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Journal of Medicinal Materials, 2022, Vol. 27, No. 6 (pp. 330 - 335)

CEMBRANOID CONSTITUENTS FROM THE SOFT CORAL *SARCOPHYTON INFUNDIBULIFORME*

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(Received July 25th, 2022)

Summary

Cembranoid Constituents from the Soft Coral *Sarcophyton infundibuliforme*

Five cembranoids were isolated from the methanolic extract of the Vietnamese soft coral *Sarcophyton infundibuliforme* using combined chromatographic experiments. Their chemical structures were elucidated as sarcrassin D (**1**), emblide (**2**), 7α,8β-dihydroxydeepoxysarcophine (**3**), lobocrasol B (**4**), and sarcophine (**5**) on the basis of detailed analysis of the 1D and 2D NMR spectroscopic data in comparison with the literature values. This is the first report of these compounds from the soft coral *Sarcophyton infundibuliforme*.

Keywords: *Sarcophyton infundibuliforme, Soft coral, Cembranoid.*

1. Introduction

Soft corals are well-known as excellent sources of marine-derived natural products. Among them, members of the genera *Sarcophyton*, *Sinularia*, and *Lobophytum* are the most prolific and especially attractive targets for marine natural product research. These marine invertebrates constitute an important group of marine invertebrates widely distributed in the coral reefs of the world oceans and have proven to be a biochemical warehouse for terpenes, particularly cembranoid diterpenes [1]. *Sarcophyton* species contain diterpenes up to 10% of their dry weight, and this large quantity

of secondary metabolites plays an important role in the survival of soft corals with defensive, competitive, reproductive, and possibly pheromonal functions [2]. Cembranoids are derived from the cyclization of geranylgeranyl pyrophosphate. They are a class of isoprenoids and consist of a fourteen-membered carbocyclic ring with an isopropyl residue at position 1, and three methyl groups at positions 4, 8, and 12. These compounds have diverse structural variations with many functional groups (lactone, epoxide, furan, ester, aldehyde, hydroxyl, and carboxyl moieties) and cyclizations [1],[2],[3],[4]. Cembranoids from soft corals exhibited various biological effects, especially anti-tumor, antibacterial, and anti-inflammatory activities [4].

Our previous investigations on Vietnamese soft corals reported cembranoids from *Sarcophyton mililatensis* [5], *S. ehrenbergi* [6], *Lobophytum laevigatum* [7], *L. crassum* [8],[9], *Sinularia digitata* [10], and *S. maxima* [11] species. In line with this, the current paper addresses the isolation and structural elucidation of five cembranoids (**1–5**, Fig. 2) from the soft coral *Sarcophyton infundibuliforme*.

2. Material and methods

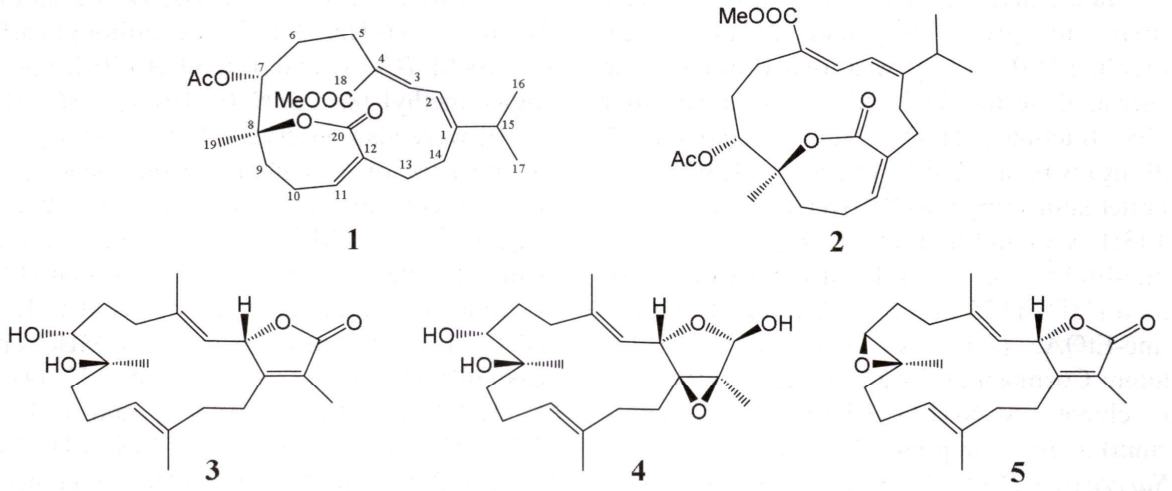
2.1. Soft coral materials

The samples of the soft coral *Sarcophyton infundibuliforme* Tixier-Durivault, 1958 (Fig. 1) were collected near Hon Cau island, Binh Thuan province, Vietnam, in June 2021. The species was identified by Prof. Do Cong Thung, Institute of Marine Environment and Resources, VAST. The voucher specimens (Hon Cau SHM-03) are deposited at the Institute of Marine Biochemistry and the Institute of Marine Environment and Resources, VAST.

Fig. 1 The soft coral *Sarcophyton infundibuliforme*

2.2. General experimental procedures

Optical rotations were determined on a JASCO P-2000 polarimeter. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE NEO 600 FT-NMR spectrometer with TMS used as an internal standard. High-resolution mass spectra were obtained using an Agilent 6530 Accurate-Mass spectrometer. Medium pressure liquid chromatography (MPLC) was carried out on a Biotage - Isolera One system. Column chromatography (CC) was performed on *silica gel* (Kieselgel 60, 70-230 mesh, and 230-400 mesh) and reversed-phase *silica gel* (ODS-A, 12 nm S-150 μm). HPLC purification was carried out on an Agilent 1260 Infinity II system. Precoated *silica gel* 60 F_{254} and RP-18 F_{254S} plates were used for TLC and the spots were visualized by spraying with aqueous 10% H_2SO_4, which was followed by heating for 3-5 min.



1 **2** **3** **4** **5**

Fig. 2. Chemical structures of compounds **1–5**

2.3. Extraction and isolation

The dried bodies of the soft coral *Sarcophyton infundibuliforme* (2.5 kg) were extracted with methanol (3 × 5 L each) under ultrasonic conditions. The resulting solutions were filtered, combined, and concentrated under reduced pressure to give the methanol residue (M, 300 g). This was suspended in water (2 L) and extracted in turn with *n*-hexane (2 × 5 L each) and CH_2Cl_2 (2 × 5 L each) to obtain extracts in *n*-hexane (H, 80 g), CH_2Cl_2 (D, 10 g), and water. On concentration, extracts H and D were combined and separated on *silica gel* MPLC with the mobile phase of *n*-hexane-acetone (gradient 50:1→1:1, v/v) to obtain eight fractions, H1-H8. Fractions H3 (10 g) and H-4 (10 g) were combined and separated into eight subfractions, H3A-H3H, by RP-18 MPLC with the mobile phase of MeOH-H_2O (gradient 1:1→15:1, v/v). Subfraction H3B (1 g) was further separated into three smaller fractions H3B1-H3B3 using *silica gel* CC with *n*-hexane-CH_2Cl_2-EtOAc (5:2:1, v/v). Purification of fraction H3B3 (150 mg) by RP-18 CC with acetone-H_2O (3:1, v/v) and then by HPLC (column: Cosmosil 5C18-MS-II, 250 × 10 mm, 5 mm; eluent: ACN-H_2O 47:53; flow rate: 2 mL/min) to give compound **4** (9.0 mg). Subfraction H3C (1.3 g) was treated in the same manner as done for H3B to obtain three smaller fractions, H3C1-H3C3. Compound **5** (20.0 mg) was purified from fraction H3C1 (500 mg) by *silica gel* CC with *n*-hexane-EtOAc (7:1, v/v). Purification of fraction H3C3 (125 mg) on RP-18 CC with acetone-H_2O (3:1, v/v) and then on HPLC (column: Cosmosil 5C18-MS-II, 250 × 10 mm, 5 mm; eluent: ACN-H_2O 62:38; flow rate: 2 mL/min) to give compound **3** (4.0 mg). Subfraction H3D (1.6 g) was treated in the same manner as done for H3B and H3C to obtain four smaller fractions, H3D1-H3D4. Compound **2** (15.0 mg) was purified from fraction H3D1 (500 mg) after subjecting it to RP-18 CC with acetone-H_2O (3:1, v/v) and then to *silica gel* CC with *n*-hexane-EtOAc (4:1, v/v). Finally, purification of fraction H3D3 (175 mg) by *silica gel* CC with *n*-hexane-EtOAc (4:1, v/v), followed by HPLC (column: Cosmosil 5C18-MS-II, 250 × 10 mm, 5 mm; eluent: ACN-H_2O 63:37; flow rate: 2 mL/min) to give compound **1** (7.5 mg).

Sarcrassin D (1): Pale yellow oil, molecular formula $C_{23}H_{32}O_6$; $[\alpha]_D^{25}$ +135 (*c* 0.05, CH_2Cl_2) [12]; ^1H (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) see Table 1.

Emblide (2): White powder, molecular formula $C_{23}H_{32}O_6$; $[\alpha]_D^{25}$ +85 (*c* 0.05, CH_2Cl_2) [12]; ^1H (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) see Table 1.

7α,8β-Dihydroxydeepoxysarcophine (3): White powder, molecular formula $C_{20}H_{30}O_4$; $[\alpha]_D^{25}$ +5 (*c* 0.05, CH_2Cl_2) [13]; ^1H (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) see Table 2.

Lobocrasol B (4): White solid, molecular formula $C_{20}H_{32}O_5$; $[\alpha]_D^{25}$ +7 (*c* 0.05, CH_2Cl_2) [9]; ^1H (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) see Table 2.

Sarcophine (5): White powder, molecular formula $C_{20}H_{28}O_3$; $[\alpha]_D^{25}$ +65 (*c* 0.05, CH_2Cl_2) [14]; ^1H (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) see Table 2.

3. Results and discussion

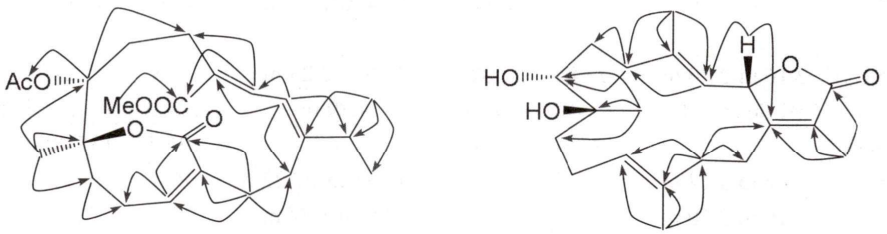
Compound **1** was isolated as a pale yellow oil. Its ^1H and ^{13}C NMR spectra reveal signals of 23 carbons including one methyl ester [δ_C 51.82 (C-21)/δ_H 3.71 (3H, s, H-21)] and one acetoxy group [δ_C 169.86 (C, C-22) and 21.05 (CH_3, C-23)/δ_H 2.03 (3H, s, H-23)]. In addition, the typical signals of three trisubstituted double bonds [δ_C 155.30 (C, C-1), 119.20 (CH, C-2), 137.09 (CH, C-3), 128.97 (C, C-4), 141.88 (CH, C-11), and 132.26 (C, C-12)/δ_H 5.92 (1H, d, J = 9.6 Hz, H-2), 7.55 (1H, d, J = 9.6 Hz, H-3), and 6.30 (1H, t, J = 4.2 Hz, H-11)], one oxymethine [δ_C 68.20 (C-7)/δ_H 5.24 (1H, br d, J = 10.8 Hz, H-7)], one tertiary oxygenated carbon [δ_C 82.10 (C-8)], one isopropyl group [δ_C 31.10 (CH, C-15), 19.86 (CH_3, C-16), and 22.90 (C-17)/δ_H 2.65 (1H, m, H-15), 1.07 (3H, d, J = 6.6 Hz, H-16), and 0.99 (3H, d, J = 6.6 Hz, H-17)], two carboxyl carbons [δ_C 168.61 (C-18) and 166.59 (C-20)], and one singlet methyl [δ_C 23.99 (C-19)/δ_H 1.36 (3H, s, H-19)] were also observed. These data suggested the presence of a cembranoid diterpene, one of the main constituents of *Sarcophyton* soft corals [1],[2]. The ^{13}C NMR data of **1** were found to be essentially identical to those of sarcrassin D [12]. Locations of the three double bonds at C-1, C-3, and C-11 were confirmed by the HMBC cross-peaks of H-2 (δ_H 5.92) with C-3 (δ_C 137.09), C-4 (δ_C 128.97), C-14 (δ_C 32.99), and C-15 (δ_C 31.10); H-13 (δ_H 3.21) with C-11 (δ_C 141.88), C-12 (δ_C 132.26), and C-14 (δ_C 32.99); and those of H-16 (δ_H 1.07) and H-17 (δ_H 0.99) with C-1 (δ_C

155.30) (Fig. 3). The methyl protons H-19 (δ_H 1.36) revealed HMBC cross-peaks with C-7 (δ_C 68.20) and C-8 (δ_C 82.10) indicating positions of the oxymethine and tertiary oxygenated carbons. Moreover, HMBC correlations of the olefinic protons H-3 (δ_H 7.55) and H-11 (δ_H 6.30) with the corresponding carbons C-18 (δ_C 168.61) and C-20 (δ_C 166.59) confirmed locations of the two carboxyl groups. The attachment of the methyl ester at C-18 was determined by an HMBC cross-peak of H-21 (δ_H 3.71) with C-18 (δ_C 168.61). From all the above observations, compound **1** was identified as sarcrassin D [12]. Its absolute configurations were confirmed by the X-ray diffraction experiment [15].

The ^{1}H and ^{13}C NMR data of **2** were similar to those of **1** except for the difference in some signals around the diene structure (Table 1). The ^{13}C NMR carbon signals at C-3 (δ_C 135.45), C-4 (δ_C 124.39), and C-14 (δ_C 27.09) of **2** were strongly shifted upfield relative to those of **1** at δ_C 137.09 (C-3), 128.97 (C-4), and 32.99 (C-14). Whereas, the ^{13}C NMR carbon signals at C-5 (δ_C 26.28), C-13 (δ_C 37.07), C-15 (δ_C 35.89), and C-16 (δ_C 21.92) of **2** were strongly shifted downfield relative to those of **1** at δ_C 20.66 (C-5), 34.22 (C-13), 31.10 (C-15), and 19.86 (C-16). An excellent agreement of the ^{13}C NMR data of **2** with those reported (Table 1) as well as the detailed analysis of the HSQC and HMBC spectra allowed the identification of this compound as emblide [12].

As in case **1** and **2**, the NMR features of **3** were also indicative of a cembranoid [1],[2]. The ^{1}H and ^{13}C NMR spectra exhibited typical signals of two oxymethines [δ_C 79.11 (C-2) and 72.89 (C-7)/δ_H 5.58 (1H, dd, J = 1.2, 10.2 Hz, H-2) and 3.50 (1H, dd, J = 0.6, 10.8 Hz, H-7)], one tertiary oxygenated carbon [δ_C 75.43 (C-8)], one fully substituted double bond [δ_C 162.64 (C, C-1) and 122.90 (C, C-15)], two trisubstituted double bonds [δ_C 121.02 (CH, C-3), 144.03 (C, C-4), 125.29 (CH, C-11), and 134.83 (C, C-12)/δ_H 4.95 (1H, d, J = 10.2 Hz, H-3) and 5.01 (1H, dd, J = 5.4, 8.4 Hz, H-11)], one lactone carbon [δ_C 174.85 (C-16)], and four singlet methyls [δ_C 8.97 (C-17), 16.545 (C-18), 24.26 (C-19), and 15.42 (C-20)/δ_H 1.83 (H-17), 1.92 (H-18), 1.20 (H-19), and 1.66 (H-20), each 3H, s]. From these observations, ^{13}C NMR data of **3** (Table 2) were found to be similar to those of 7α,8β-dihydroxydeepoxysarcophine [13]. The locations of the three double bonds at C-1/C-15, C-3/C-4, and C-11/C-12 and lactone carbon at C-16 were confirmed by the HMBC cross-peaks of H-2 (δ_H 5.58) with C-1 (δ_C 162.64) and C-3 (δ_C 121.02); H-13 (δ_H 2.05 and 2.14) with C-1 (δ_C 162.64), C-11 (δ_C 125.29), C-12 (δ_C 134.83), and C-14 (δ_C 26.85); H-17 (δ_H 1.83) with C-1 (δ_C 162.64), C-15 (δ_C 122.90), and C-16 (δ_C 174.85); H-18 (δ_H 1.92) with C-3 (δ_C 121.02), C-4 (δ_C 144.03), and C-5 (δ_C 35.56); and those of H-20 (δ_H 1.66) with C-11 (δ_C 125.29), C-12 (δ_C 134.83), and C-13 (δ_C 36.58) (Fig. 3). In addition, the HMBC correlations of H-5 (δ_H 2.21 and 3.42) with C-7 (δ_C 72.89) and H-19 (δ_H 1.20) with C-7 (δ_C 72.89), C-8 (δ_C 75.43), and C-9 (δ_C 37.21) clearly confirmed positions of the oxymethine at C-7 and tertiary oxygenated carbon at C-8. Thus, compound **3** was identified as 7α,8β-dihydroxydeepoxysarcophine [13].

Similarly, the detailed analysis of the 1D (^{1}H and ^{13}C NMR) and 2D (HSQC and HMBC) NMR spectroscopic data in comparison with those reported, the remaining compound was identified as lobocrasol B (**4**) [9] and sarcophine (**5**) [14]. In our previous investigations, we have already isolated compounds **2** from *Lobophytum laevigatum* [7] and *Sinularia digitata* [10]; **4** from *Lobophytum crassum* [9]; and **5** from *Sarcophyton mililatensis* [5], *Lobophytum laevigatum* [7], and *Sinularia digitata* [10]. However, this is the first report of **1**–**5** from the species *S. infundibuliforme*.



1 **3**

Fig. 3: Key HMBC correlations of **1** and **3**

Table 1. ^{1}H (600 MHz) and ^{13}C NMR (150 MHz) spectroscopic data of **1** and **2** in $CDCl_3$

C	δ_C[a]	**1**		δ_C[b]	**2**	
		δ_C	δ_H mult. (*J* in Hz)		δ_C	δ_H mult. (*J* in Hz)
1	155.3	155.30	-	155.2	155.24	-
2	119.2	119.20	5.92 d (9.6)	120.8	120.83	7.16 d (12.0)
3	137.1	137.09	7.55 d (9.6)	135.4	135.45	6.27 d (12.0)
4	129.0	128.97	-	124.4	124.39	-
5	20.7	20.66	2.47 m/2.79 m	26.2	26.28	2.36 m/2.46 m
6	26.0	25.88	1.78 m/2.20 m	25.2	25.19	1.84 m/2.18 m
7	68.3	68.20	5.24 br d (10.8)	68.2	68.12	5.40 dd (2.4, 9.0)
8	82.1	82.10	-	82.4	82.41	-
9	34.3	34.28	1.87 dd (5.4, 15.6)/2.03 m	34.5	34.48	2.00 m/2.06 m
10	27.3	27.29	2.30 m/2.88 m	27.1	27.13	2.30 m/2.50 m
11	141.8	141.88	6.30 t (4.2)	142.2	142.25	6.12 t (4.2)
12	132.3	132.26	-	131.9	131.99	-
13	34.2	34.22	2.30 m/3.21 dt (4.2, 13.2)	37.1	37.07	1.89 br t (12.6)/3.17 m
14	33.0	32.99	2.35 m/2.60 m	27.1	27.09	2.13 m/2.66 br t (12.6)
15	31.1	31.10	2.65 m	35.9	35.89	2.38 m
16	19.8	19.86	1.07 d (6.6)	21.9	21.92	1.30 d (6.6)
17	22.8	22.90	0.99 d (6.6)	22.6	22.67	1.09 d (6.6)
18	168.6	168.61	-	168.2	168.21	-
19	24.0	23.99	1.36 s	23.7	23.68	1.48 s
20	166.5	166.59	-	166.3	166.35	-
21	51.7	51.82	3.71 s	51.2	51.22	3.73 s
22	169.8	169.86	-	169.6	169.61	-
23	21.0	21.05	2.03 s	20.9	20.87	2.03 s

[a]δ_C of sarcrassin D [12] and [b]δ_C of emblide [12].

Table 2. ^{1}H (600 MHz) and ^{13}C NMR (150 MHz) spectroscopic data of **3**–**5** in $CDCl_3$

C	δ_C[a]	**3**		δ_C[b]	**4**		δ_C[c]	**5**	
		δ_C	δ_H mult. (*J* in Hz)		δ_C	δ_H mult. (*J* in Hz)		δ_C	δ_H mult. (*J* in Hz)
1	163.2	162.64	-	71.19	71.13	-	162.2	162.32	-
2	79.3	79.11	5.58 dd (1.2, 10.2)	77.50	77.78	4.89 d (10.8)	78.8	78.75	5.58 dd (1.8, 10.2)
3	120.6	121.02	4.95 d (10.2)	125.28	125.40	5.45 d (10.8)	120.6	120.53	5.03 dd (1.8, 10.2)
4	144.2	144.03	-	139.22	139.60	-	144.0	143.93	-
5	35.3	35.56	2.21 m 2.42 dt (2.4, 12.6)	34.95	35.37	2.10 m 2.46 dt (1.8, 12.6)	37.4	37.26	2.37 m
6	26.7	27.03	1.55 m/1.89 m	26.52	26.67	1.51 m/1.85 m	25.2	25.18	1.66 m/1.89 m
7	72.5	72.89	3.50 dd (0.6, 10.8)	72.87	72.75	3.52 dd (1.2, 11.4)	61.5	61.27	2.68 t (4.2)
8	75.4	75.43	-	75.83	75.70	-	59.9	59.82	-
9	36.8	37.21	1.75 m/1.78 m	37.00	36.84	1.64 m/1.85 m	39.0	38.85	1.11 dt (3.0, 13.2) 2.07 m
10	23.5	23.58	2.16 m/2.20 m	23.84	23.82	2.06 m/2.23 m	23.3	23.21	1.93 m/2.24 m
11	125.2	125.29	5.01 dd (5.4, 8.4)	124.62	124.51	4.89 m	124.9	124.87	5.15 dd (4.5, 6.0)
12	134.5	134.83	-	134.84	135.03	-	135.5	135.40	-
13	36.4	36.58	2.05 m/2.14 m	35.40	35.33	1.96 t (12.6)/2.25 m	36.4	36.21	2.04 m/2.18 m
14	26.8	26.85	2.10 m/2.70 m	26.27	26.53	1.70 m/1.84 m	27.5	27.43	2.10 m/2.75 m
15	122.4	122.90	-	68.21	68.32	-	122.9	122.73	-
16	175.1	174.85	-	98.30	98.60	5.25 s	175.0	174.57	-

C	δ_C[a]	3		δ_C[b]	4		δ_C[c]	5	
		δ_C	δ_H mult. (*J* in Hz)		δ_C	δ_H mult. (*J* in Hz)		δ_C	δ_H mult. (*J* in Hz)
17	8.8	8.97	1.83 s	11.20	11.36	1.49 s	8.9	8.90	1.85 t (1.8)
18	16.4	16.45	1.92 s	15.82	15.95	1.85 s	16.1	16.06	1.90 d (1.8)
19	24.2	24.26	1.20 s	24.33	24.45	1.21 s	17.7	17.12	1.28 s
20	15.2	15.42	1.66 s	15.00	15.14	1.60 s	15.5	15.39	1.62 br s

[a]δ_C of 7α,8β-dihydroxydeepoxysarcophine [13], [b]δ_C of lobocrasol B [9], and [c]δ_C of sarcophine [14].

4. Conclusion

From the Vietnamese soft coral *S. infundibuliforme* five cembranoid diterpenes were isolated by using various chromatographic experiments. The structures were elucidated as sarcrassin D (**1**), emblide (**2**), 7α,8β-dihydroxydeepoxysarcophine (**3**), lobocrasol B (**4**), and sarcophine (**5**) by detailed analysis of their 1D and 2D NMR spectral data in comparison with the literature values. Compounds **1**–**5** were reported here for the first time from the species *S. infundibuliforme*.

Acknowledgments: *This research was supported by the Vietnam Academy of Science and Technology (grant number TĐDLB0.02/2022.*

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