

Supporting Information

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A New Organic Acid Derivative from the Fruits of *Rosa roxburghii*

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CL-7 #74 RT: 0.33 AV: 1 NL: 4.00E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

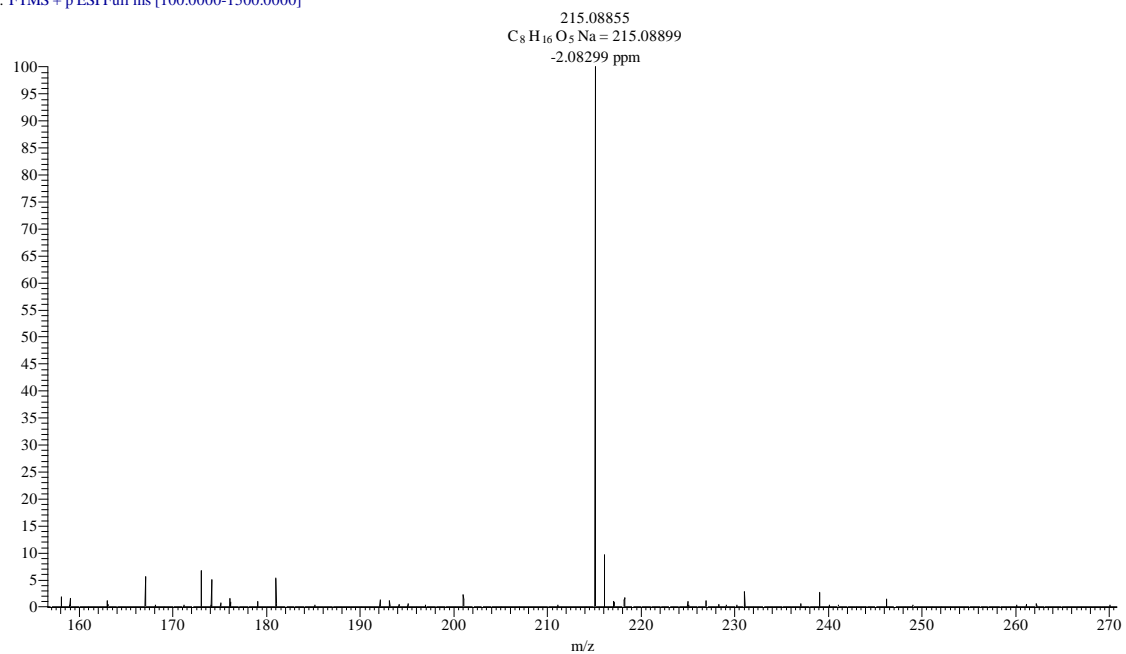


Figure S1: HR-ESI-MS spectrum of **1** (Roxbuacidester A)

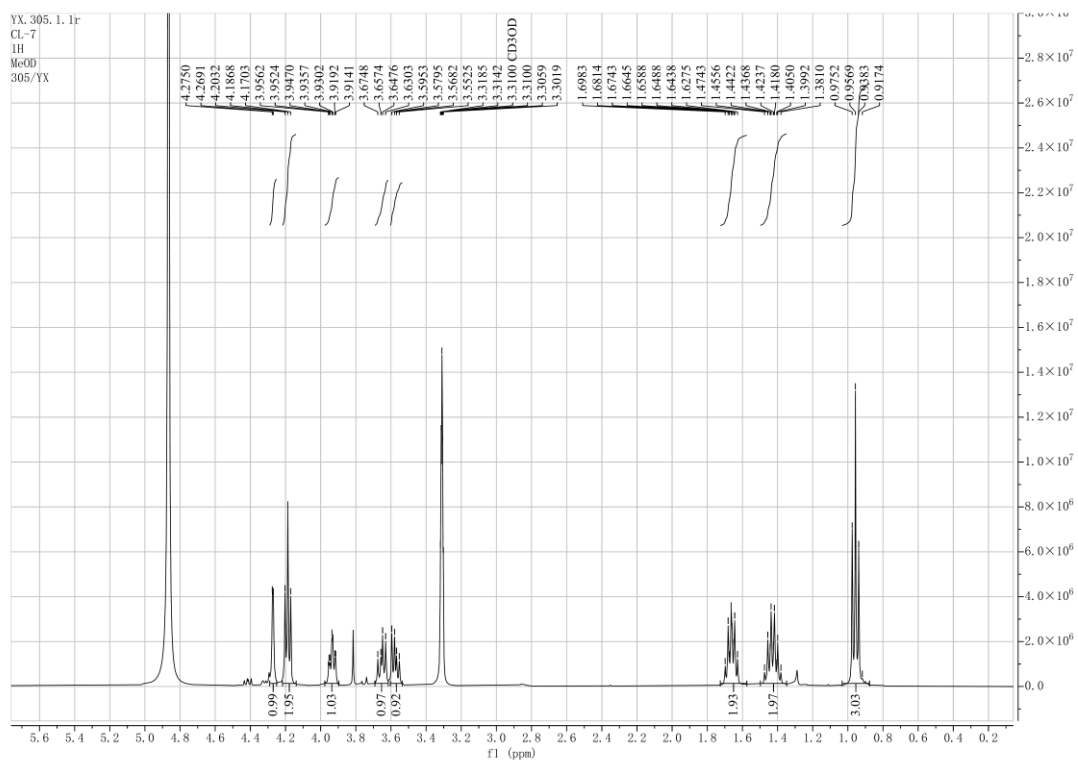


Figure S2: $^1\text{H-NMR}$ (400 MHz, CD_3OD) spectrum of **1** (Roxbuacidester A)

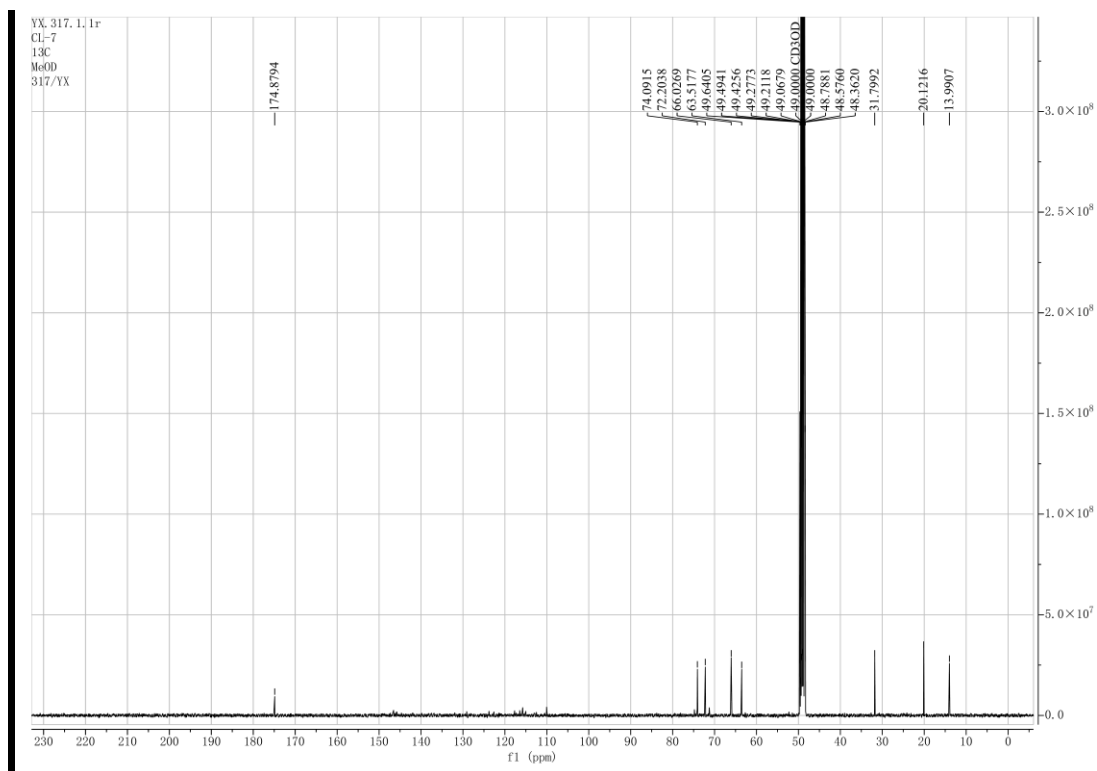


Figure S3: ^{13}C -NMR (100 MHz, CD_3OD) spectrum of **1** (Roxbuacidester A)

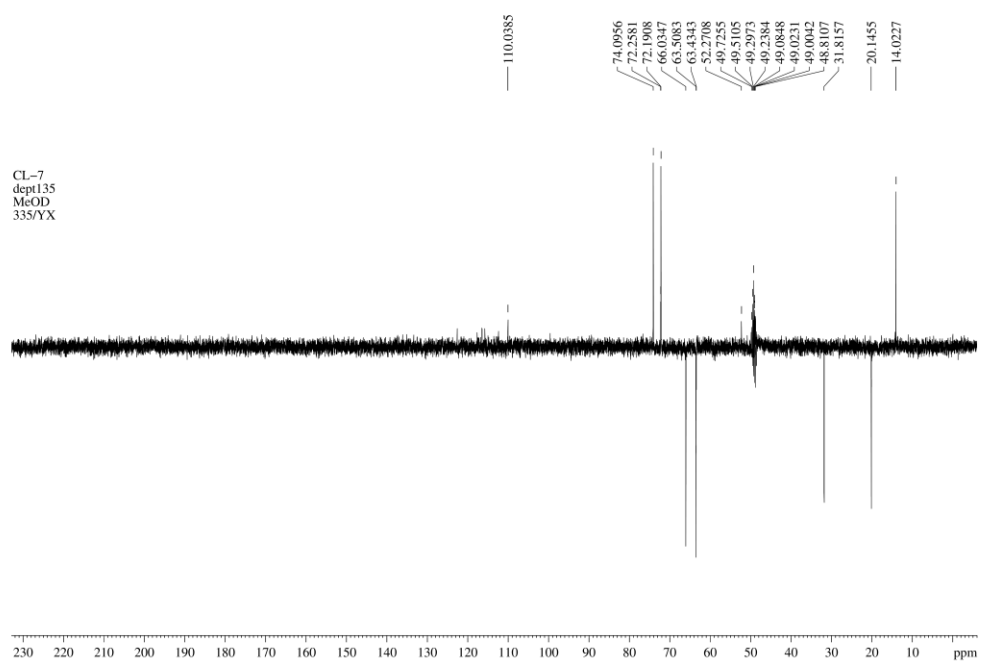


Figure S4: DEPT135 (100 MHz, CD₃OD) spectrum of **1** (Roxbuacidester A)

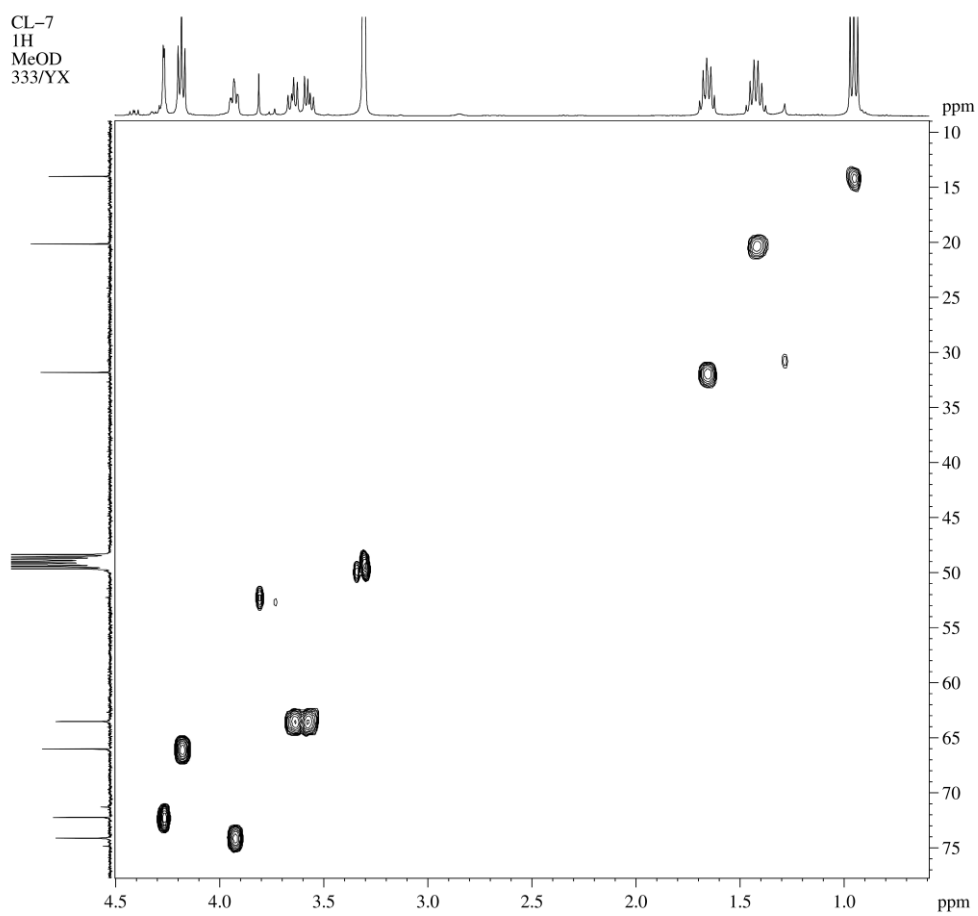


Figure S5: HSQC spectrum of **1** (Roxbuacidester A)

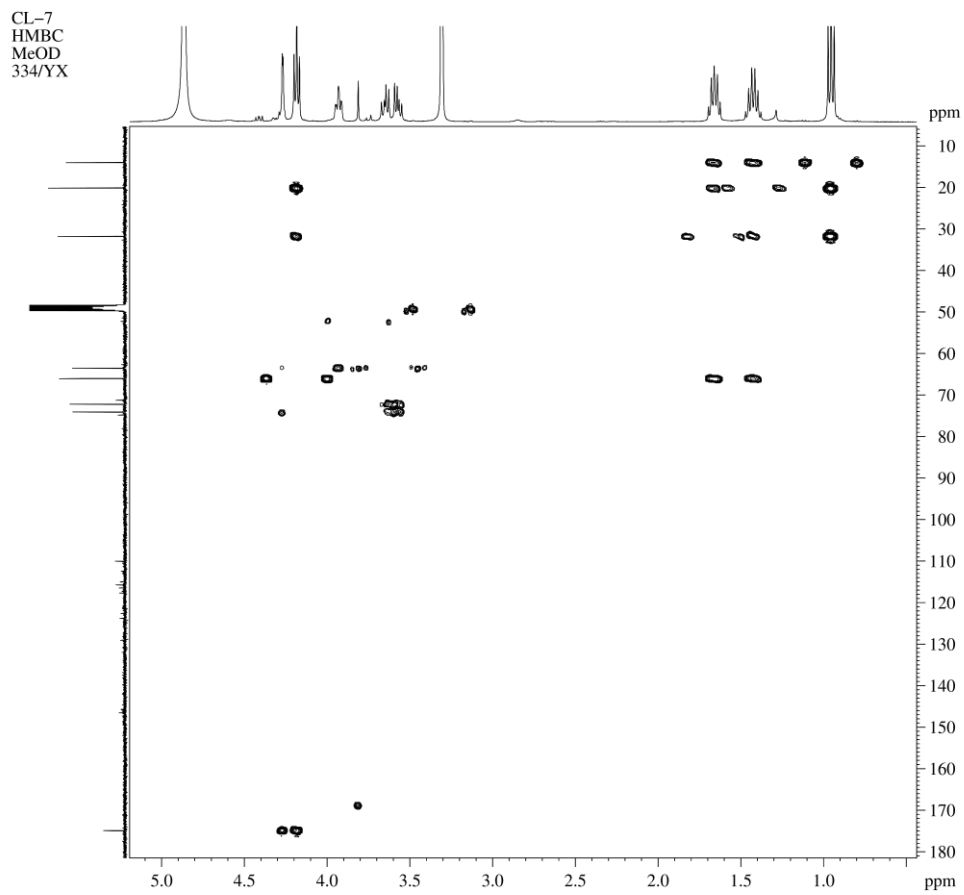


Figure S6: HMBC spectrum of **1** (Roxbuacidester A)

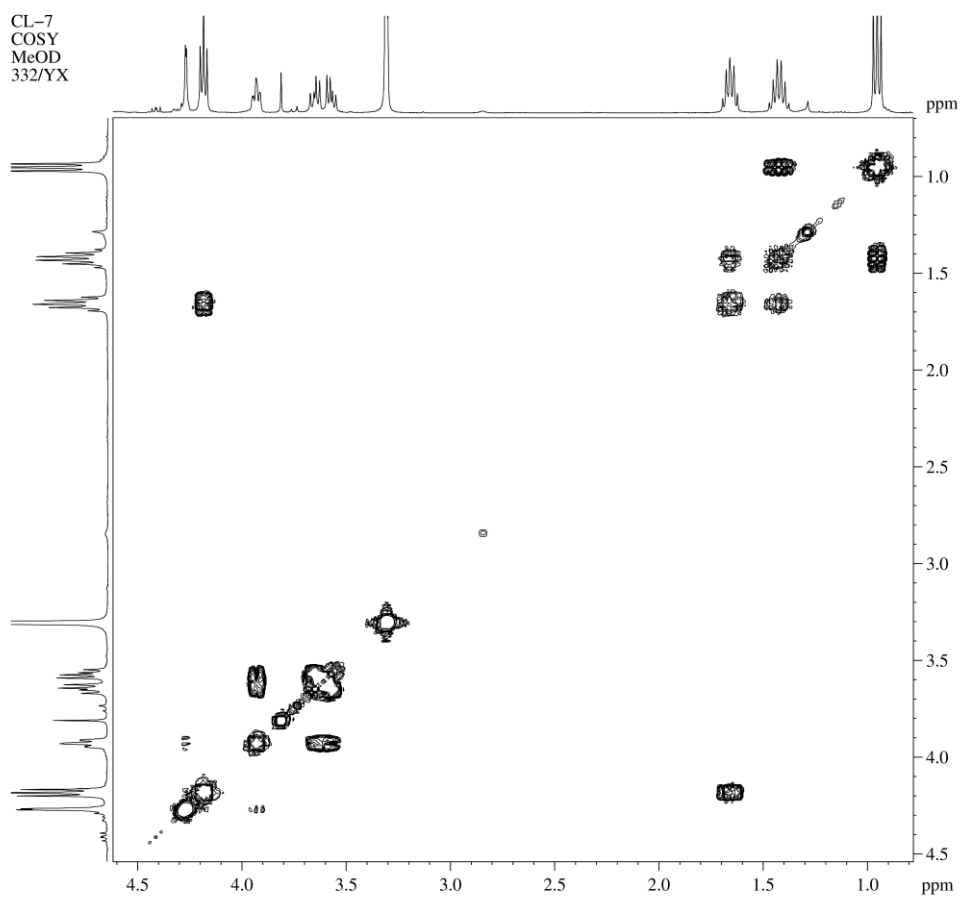
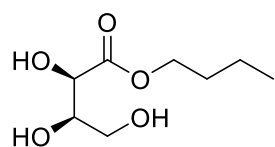


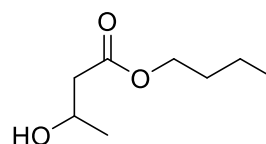
Figure S7: ^1H - ^1H COSY spectrum of **1** (Roxbuacidester A)

Table S1: ¹³C-NMR data of Compounds (2-7) (100 MHz, in CD₃OD)

Position	Compound 2	Compound 3	Compound 4	Compound 5	Compound 6	Compound 7
1	174.5	123.2	121.5	127.9	127.1	128.1
2	160.3	115.8	110.1	115.1	131.0	133.1
3	125.7	146.1	146.3	146.8	116.8	115.8
4	109.5	151.8	139.8	149.4	161.1	159.5
5	36.9	117.8	146.3	116.5	116.8	115.8
6	23.8	123.9	110.1	122.8	131.0	133.1
7	32.7	170.4	169.1	146.8	146.3	141.7
8	23.5			116.0	116.2	116.8
9	14.3			171.3	168.5	170.5
10	10.8					
11	8.2					
OCH₃			52.4			



Roxbuacidester A (1)



Butyl 3-hydroxybutanoate

Table S2: ^1H and ^{13}C NMR data for Roxbuacidester A (1) and Butyl 3-hydroxybutanoate^[1]

Position	Roxbuacidester A (1) ^a		butyl 3-hydroxybutanoate ^b	
	δ_{C}	δ_{H} (J in Hz)	δ_{C}	δ_{H} (J in Hz)
1	174.9 (C)	-	172.8(C)	-
2	72.2 (CH)	4.27(1H, d, 2.1)	42.8(CH ₂)	2.38(1H,dd, 16.6, 8.5) 2.45(1H,dd, 16.6, 3.7)
3	74.1 (CH)	3.93(1H, ddd, 7.0, 6.3, 2.1)	64.2(CH)	4.16(1H, m)
4	63.5(CH ₂)	3.65(1H, dd, 10.8, 7.0) 3.57(1H, dd, 10.8, 6.3)	22.4(CH ₃)	1.19(3H, t, 6.3)
1'	66.0(CH ₂)	4.18(2H, t, 6.6)	64.5(CH ₂)	4.08(2H, t, 6.7)
2'	31.8(CH ₂)	1.67(2H, m)	30.6(CH ₂)	1.58(2H,m)
3'	20.1(CH ₂)	1.42(2H, m)	19.0(CH ₂)	1.35(2H,m)
4'	14.0(CH ₃)	0.95(3H, t, 7.4)	13.6(CH ₃)	0.92(3H, t, 7.0)

^a Measured in CD₃OD

^b Measured in CDCl₃

[1] D. Krajewski, C. Duque and P. Schrejer (1997). Aliphatic β -D-glucosides from fruits of *Carica pubescens*, *Phytochemistry* **45(8)**, 1627-1631.