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*Research Article*

# Chemical investigation of the *n*-hexane extract of *Marchantia polymorpha* L.

**Nguyen Tran Huynh Le[1], Nguyen Cong Thai Son[1], Tran Quoc Tan[2], Quach Ngo Diem Phuong[2], Nguyen Kim Phi Phung[3], Nguyen Thi Hoai Thu[4,*]**

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**ABSTRACT**

**Introduction:** *Marchantia polymorpha* belongs to the liverwort family. *Marchantia* species are known to possess diverse chemical constituents and bioactivities. As part of a chemically systematic study of liverworts, the isolation and structural elucidation of six compounds from *Marchantia polymorpha* were reported. **Method:** A dried powder of *Marchantia polymorpha* was macerated in methanol to prepare the crude extract. Then, the liquid–liquid partition method was applied to this extract to separate it into different polar extracts, including *n*-hexane, ethyl acetate extracts, and residue. The Sephadex LH-20 and silica gel column chromatography and recrystallization methods were used to isolate organic compounds. Their chemical structures were determined by usual techniques such as MS and NMR spectra interpretation in comparison with the experimentally spectroscopic data reported. **Results:** Six compounds consisting of marchantin G (**1**), quercetin (**2**), kaempferol (**3**), hexaconazole (**4**), indole-3-carboxylic acid (**5**), and sitosterol 3-O-$\beta$-D-glucopyranoside (**6**) were isolated. **Conclusion:** To the best of our knowledge, although all isolated compounds were known to be present in other species, they were reported from this species for the first time.

**Key words:** Marchantia polymorpha, chemical constituents, bis-bibenzyl, flavonol, alkaloid, phytosterol

[1]*Sai Gon University, Ho Chi Minh City, Vietnam*

[2]*Faculty of Biology and Biotechnology, University of Science, Vietnam National University-Ho Chi Minh City, Ho Chi Minh City, Vietnam.*

[3]*Faculty of Chemistry, University of Science, Vietnam National University-Ho Chi Minh City, Ho Chi Minh City, Vietnam.*

[4]*Faculty of Basic Sciences, University of Medicine and Pharmacy at Ho Chi Minh City, Ho Chi Minh City, Vietnam.*

**Correspondence**

**Nguyen Thi Hoai Thu**, Faculty of Basic Sciences, University of Medicine and Pharmacy at Ho Chi Minh City, Ho Chi Minh City, Vietnam.

Email: nguyenthihoaithu@ump.edu.vn

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## INTRODUCTION

*Marchantia polymorpha* L. (Marchantiaceae) belongs to liverworts. It is known as a traditional medicine to cure poisonous snake bites, insect bites, inflammation, cuts, fractures, etc.[1]. In biological studies, *M. polymorpha* possessed inhibition of the enzymes $\alpha$-glucosidase and tyrosinase, antibacterial and antioxidant activities, and cytotoxicity against the MCF-7 cell line[2]. In phytochemical studies, *M. polymorpha* was reported to contain many types of compounds comprising bis-bibenzyl, sesquiterpenoid[3], flavonoid[4], glycoside[5], phenolic and coumarin[6]. Our previous study on the ethyl acetate extract of this species led to the isolation of one bibenzyl (lunularin), two bis-bibenzyl compounds (marchantin A and isoriccardin C), and two flavonoids (luteolin and apigenin). The antibacterial, antioxidant, and cytotoxic activities were evaluated. The compound lunularin showed an $IC_{50}$ value of 4.59 $\pm$ 0.38 $\mu$g/mL and an $SC_{50}$ of 3.99 $\pm$ 0.47 $\mu$g/mL in the experiments against MCF-7 cancer cells and DPPH radical scavenging activity, respectively. In comparison, isoriccardin C showed remarkable antibacterial activity against *Staphylococcus epidermidis* with an inhibition zone of 12.67 mm at a concentration of 50 $\mu$g/well[7]. This paper reports a continuous chemical study of the *n*-hexane extract of this species.

## MATERIALS AND METHODS

### General experimental procedures

The NMR and MS spectra were registered at the Institute of Chemistry, Vietnam Academy of Science and Technology on Bruker Avance at 500 MHz for $^1$H-NMR and 125 MHz for $^{13}$C-NMR and on an X500$_R$ QTOF for HR-ESI-MS.

### Plant material

*Marchantia polymorpha* L. was collected in Da Lat city, Lam Dong Province, Vietnam, in October 2018. The scientific name of this species was identified by Msc. Luong Thien Tam, Faculty of Biology and Biotechnology, University of Science, VNUHCM.

### Extraction and isolation

The dried *Marchantia polymorpha* L. (2.0 kg) was ground into powder and macerated in methanol (3x7 L) at room temperature. The filtrated solution was then evaporated at reduced pressure to give a crude

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extract (110.0 g). This crude extract was separated into different polar fractions by a liquid–liquid partition method with *n*-hexane and ethyl acetate.

The *n*-hexane extract (31.3 g) was subjected to normal-phase silica gel column chromatography. The solvent systems used to elute this column were *n*-hexane:ethyl acetate (stepwise, 99:1, 98:2, 95:5, 90:10, 50:50, 0:100) and ethyl acetate:methanol (1:1) to give eight subfractions (H1–H8). A silica gel column chromatography was applied for fraction H3 (4.6 g), eluted with *n*-hexane:ethyl acetate (stepwise, 99:1, 98:2, 95:5, 90:10, 50:50, 0:100) to give seven subfractions (H3.1–H3.7). Subfraction H3.3 (650 mg) was then subjected to silica gel column chromatography and eluted with *n*-hexane:ethyl acetate as the abovementioned eluent to afford six fractions (H3.3.1–H3.3.6). Compound **4** (10.3 mg) was obtained from fraction H3.3.2 (110 mg) after applying this fraction to Sephadex-LH20 eluted with chloroform:methanol (1:4). Three compounds, **2** (5.6 mg), **3** (6.1 mg), and **5** (12.2 mg), were obtained from subfraction H3.4 (350 mg) by silica gel column chromatography eluted with *n*-hexane:ethyl acetate (6:4) and further purified by Sephadex-LH20 chromatography eluted with a chloroform:methanol (1:4) solvent system. Fraction H4 (5.1 g) was separated into six subfractions (H4.1–H4.6) by silica gel column chromatography and eluted with *n*-hexane:ethyl acetate as described above. Compound **1** was then isolated from subfraction H.4.2 (1.2 g) by silica gel column chromatography eluted with *n*-hexane:ethyl acetate (65:35), followed by Sephadex-LH20 chromatography eluted with chloroform:methanol (1:4). Fraction H8 (3.0 g) was subjected to silica gel column chromatography and then eluted with *n*-hexane:ethyl acetate and then ethyl acetate:methanol as previously described. A precipitate (220 mg) appeared when the column chromatography of fraction H8 was eluted with ethyl acetate:methanol (50:50), which was then recrystallized in ethyl acetate to afford **6** (16.6 mg).

## RESULTS

From the *n*-hexane extract of *Marchantia polymorpha* L., collected in Da Lat city, Lam Dong Province, six compounds, **1** (7.8 mg), **2** (5.6 mg), **3** (6.1 mg), **4** (10.3 mg), **5** (12.2 mg) and **6** (16.6 mg), were isolated. Their physical properties and spectroscopic data were obtained as follows (**Figure 1**).

**Marchantin G (1)**: A yellowish solid. HR-ESI-MS: *m/z* 453.1352 $[M-H]^-$. $^1$H-NMR (DMSO-$d_6$) (*J* in Hertz): $\delta_H$ 6.60 (*d*, 8.5, H-2/H-6), 6.98 (*d*, 8.5, H-3/H-5), 3.01 (*brs*, H-7/H-8), 7.03 (*d*, 5.0, H-12), 6.74 (*dd*, 5.0, 4.5, H-13), 7.03 (*d*, 5.0, H-14), 6.47 (*d*, 2.0, H-3'), 7.09 (*d*, 2.0, H-5'), 3.76 (*s*, H-8'), 6.08 (*brs*, H-10'), 6.82 (*dd*, 8.0, 2.0, H-12'), 7.11 (*dd*, 8.5, 8.0, H-13'), and 6.43 (*br d*, 8.0, H-14'). $^{13}$C-NMR (DMSO-$d_6$): $\delta_C$ 153.3 (C-1), 119.6 (C-2/C-6), 129.6 (C-3/C-5), 137.1 (C-4), 33.4 (C-7), 28.5 (C-8), 134.0 (C-9), 137.4 (C-10), 149.5 (C-11), 125.0 (C-12), 114.3 (C-13), 119.6 (C-14), 140.7 (C-1'), 145.9 (C-2'), 111.5 (C-3'), 137.1 (C-4'), 108.4 (C-5'), 158.0 (C-6'), 195.6 (C-7'), 46.0 (C-8'), 136.5 (C-9'), 113.8 (C-10'), 157.7 (C-11'), 114.1 (C-12'), 129.1 (C-13'), and 119.4 (C-14'). Selected COSY and HMBC correlations: see **Figure 2**.

**Quercetin (2)**: A yellowish solid. HR-ESI-MS: *m/z* 301.0353 $[M-H]^-$. $^1$H-NMR (DMSO-$d_6$) (*J* in Hertz): $\delta_H$ 6.18 (*d*, 1.5, H-6), 6.40 (*d*, 1.5, H-8), 7.67 (*d*, 2.0, H-2'), 6.88 (*d*, 7.0, H-5'), 7.53 (*d d*, 7.0, 2.0, H-6'), and 12.49 (1H, *s*, 5-OH). $^{13}$C-NMR (DMSO-$d_6$): $\delta_C$ 146.8 (C-2), 135.7 (C-3), 175.8 (C-4), 160.7 (C-5), 98.1 (C-6), 163.9 (C-7), 93.3 (C-8), 156.1 (C-9), 103.0 (C-10), 121.9 (C-1'), 115.0 (C-2'), 145.0 (C-3'), 146.8 (C-4'), 115.6 (C-5'), and 119.9 (C-6'). Selected HMBC correlations: see **Figure 2**.

**Kaempferol (3)**: A yellowish solid. $^1$H-NMR (DMSO-$d_6$) (*J* in Hertz): $\delta_H$ 6.19 (*s*, H-6), 6.44 (*s*, H-8), 8.04 (*d*, 9.0, H-2'/H-6'), 6.93 (*d*, 8.5, H-3'/H-5'), and 12.46 (*s*, 5-OH). $^{13}$C-NMR (DMSO-$d_6$): $\delta_C$ 146.7 (C-2), 135.5 (C-3), 175.8 (C-4), 156.1 (C-5), 98.1 (C-6), 163.8 (C-7), 93.4 (C-8), 160.6 (C-9), 102.9 (C-10), 121.6 (C-1'), 129.4 (C-2'/C-6'), 115.4 (C-3'/C-5'), and 159.1 (C-4').

**Hexaconazole (4)**: White solid. HR-ESI-MS: *m/z* 314.0819 $[C_{14}H_{17}{}^{35}Cl_2N_3O+H]^+$, 316.0792 $[C_{14}H_{17}{}^{35}Cl^{37}ClN_3O+H]^+$, and 318.0773 $[C_{14}H_{17}{}^{37}Cl_2N_3O+H]^+$. $^1$H-NMR (DMSO-$d_6$) (*J* in Hertz): $\delta_H$ 4.83 (*d*, 14.5, H-1a), 4.54 (*d*, 14.5, H-1b), 2.47 (*dd*, 14.0, 5.5, H-3a), 1.61 (*ddd*, 14.5, 12.5, 4.5, H-3b), 1.25 (*m*, H-4a), 0.70 (*m*, H-4b), 1.16 (*m*, H-5), 0.77 (*t*, 7.0, H-6), 7.73 (*s*, H-3'), 8.26 (*s*, H-5'), 7.52 (*d*, 2.5, H-3"), 7.29 (*dd*, 8.5, 2.0, H-5"), 7.53 (*d*, 8.0, H-6"), and 5.71 (*s*, 2-OH $^{13}$C-NMR (DMSO-$d_6$): $\delta_C$ 56.1 (C-1), 75.5 (C-2), 35.7 (C-3), 25.1 (C-4), 22.3 (C-5), 13.8 (C-6), 150.3 (C-3'), 144.7 (C-5'), 139.0 (C-1"), 132.3 (C-2"), 129.7 (C-3"), 130.9 (C-4"), 126.8 (C-5"), and 131.0 (C-6"). Selected COSY and HMBC correlations: see **Figure 2**.

**Indole-3-carboxylic acid (5)**: White powder. HR-ESI-MS: *m/z* 162.0557 $[M+H]^+$. $^1$H-NMR (DMSO-$d_6$) (*J* in Hertz): $\delta_H$ 7.98 (*d*, 3.0, H-2), 8.00 (*d*, 7.0, H-4), 7.14 (*ddd*, 8.0, 7.0, 1.0, H-5), 7.18 (*ddd*, 8.0, 7.0, 1.5, H-6), 7.45 (*dd*, 7.0, 1.0, H-7), and 11.77 (1H, *brs*, NH). $^{13}$C-NMR (DMSO-$d_6$): $\delta_C$ 132.2 (C-2), 107.3 (C-3), 120.5 (C-4), 121.0 (C-5), 122.1 (C-6), 112.2 (C-7), 136.2 (C-8), 126.0 (C-9), and 165.9 (C-10). Selected COSY and HMBC correlations: see **Figure 2**.

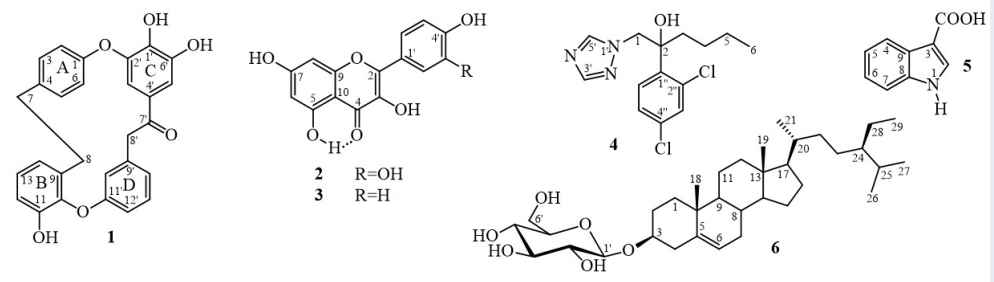


**Figure 1**: **The chemical structures of isolated compounds 1-6**

**Sitosterol 3-*O*-$\beta$-D-glucopyranoside (6)**: White powder. $^1$H-NMR (DMSO-$d_6$) (*J* in Hertz): $\delta_H$ 3.45 (*m*, H-3), 5.32 (*brd*, 4.5, H-6), 0.65 (*s*, H-18), 0.95 (*s*, H-19), 0.90 (*d*, 6.5, H-21), 0.81 (*d*, 7.0, H-26), 0.79 (*d*, 7.0, H-27), 0.82 (*t*, 7.0, H-29), 4.22 (*d*, 7.5, H-1'), 2.91 (*m*, H-2'), 3.12 (*dd*, 9.0, 9.0, H-3'), 3.01 (*dd*, 9.0, 9.0, H-4'), 3.07 (*m*, H-5'), 3.64 (*dd*, 10.0, 5.5, H-6'a), and 3.41 (*dd*, 11.5, 6.0, H-6'b). The $^{13}$C-NMR (DMSO-$d_6$): $\delta_C$ 36.8 (C-1), 31.3 (C-2), 76.9 (C-3), 38.3 (C-4), 140.5 (C-5), 121.2 (C-6), 31.4 (C-7), 31.3 (C-8), 49.6 (C-9), 35.4 (C-10), 20.6 (C-11), 39.2 (C-12), 41.8 (C-13), 56.2 (C-14), 23.8 (C-15), 27.7 (C-16), 55.4 (C-17), 11.6 (C-18), 18.9 (C-19), 36.2 (C-20), 18.6 (C-21), 33.3 (C-22), 25.5 (C-23), 45.1 (C-24), 28.7 (C-25), 19.1 (C-26), 19.7 (C-27), 22.6 (C-28), 11.8 (C-29), 100.8 (C-1'), 73.5 (C-2'), 76.8 (C-3'), 70.1 (C-4'), 76.9 (C-5'), and 61.1 (C-6').

## DISCUSSION

Compound **1** was isolated as a yellowish powder. Its HR-ESI-MS showed a deprotonated ion peak at *m/z* 453.1352 $[M-H]^-$ (calcd. for $C_{28}H_{22}O_6$–H, 453.1338). The $^1$H-NMR spectrum of **1** showed two doublet proton signals with a large coupling constant of 8.5 Hz, each integrated two protons at $\delta_H$ 6.60 (H-2/H-6) and 6.98 (H-3/H-5) of a *para*-disubstituted benzene ring (ring A), as shown in **Figure 1**. A set of three aromatic protons at $\delta_H$ 7.03 (*d*, 5.0 Hz, H-12), 6.74 (*dd*, 5.0, 4.5 Hz, H-13), and 7.03 (*d*, 5.0 Hz, H-14) were assigned for a 1,2,3-trisubstituted benzene ring (ring B). The connection of H-12/H-13/H-14 was confirmed by COSY correlations. Two *meta*-coupling doublet proton signals at $\delta_H$ 6.47 (*d*, 2.0 Hz, H-3') and 7.09 (*d*, 2.0 Hz, H-5') belonged to a 1,3,4,5-tetrasubstituted benzene ring (ring C). The four remaining aromatic proton signals at $\delta_H$ 6.08 (*brs*, H-10'), 6.82 (*dd*, 8.0, 2.0 Hz, H-12'), 7.11 (*dd*, 8.5, 8.0 Hz, H-13'), and 6.43 (*br d*, 8.0, H-14') along with the COSY connections H-12'/H-13'/H-14' confirmed the presence of *meta*-disubstituted benzene (ring D). In the higher magnetic resonance zone, there were signals of three methylene groups at $\delta_H$ 3.01 (*brs*, H-7/H-8) and 3.76 (*s*, H-8'). From the above information, **1** was suggested to possess four benzene rings and three methylene groups. These corresponded to the presence of three carbon signals at the high magnetic field at $\delta_C$ 33.4 (C-7), 28.5 (C-8), and 46.0 (C-8') of three methylene groups in the $^{13}$C-NMR spectrum. In the higher frequency range, twenty-two carbon signals at 108–158 ppm, including two signals at $\delta_C$ 119.6 (C-2/C-6) and 129.6 (C-3/C-5) appearing in the double intensity of a *para*-disubstituted benzene ring, were assigned to four benzene rings. The last carbon signal at $\delta_C$ 195.6 was assigned to a conjugated carbonyl carbon. Therefore, **1** was suggested to be a bis-bibenzyl compound type that possessed two dihydrostilbenoid units, as normally found in *Marchantia* species. HMBC correlations of protons H-3/H-5 with carbons at $\delta_C$ 153.3 (C-1) and 33.4 (C-7) demonstrated the position of ring A at C-7. The HMBC cross-peaks of proton H-8 with carbons at $\delta_C$ 134.0 (C-9), 137.4 (C-10), and 119.6 (C-14) suggested the position of ring B at C-8. Additionally, HMBC cross-peaks of both protons H-3' and H-5' with the carbonyl carbon at $\delta_C$ 195.6 (C-7'), along with correlations of proton H-8' with carbons at $\delta_C$ 195.6 (C-7'), 113.8 (C-10'), 119.4 (C-14'), confirmed the position of two remaining dibenzyl units. From all the above MS and NMR analyses as well as the good compatibility of the NMR data of **1** with published data[8,9], the chemical structure of **1** was suggested to be marchantin G.

Compound **2** was isolated as a yellowish powder. The molecular formula of **2** was identified to be $C_{15}H_{10}O_7$ based on a quasi-molecular ion peak at *m/z* 301.0353 $[M-H]^-$ (calcd. for $C_{15}H_{10}O_7$–H, 301.0348) on the HR-ESI-MS spectrum. The proton spectrum of **2** showed the characteristic signals of a flavonoid, comprising a singlet proton signal at $\delta_H$

12.49 (1H, *s*) of a chelated hydroxy group at C-5 as usual, two doublet proton signals with a small coupling constant value of 1.5 Hz at $\delta_H$ 6.18 (H-6), 6.40 (H-8), and a set of three aromatic proton signals [at $\delta_H$ 7.67 (*d*, 2.0 Hz, H-2'), 6.88 (*d*, 7.0 Hz, H-5'), and 7.53 (*d d*, 7.0, 2.0 Hz, H-6')] of a 1,3,4-trisubstituted benzene ring. This corresponded to the presence of 15 carbon signals in the $^{13}$C-NMR spectrum and the molecular formula of $C_{15}H_{10}O_7$ assigned by the HR-ESI-MS spectrum as above. The observation of the upfield shifted carbonyl carbon C-4 at $\delta_C$ 175.8 along with the carbon C-3 at $\delta_C$ 135.7 suggested **2** to be a flavonol type. The HMBC spectrum of **2** revealed the correlations of protons H-6, H-8, H-2', H-5', and H-6' with carbons via two or three bonds, as shown in **Figure 2**. Compound **2** was elucidated as quercetin by the good compatibility of its NMR data of **2** with those of quercetin [10].

Compound **3** was obtained as a yellowish powder. The comparison of the NMR spectra of **2** and **3** revealed that **3** was also a flavonol. The only difference between **2** and **3** was the presence of a pair signals at $\delta_H$ 8.04 (*d*, 9.0 Hz, H-2'/H-6'), 6.93 (*d*, 8.5 Hz, H-3'/H-5') of a *para*-disubstituted benzene ring in **3**, instead of signals of the 1,3,4-trisubstituted ring in **2**. The $^{13}$C-NMR spectrum of **3** displayed 15 carbon signals, including two carbon signals at $\delta_C$ 129.4 (C-2'/C-6') and 115.4 (C-3'/C-5') appearing in double intensity in a symmetrical benzene ring possessing two substitutions at the *para* position. Therefore, **3** was determined to be kaempferol due to the good compatibility of its NMR data with those published in the literature [11].

Compound **4** was a white powder. HR-ESI-MS showed three protonated ion peaks at *m/z* 314.0819, 316.0792, and 318.0773 with a relative intensity ratio of 9:6:1, which were calculated for ($C_{14}H_{17}{}^{35}Cl_2N_3O$+H, 314.0827), ($C_{14}H_{17}{}^{35}Cl^{37}ClN_3O$+H, 316.0797), and ($C_{14}H_{17}{}^{37}Cl_2N_3O$+H, 318.0768), respectively. These results suggested that **4** possessed two chlorine atoms in the molecular formula. In the high magnetic zone, the proton spectrum of **4** showed signals of a terminal methyl ($\delta_H$ 0.77, *t,* 7.0 Hz, H-6), three methylene groups ($\delta_H$ 2.47, *dd*, 14.0, 5.5 Hz, H-3a; 1.61, *ddd*, 14.5, 12.5, 4.5 Hz, H-3b; 1.25, *m*, H-4a; 0.70, *m*, H-4b; 1.16, *m*, H-5). The COSY spectrum showed a connection of H6/H5/H4/H3 (**Figure 2**). These NMR data suggested that they belonged to an *n*-butyl group linked to a certain chiral quaternary carbon. In the mediated magnetic zone, the proton spectrum also showed two doublet signals at $\delta_H$ 4.83 (*d*, 14.5 Hz, H-1a) and 4.54 (*d*, 14.5 Hz, H-1b) whose carbon signal was at $\delta_C$ 56.1 (C-1) via an HSQC experiment. These two nonequivalent hydrogens should be between a nitrogen atom and a certain quaternary carbon. The HMBC experiment showed cross-peaks of protons $H_2$-1 to C-3 and a quaternary carbon, of $H_2$-3 to C-1, and to the same quaternary carbon; therefore, this quaternary carbon should be C-2 ($\delta_C$ 75.5). Up to this point, compound **4** contained a six-carbon chain and a 2-hydroxyhexyl moiety. At a low magnetic field, the proton spectrum displayed a set of three aromatic signals at $\delta_H$ 7.52 (*d*, 2.5 Hz, H-3"), 7.29 (*dd*, 8.5, 2.0 Hz, H-5"), and 7.53 (*d*, 8.0 Hz, H-6") of a 1,2,4-trisubstituted benzene ring. The HMBC experiment revealed cross-peaks of proton H-6" to C-2 and of the hydroxy proton ($\delta_H$ 5.71,2-OH) to C-1"; therefore, this benzene ring joined to the abovementioned six-carbon chain at its C-2. In the proton spectrum, two left signals at $\delta_H$ 7.73 (1H, *s*, H-3') and 8.26 (1H, *s*, H-5'), which showed HSQC correlations to carbons C-3' ($\delta_C$ 150.3) and C-5' ($\delta_C$ 144.7), respectively, were hydrogens of a 1,2,4-triazole ring. The HMBC cross-peak of $H_2$-1 of the six-carbon chain to C-5' proved that this five-membered heterocyclic moiety was linked to C-1 of the chain. All mentioned data were in agreement, as shown in **Figure 2**. The chemical structure of **4** was determined to be hexaconazole by comparing its NMR data with those reported in the literature [12]. Although local residents used fungicides to kill parasitic fungi, the material was washed carefully before extraction. Therefore, hexaconazole, a triazole fungicide, isolated from this species could be an artifact that was absorbed by this liverwort. This noted that the bioactivities of extracts of *M. polymorpha*, such as antibacterial activity in a previous preliminary study [2], could be a result of either the second metabolites of this species or the artifact. Therefore, the chemical investigation was meaningful to understanding the bioactivities of the surveyed species.

Compound **5** was isolated as a white powder. Its HR-ESI-MS spectrum showed a pseudomolecular ion peak at *m/z* 162.0557 $[M+H]^+$ (calcd. for $C_9H_7O_2N$+H, 162.0555). The proton spectrum of **5** showed a set of four signals at 8.00 (*d*, 7.0 Hz, H-4), 7.14 (*ddd*, 8.0, 7.0, 1.0 Hz, H-5), 7.18 (*ddd*, 8.0, 7.0, 1.5 Hz, H-6), and 7.45 (*dd*, 7.0, 1.0 Hz, H-7) of a 1,2-disubstituted benzene ring, which was further confirmed by the COSY correlations of H-4/H-5/H-6/H-7. In addition, the $^1$H-NMR spectrum of **5** displayed an olefin methine proton at $\delta_H$ 7.98 (1H, *d*, 3.0 Hz, H-2) and an amino proton at $\delta_H$ 11.77 (1H, *brs*, NH). The

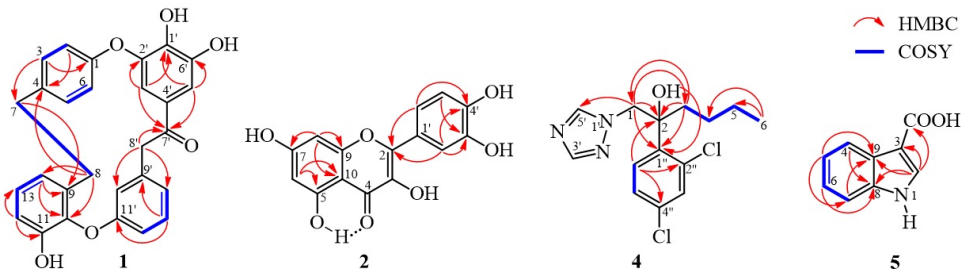


**Figure 2: Selected COSY and HMBC correlations of 1, 2, 4, and 5**

$^{13}$C-NMR spectrum revealed nine carbon signals, including six signals belonging to the benzene ring, two olefinic carbons at $\delta_C$ 132.2 (=CH-, C-2) and 107.3 (=C<, C-3) of a double bond -CH=C<, and one carboxyl carbon at $\delta_C$ 165.9. The HMBC cross-peaks of the olefinic proton (H-2) with both quaternary carbons C-8 and C-9 of the benzene ring suggested the presence of an indole skeleton. The good compatibility of its NMR data with those published in the literature[13] confirmed the chemical structure of **5** to be indole-3-carboxylic acid.

Compound **6** was a white powder. NMR spectra of **6** showed signals characterized for a sitosterol 3-*O*-$\beta$-D-glucopyranoside. The $^{13}$C-NMR spectrum displayed two olefinic carbons at $\delta_C$ 121.2 (=C<) and 140.5 (=CH-) of a double bond at C-5, an oxygenated carbon at $\delta_C$ 76.9 of C-3 as usual, one anomeric carbon at $\delta_C$ 100.8 (C-1') and five oxygenated carbons from 61.0 to 77.0 ppm of a sugar unit. Moreover, the proton spectrum showed signals supported for sitosterol 3-*O*-$\beta$-D-glucopyranoside, comprising one olefinic methine proton at $\delta_H$ 5.32 (*brd*, 4.5 Hz, H-6), one oxygenated methine proton at $\delta_H$ 3.45 (*m*, H-3), two singlet, three doublet and a triplet proton signals from 0.65 to 0.95 ppm of six methyl groups in the sitosterol skeleton. An anomeric proton signal at $\delta_H$ 4.22 (1H, *d*, 7.5 Hz) and oxygenated proton signals from 2.9 to 3.7 ppm belonged to a $\beta$-D-glucose unit. **6** was thus determined to be sitosterol 3-*O*-$\beta$-D-glucopyranoside by comparing its NMR data with those reported in the literature[14].

## CONCLUSION

From the *n*-hexane extract of *Marchantia polymorpha* L., six compounds were isolated, consisting of one bis-dibenzyl (marchantin G), two flavonols (quercetin and kaempferol), two alkaloids (hexaconazole and indole-3-carboxylic acid), and a phytosterol (sitosterol 3-*O*-$\beta$-D-glucopyranoside). Their chemical structures were elucidated by NMR and HR-MS data analysis in comparison with published data. This was the first time that the full NMR data of compound **1** were published.

## ABBREVIATIONS

**HR-ESI-MS:** High resolution electrospray ionization-Mass spectrometry
**$^1$ H-NMR:** Proton nuclear magnetic resonance
**$^{13}$ C-NMR:** Carbon-13 nuclear magnetic resonance
**COSY:** Homonuclear correlation spectroscopy
**HSQC:** Heteronuclear single quantum coherence
**HMBC:** Heteronuclear multiple bond correlation
***s***: singlet
***brs***: broad singlet
***d***: doublet
***dd***: doublet of doublets
***ddd***: doublet of doublet of doublets
***brd***: broad doublet
***t***: triplet
***m***: multiplet
**calcd.:** calculated
**DMSO:** dimethyl sulfoxide

## COMPETING INTEREST

The authors declare no competing financial interest.

## AUTHORS' CONTRIBUTION

Nguyen T.H.L., Tran Q.T. contributed to conducting the experiments and acquiring the data. Nguyen C.T.S., Nguyen K.P.P. interpreted NMR and MS data. Quach N.D.P., Nguyen T.H.T. provided final approval of the manuscript to be submitted.

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