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Thiophene compounds from *Eclipta prostrata* (L.) L.

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ABSTRACT
Eclipta prostrata (L.) L. is a medicinal plant widely distributed in South America, Oceania, and Asia, and is commonly used in traditional medicine for the treatment of various diseases, particularly respiratory disorders and hemorrhagic conditions. Recent studies have demonstrated that this species possesses diverse biological activities, including anticancer, hypoglycemic, hepatoprotective, antioxidant, and anti-inflammatory effects. In this study, three thiophene compounds were isolated from the methanolic extract of the aerial parts of Eclipta prostrata using chromatographic techniques such as thin-layer chromatography (TLC), column chromatography (CC), and high-performance liquid chromatography (HPLC). The isolated compounds were identified as 5-(4-isovaleroyloxybut-1-ynyl)-2,2'-bithiophene (1), 5-(but-3-en-1-yn-1-yl)-5'-(hydroxymethyl dimethylacrylate)-2,2'-bithiophene (2), and 5'-tigloyloxymethyl-5-(but-3-en-1-yn-1-yl)-2,2'-bithiophene (3). Their structures were elucidated based on HR-ESI-MS and NMR spectroscopic analyses (^{1}H, ^{13}C, HSQC, and HMBC), in combination with comparison to literature data. Notably, the complete spectroscopic data of compounds (1) and (3) are reported here for the first time.

Keywords: **Eclipta, Eclipta prostrata,** ***lignan, thiophene, senecioester.***

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I. INTRODUCTION

Eclipta prostrata (L.) L. is a medicinal herb belonging to the family Asteraceae (Eclipta), widely distributed across South America, Oceania, and Asia, including India, China, Japan, Cambodia, Malaysia, Indonesia, Brazil, Mexico, Colombia, Nigeria, Kenya, … [1]. In traditional medicine, this species is used to treat various conditions such as burns and skin fungi. In India, the plant is employed in the treatment of respiratory disorders, skin diseases, fever, hair loss, premature graying, diabetes, and jaundice. In Vietnam, it is used to treat hemoptysis, epistaxis, hepatitis, dengue fever, uterine hemorrhage, enteritis, and fever. In Thailand, different parts of the plant serve various purposes: the leaves are used for gray hair and skin diseases; the stems for tuberculosis, asthma, and as a blood tonic; the roots possess antibacterial and hepatoprotective properties; and the whole plant is used as a treatment for HIV [2, 3]. Given its diverse applications in traditional medicine, *Eclipta prostrata* has been extensively studied regarding its chemical constituents and biological activities. Research results indicate that the plant exhibits notable activities, including anti-inflammatory, antibacterial, anticancer, hypoglycemic, hepatoprotective, and antioxidant effects [4-10]. Numerous compounds have been isolated and structurally identified, including thiophenes, triterpenoids, flavonoids, phenolics, and lignans [4, 9, 11-15]. In this study, from the methanol extract of *Eclipta prostrata*, we conducted the isolation and structural determination of compounds belonging to the thiophene and lignan groups.

II. EXPERIMENTAL SECTION

2.1. General experimental procedures

All NMR spectra, including ^{1}H-NMR (600 MHz), ^{13}C-NMR (150 MHz), HSQC, and HMBC, were recorded on a Bruker AM600 FT-NMR spectrometer using TMS as an internal standard. Optical rotation was measured on a Jasco DIP-370 automatic polarimeter. Column chromatography (CC) was carried out using silica gel (Kieselgel 60, 70–230 mesh and 230–400 mesh, Merck) or RP-18 resin (30–50 µm, Fuji Silysia Chemical Ltd.). Thin-layer chromatography (TLC) was performed on pre-coated silica gel 60 F_{254} (0.25 mm, Merck) and RP-18 $F_{254}S$ (0.25 mm, Merck) plates. HPLC was conducted on an Agilent 1100 system equipped with a J'sphere H-80 column (250 × 20 mm), using a flow rate of 3.0 mL/min and a DAD detector.

2.2. Plant material

The aerial parts of *Eclipta prostrata* (L.) L. were collected in Thai Nguyen, Vietnam, in December 2025. The scientific name was authenticated by Dr. Pho Thi Thuy Hang, Thai Nguyen University of Medicine and Pharmacy, Vietnam (Figure 1).

Figure 1. *Eclipta* prostrata (L.) L.

2.3. Extraction and isolation

The dried aerial parts of *Eclipta prostrata* were powdered (2.2 kg) and extracted with methanol using an ultrasonic apparatus (3 × 10 L, 50 °C, 1 h each). The combined extracts were filtered and concentrated under reduced pressure to yield 124 g of crude methanol extract. The residue was suspended in 1 L of distilled water and successively partitioned with organic solvents of increasing polarity, including n-hexane, CH_2Cl_2, and EtOAc, to afford the corresponding fractions: n-hexane (PL1, 42.6 g), CH_2Cl_2 (PL2, 4.2 g), EtOAc (PL3, 3.8 g), and the remaining aqueous fraction (PL4), after removal of the organic solvents under reduced pressure. Fraction PL1 was evenly dispersed in *n*-hexane, adsorbed onto silica gel, evaporated to dryness to remove the solvent, finely ground, and subjected to silica gel column chromatography using a gradient elution system of *n*-hexane:acetone (100:0 → 1:1, *v/v*), yielding three subfractions: PL1A (2.6 g), PL1B (9.1 g), and PL1C (13.2 g). Subfraction PL1B was further separated on a silica gel column using CH_2Cl_2:acetone (2.5:1, *v/v*) as the eluent to give three fractions: PL1B1 (0.7 g), PL1B2 (3.2 g), and PL1B3 (2.3 g). Fraction PL1B2 was then chromatographed on an RP-18 column with MeOH:water (3:1, *v/v*) to afford two subfractions: PL1B2A (0.92 g) and PL1B2B (0.76 g). Compound 1 (3.7 mg, t_R 40.7 min) was obtained by purification of PL1B2B using HPLC with 93% acetonitrile in water as the mobile phase. Purification of PL1B2A by HPLC yielded compound 3 (4.3 mg, t_R 30.5 min) using 95% acetonitrile in water as the mobile phase, and compound 2 (5.4 mg, t_R 38.2 min) using 93% acetonitrile in water as the mobile phase.

5-(4-isovaleroyloxybut-1-ynyl)-2,2′-bithiophene (1): brown oil; HR-EI-MS m/z 319.0829 $[M + H]^+$ (calcd for $C_{17}H_{19}O_2S_2$, 319.0821); ^{1}H-NMR and ^{13}C-NMR data, see Table 1.

5-(but-3-en-1-yn-1-yl)-5′-(hydroxymethyl dimethylacrylate)-2,2′-bithiophene (2): brown oil; HR-ESI-MS m/z 351.0484 $[M + Na]^+$ (calcd for $C_{18}H_{16}O_2S_2Na$, 351.0489); ^{1}H-NMR and ^{13}C-NMR data, see Table 1.

5′-tigloyloxymethyl-5-(but-3-en-1-yn-1-yl)-2,2′-bithiophene (3): brown oil; ^{1}H-NMR and ^{13}C-NMR data, see Table 2.

III. RESULTS AND DISCUSSION

Compound 1 was obtained as a brown oil. Its molecular formula was established as $C_{17}H_{18}O_2S_2$ based on HR-ESI-MS, which showed a pseudomolecular ion peak at *m/z* 319.0829 $[M + H]^+$ (calcd for $C_{17}H_{19}O_2S_2$, 319.0821). The ^{1}H-NMR spectrum of 2 displayed signals for five aromatic protons at δ_H 6.99 (1H, d, J = 3.6 Hz, H-3), 7.02 (1H, d, J = 3.6 Hz, H-4); 7.15 (1H, dd, *J* = 1.2, 4.2 Hz, H-3′), 7.01 (1H, dd, *J* = 4.2, 5.4 Hz, H-4′), and 7.22 (1H, dd, *J* = 1.2, 5.4 Hz, H-5′). In addition, one methine proton was observed at δ_H 2.14 (1H, m, H-3″), two methylene groups at δ_H 2.23 (2H, d, *J* = 7.2 Hz, H-2″) and 2.78 (2H, t, *J* = 7.2 Hz, H-8), one oxygenated methylene at δ_H 4.24 (2H, t, *J* = 7.2 Hz, H-9), and two methyl groups at δ_H 0.98 × 2 (each 3H, d, *J* = 6.6 Hz, H-4″ and H-5″). The ^{13}C-NMR and HSQC spectra revealed 17 carbon signals, including one carbonyl carbon at δ_C 172.9; five quaternary carbons at δ_C 138.0, 122.2, 75.1, 90.7, and 136.8; five methine carbons at δ_C 123.2, 132.3, 124.1, 127.8, and 25.7; two methylene carbons at δ_C 20.3 and 43.3; one oxygenated methylene carbon at δ_C 61.8; and two methyl carbons at δ_C 22.4 × 2 (Table 1). Analysis of the NMR data suggested that compound 1 is a bithiophene derivative. This was supported by HMBC correlations from H-3 (δ_H 6.99) to C-4 (δ_C 132.3), C-5 (δ_C 122.1), and C-2′ (δ_C 136.8); from H-4 (δ_H 7.02) to C-2 (δ_C 138.0); and from H-3′ (δ_H 7.15) to C-2′ (δ_C 136.8), C-5′ (δ_C 124.8), and C-2 (δ_C 138.0). Further HMBC correlations between H-2″ (δ_H 2.23) and C-1″ (δ_C 172.9), C-3″ (δ_C 25.7), C-4″ (δ_C 22.4), and C-5″ (δ_C 22.4); between H-9 (δ_H 4.24) and C-1″ (δ_C 172.9), C-7 (δ_C 90.7), and C-8 (δ_C 20.3); and between H-8 (δ_H 2.78) and C-6 (δ_C 75.1), C-7 (δ_C 90.7), and C-9 (δ_C 61.8) indicated the presence of a 4-isovaleroyloxybut-1-yn-1-yl moiety (Figure 2). The HMBC correlation between H-4 (δ_H 7.02) and C-6 (δ_C 75.1) established the attachment of this moiety at C-5 of the bithiophene ring. Comparison of the NMR data of 1 with those reported for 5-(4-isovaleroyloxybut-1-ynyl)-2,2′-bithiophene [16] showed good agreement. Therefore, compound 2 was identified as 5-(4-isovaleroyloxybut-1-ynyl)-2,2′-bithiophene (Figure 2).

Compound 2 was obtained as a brown oil. Its molecular formula was established as $C_{18}H_{16}O_2S_2$ based on the pseudomolecular ion peak at m/z 351.0484 $[M + Na]^+$ in the HR-ESI-MS spectrum (calcd for $C_{18}H_{16}O_2S_2Na$, 351.0489). The ^{1}H-NMR spectrum of 3 showed signals for four aromatic protons at δ_H 6.97 (1H, d, *J* = 3.6 Hz, H-4′), 7.00 (1H, d, *J* = 3.6 Hz, H-3), 7.02 (1H, d, *J* = 3.6 Hz, H-3′), and 7.08 (1H, d, *J* = 3.6 Hz, H-4); three olefinic protons of a vinyl group at δ_H 5.55 (1H, dd, *J* = 1.8, 11.4 Hz, H-9), 5.73 (1H, dd, *J* = 1.8, 17.4 Hz, H-9), and 6.02 (1H, dd, *J* = 11.4, 17.4 Hz, H-8); one additional olefinic proton at δ_H 5.70 (1H, s,H-2″); one oxygenated methylene

at $\delta\delta_H$ 5.23 (2H, s, H-6′); and two methyl groups at δ_H 1.89 (3H, s,H-4″) and 2.18 (3H, s, H-5″). The ^{13}C-NMR and HSQC spectra revealed 18 carbon signals, including eight quaternary carbons at δ_C 83.2, 93.1, 122.1, 137.8, 138.3, 138.8, 158.0, and 166.1; six methine carbons at δ_C 115.5, 116.8, 123.7, 123.7, 128.7, and 132.8; one oxygenated methylene carbon at δ_C 59.7; and two methyl carbons at δ_C 20.4 and 27.5. Analysis of the NMR data indicated that compound 2 is a bithiophene derivative. This was supported by HMBC correlations from H-3 (δ_H 7.00) to C-2 (δ_C 138.8), C-4 (δ_C 132.8), C-5 (δ_C 122.1), and C-2′ (δ_C 137.8), and from H-3′ (δ_H 7.02) to C-2′ (δ_C 137.8), C-4′ (δ_C 128.7), C-5′ (δ_C 138.3), and C-2 (δ_C 138.8), confirming the presence of a bithiophene core. HMBC correlations from H-9 (δ_H 5.55 and 5.73) to C-8 (δ_C 116.8) and C-7 (δ_C 93.1), and from H-8 (δ_H 6.02) to C-9 (δ_C 127.0) and C-6 (δ_C 83.2), indicated the presence of a but-3-en-1-yn-1-yl moiety. The HMBC correlation from H-4 (δ_H 7.08) to C-6 (δ_C 83.2) established its attachment at C-5 of the bithiophene ring. Further HMBC correlations from H-4″ (δ_H 1.89) and H-5″ (δ_H 2.18) to C-2″ (δ_C 115.5) and C-3″ (δ_C 158.0), and from H-6′ (δ_H 5.23) to C-1″ (δ_C 166.1), C-4′ (δ_C 128.7), and C-5′ (δ_C 138.3), established the presence of a hydroxymethyl dimethylacrylate moiety at C-5′ of the bithiophene unit (Figure 3). Based on these spectroscopic analyses, compound 2 was identified as 5-(but-3-en-1-yn-1-yl)-5′-(hydroxymethyl dimethylacrylate)-2,2′-bithiophene (Figure 2). A search in the SciFinder database indicated that the NMR spectroscopic data of this compound are reported here for the first time.

Table 1. ^{1}H-NMR and ^{13}C-NMR spectroscopic data of compounds 1 and 2

	1		2	
C	δ_C	δ_H **(mult., *J* in Hz)**	δ_C	δ_H **(mult., *J* in Hz)**
2	138.0	-	138.8	-
3	123.2	6.99 (d, 3.6)	123.7	7.00 (d, 3.6)
4	132.3	7.02 (d, 3.6)	132.8	7.08 (d, 3.6)
5	122.1	-	122.1	-
6	75.1	-	83.2	-
7	90.7	-	93.1	-
8	20.3	2.78 (t, 7.2)	116.8	6.02 (dd, 11.4, 17.4)
9	61.8	4.25 (t, 7.2)	127.0	5.55 (dd, 1.8, 11.4)/5.73 (dd, 1.8, 17.4)
2′	136.8	-	137.8	-
3′	124.1	7.15 (dd, 1.2, 4.2)	123.7	7.02 (d, 3.6)
4′	127.8	7.01 (dd, 4.2, 5.4)	128.7	6.97 (d, 3.6)
5′	124.8	7.22 (dd, 1.2. 5.4)	138.3	-
6′			59.7	5.23 (s)
1″	172.9	-	166.1	-
2″	43.3	2.23 (d, 7.2)	115.5	5.70 (s)
3″	25.7	2.13 (m)	158.0	-
4″	22.4	0.98 (d, 6.6)	27.5	1.89 (s)
5″	22.4	0.98 (d, 6.6)	20.4	2.18 (s)

Compound 3 was obtained as a brown oil. The ^{1}H-NMR spectrum of 1 displayed signals for four aromatic protons at δ_H 6.99 (1H, d, J = 3.6 Hz, H-4′), 7.03 (1H, d, J = 3.6 Hz, H-3), 7.03 (1H, d, J = 3.6 Hz, H-3′), and 7.08 (1H, d, J = 3.6 Hz, H-4). In addition, three olefinic protons of a vinyl group were observed at δ_H 5.55 (1H, dd, J = 1.8, 11.4 Hz, H-9), 5.73 (1H, dd, J = 1.8, 17.4 Hz, H-9), and 6.03 (1H, dd, J = 11.4, 17.4 Hz, H-8). A methylene group directly attached to oxygen appeared at δ_H 5.29 (2H, s), along with signals corresponding to a tigloyl moiety at δ_H 1.9 (3H, t, J = 1.8 Hz, H-5″), 2.0 (3H, dd, J = 1.8, 7.8 Hz, H-4″), and 6.10 (1H, m, H-3″). The ^{13}C-NMR spectrum exhibited 18 carbon signals, including one carbonyl carbon at δ_C 167.6; seven quaternary carbons at δ_C 83.1, 93.1, 122.1, 127.4, 137.9, 138.1, and 138.7; six methine carbons at δ_C 116.8, 123.7, 123.7, 128.7, 132.8, and 138.9; two methylene carbons at δ_C 60.3 and 127.1; and two methyl carbons at δ_C 15.9 and 20.5 (Table 2). Based on the above spectroscopic analysis, compound 3 was identified as 5′-tigloyloxymethyl-5-(but-3-en-1-yn-1-yl)-2,2′-bithiophene, also known as a tiglinsaureester (Figure 2). A search of the SciFinder database indicated that the spectroscopic data of compound 3 are reported here for the first time.

Table 2. ^{1}H-NMR and ^{13}C-NMR spectroscopic data of compound 3

C	δ_C	δ_H **(mult., *J* in Hz)**	**C**	δ_C	δ_H **(mult., *J* in Hz)**
2	138.7	-	3′	123.7	7.03 (d, 3.6)
3	123.7	7.03 (d, 3.6)	4′	128.7	6.99 (d, 3.6)
4	132.8	7.08 (d, 3.6)	5′	138.1	-
5	122.1	-	6′	60.3	5.29 (s)
6	83.1	-	1″	167.6	-
7	93.1	-	2″	127.4	-
8	116.8	6.03 (dd, 11.4, 17.4)	3″	138.9	6.10 (m)
9	127.1	5.55 (dd, 1.8, 11.4)/5.73 (dd, 1.8. 17.4)	4″	15.9	2.0 (dd, 1.8, 7.8)
2′	137.9	-	5″	20.5	1.9 (t, 1.8)

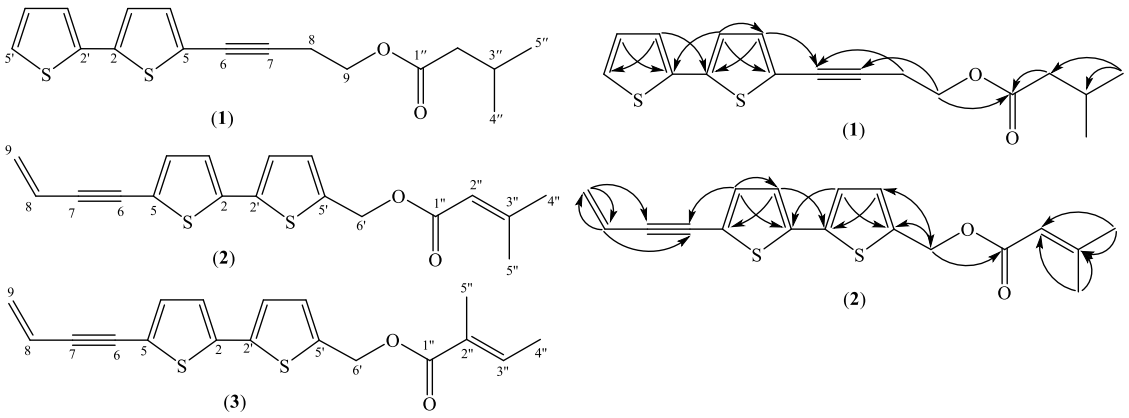

Figure 2. Chemical structures and HMBC correlations of compounds 1–3 isolated from *Eclipta prostrata*

IV. CONCLUSION

Using modern chromatographic techniques, including thin-layer chromatography, column chromatography, and high-performance liquid chromatography, one lignan and two thiophene derivatives were isolated from the methanolic extract of the aerial parts of *Eclipta prostrata*. Based on comprehensive spectroscopic analyses, including HR-ESI-MS, ^{1}H-NMR, ^{13}C-NMR, HSQC, and HMBC, together with comparison with literature data, the structures of the isolated compounds were elucidated as 5-(4-isovaleroyloxybut-1-ynyl)-2,2′-bithiophene (1), and 5-(but-3-en-1-yn-1-yl)-5′-(hydroxymethyl dimethylacrylate)-2,2′-bithiophene (2), and 5′-tigloyloxymethyl-5-(but-3-en-1-yn-1-yl)-2,2′-bithiophene (3). Notably, the complete spectroscopic data of compounds (1) and (3) are reported here for the first time.

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