SUPPLEMENTARY MATERIAL

Three new acyltyramines from *Anisodus luridus* Link et Otto (Solanaceae)

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Abstract

Three new acyltyramines, *N*-[2-(4-hydroxyphenyl)ethyl]hentriacontanamide (1), *N*-[2-(4-hydroxyphenyl)ethyl]nonacosanamide (2) and *N*-[2-(4-hydroxyphenyl)ethyl]heneicosanamide (3) have been isolated from *n*-hexane extract of leaves of *Anisodus luridus* (Solanaceae). Successive extraction of defatted leaves of *A. luridus* with methanol afforded a residue on removal of solvent under reduced pressure. Residue was partitioned by means of chloroform and *n*-butanol. Chromatographic resolution of *n*-BuOH extract afforded six known compounds, apigenin (4), luteolin (5), quercetin (6), quercetin-3-*O*- α -L-rhamnoside (7), kaempferol 3-*O*- α -rhamnoside (8) and quercetin 3-*O*- α -L-rhamnopyranosyl-(1 $\rightarrow$ 6)- β -D-glucopyranoside (9). The structures of the isolated compounds were assigned with the help of spectroscopic techniques. This is the first report of isolation of these compounds from this plant.

Keywords: *Anisodus luridus*, acyltyramines, leaves, Solanaceae

Table S1: ^1H and ^{13}C NMR spectral data of compounds **1**, **2** and **3**

Position	Table 1S - ^1H and ^{13}C NMR [#] spectral data of compounds 1 , 2 and 3					
	Compound 1		Compound 2		Compound 3	
	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}
2	34.6	2.11 t (7.5, 8 Hz)	34.6	2.11 t (10, 5 Hz)	34.6	2.11 t (7.5 Hz)
3	25.7	1.25 br s	25.7	1.57 t (5, 10 Hz)	25.7	1.25 br s
21	*	*	*	*	13.9	0.88 t (6.5, 7 Hz)
29	*	*	13.9	0.88 t (5 Hz)	-	-
31	13.9	0.88 t (7 Hz)	-	-	-	-
1'	40.6	3.47 q (6.5 Hz)	40.6	3.43 q (6.6 Hz)	40.8	3.47 q (6.5 Hz)
2'	36.6	2.74 t (7 Hz)	36.6	2.71 t (5, 10 Hz)	36.6	2.74 t (7, 6.5 Hz)
3'	129.7	-	129.7	-	129.7	-
4',8'	129.6	7.05 d (8 Hz)	129.6	7.02 d (10 Hz)	129.6	7.05 d (8.5 Hz)
5',7'	115.3	6.78 d (8 Hz)	115.3	6.77 d (10 Hz)	115.3	6.78 d (8.5 Hz)
6'	155.2	-	155.2	-	155.2	-

* Chemical shifts for methylenes of respective acyltyramine are shown in experimental section for the sake of proper depiction of data in the table.

[#] δ_{H} (500 MHz, CDCl_3) ; δ_{C} (125 MHz, CDCl_3 / $\text{CDCl}_3\text{-CD}_3\text{OD}$)

Table S2: ¹H NMR spectral data of compounds **4-9**

Posit ion	Table 2S: ¹ H NMR spectral data of compounds 4-9											
	Compound 4 *		Compound 5		Compound 6		Compound 7		Compound 8		Compound 9	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}
2	-	157.3	-	164.4	-	146.4	-	157.0	-	155.9	-	156.8
3	6.97, s	103.7	6.78, s	103.2	-	135.4	-	134.4	-	133.3	-	133.5
4	-	181.6	-	182.0	-	175.5	-	172.2	-	176.9	-	177.6
5	-	163.7	-	99.1	-	160.7	-	161.3	-	158.8	-	161.4
6	5.88, s	98.9	6.29, d, 1.9 Hz	164.2	6.17, , d, 1.8 Hz	98.2	6.21, d, 1.8 Hz	99.1	6.22, d, 1.8 Hz	97.2	6.15, s	99.1
7	-	164.6	-	94.2	-	164.0	-	164.6	-	163.1	-	164.8
8	6.03, s	94.0	6.55, d, 1.9 Hz	157.6	6.42, , d, 1.8 Hz	93.5	6.39, d, 1.8 Hz	94.1	6.39, d, 1.8 Hz	92.2	6.35, s	94.6
9	-	157.3	-	104.6	-	156.4	-	156.9	-	156.6	-	156.9
10	-	103.4	-	161.8	-	103.2	-	104.0	-	103.3	-	104.1
1'	-	121.1	-	121.8	-	122.1	-	121.2	-	120.0	-	121.9
2'	7.70, d, 8.8 Hz	128.4	7.54, dd, 7.5 & 2.0 Hz	113.7	7.64, , d, 2.1 Hz	115.3	7.30, d, 1.9 Hz	115.9	6.95, d, 7.0 Hz	129.2	7.51, s	116.5
3'	6.57, d, 8.8 Hz	116.0	-	146.6	-	144.9	-	145.6	7.77, d, 7.0 Hz	113.9	-	145.0
4'	-	161.2	-	150.0	-	148.1	-	148.5	-	160.4	-	148.0
5'	6.57,	116.0	7.00,	116.3	6.88	115.6	6.86,	116.1	7.77,	113.9	6.83,	115.5

	d,		d,		, d,		d,		d,		d,	
	8.8		7.5		8.7		8.8		7.0		9.1	
	Hz		Hz		Hz		Hz		Hz		Hz	
6'	7.70,	128.4	7.52,	119.3	7.63	121.7	7.25,	121.2	6.95,	129.2	7.53,	121.4
	d,		dd,		, dd,		dd,		d,		d,	
	8.8		7.5		8.7		8.8		7.0		9.1	
	Hz		&		&		&		Hz		Hz	
			2.0		2.1		1.9					
			Hz		Hz		Hz					
1"	-	-	-	-	-	-	5.25,	102.3	5.39,	100.8	101.	101.5
							d,		d,		5	
							1.8		1.2			
							Hz		Hz			
2"	-	-	-	-	-	-	3.69	78.8	4.0-	69.4	4.5-	74.3
							-		3.0,		3.0,	
							3.10,		m		m	
							m					
3"	-	-	-	-	-	-	3.69	78.8	4.0-	69.5	4.5-	76.7
							-		3.0,		3.0,	
							3.10,		m		m	
							m					
4"	-	-	-	-	-	-	3.69	71.7	4.0-	70.6	4.5-	70.3
							-		3.0,		3.0,	
							3.10,		m		m	
							m					
5"	-	-	-	-	-	-	3.69	70.5	4.0-	69.3	4.5-	76.1
							-		3.0,		3.0,	
							3.10,		m		m	
							m					
6"	-	-	-	-	-	-	0.85,	17.9	0.94,	14.9	4.5-	67.3
							d,		d,		3.0,	
							6.0		6.9		m	
							Hz		Hz			

1'''	-	-	-	-	-	-	-	-	-	-	4.5- 3.0, m	101.6
2'''	-	-	-	-	-	-	-	-	-	-	4.5- 3.0, m	70.8
3'''	-	-	-	-	-	-	-	-	-	-	4.5- 3.0, m	70.6
4'''	-	-	-	-	-	-	-	-	-	-	4.5- 3.0, m	72.1
5'''	-	-	-	-	-	-	-	-	-	-	4.5- 3.0, m	68.5
6'''	-	-	-	-	-	-	-	-	-	-	4.5- 3.0, m	17.9

Figure S1: FT-IR spectra of alkyltyramines 1-3

Figure S2: ¹H NMR spectrum of compound **1** (*N*-hentriacontanoyltyramine)

Figure S3: ¹H NMR spectrum of compound **2** (*N*-nonacosanoyltyramine)

Figure S4: ¹H NMR spectrum of compound **3** (*N*-heneicosanoyltyramine)

Figure S5: ¹³C NMR spectrum

YF1591/ALR-H4,in CDCl₃, H-H cosy, 500 MHz, 256*256, ti 1, 2013/4/3

Figure S6: ¹H-¹H COSY spectrum