 1.00 (d, 6.0) |
| 6α | 28.6 (t) | 2.5 [c] | 22α | 36.3 (t) | 1.65 [c] |
| 6β | | 2.03 (m) | 22β | | 1.24 [c] |
| 7 | 117.8 (d) | 5.22 (brs) | 23α | 27.0 (t) | 2.73 (m) |
| 8 | 142.7 (s) | | 23β | | 2.86 (m) |
| 9 | 137.5 (s) | | 24 | 142.1 (d) | 6.03 (t, 6.8) |
| 10 | 36.7 (s) | | 25 | 128.7 (s) | |
| 11 | 120.5 (d) | 5.33 (brs) | 26 | 170.7 (s) | |
| 12α | 38.9 (t) | 2.14 [c] | 27 | 21.6 (q) | 2.13 (s) |
| 12β | | 2.14 [c] | 28 | 24.3 (q) | 0.93 (s) |
| 13 | 44.6 (s) | | 29 | 22.2 (q) | 1.73 (s) |
| 14 | 50.5 (s) | | 30α | 112.2 (t) | 4.36 (brs) |
| 15α | 31.3 (t) | 1.66 [c] | 30β | | 4.82 (brs) |
| 15β | | 1.31 [c] | | | |

[a] At 100 MHz; [b] at 400 MHz; [c] overlap.

*Extraction and isolation*

The dried powdered sclerotia of *P. cocos* (5.0 kg) were extracted with 95% EtOH (three times, each 20 L) at room temperature. The solvent was removed and the EtOH extract was suspended in distilled water and successively partitioned between petroleum ether, EtOAc and n-BuOH successively (three times, each 1.5 L). The EtOAc extract (65 g) was applied to a silica gel column, and eluted with chloroform containing increasing amounts of methanol. The fractions obtained from petroleum ether-EtOAc (1:1) elution were combined and subjected to repeated column chromatography and further purified by HPLC to yield pure compounds **1** (4 mg), **2** (8 mg), and **3** (5 mg).

*3,4-Secolanosta-4(28),7,9,24Z- teraen-3,26-dioic acid* (**1**): White solid; $[\alpha]^{20}_{D}$ + 30.9° (*c* 0.4, MeOH); UV ($CHCl_3$) $\lambda_{max}$ (log ε) 241 (1.81), 267 (1.75) nm; IR (KBr): 2933, 1696, 1639, 1454, 1437, 1415, 1379, 1306, 1202, 1149 $cm^{-1}$; HR-ESIMS: revealed *m/z*: 467.3159, requires *m/z*: 467.3161 for $C_{30}H_{43}O_4$); $^{1}H$ and $^{13}C$ NMR: see Table.

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