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TRITERPENOIDS AND BENZOIC ACID DERIVATIVES FROM THE FLOWERS OF *SYZYGIUM CUMINI*

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Summary

Triterpenoids and Benzoic Acid Derivatives from the Flowers of *Syzygium cumini*

From the flowers of *Syzygium cumini* (L.) Skeels, twelve known compounds (seven triterpenoids and five benzoic acid derivatives) were isolated, including friedelin (**1**), epifriedelanol (**2**), ursolic acid (**3**), corosolic acid (**4**), arjunolic acid (**5**), lupeol (**6**), betulinic acid (**7**), gallic acid (**8**), 3,5-dihydroxy-4-methoxybenzoic acid (**9**), syringic acid (**10**), protocatechuic acid (**11**), and isovanillic acid (**12**). The structures of the isolates were determined by spectroscopic analyses including MS and NMR data. Among them, compounds **4-6**, **9**, and **11** were first isolated from the flowers of *S. cumini*. Also, this is the first report of the chemical constituents from *S. cumini* in Vietnam.

Keywords: *Syzygium cumini,* Myrtaceae, *Triterpenoid, Phenolic.*

1. Introduction

Syzygium cumini is a flowering plant from the Myrtaceae family with notable pharmaceutical, and industrial applications. *Syzygium* species are commonly found in tropical and subtropical regions around the world [1]. Traditionally, *S. cumini* has been used as a folk remedy for treating stomach issues, diabetes, and bronchitis [1],[2]. Chemical investigations of *Syzygium* species have identified compounds such as flavonoids, glycosides, triterpenoids, and saponins, which exhibited various bioactivities, including antidiabetic, antifungal, anti-inflammatory, antibacterial, antioxidant, and cytotoxic properties, etc [1], [3]. As part of our study in the search for new bioactive compounds from plants in Vietnam, an EtOAc extract of *S. cumini* flowers inhibited 31.8% of the KB cell lines at a concentration of 1.0 µg/mL. Thus, this species was selected for further investigation of the chemical constituents and bioactivities. In this paper, we report the isolation and structural elucidation of seven known triterpenoids and five known benzoic acid derivatives (compounds **1-12**, Fig. 1) from *S. cumini* flowers.

2. Materials and methods

2.1. General experiment procedures

The ESI-MS were recorded on an Agilent 1100 LC-MSD Trap spectrometer. Optical rotations were recorded on a JASCO P-2000 polarimeter, using a sodium (589, D line) lamp. The NMR spectra were recorded on a Bruker 600 MHz spectrometer and tetramethylsilane (TMS) was used as an internal standard. Thin layer chromatography used pre-coated *silica gel* Merck 60 F_{254}. Column chromatography (CC) was performed on *silica gel* (Kieselgel 60, 70-230 mesh and 230-400 mesh), or Sephadex LH-20 resins (Sigma-Aldrich, USA). Medium-pressure liquid chromatography (MPLC) was performed on a Biotage-Isolera One system (Sweden).

2.2. Material

The flowers of *Syzygium cumini* (L.) Skeels (VN1236-Fl) were collected in Vinh Linh district, Quang Tri province, in November 2022 and identified by Dr. Nguyen The Cuong of the Institute of Ecology and Biological Resources, Vietnam Academy of Science and Technology (VAST). A voucher specimen (VN1236-Fl) was deposited at the Institute of Marine Biochemistry (IMBC), VAST.

2.3. Extraction and isolation of the flowers of S. cumini

A total of 0.3 kg of dried and powdered *S. cumini* flowers was extracted with MeOH (1 L x 5) under ultrasonic conditions at 45-50°C. The MeOH extract was then filtered and evaporated under reduced pressure to get 34.3 g of extract, which was suspended in 200 mL of distilled water (H_2O) and then partitioned with CH_2Cl_2

and EtOAc. The concentration of these organic solutions *in vacuo* yielded 11.3 g of the CH_2Cl_2 extract and 6.5 g of the EtOAc extract. The CH_2Cl_2 crude extract (11.3 g) was subjected to chromatography on a *silica gel* column, eluted with the solvent mixtures of *n*-hexane/acetone gradient (100/0 to 0/100, *v/v*) to yield seven fractions (C1 to C7). Fraction C2 (2.2 g) was chromatographed on a *silica gel* column using *n*-hexane/ EtOAc gradient (100/0 to 0/100, *v/v*) to obtain three subfractions (C2.1-C2.3). Subfraction C2.2 (0.3 g) was applied to a *silica gel* column chromatography (CC) using *n*-hexane/acetone (20/1, *v/v*) to give compound **1** (12 mg). Fraction C3 (1.02 g) was purified by CC on *silica gel*, eluted with *n*-hexane/acetone gradient (100/0 to 0/100, *v/v*) to yield compounds **2** (5 mg) and **6** (8 mg). Fraction C4 (1.03 g) was separated into four subfractions (C4.1-C.4.4) by CC on *silica gel* using the solvent mixtures of CH_2Cl_2/acetone (9/1, *v/v*). Subfractions C4.1 (210 mg) and C4.3 (148 mg) were recrystallized in a solvent mixture of CH_2Cl_2/MeOH (9/1, *v/v*) to afford compounds **3** (32 mg) and **7** (24 mg), respectively. Fraction C6 (183 mg) was subjected to CC on Sephadex LH-20 (CH_2Cl_2/MeOH (2/8, *v/v*), followed by CC on *silica gel* (CH_2Cl_2/acetone (9/1, 85/15, *v/v*) to afford compounds **12** (8 mg) and **10** (9 mg). The EtOAc extract (6.5 g) was chromatographed over a *silica gel* column (eluted with a CH_2Cl_2/MeOH solvent system) CC on MPLC equipment to give six fractions (E1-E6). Fraction E2 (647 mg) was subjected to a *silica gel* column and eluted with CH_2Cl_2/MeOH gradient (100/0 to 10/90, *v/v*) to yield four subfractions (E2.1 to E2.4). Compound **4** (15 mg) was obtained from the purification of subfraction E2.2 (213 mg) by recrystallizing in a solvent mixture of CH_2Cl_2/MeOH (9/1, *v/v*). Purification of fraction E2.3 (245 mg) by CC on Sephadex LH-20 using MeOH (95%) and column chromatography (CC) on *silica gel* with CH_2Cl_2/MeOH (9/1, 8/2, *v/v*) yielded compounds **9** (21 mg) and **11** (13 mg). Compound **8** (15 mg) was obtained from the purification of fraction E3 (312 mg) by column CC on *silica gel*, eluted with CH_2Cl_2/MeOH (9/1, 85/15, *v/v*). Fraction E6 (279 mg) was subjected to CC on Sephadex LH-20 (CH_2Cl_2/MeOH (2/8, *v/v*), followed by CC on a *silica gel* column (dichloromethane/ methanol (4/1, 3/1, *v/v*) to afford compound **5** (8 mg).

Friedelin (1): White solid, m.p 264-265 °C, α_D^{25} -31.5° (*c* 0.52; $CHCl_3$), ESI-MS: *m/z* 449 $[M+Na]^+$, ^{1}H-NMR (600 MHz, $CDCl_3$): δ_H 1.69 m (1H, m, H-1α), 1.96 (1H, m, H-1β), 2.30 (1H, m, H-2α), 2.39 (1H, m, H-2β), 2.25 (1H, q, *J* = 6.6 Hz, H-4), 1.29 (1H, m, H-6α), 1.75 (1H, m, H-6β), 1.38 (1H, m, H-7α), 1.49 (1H, m, H-7β), 1.40 (1H, m, H-8), 1.56 (1H, m, H-10), 1.25 (1H, m, H-11α), 1.45 (1H, m, H-11β), 1.33 (2H, m, H-12), 1.31 (1H, m, H-15α), 1.51 (1H, m, H-15β), 1.34 (1H, m, H-16α), 1.58 (1H, m, H-16β), 1.55 (1H, m, H-18), 1.22 (1H, m, H-19α), 1.38 (1H, m, H-19β), 1.27 (1H, m, H-21α), 1.46 (1H, m, H-21β), 0.96 (1H, m, H-22α), 1.55 (1H, m, H-22β), 0.88 (3H, d, *J* = 6.6 Hz, H-23), 0.73 (3H, s, H-24), 0.87 (3H, s, H-25), 1.01 (3H, s, H-26), 1.05 (3H, s, H-27), 0.96 (3H, s, H-29), 1.00 (1H, s, H-30), 1.18 (3H, s, H-28). ^{13}C-NMR (150 MHz, $CDCl_3$): see Table 1.

Epifriedelanol (2): White solid, m.p 281-282°C, α_D^{25}+19.5° (*c* 0.2; $CHCl_3$), ESI-MS: *m/z* 429 $[M+H]^+$, ^{1}H-NMR (600 MHz, $CDCl_3$): δ_H 1.43 (1H, m, H-1α), 1.54 (1H, m, H-1β), 1.89 (1H, br dt, *J* = 10.2 Hz, H-2α), 1.57 (1H, overlapped, H-2β), 3.73 (1H, br d, *J* = 2.4 Hz, H-3), 1.26 (1H, m, H-4), 0.98 (1H, m, H-6α), 1.75 (1H, dt, *J* = 9.6, 3.0 Hz, H-6β), 1.36 (2H, m, H-7), 1.25 (1H, m, H-8), 0.87 (1H, m, H-10), 1.19 (1H, m, H-11α), 1.34 (1H, m, H-11β), 1.29 (1H, m, H-12α), 1.33 (1H, m, H-12β), 1.27 (1H, m, H-15α), 1.46 (1H, m, H-15β), 1.31 (1H, m, H-16α), 1.51 (1H, m, H-16β), 1.49 (1H, m, H-18), 1.10 (1H, m, H-19α), 1.42 (1H, m, H-19β), 1.25 (1H, m, H-21α), 1.45 (1H, m, H-21β), 1.46 (1H, m, H-22α), 0.93 (3H, d, *J* = 8.4 Hz, H-23), 0.97 (3H, s, H-24), 0.85 (3H, s, H-25), 0.99 (3H, s, H-26), 1.01 (3H, s, H-27), 0.99 (3H, s, H-28), 0.94 (3H, s, H-9), 1.17 (1H, s, H-30). ^{13}C-NMR (150 MHz, $CDCl_3$): see Table 1.

Ursolic acid (3): White powder, m.p 257-258°C, α_D^{25}+57.5° (*c* 0.40; MeOH), ESI-MS: *m/z* 479 $[M+Na]^+$. ^{1}H-NMR (600 MHz, CD_3OD + $CDCl_3$): δ_H 5.23 (1H, t, *J* = 3.6 Hz, H-12), 3.17 (1H, dd, *J* = 11.4, 4.2 Hz, H-3), 2.18 (1H, d, *J* = 7.2 Hz, H-18), 1.17 (3H, s, H-27), 1.00 (3H, s, H-23), 0.99 (3H, d, *J* = 6.0 Hz, H-30), 0.98 (3H, s, H-25), 0.90 (3H, d, *J* = 6.6 Hz, H-29), 0.87 (3H, s, H-26), 0.80 (3H, s, H-24), 0.76 (1H, br d, *J* = 11.4 Hz, H-5α). ^{13}C-NMR (150 MHz, CD_3OD + $CDCl_3$): see Table 1.

Corosolic acid (4): White powder, m.p 244-245°C, ESI-MS: *m/z* 495 $[M+Na]^+$. ^{1}H-NMR (600 MHz, CD_3OD): δ_H 5.26 (1H, t, *J* = 3.6 Hz, H-12), 3.64 (1H, m, H-2), 2.93 (1H, d, *J* = 9.6 Hz, H-3), 2.23 (1H, br d, *J* = 10.8 Hz, H-18), 1.15 (3H, s, H-27), 1.04 (6H, s, H-23 and H-25), 0.96 (3H, d, *J* = 6.6 Hz, H-30), 0.90 (3H, d, *J* =

6.6 Hz, H-29), 0.86 (3H, s, H-26), 0.83 (3H, s, H-24). ^{13}C-NMR (150 MHz, CD_3OD): see Table 1.

Arjunolic acid (5): White solid, ESI-MS: *m/z* 489 $[M+H]^+$, ^{1}H-NMR (600 MHz, CD_3OD): δ_H 5.27 (1H, m, H-12), 3.72 (1H, m, H-2), 3.53 (1H, d, J = 10.8 Hz, H-23β), 3.37 (1H, d, J = 9.6 Hz, H-3), 3.29 (1H, d, J = 10.8 Hz, H-23α), 1.20 (3H, s, H-27), 1.06 (3H, s, H-26), 0.97 (3H, s, H-30), 0.92 (3H, s, H-29), 0.84 (3H, s, H-25), 0.72 (3H, s, H-24). ^{13}C-NMR (150 MHz, CD_3OD): see Table 1.

Lupeol (6): White powder, m.p 214-215°C, ESI-MS: *m/z* 427 $[M+H]^+$, ^{1}H-NMR (600 MHz, $CDCl_3$): δ_H 4.69 (1H, d, J = 2.4, H_1-29), 4.57 (1H, d, J = 0.6 Hz, H_2-29), 3.18 (1H, dd, J = 4.8, 11.4 Hz, H-3), 2.38 (1H, m, H-19), 1.67 (3H, s, H-30), 1.03 (3H, s, H-26), 0.94 (3H, s, H-27), 0.92 (3H, s, H-23), 0.83 (3H, s, H-35), 0.79 (3H, s, H-28), 0.76 (3H, s, H-24). ^{13}C-NMR (150 MHz, CD_3OD): see Table 1.

Betulinic acid (7): White powder, α_D^{25} +11.2° (*c* 0.15, MeOH), ESI-MS: *m/z* 479 $[M+Na]^+$, ^{1}H-NMR (600 MHz, CD_3OD + $CDCl_3$): δ_H4.73 (1H, d, J = 1.8 Hz, H_1-29), 4.60 (1H, dd, J = 1.8, Hz, H_2-29); 3.16 (1H, dd, J = 11.4; 4.8 Hz, H-3α); 3.01 (1H, ddd, J = 11.4; 4,8 Hz, H-19); 1.69 (3H, s, H_3-30), 0.99 (3H, s, H_3-27); 1.97 (3H, s, H_3-26); 0.95 (3H, s, H_3-23), 0.83 (3H, s, H_3-25); 0.75 (3H, s, H_3-24); 0.69 (1H, m, H-5). ^{13}C-NMR (150 MHz, CD_3OD + $CDCl_3$): see Table 1.

Gallic acid (8): Brown solid. ^{1}H-NMR (600 MHz, CD_3OD): δ_H 7.09 (2H, s, H-2 and H-6).

3,5-Dihydroxy-4-methoxybenzoic acid (9): brown solid. ^{1}H-NMR (600 MHz, CD_3OD): δ_H 7.06 (2H, s, H-2, H-6), 3.83 (3H, s, OCH_3).

Syringic acid (10): Brown solid. ^{1}H-NMR (600 MHz, acetone-d_6): δ_H 3.89 (6H, s, 3,5-OCH_3), 7.33 (2H, s, H-2 and H-6). ^{13}C-NMR (150 MHz, acetone-d_6): δ_C 56.7 (3,5-OCH_3), 108.2 (C-2 and C-6), 121.5 (C-1), 141.5 (C-4), 148.3 (C-3 and C-5), 167.4 (C=O).

Protocatechuic acid (11): Brown solid. ^{1}H-NMR (600 MHz, CD_3OD): δ_H 6.82 (1H, d, J = 8.4 Hz, H-5), 7.45 (1H, dd, J = 1.8, 7.8 Hz, H-6), 7.46 (1H, d, J = 1.8 Hz, H-2). ^{13}C-NMR (150 MHz, CD_3OD): δ_C 115.8 (C-5), 117.1 (C-2), 123.1 (C-1), 123.9 (C-6), 146.0 (C-3), 151.4 (C-4), 170.3 (C=O).

Isovanillic acid (12): Brown solid. ^{1}H-NMR (600 MHz, CD_3OD): δ_H 3.90 (3H, s, OCH_3), 6.77 (1H, d, J = 7.8 Hz, H-5), 7.49 (1H, dd, J = 7.5, 2.4 Hz, H-6), 7.60 (1H, d, J = 1.8 Hz, H-2). ^{13}C-NMR (150 MHz, CD_3OD): δ_C 54.9 (OCH_3), 112.7 (C-5), 113.7 (C-2), 122.8 (C-1), 129.3 (C-6), 146.7 (C-3), 148.5 (C-4), 172.0 (C=O).

3. Results and discussion

Compound **1** was obtained as a white solid and optically active α_D^{25}-31.5° (*c* 0.52; $CHCl_3$). The ESI-MS spectrum of compound **1** showed the pseudomolecular ion peak at *m/z* 449 $[M+Na]^+$. The ^{1}H NMR spectrum showed the presence of eight methyl groups (seven singlets and one doublet) at δ_H 0.73 (3H, s, H-24), 0.87 (3H, s, H-25), 1.01 (3H, s, H-26), 1.05 (3H, s, H-27), 0.96 (3H, s, H-29), 1.00 (1H, s, H-30), 1.18 (3H, s, H-28), 0.88 (3H, d, J = 6.6 Hz, H-23), and other signals of overlapped aliphatic protons. The ^{13}C-NMR and DEPT spectra of **1** showed the signals of 30 carbons, including 8 methyls, 4 sp^3 methines, 11 methylenes, 6 sp^3 quaternary carbons, and one carbonyl (δ_C 213.1). These observations indicated compound **1** was a pentacyclic triterpenoid. The structure of compound **1** was confirmed by the comparison with the reported ^{1}H-NMR and ^{13}C-NMR spectra data [3],[4], which corresponded to those described for friedelin.

Compound **2** was obtained as a white solid, and optically active α_D^{25}+19.5° (*c* 0.2; $CHCl_3$). The ESI-MS spectrum indicated the pseudomolecular ion peak at *m/z* 429 $[M+H]^+$. The ^{1}H, ^{13}C NMR and DEPT spectra of compound **2** showed the typical signals of a pentacyclic triterpenoid, which were similar to those of compound **1**. However, in the structure of compound **2**, the disappearance of the carbonyl group at C-3 was observed, and instead, an additional sp^3 oxymethine group at δ_H 3.73 (br d, J = 2.4 Hz, H-3), δ_C 72.8 was noted in the structure of **2**. The spin-spin coupling constant (J value) of the proton H-3 was 2.4 Hz, confirming its equatorial position and the β orientation of the hydroxyl group at C-3. Based on the above analyses and the comparison with literature data [3],[5], the structure of compound **2** was determined to be epifriedelanol.

Compound **3** was obtained as a white solid, m.p 257-258 °C, and optically active α_D^{25}+57.5° (*c* 0.40; MeOH). The ESI-MS spectrum of **3** exhibited an ion peak at *m/z* 479 $[M+Na]^+$. The ^{1}H NMR spectrum of compound **3** indicated the presence of seven methyl groups (five singlet methyl groups and two doublet methyl groups), one olefinic proton at δ_H 5.23 (t, J = 3.6 Hz, H-12), and one oxygenated methine at δ_H 3.17 (dd, J = 11.4, 4.2 Hz, H-3). The ^{13}C NMR and HSQC spectra of compound **3** displayed the signals of 30 carbons, including 7 methyl groups, 9 methylene groups, 6 sp^3 methines (one

oxygenated methine at δ_C 79.8), a double bond (δ_C 126.3 and 140.2), 5 sp^3 quaternary carbons and a carboxylic (δ_C 181.5). These NMR data suggested compound **3** was a pentacyclic triterpenoid belonging to an ursane skeleton. H-3 was confirmed to be an axial disposition by its large proton coupling constant J = 11.4 Hz. The combination of NMR data, MS, optical rotation value, and comparison with the reported literature confirmed the structure of compound **3** as ursolic acid [6],[7].

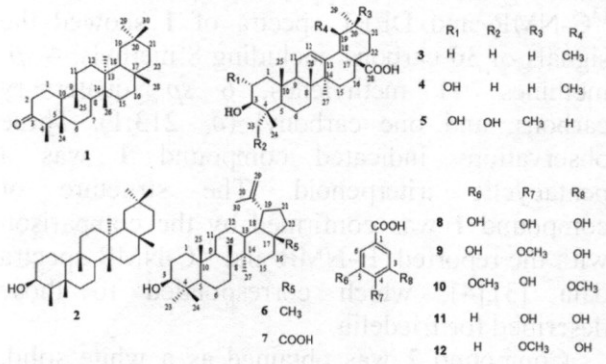

Fig. 1. Structures of the isolated compounds **1-12**

Compound **4** was obtained as a white solid. Comparison of the 1D-NMR spectra of compound **4** with those of **3** indicated that compound **4** had the same ursane skeleton as compound **3**. Unlike compound **3**, the 1D NMR of compound **4** indicated the presence of two oxymethine groups at δ_H 2.93 (d, J = 9.6 Hz, H-3), 3.64 (m, H-2), and δ_C 84.5 (C-3), 79.8 (C-2). The spin-spin coupling constant (J value) of the H-3 was 9.6 Hz, confirming its α position. Additionally, the oxymethine group at δ_H 3.64 (m, H-2) and δ_C 79.8 (C-2) suggested the presence of a methine group instead of a methylene group at the C-2 position of the ursane skeleton. The ESI-MS spectrum of **4** exhibited a molecular ion peak at m/z 495 $[M+Na]^+$. Through analyses of the 1D-NMR data of **4** and comparison with the reported data, compound **4** was identified as corosolic acid [8], which had a chemopreventive effect on HepG2 cells by apoptosis [9] and inhibited TNF-α-stimulated IL-8 secretion from HT29 cell line [8].

Compound **5** was obtained as a white solid. The ^{1}H NMR along with HSQC spectra of compound **5** indicated the presence of six singlet methyl groups at δ_H 1.20 (s, H-27), 1.06 (s, H-26), 0.97 (s, H-30), 0.92 (s, H-29), 0.84 (s, H-25), 0.72 (s, H-24), an olefinic proton at δ_H 5.27 (1H, m, H-12), two oxygenated methine groups at δ_H 3.72 (m, H-2), 3.37 (d, J = 9.6 Hz, H-3) and one oxygenated methylene at δ_H 3.53 (1H, d, J = 10.8 Hz, H-23β), 3.29 (1H, d, J = 10.8 Hz, H-23α) and other signals of overlapped aliphatic protons. The ^{13}C NMR and HSQC spectra of compound **5** displayed the signals of 30 carbons, including ten sp^3 methylene groups (one oxygenated methylene), six singlet methyl groups, five sp^3 methine groups (two oxygenated methine groups), six sp^3 quaternary carbons, one double bond, and one carbonyl group. These NMR data suggested compound **5** was a pentacyclic triterpenoid belonging to the oleane skeleton. Based on the ^{1}H, ^{13}C NMR data analyses, the structure of compound **5** is similar to that of compound **4**, containing two oxygenated methine groups at the C-2 and C-3 positions of the pentacyclic triterpenoid. The large coupling constant between H-2 and H-3 (J = 9.6 Hz) indicated their axial orientations and suggested the equatorial arrangement of the hydroxyl groups at C-2 and C-3 (2α, 3β orientation). Additionally, it was suggested that the oxygenated methylene group at δ_C 66.4 was instead of a methyl group at the C-23 position of the oleane skeleton. Thus, through analyses of the NMR data of compound **5** and comparison with reported data [10], compound **5** was identified as arjunolic acid [11],[12].

Compound **6** was obtained as a white solid. Its ^{1}H NMR spectrum showed the signals of seven methyl groups, two olefinic protons [δ_H 4.69 (d, J = 2.4, H_1-29), 4.57 (d, J = 0.6 Hz, H_2-29)], an oxymethine [δ_H 3.18 (dd, J = 4.8, 11.4 Hz, H-3)] and overlapping aliphatic proton signals. The ^{13}C NMR and DEPT spectra of compound **6** showed 30 carbon signals, including seven methyl groups, ten sp^3 methylene groups, six sp^3 methine groups, five sp^3 quaternary carbons, and an exocyclic double bond. The chemical shifts of methyl CH_3-30 (δ_H 1.67 (s), δ_C 19.3) suggested its linkage to a double bond. These analyses of NMR data suggested that compound **6** was a terpenoid belonging to the lupane skeleton. Thus, compound **6** has been identified as lupeol based on NMR data analysis and comparison with literature values [7],[13].

Compound **7** was isolated as a white solid and optically active α_D^{25} +11.2° (c 0.15, MeOH). The ^{1}H NMR, ^{13}C NMR, and HSQC spectra of **7** displayed the characteristic signals of the lupane skeleton as compound **6**, except for the absence of one singlet methyl signal compared to compound **6**. In addition, the signal of a carboxylic group at δ_C 180.1 was observed in the ^{13}C NMR spectrum of compound **7**. This analysis suggested that one methyl group of compound **6**

was oxidized into a carboxylic functional group at C-28 (δ_C 180.1). Additionally, the axial disposition of H-3 was confirmed by its coupling constant J = 11.4 Hz. Based on the above evidence and by comparison with those reported in the reference [14], compound **7** was determined to be betulinic acid which displayed cytotoxic effects on three cancer lines HCT116 (IC_{50} 11.1 μM), NIC-N187 (IC_{50} 18.7 μM) [7], MCF7 (IC_{50} 13.5 μg/mL) [15].

Table 1. ^{13}C NMR data for compounds **1-7**

Positions	1	2	3	4	5	6	7
1	22.3	15.8	40.0	48.1	47.7	38.9	40.1
2	41.5	35.2	27.9	69.5	69.7	27.5	28.0
3	213.1	72.8	79.8	84.5	78.3	79.0	79.7
4	58.2	49.2	39.8	40.7	44.1	38.7	40.0
5	42.1	37.1	56.8	56.6	48.6	55.3	56.9
6	41.3	41.8	19.5	19.5	19.1	18.3	19.3
7	18.3	17.6	34.4	40.6	33.7	34.3	35.6
8	53.1	53.2	40.8	33.8	40.6	40.9	41.9
9	37.5	38.4	49.0	48.8	48.2	50.5	52.0
10	59.5	61.4	38.1	39.2	39.0	37.2	38.3
11	35.6	35.4	24.4	23.9	24.0	20.9	22.1
12	30.5	30.7	126.3	126.2	123.4	25.2	26.9
13	39.7	37.9	140.2	140.1	145.4	38.1	39.7
14	38.3	39.7	43.3	43.3	42.8	42.8	43.6
15	32.4	32.4	29.5	29.3	29.2	27.4	30.8
16	36.0	36.1	25.6	25.5	24.5	35.6	33.4
17	30	30.1	48.9	48.6	47.3	43.0	57.5
18	42.8	42.9	54.7	54.5	43.0	48.3	50.5
19	35.4	35.6	40.7	40.4	44.1	48.0	48.6
20	28.2	28.2	40.4	40.3	31.6	151.0	152.1
21	32.8	32.9	32.1	31.9	33.8	29.9	31.6
22	39.3	39.3	38.4	38.2	33.4	40.0	38.1
23	6.8	11.6	28.8	29.3	66.4	28.0	28.3
24	14.7	16.4	16.4	17.5	13.8	15.4	16.1
25	17.9	18.3	16.0	17.2	17.8	16.1	16.5
26	20.3	18.7	18.1	18.0	17.5	16.0	16.7
27	18.7	20.1	24.1	24.1	26.5	14.6	15.1
28	32.1	31.8	181.5	181.3	181.9	18.0	180.1
29	35.0	35.0	17.8	17.7	31.8	109.3	110.2
30	31.8	32.1	21.7	21.7	24.6	19.3	19.2

Based on 1D NMR data and comparison with the literature values, the remaining compounds were identified as gallic acid (**8**) [16], 3,5-dihydroxy-4-methoxybenzoic acid (**9**) [17], syringic acid (**10**) [18], protocatechuic acid (**11**) [19],[20], isovanillic acid (**12**) [21]. Accordingly, compounds **1**, **2**, **7**, and **8** were reported to be previously isolated from the leaves of *S. cumini* [22],[23], compounds **3-5** were previously isolated from the stem barks of *S. cumini* [24],[25], compounds **11-12** were previously isolated from the fruits of *S. cumini* [26],[27]. To the best of our knowledge, compounds **4-6**, **9**, and **11** were first isolated from the flowers of this species. Thus, it could be seen that the isolated triterpenoids and benzoic acid derivatives from the flowers of *S. cumini* were consistent with those of compound classes reported from the *Syzygium* genus.

4. Conclusion

In summary, from the flowers of *S. cumini*, seven triterpenoids and five benzoic acid derivatives were isolated and structurally determined by the spectroscopic analyses of the MS and NMR data and the comparison with the literature. These compounds included friedelin (**1**), epifriedelanol (**2**), ursolic acid (**3**), corosolic acid (**4**), arjunolic acid (**5**), lupeol (**6**), betulinic acid (**7**), gallic acid (**8**), 3,5 dihydroxyl-4-methoxy benzoic acid (**9**), syringic acid (**10**), protocatechuic acid (**11**), and isovanillic acid (**12**). Among them,

compounds **4-6**, **9**, and **11** were first isolated from the flowers of *S. cumini*, and this was also the first report of the isolation and structural elucidation from the flowers of *S. cumini* in Vietnam. Further studies on the phytochemical constituents and bioactivities of the remaining extract of *S. cumini* should be conducted to strengthen the chemical and pharmacological knowledge of this species.

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