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Isolation and structural elucidation of xanthone derivatives from the pericarp of *Garcinia mangostana* L.

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Abstract:

In Vietnam, *Garcinia mangostana* L. is commonly referred to as "Mang Cut" in Vietnamese, renowned not only as the "queen of fruits" but also for its various medicinal properties, particularly the shell of the mangosteen fruit. In traditional medicine, the shell of *G. mangostana* has long been employed to treat infections, diarrhoea, dysentery, and inflammation. Previous studies have shown that it possesses a variety of bioactive properties, including antibacterial, antifungal, anti-allergic, anti-inflammatory, anti-tumour, and antiviral effects, attributed to xanthones. In our research, a phytochemical analysis of the ethyl acetate extract from the shell of *G. mangostana* led to the identification of several compounds, including garcinone C (1), garcinone D (2), bannaxanthone A (3), 8-deoxygartanin (4), and mangostanol (5). Their structures were elucidated through a comprehensive examination of ESIMS, 1D, and 2D NMR spectroscopic data. This study reports for the first time of bannaxanthone A (3) being isolated from this plant. These findings contribute to our understanding of *G. mangostana* and highlight its potential as a valuable herbal resource that may provide secondary compounds for the treatment of non-communicable diseases in the future.

Keywords: **bannaxanthone A, *Garcinia mangostana,* garcinone C, garcinone D, mangostanol.**

Classification numbers: **2.2, 3.3, 3.5**

1. Introduction

Garcinia mangostana belongs to the genus *Garcinia*, which is primarily distributed in tropical regions of Southeast Asia, including Thailand, the Philippines, Indonesia, Malaysia, and Vietnam [1, 2]. The shell of this species has been used in traditional medicine to cure conditions like ulcers, inflammation, diarrhoea, and dysentery [2-4]. Previous publications have indicated that it contains a variety of secondary compounds, including triterpenoids, flavonoids, benzophenones, and anthocyanins, particularly prenylated and oxygenated xanthones [2, 3]. Xanthones are the main chemical constituents that exhibit numerous biological activities, including activities against breast cancer, cardiovascular disorders, diabetes mellitus, inflammation, antioxidant, antitumoral, anti-inflammatory, antiallergy, and antibacterial properties [3, 5]. Previous research has shown that two compounds, γ-mangostin and α-mangostin, were the principal components and are considered important markers for chemotaxonomy [6, 7]. Continuing our study of ethyl acetate extract, we isolated five known xanthones, garcinone C (**1**), garcinone D (**2**), bannaxanthone A (**3**), 8-deoxygartanin (**4**), and mangostanol (**5**) with bannaxanthone A reported from *G. xipshuanbannaensis* [8].

2. Materials and methods

2.1. General experimental procedures

Thin-layer chromatography spots are visualised using ultraviolet light at 254 and 365 nm, followed by immersion in a 10% aqueous solution of H_2SO_4 (v/v) and subsequent heating. Column chromatography (CC) was performed using adsorption materials such as silica gel size 0.063-0.200 mm, reverse phase powder RP-18 (YMC, Japan), and Diaion HP-20 resin (0.25-0.85 mm, Mitsubishi Chemical Corp., Japan). A JASCO P-2000 polarimeter was used to measure optical rotations. NMR spectral data were recorded using a Bruker AM600 FT-NMR spectrometer. Electrospray ionisation mass spectrometry (ESIMS) was conducted with a Waters Q-Tof micro mass spectrometer.

2.2. Plant materials

The shells of *Garcinia mangostana* L. were collected from Can Tho province, Vietnam, in 2018 and identified by Nguyen Quoc Binh at the Vietnam National Museum of Nature, Vietnam Academy of Science and Technology. The received specimens (code: GM0618) were described in the literature [6].

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2.3. Extraction and isolation

A dry powder from the shell of *G. mangostana* (4.0 kg) was extracted with methanolic solvent at room temperature (3×12 litres). The solvent was removed under decreased pressure to produce a crude residue (400.1 g), which was dispersed in water (1000 ml) and sequentially partitioned with n-hexane (yielding 8 g) and ethyl acetate (EtOAc; yielding 30.2 g), respectively. The EtOAc extract (30.2 g) was subjected to silica gel column chromatography and eluted with DCM:MeOH (100:0-0:100; v:v) to produce four fractions, GME1-GME4. Fraction GME1 (400.0 mg) was loaded onto a silica gel column and eluted with a solvent system n-hexane:EtOAc (2:1, v:v) to obtain fraction GM5. 8-deoxygartanin (4) (16.0 mg) was purified on a reversed-phase silica gel column from fraction GM5 and washed with MeOH:H_2O (2:0.5; v:v). Fraction GME2 (21.0 g) was subjected to silica gel column chromatography, eluted with n-hexane:EtOAC (0.2:2, v:v), yielding garcinone D (2) (10.0 mg). Fraction GME3 (2.6 g) was segregated on a reversed-phase silica gel column and washed with MeOH:H_2O (2:0.5; v:v) to yield garcinone C (1) (30.0 mg) and mangostanol (5) (70.0 mg). Fraction GME4 (2.7 g) was detached on a reversed-phase silica gel column and washed with MeOH:H_2O (2:0.5; v:v) to obtain bannaxanthone A (3) (6.0 mg).

Garcinone C **(1)**: A yellow powder, melting point: 216-218°C, molecular formula $C_{23}H_{26}O_7$, ESIMS (*m/z* 415.9) $[M+H]^+$, ^{1}H NMR (600 MHz, CD_3OD), carbon-13 nuclear magnetic resonance (^{13}C NMR) (150 MHz, CD_3OD).

Garcinone D **(2)**: A yellow powder, melting point: 150-154°C, molecular formula $C_{24}H_{28}O_7$, ESIMS (*m/z* 413.0) $[M-H]^-$, ^{1}H NMR (600 MHz, CD_3OD), ^{13}C NMR (150 MHz, CD_3OD).

Bannaxanthone A **(3)**: A yellow powder, molecular formula $C_{23}H_{25}O_7$, ESIMS (*m/z* 414.0) $[M+H]^+$, ^{1}H-NMR (500 MHz, CD_3OD), ^{13}C NMR (150 MHz, CD_3OD).

8-deoxygartanin **(4)**: A yellow powder, melting point: 165.5°C, molecular formula $C_{23}H_{24}O_5$, ESIMS (*m/z* 380.9) $[M+H]^+$, ^{1}H NMR (500 MHz, CD_3OD), ^{13}C NMR (150 MHz, CD_3OD).

Mangostanol **(5)**: A yellow powder, melting point: 164-166°C, $[\alpha]^{28}_D = +16.3$ (*c* 0.1, MeOH), molecular formula $C_{24}H_{26}O_7$, ESIMS (*m/z* 425.9) $[M-H]^-$, ^{1}H NMR (600 MHz, CD_3OD), ^{13}C NMR (150 MHz, CD_3OD).

3. Results and discussion

Compound **1** was purified as a yellow powder from the EtOAc extract. Its molecular formula was determined to be $C_{23}H_{26}O_7$ based on the pseudo-molecular ion peak at (*m/z* 415.9) $[M+H]^+$ on the ESIMS spectrum. The ^{1}H-NMR spectrum of **1** exhibited two singlet signals of aromatic rings at δ_H 6.67 (1H, s, H-5), and 6.24 (1H, s, H-4). In addition, two multiple signals of methylene at δ_H 3.43 (2H, m, H-15) and 1.77 (2H, m, H-16) and a singlet signal of two methyls at δ_H 1.32 (6H, s, H-18, H-19) indicating the presence of a saturated prenyl moiety. Moreover, the ^{1}H-NMR spectrum of **1** showed a signal of a double bond proton at δ_H 5.23 (1H, m, H-11), one signal of methylene at δ_H 3.30 (2H, m, H-10), together with two singlet signals of methyl at δ_H 1.66 (3H, d, J=0.6 Hz, H-14) and 1.78 (3H, *br s*, H-13), which exhibited a prenyl-unsaturated moiety. Moreover, ^{13}C NMR, and distortionless enhancement by polarisation transfer (DEPT) of **1** revealed a total of 23 carbon signals, including four methyls (4×CH_3), three methylenes (3×CH_2), three methines (3×CH), and 13 quaternary carbons (13×Cq). Comparing the spectra of compound **1** with the literature [9] confirmed compound **1**'s identity as a xanthone named garcinone C (Fig. 1).

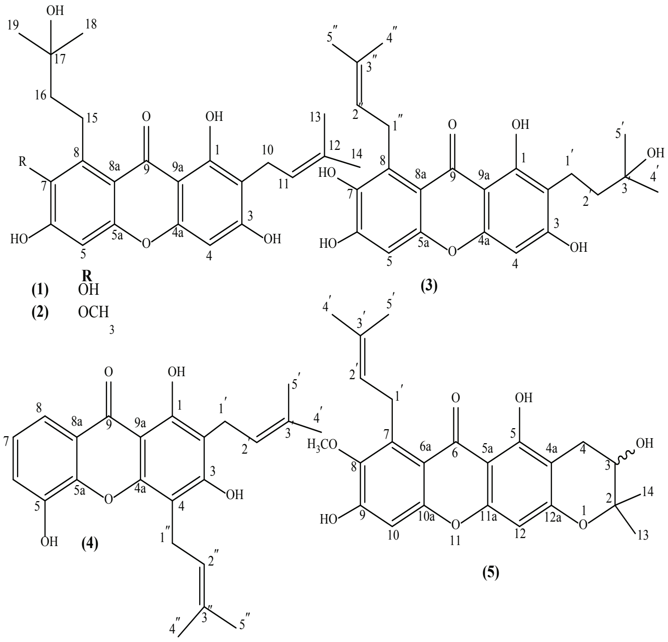

Fig. 1. Some compounds from pericarp of *G. mangostana*.

Compound **2** was isolated from the EtOAc extract as a yellow powder. The ^{1}H- and ^{13}C NMR of **2** were similar those of **1**, except for the appearance of one methoxy group δ_H 3.86 (3H, s, 7-OCH_3)/δ_C 61.5. Moreover, a chemical shift of C-7 moved from strong field in **1** δ_C 141.9 (C-7) to down field in **2** δ_C 144.7 (C-7). These data displayed that compound **2** is a methoxylated derivative of compound **1** and that compound **2** was resulted from replacement the hydrogen atom in the hydroxyl group at C-7 in **1** by a methyl group. Compound **2** was therefore identified as garcinone D [10].

Compound **3** was purified as a yellow powder from the EtOAc extract. The ^{1}H-NMR of compound **3** exhibited two singlet signals, which are characteristic of a benzene ring at δ_H 6.68 (1H, s, H-5) and 6.26 (1H, s, H-4), along with a multiplet signal for double bond at δ_H 5.29 (1H, m, H-2”), one doublet of methylene at δ_H 4.14 (2H, d, J=6.6 Hz, H-1”), and two singlet signals of methyl at δ_H 1.68 (3H, s, H-4”) and 1.86 (3H, s, H-5”), which indicated a prenyl moiety. In addition, multiple signals at δ_H 1.70 (2H, m, H-2’), 2.71 (2H, m, H-1’), along with a singlet signal of two methyls at δ_H 1.29 (6H, s, H-4’, H-5’), confirmed a 2-methylbutan-2-ol moiety. Analysis of ^{13}C NMR and DEPT spectra revealed 23 carbon signals, including four methyls (4×CH_3) at δ_C 26.0 (C-4”), 18.3 (C-5”), and 29.0 (C-4’ and C-5’), three methylenes (3×CH_2) at δ_C 18.4 (C-1’), 26.6 (C-1”), and 43.4 (C-2’), three methines (3×CH) at δ_C 92.9 (C-4), 100.9 (C-5), and 124.9 (C-2”), 12 quaternary carbons at δ_C 161.5 (C-1), 111.9 (C-2), 163.3 (C-3), 156.3 (C-4a), 154.2 (C-5a), 153.9 (C-6), 142.2 (C-7), 129.2 (C-8), 111.8 (C-8a), 103.8 (C-9a), 71.8 (C-3’), and 131.7 (C-3”), and one carbon of carbonyl at δ_C 183.5 (C-9). These data suggest that the structure of compound **3** was a xanthone skeleton bonded with two moieties as a prenyl and a 2-methylbutan-2-ol, however the linkage positions differed from compound **1**. Comparing spectroscopic data with another report allowed for the identification of compound **3** as bannaxanthone A [8]. ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR data of compound 3 in CD_3OD are presented in Table 1.

Compound **4** was isolated from the EtOAc extract as a yellow powder. The ^{1}H NMR revealed characteristic signals of the appearance of a benzene ring at δ_H 7.60 (1H, dd, J=7.8, 1.2 Hz, H-8), 7.20 (1H, d, J=7.2 Hz, H-6), and 7.15 (1H, t, J=7.8 Hz, H-7) together with double bond proton signal at δ_H 5.30 (1H, m, H-2′), 5.23 (1H, m, H-2″). In addition, some signals indicated the presence of two prenyl units, including four methyls at δ_H 1.89 (3H, s, H-5′), 1.81 (3H, s, H-5″), 1.69 (6H, s, H-4′ and H-4″), and two doublets of methylene proton signals at δ_H 3.60 (2H, d, J=7.2 Hz, H-1″), 3.37 (2H, d, J=7.2 Hz, H-1′). Analysis of ^{13}C NMR, and DEPT showed 23 carbon signals, including four methyls (4×CH_3) at δ_C 18.0 (C-5″), 25.9 (C-4″), 18.1 (C-5′), and 26.0 (C-4′), five methines at δ_C 120.9 (C-6), 124.4 (C-7), 116.2 (C-8), 123.3 (C-2″), and 123.4 (C-2′), two methylenes at δ_C 22.4 (C-1″), and 22.6 (C-1′), one carbon carbonyl at δ_C 182.5 (C-9), and 11 quaternary carbons at δ_C 159.2 (C-1), 111.7 (C-2), 162.2 (C-3), 108.0 (C-4), 153.9 (C-4a), 147.7 (C-5), 146.9 (C-5a), 122.4 (C-8a), 104.0 (C-9a), 132.7 (C-3″), and 132.9 (C-3′). Based on spectroscopic NMR, ESIMS spectra data, and comparison with the literature [11], compound **4** was identified as a xanthone named 8-deoxygartanin.

Table 1. ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR data of compound 3 in CD_3OD.

No	$^{a,b}\delta_H$ (J/Hz)	$^{a,c}\delta_C$	d_C**
1	-	161.5	161.4
2	-	111.9	111.8
3	-	163.3	162.6
4	6.26 (1H, s, H-4)	92.9	92.9
4a	-	156.3	155.4
5	6.68 (1H, s, H-5)	100.9	100.8
5a	-	154.2	153.2
6	-	153.9	152.1
7	-	142.2	141.4
8	-	129.2	128.8
8a	-	111.8	111.8
9	-	183.5	182.9
9a	-	103.8	103.4
1′	2.71 (2H, m, H-1′)	18.4	17.5
2′	1.70 (2H, m, H-2′)	43.4	42.9
3′	-	71.8	70.3
4′	1.29 (3H, s, H-4′)	29.0	29.0
5′	1.29 (3H, s, H-5′)	29.0	29.0
1″	4.14 (2H, d, J=6.6 Hz, H-1″)	26.6	26.1
2″	5.29 (1H, m, H-2″)	124.9	124.1
3″	-	131.7	131.0
4″	1.68 (3H, s, H-4″)	26.0	25.7
5″	1.86 (3H, s, H-5″)	18.3	18.0

^{a}: Recorded in CD_3OD; ^{b}: 600 MHz; ^{c}: 125 MHz, **: Recorded in $(CD_3)_2CO$.

Compound **5** was separated from the EtOAc extract as a yellow powder. Its molecular formula was determined as $C_{24}H_{26}O_7$ from its molecular ion peak at (m/z 425.9) $[M-H]^-$ on the ESI-MS spectrum. The ^{1}H-NMR of compound **5** displayed two singlet signals from a benzene ring at δ_H 6.66 (1H, s, H-10), 6.32 (1H, s, H-12), together with characteristic signals of a prenyl moiety such as two singlet signals of methyl at δ_H 1.83 (3H, s, H-4’) and 1.68 (3H, d, J=0.6 Hz, H-5’), one double bond proton signal at δ_H 5.30 (1H, m, H-2’), and a signal of methylene at δ_H 4.06 (1H, m, H-1’). In addition, the ^{1}H-NMR of compound **5** lacked the signals of a 2-methylbutan-2-ol unit in **3** however, it did exhibit three doublet signals at δ_H 2.93 (1H, dd, *J*=16.8, 5.4 Hz, H-4a), 2.57 (1H, dd, *J*=16.8, 7.2 Hz, H-4b), and 3.80 (1H, dd, *J*=7.2, 5.4 Hz, H-3), together with two singlet signals of methyl at δ_H 1.48 (3H, s, H-14), and 1.36 (3H, s, H-13). Combined analysis of ^{13}C NMR and HSQC spectra of compound **5** expressed a total of 24 carbon signals, including four methyls at δ_C 20.6 (C-13), 25.6 (C-14), 18.3 (C-4'), and 26.0 (C-5'), one methoxy at δ_C 61.2 (OCH_3), four methines at δ_C 102.2 (C-10), 94.4 (C-12), 69.6 (C-3), and 125.7 (C-2'), one carbon carbonyl at δ_C 178.8 (C-6), two methylenes at δ_C 27.0 (C-1' and C-4), and 12 quaternary carbons at δ_C 79.5 (C-2), 105.3 (C-4a), 156.1 (C-5), 107.5 (C-5a), 114.8 (C-6a), 138.2 (C-7), 144.7 (C-8), 155.6 (C-9), 156.8 (C-10a), 158.3 (C-11a), 162.1 (C-12a), and 131.3 (C-3'). By comparison of its ^{1}H and ^{13}C NMR spectral data with [12], compound **5** was identified as a xanthone named mangostanol.

4. Conclusions

Five compounds were separated from the ethyl acetate extract of *G. mangostana* husk, comprising garcinone C (**1**), garcinone D (**2**), bannaxanthone A (**3**), 8-deoxygartanin (**4**), mangostanol (**5**). Structures of compounds **1-5** were elucidated by ESIMS and NMR spectroscopy. Notably, bannaxanthone A was isolated from this plant for the first time.

CRediT author statement

Nguyen Thi Hien: Conceptualisation, Methodology, Formal analysis, Writing original draft; Giang Thi Kim Lien: Investigation, Formal analysis; Dao Thi Thu Ha: Investigation, Formal analysis; Pham Thanh Huyen: Conceptualisation, Formal analysis, Resources; Nguyen Minh Khoi: Investigation, Formal analysis, Resources; Nguyen Van Tai: Supervision, Funding acquisition, Data curation; Dang Viet Hau: Data curation, Principal investigator, Writing original draft.

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COMPETING INTERESTS

The authors declare that there is no conflict of interest regarding the publication of this article.

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