Structures and Bioactivities of New Dihydrochalcones from Metrodorea stipularis

Marcela Carmen de Melo Burger,[†] João Batista Fernandes,[†] Maria Fátima das Graças Fernandes da Silva,[†] Aster Escalante, [‡] Jacques Prudhomme, [‡] Karine G. Le Roch,[‡] Mario Augusto Izidoro,[§] and Paulo Cezar Vieira.[†],*

[†]Departamento de Química, Universidade Federal de São Carlos, Rod. Washington Luís, Km 235, 13565-905 São Carlos, SP, Brazil

^{*}Department of Cell Biology & Neuroscience, University of California Riverside, 900 University Ave, Riverside, CA 92521, USA

[§]Universidade Federal de São Paulo, Rua Pedro de Toledo, 650, 04039-002, São Paulo, SP, Brazil.

AUTHOR INFORMATION

Corresponding Author

* Tel/Fax: 55-16-33518350. E-mail: dpcv@ufscar.br.

SUPPORTING INFORMATION

Compound 1			
Position	$\delta_{\rm C}$," type	$\delta_{\rm H}$ (J in Hz)	HMBC
1	205.0, qC		
2	47.4, CH ₂	3.25, t (8.4)	1, 1''', 3
3	31.6, CH ₂	2.84, t (8.4)	1"",2"", 6"", 3
1'	104.0, qC		
2'	164.0, qC		
3'	107.0, qC		
4'	161.0, qC		
5'	94.9, CH	5.87, s	1', 3',4', 6'
6'	163.0, qC		
1"	21.8, CH ₂	3.18, brd	2"", 3"", 2", 3"
2"	124.7, CH	5.17, m	
3"	134.6, qC		
4"	$27.7, CH_2$	2.03, t (6.9)	2", 3", 5", 8"
5"	40.7, CH ₂	1.93, t (6.9)	4", 6", 7"
6"	125.3, CH	5.05, m	
7"	131.4, qC		
8"	16.1, CH ₃	1.73, s	2", 3", 4"
9"	17.4, CH ₃	1.54, s	6", 7", 10"
10"	25.4, CH ₃	1.60, s	6", 7", 9"
1'''	133.2, qC		
2'''	116.0, CH	6.68, d (8.6)	4''', 6''', 3
3'''	130.2, CH	7.03, d (8.6)	1"', 4"', 5"'
4'''	156.0, qC		
5'''	130.2, ĈH	7.03, d (8.6)	1''', 3''', 4'''
6'''	116.0, CH	6.68, d (8.6)	2"', 4"', 3

^{*a* 13}C values obtained from projections of the *HSQC* e *HMBC* (100 MHz, Methanol-d₆).

 Table 1. NMR Spectroscopic Data (400 MHz, Metanol-d₆) for compound 1



Figure 1. ¹H NMR (400 MHz, Methanol-d₆) spectrum of the new compound 1



Figure 2. COSY (400 MHz, Methanol-d₆) spectrum of the new compound 1.



Figure 3. HSQC (400 MHz, Methanol-d₆) spectrum of the new compound 1



Figure 4. HMBC (400 MHz, Methanol-d₆) spectrum of the new compound 1



Figure 5. ¹H NMR (400 MHz, Acetone-d₆) spectrum of the new compound 2.



Figure 6. (A) COSY (400 MHz, Acetone-d6) spectrum of the new compound **2. (B)** Expansion of the methyl and methylenic region of the COSY spectrum of the new compound

2.



Figure 7. HSQC (400 MHz, Acetone-d6) spectrum of the new compound 2.



Figure 8. (A) HMBC (400 MHz, Acetone-d6) spectrum of the new compound 2. (B) Expansion of the methyl and methylenic region of the HMBC spectrum of the new compound 2.



Figure 9. ¹H NMR (400 MHz, Methanol-d₆) spectrum of the new compound 3.



Figure 10. COSY (400 MHz, Methanol-d₆) spectrum of the new compound 3.



Figure 11. HSQC (400 MHz, Methanol-d₆) spectrum of the new compound **3**.



Figure 12. HMBC (400 MHz, Methanol-d₆) spectrum of the new compound 3.



Figure 13. ¹H NMR (400 MHz, Methanol-d₆) spectrum of the new compound 4.



Figure 14. COSY (400 MHz, Methanol- d_6) spectrum of the new compound 4.



Figure 15. HSQC (400 MHz, Methanol-d₆) spectrum of the new compound 4.



Figure 16. HMBC (400 MHz, Methanol-d₆) spectrum of the new compound 4.