## SUPPLEMENTAL MATERIAL

### Chemical constituents from leaves and trunk bark of Rinorea oblongifolia (Violaceae)

Munvera Mfifen Aristide<sup>a</sup>, Ouahouo Wache Blandine Marlyse<sup>a</sup>, Mkounga Pierre<sup>a</sup>, Mbekou Kanko Michelle Ines<sup>b</sup>, Nuzhat Shehla<sup>c</sup>, Iqbal Choudhary Muhammad<sup>c</sup> and Nkengfack Augustin Ephrem<sup>a\*</sup>

<sup>a</sup> Department of Organic Chemistry, Faculty of Science, University of Yaounde I, P.O. Box 812, Yaounde, Cameroon

<sup>b</sup> Department of Biochemistry, Faculty of Science, University of Yaounde I, P.O. Box 812, Yaounde, Cameroon

<sup>c</sup> H.E.J. Research Institute of Chemistry, International Center for Chemical and biological Science (ICCBS), University of Karachi, Karachi-

# 75270, Pakistan

#### Abstract:

Two new coruleoellagic acid derivatives, 3,4',5,5',-tetramethylcoruleoellagic acid (1) ; 3',4,4',5,5'-pentamethylcoruleoellagic acid (2) and a new friedelanetype triterpene derivative rinol (5), were isolated from leaves and trunk bark of *Rinorea oblongifolia* (Violaceae) along with seven known compounds including 3,3',4,4',5'-pentamethylcoruleoellagic acid (3), hexamethylcoruleoellagic acid (4), 28-hydroxyfriedelin (6), friedelin (7), friedelan-3-ol (8), scopoletin (9) and β-Sitosterol-3-*O*-β-D-glucopyranoside (10). Their structures were elucidated by means of spectroscopic methods including IR, 1D and 2D NMR in conjunction with mass spectrometry. Crude extracts of leaves and trunk bark as well as compounds **1- 4** were evaluated for their antibacterial activities against 7 pathogenic bacterial strains (*Streptococcus pneumoniae* ATCC49619, *Staphylococcus aureus* ATCC 43300, *Klepsiella pneumoniae* ATCC 700603, *Haemophilus influenza* ATCC 49247, *Escherichia coli* ATCC 25922, *Pseudomonas aeruginosa* HM601, *Staphylococcus aureus* BAA 977). Compound (3) displayed noteworthy activity against *Haemophilus influenza* with MIC value of 9.38 µg/mL.

Keywords: Rinorea oblongifolia; coruleoellagic acid; friedelane-type triterpene; antibacterial activity



Figure S1: HR ESI Mass Spectrum of compound 1



Figure S2: <sup>1</sup>H NMR spectrum (DMSO, 300 MHz) of compound 1



Figure S3: <sup>13</sup>C NMR spectrum ((DMSO, 125 MHz) of compound 1



Figure S4: DEPT spectrum (DMSO, 125 MHz) of compound 1



Figure S5: DEPT- HSQC spectrum (DMSO, 500 MHz) of compound 1



Figure S6: HMBC spectrum (DMSO, 500 MHz) of compound 1



# Figure S32: HMBC and NOESY correlation of compound 1



Figure S7: NOESY spectrum (DMSO, 500 MHz) of compound 1



Figure S8: IR spectrum of compound 1



Figure S9: UV spectrum of compound 1



Figure S10: Spectrum of compound 1 after Methylation



Figure S11: EI-Mass Spectrum of compound 2



Figure S12: <sup>1</sup>H NMR Spectrum ((CD<sub>3</sub>)<sub>2</sub>CO, 500MHz) of compound 2



Figure S13: <sup>13</sup>C NMR BB spectrum ((CD<sub>3</sub>)<sub>2</sub>CO, 125MHz) of compound 2



Figure S14: DEPT 135 spectrum ((CD<sub>3</sub>)<sub>2</sub>CO, 125MHz) of Compound 2



Figure S15: HSQC spectrum ((CD<sub>3</sub>)<sub>2</sub>CO, 500MHz) of Compound 2



Figure S16: HMBC spectrum ((CD<sub>3</sub>)<sub>2</sub>CO, 500MHz) of Compound 2



Figure S33: HMBC and NOESY correlation of compound 2



Figure S17: NOESY Spectrum ((CD<sub>3</sub>)<sub>2</sub>CO, 500MHz) of compound 2



Figure S18: IR spectrum of compound 2



Figure S19: UV spectrum of compound 2



Figure S20: <sup>1</sup>H NMR spectrum (CDCl3, 500 MHz) of compound 2 after acetylation



Figure S21: +FAB-MASS spectrum of compound 5



Figure S22: <sup>1</sup>H NMR spectrum (C5D5N, 800 MHz) of compound 5



Figure S23: <sup>13</sup>C NMR BB spectrum (C5D5N, 200 MHz) of compound 5

BB .



Figure S24: DEPT 135 spectrum of (C5D5N, 200 MHz) compound 5 (part 1)



Figure S25: DEPT 135 spectrum of (C5D5N, 200 MHz) compound 5 (part 2)

Dept 135



Figure S26: DEPT 90 spectrum of (C5D5N, 200 MHz) compound 5



Figure S27: COSY spectrum of (C5D5N, 800 MHz) compound 5



Figure S28: HSQC spectrum of (C5D5N, 800 MHz) compound 5



Figure S34: HMBC correlation of compound 5



Figure S29: HMBC spectrum of (C5D5N, 800 MHz) compound 5



Figure S35: NOESY correlation of compound 5



Figure S30: NOESY spectrum of (C5D5N, 800 MHz) compound 5



Figure S31: IR spectrum of compound 5

	Compound 1 (DMSO-d <sub>6</sub> , 500MHz)			<b>Compound 2</b> (Acetone-d <sub>6</sub> , 500MHz)			
	<sup>1</sup> H NMR	<sup>13</sup> C NMR	HMBC	<sup>1</sup> H NMR	<sup>13</sup> C NMR	HMBC	
1		113.2					
2		128.8					
3		142.0		(OH)	155.6		
4	(OH)	155.2			141.5		
5		140.0			147.4		
6		111.6					
7		158.3					
1'		112.0					
2'		128.0					
3'	(OH)	155.2			147.6		
4'		152.7			148.9		
5'		146.4			153.0		
6'		107.5					
7'		158.3					
5 - OCH <sub>3</sub>	4.02	60.8	C-5	4.20	62.2	C-5	
4 - OCH <sub>3</sub>				4.15	61.8	C-4	
3 - OCH <sub>3</sub>	4.13	61.8	C-3				
5'- OCH <sub>3</sub>	3.99	61.9	C-5'	3.96	62.4	C-5'	
4'- OCH <sub>3</sub>	3.89	62.0	C-4'	3.99	62.3	C-4'	
3'- OCH <sub>3</sub>				3.95	62.4	C-3'	

 Table S1: The NMR spectral data of compounds 1 and 2.

Position	NMR Proton	NMR Carbon
1	1,63 ; H1a ; m	20.5
	1,88 ; H1b ; m	
2	2.00 ; H2a, m	39.2
	2,24 ; H2b, dd ( <i>J</i> = 6.4 ; 12 Hz)	
3		106.4
4	1,59 ; m	54.0
5		47.5
6	1.36 ; H6a ; m	35.1
	1.43 ; H6b ; m	
7	0.96 ; H7a ; m	19.6
	1.01 ; H7b ; m	
8	1,23 ; m	52.8
9		37.6
10	1, 23 ; m	57.4
11	1,18 ; H11a ; m	35.5
	1,23 ; H11b ; m	
12	1.23 ; m	30.4
13		39.8
14		38.2
15	1.28 ; H15a ; m	32.7
	1.52 ; H15b ; m	
16	1.31 ; H16a ; m	36.3
	1.56 ; H16b ; m	
17		30.1
18	1.52 ; m	43.0
19	1.38 ; H19a ; m	34.1
	1.71 ; H19b ; m	
20		28.3
21	1,23 ; 21Ha ; m	33.2
	1,41 ; 21Hb ; m	
22	0.91 ; H22a ; m	39.4
	1.46 ; H22b ; m	
23	1,23, bd	8.6
24	3.74 ; H24a ; d, <i>J</i> = 8 Hz	73.1
	4.27 ; H24b ; d, <i>J</i> = 8 Hz	
25	0.85, s	16.4
26	0.92, s	20.6
27	1.02, s	18.8
28	1.16, s	32.2
29	0.99, s	35.0

 Table S2: The NMR spectral data of compounds 5.

Table S3: Results of antibacterial activity of compound 1-4	and crude extracts

MIC in µg/mL								
	Streptococcus pneumoniae ATCC49619	Staphylococcus aureus ATCC 43300	Klepsiella pneumoniae ATCC 700603	Haemophilus influenza ATCC 49247	Escherichia coli ATCC 25922	Pseudomonas aeruginosa HM601	Staphylococcus aureus BAA 977	
1	>50	>50	>50	$25 \pm 0.00$	>50	>50	>50	
2	>50	>50	>50	>50	>50	>50	50±0.00	
3	50	>50	>50	$9.38 \pm 4.42$	>50	>50	>50	
4	>50	>50	>50	$50\pm0.00$	>50	>50	>50	
Extract of leaves	>500	>500	>500	$500 \pm 0.00$	>500	>500	>500	
Extract of trunk bark	>500	>500	>500	$500\pm0.00$	>500	>500	>500	
Ciprofloxacin	$8\pm0.00$	$8\pm0.00$	$0.5 \pm 0.00$	$1 \pm 0.00$	$4\pm0.00$	$1 \pm 0.00$	$16\pm0.00$	