SUPPLEMENTARY MATERIAL

Isolation and characterization of three new anthraquinone secondary metabolites from *Symplocos racemosa*

Umar Farooq^{*a}), Sadia Naz^a), Ajmal Khan^{**a}) Sara Khan^a) Afsar Khan^{**a}), Mumtaz Ali^b) Saleha Suleman Khan^c)

a) *Department of Chemistry, COMSATS Institute of Information Technology, Abbottabad-22060, Pakistan*

b) *Department of Chemistry, University of Malakand, Chakdara, Dir (L), Pakistan*

c) *H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan*

Abstract

Three new anthraquinone secondary metabolites were isolated from *Symplocos racemosa*; a small tree of family symplocaceae. The structure of compounds (**1-3**) were elucidated to be 1,4-dihydroxy-6-(ethoxymethyl)-8-propylanthracene-9,10-dione (**1**), 1,4-dihydroxy-6-(hydroxymethyl)-8-butyl anthracene-9,10-dione (**2**) and 1,4-dihydroxy-6-(hydroxymethyl)-8-propyl anthracene-9,10-dione (**3**) by using their spectral data i.e. through IR, UV, ¹H NMR, ¹³C NMR and two-dimensional (2D) NMR techniques including Heteronuclear Multiple Quantum Coherence (HMQC), Heteronuclear Multiple Bond Correlation (HMBC) and Correlation Spectroscopy (COSY).

Keywords:

Anthraquinone

Symplocos racemosa

Symplocaceae

SUPPLEMENTARY MATERIAL

Supplementary material is accompanied with this article.

Captions

Table S1. ^1H NMR (500MHz) of Compound **1-3** in CDCl_3 (δ_{H} , J in Hz)

Table S2. ^{13}C NMR (125MHz) of Compound **1-3** in CDCl_3 (δ_{C} , J in Hz)

Figure S1. Important HMBC and COSY correlations of Compound **1**

Table S1. ^1H -NMR (500MHz) of Compound **1-3** in CDCl_3 (δ_{H} , J in Hz)

Carbon No	Compound 1 ^1H -NMR (δ_{H} ppm)	Compound 2 ^1H -NMR (δ_{H} ppm)	Compound 3 ^1H -NMR (δ_{H} ppm)
1	-	-	-
2	7.20 (1H, d, $J = 9.5$)	7.20 (1H, d, $J = 9.4$)	7.15 (1H, d, $J = 10.1$)
3	7.16 (1H, d, $J = 9.5$)	7.16 (1H, d, $J = 9.4$)	7.10 (1H, d, $J = 10.1$)
4	-	-	-
4a	-	-	-
5	8.10 (1H, d, $J = 2.1$)	8.10 (1H, d, $J = 2.1$)	8.01 (1H, d, $J = 1.9$)
6	-	-	-
7	7.52 (1H, d, $J = 2.1$)	7.58 (1H, d, $J = 2.1$)	7.48 (1H, d, $J = 1.9$)
8	-	-	-
8a	-	-	-
9	-	-	-
9a	-	-	-
10	-	-	-
10a	-	-	-
1'	3.20 (2H, t, $J = 7.9$)	3.18 (2H, t, $J = 8.4$)	3.21 (2H, t, $J = 8.2$)
2'	1.75 (2H, m)	1.68 (2H, m)	1.82 (2H, m)
3'	1.10 (3H, t, $J = 7.7$)	1.52 (2H, m)	1.18 (3H, t, $J = 8.1$)
4'	-	1.12 (3H, t, $J = 7.6$)	-
1''	4.85 (2H, s)	5.18 (2H, br s)	5.10 (2H, br s)
2''	3.80 (2H, q, $J = 6.8$)	-	-
3''	1.30 (3H, t, $J = 8.2$)	-	-

Note: δ_{H} values at H-2 and H-3 may be reversed.

Table S2. ^{13}C NMR (125MHz) of Compound **1-3** in CDCl_3

Carbon No	^{13}C -NMR (δ_{C} ppm)	^{13}C -NMR (δ_{C} ppm)	^{13}C -NMR (δ_{C} ppm)
1	162.7	160.1	161.2
2	133.4	131.5	133.4
3	133.1	130.9	132.6
4	162.1	160.7	160.1
4a	118.6	118.7	119.8
5	130.2	123.2	125.1
6	149.4	151.4	150.4
7	137.4	136.5	137.1
8	156.1	155.1	156.1
8a	128.1	125.4	127.1
9	190.1	192.1	190.7
9a	119.1	118.1	120.1
10	189.1	191.5	190.1
10a	140.1	142.5	140.1
1'	44.1	39.1	44.1
2'	29.9	36.4	29.1
3'	20.6	28.1	20.1
4'	-	19.3	-
1''	67.3	61.3	62.3
2''	72.5	-	-
3''	19.4	-	-

Note: δ_{C} values at C-1 and C-4, C-2 and C-3, C-4a and C-9a may be reversed.

Figure S1. Important HMBC and COSY correlations of Compound **1**