SUPPLEMENTARY MATERIAL

Novel skeleton sesquiterpenoids isolated from guava leaves

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Abstract: A chemical investigation of the plant *Psidium guajava* L., collected in Guangdong province, afforded two novel skeleton sesquiterpenoids **1** and **2**. Compound **2** also known as isocaryolan-9-one was a new natural product. The structure of the novel compound **1** was determined as guavacid A by various spectroscopic methods. A possible biosynthetic pathway for **1** and **2** was proposed.

Keywords: *Psidium guajava* L.; sesquiterpenoid; guavacid A; isocaryolan-9-one.

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Table S1. NMR Data of compounds **1** and **2** (CDCl₃, δ in ppm, *J* in Hz)

Position	1		2	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1		41.9		31.7
2	1.62 (1H, m)	46.0	1.65 (1H, m)	42.1
3	1.36 (1H, m, H-3 β)	37.2	1.48 (1H, m, H-3 β)	35.9
	1.58 (1H, m, H-3 α)		1.56 (1H, m, H-3 α)	
4		33.5		32.9
5	1.55 (1H, m)	48.9	1.62 (1H, m)	46.3
6	1.36 (1H, m, H-6 α)	25.8	1.34 (1H, m, H-6 α)	25.6
	1.66 (1H, m, H-6 β)		1.46 (1H, m, H-6 β)	
7	1.66 (1H, m, H-7 β)	34.3	1.17 (1H, m, H-7 α)	29.8
	1.80 (1H, dd, <i>J</i> =13.0, 6.0, H-7 α)		2.28 (1H, m, H-7 β)	
8		52.6	2.51 (1H, m)	44.9
9	1.70 (1H, m, H-9 β)	29.5		215.8
	2.17 (1H, dd, <i>J</i> =14.0, 8.5, H-9 α)			
10	1.46 (1H, m, H-10 β)	45.4	2.45 (2H, m)	36.7
	1.55 (1H, m, H-10 α)			
11	1.62 (1H, m, H-11 α)	48.9	1.64 (1H, m, H-11 α)	36.7
	1.95 (1H, dd, <i>J</i> =13.0, 2.5, H-11 β)		1.72 (1H, m, H-11 β)	
12		184.5	1.74 (1H, m, H-12 α)	42.0
			2.04 (1H, dd, <i>J</i> =14.4, 8.4, H-12 β)	
13	0.95 (3H, s)	22.0	0.90 (3H, s)	26.0
14	1.01 (3H, s)	20.3	0.94 (3H, s)	21.8
15	1.01 (3H, s)	30.5	0.98 (3H, s)	30.5

Figure S1. ¹H-NMR spectrum of compound 1

Figure S2. ¹H-NMR spectrum of compound 1 (expansion)

Figure S3. ^{13}C -NMR spectrum of compound **1**

Figure S4. ^{13}C -NMR spectrum of compound **1** (expansion)

Figure S5. 2D HSQC NMR spectrum of compound **1**

Figure S6. Key HMBC and ^1H - ^1H COSY correlations of compound **1**

Figure S7. 2D ^1H - ^1H COSY NMR spectrum of compound **1**

Figure S8. 2D HMBC NMR spectrum of compound **1**

Figure S9. 2D HMBC NMR spectrum of compound **1** (expansion-1)

Figure S10. 2D HMBC NMR spectrum of compound **1** (expansion-2)

Figure S11. Key NOESY correlations of **1**

Figure S12. 2D NOESY NMR spectrum of compound **1**

test01_150429201916#38 RT: 1.07 AV: 1 NL: 8.75E2
T: - c Full ms [100.00-500.00]

Figure S13. ESI-MS of compound **1**

Figure S14. The total ion current of compound **1**

Figure S15. EI-MS of compound **1**

Figure S16. ^1H -NMR spectrum of compound **2**

Figure S17. ^1H -NMR spectrum of compound **2** (expansion)

Figure S18. ^{13}C -NMR spectrum of compound **2**

Figure S19. ^{13}C -NMR spectrum of compound **2** (expansion-1)

Figure S20. ^{13}C -NMR spectrum of compound **2** (expansion-2)

Figure S21. DEPT-135 spectrum of compound **2**

Figure S22. 2D HSQC NMR spectrum of compound **2**

Figure S23. 2D HMBC NMR spectrum of compound **2**

Figure S24. 2D HMBC NMR spectrum of compound **2** (expansion-1)

Figure S25. 2D HMBC NMR spectrum of compound **2** (expansion-2)

Figure S26. 2D ^1H - ^1H COSY NMR spectrum of compound **2**

Figure S27. 2D ^1H - ^1H COSY NMR spectrum of compound **2** (expansion-1)

Figure S28. 2D ^1H - ^1H COSY NMR spectrum of compound **2** (expansion-2)

Figure S29. 2D NOESY NMR spectrum of compound **2**

Figure S30. The total ion current of compound **2**

Figure S31. EI-MS of compound **2**