

**A New Antifungal Phenolic Glycoside Derivative and Iridoids and Lignans  
from *Alibertia sessilis* (Vell.) K. Schum. (Rubiaceae)**

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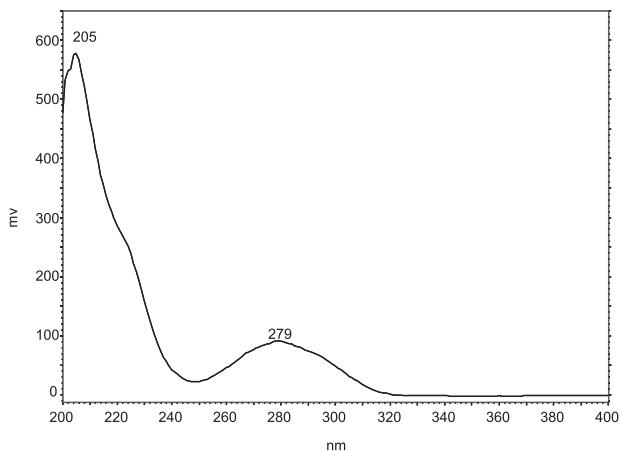


Figure S1. UV spectrum of compound 1 (MeOH).

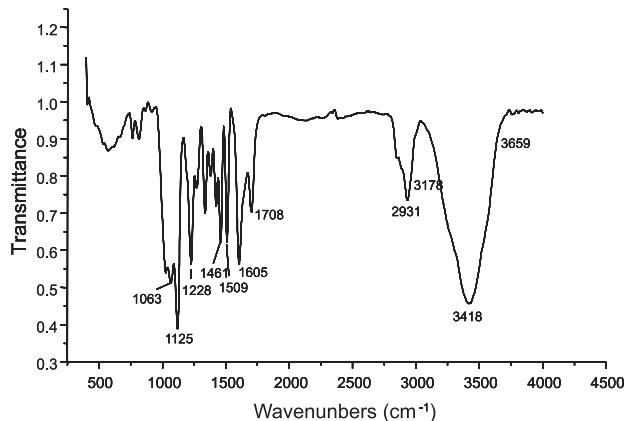
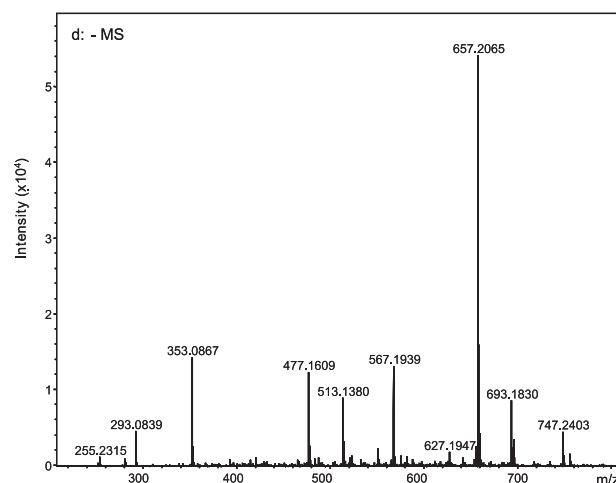
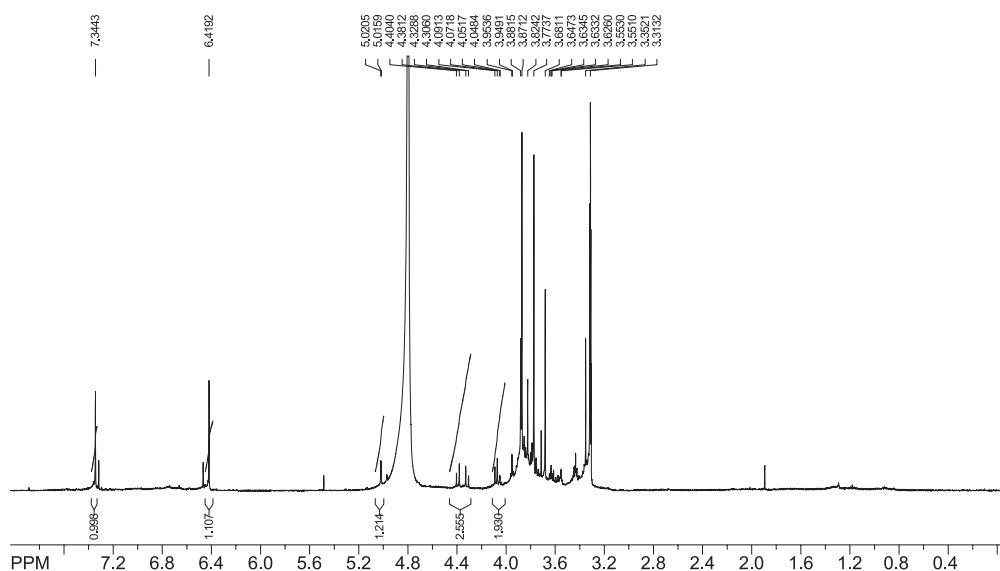


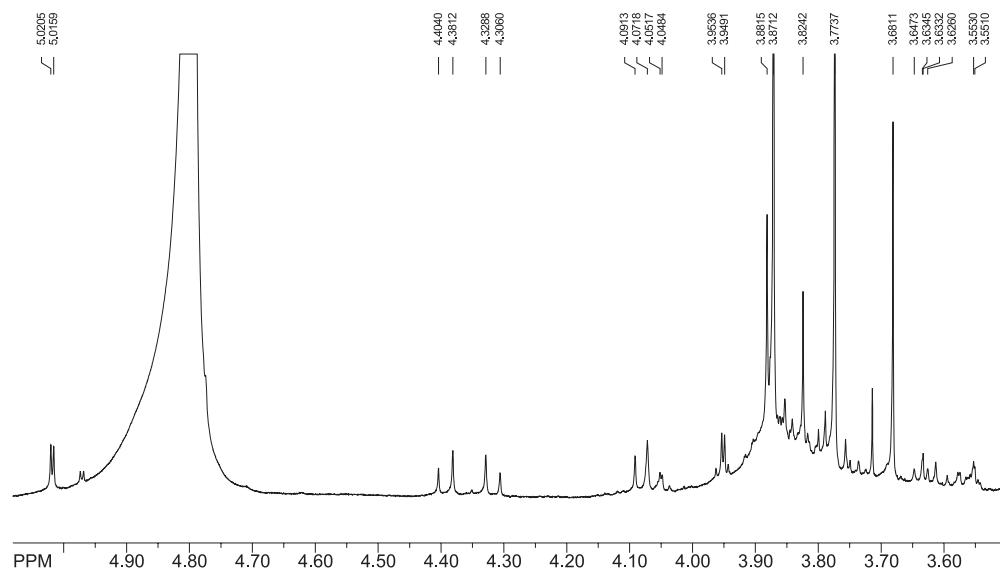
Figure S2. IR spectrum of compound 1 (KBr).



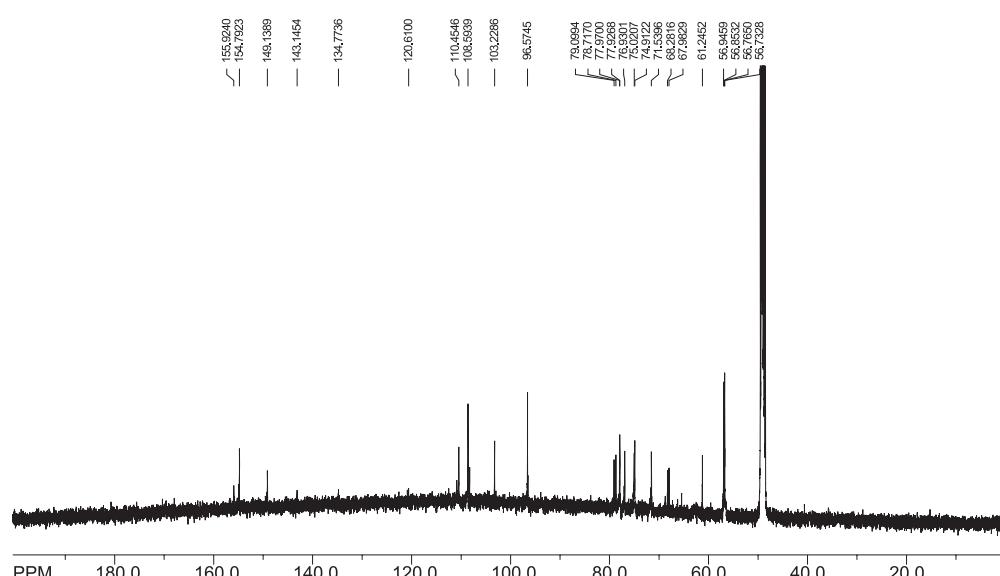
**Figure S3.** HRESIMS spectrum of compound 1 (negative mode).



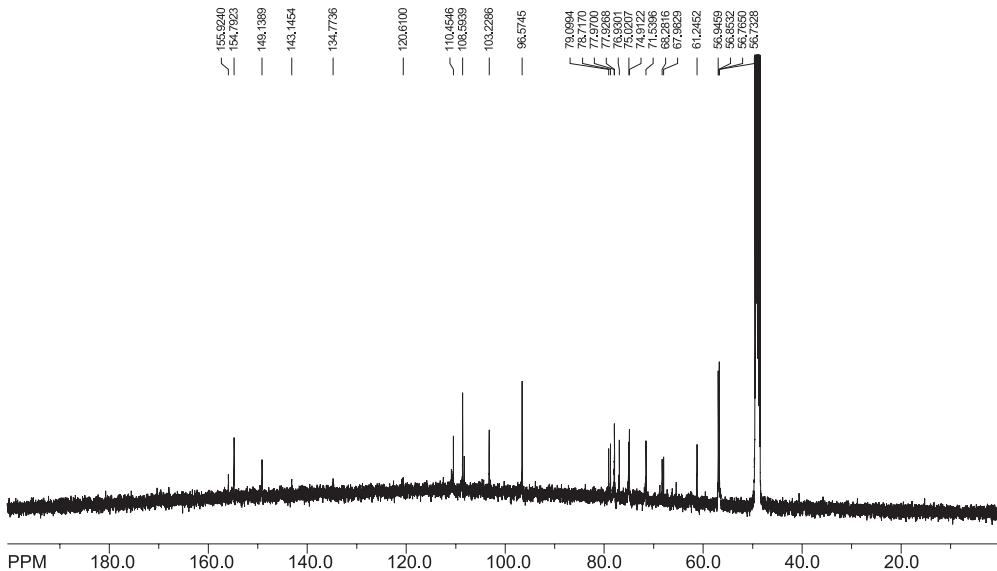
**Figure S4.**  $^1\text{H}$  NMR spectrum of compound 1 ( $\text{CD}_3\text{OD}$ , 500 MHz).



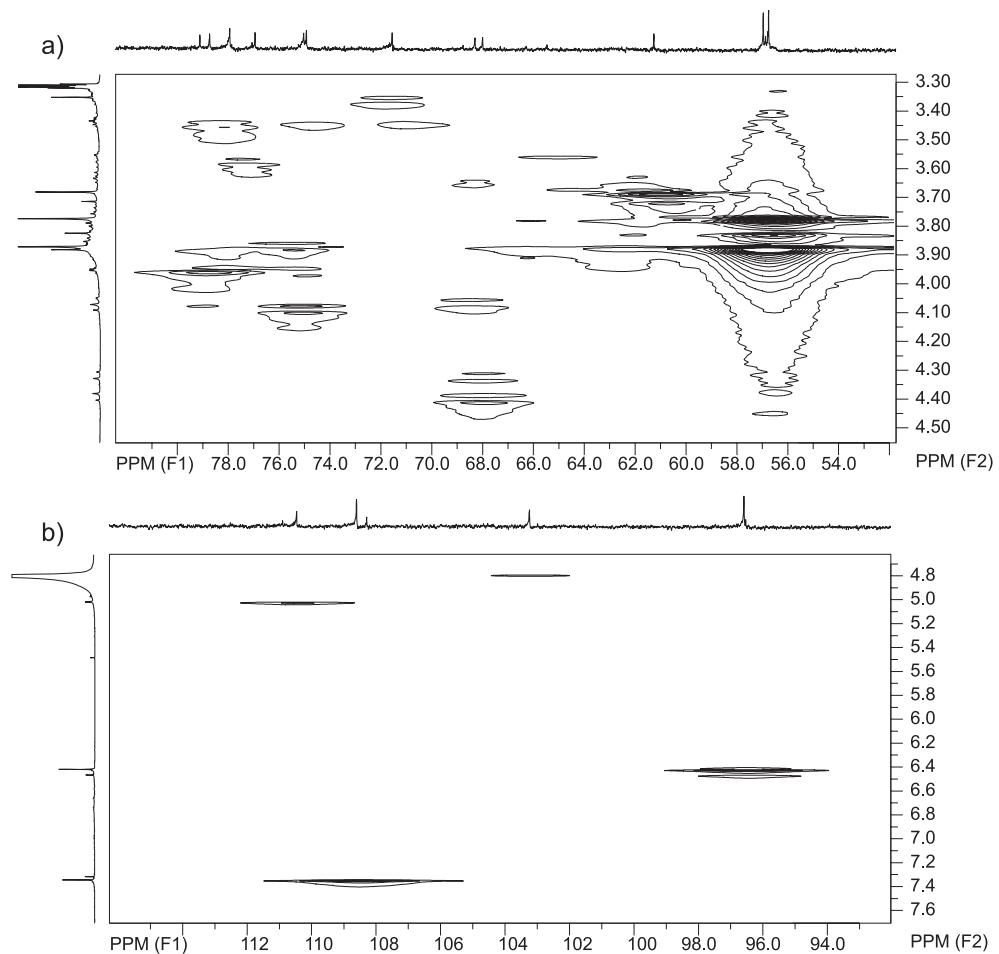
**Figure S5.** Expansion of <sup>1</sup>H NMR spectrum of compound **1** (CD<sub>3</sub>OD, 500 MHz).



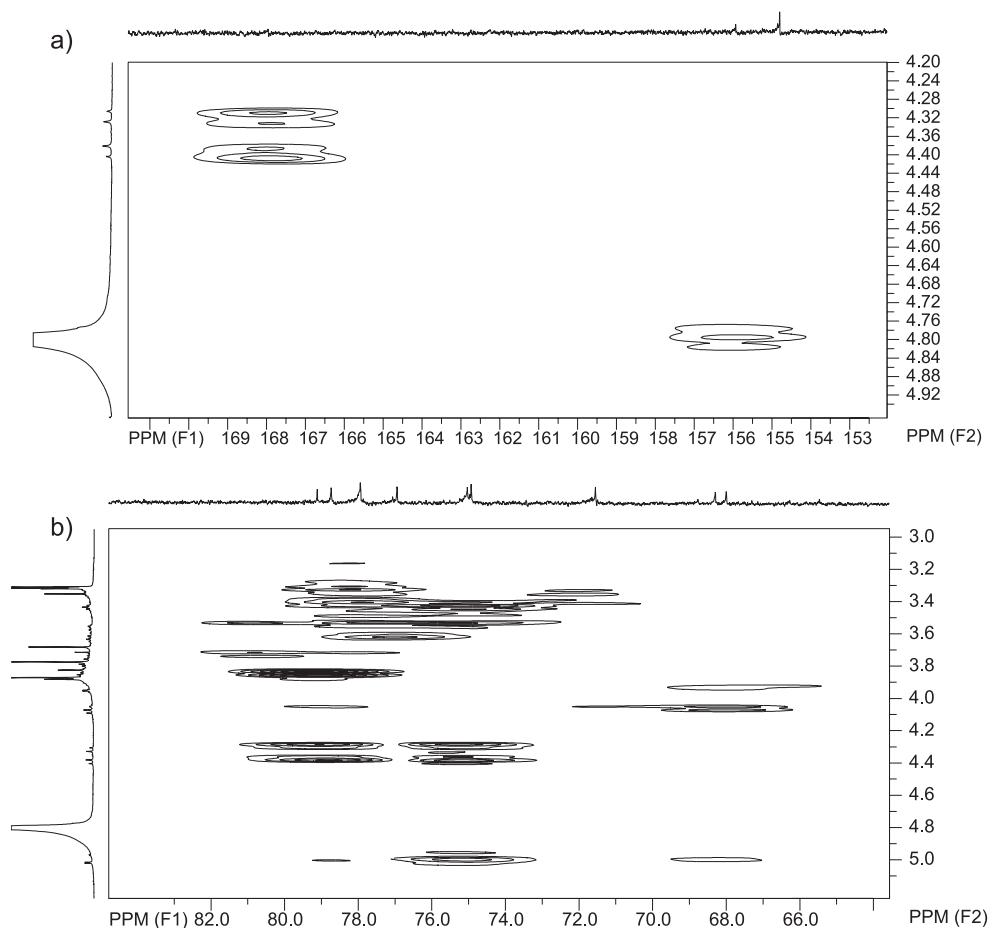
**Figure S6.** TOCSY spectrum of compound **1** (CD<sub>3</sub>OD, 500 MHz).



**Figure S7.**  $^{13}\text{C}$  NMR spectrum of compound **1** ( $\text{CD}_3\text{OD}$ , 126 MHz).



**Figure S8.** Expansions of the gHMQC spectrum of compound **1** ( $\text{CD}_3\text{OD}$ , 500 MHz).



**Figure S9.** Expansions of the gHMBC spectrum of compound 1 ( $\text{CD}_3\text{OD}$ , 500 MHz).

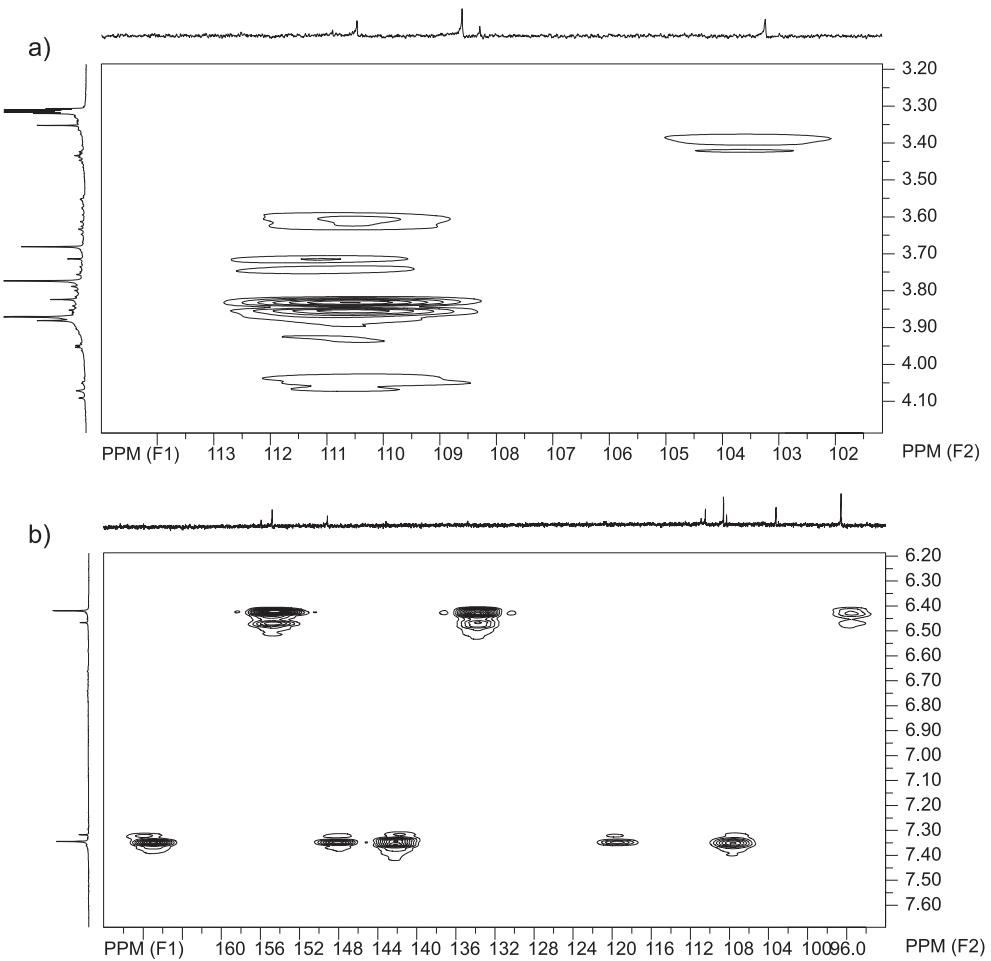


Figure S10. Expansions of the gHMBC spectrum of compound 1 ( $\text{CD}_3\text{OD}$ , 500 MHz).

**Table S1.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR data of analogous compounds of **1** in literature

position	1	A	B	C	D	E
1	155.9	153.1	153.6	155.9	156.0	
2,6	96.5/ 6.41 s 110.1/ 6.39 dd (2.6, 8.6)	103.7/ 6.60 d (2.6)	94.0/ 6.26 s	96.7/ 6.43 s	96.4/ 6.45 s	
3,5	154.7	149.9116.7/ 6.50 d (8.6)	153.0	154.8	154.8	
4	134.7	143.4	132.4	134.8	134.6	
1'	103.2/ 4.79 d (7.5)	102.5/ 4.77 d (7.2)	99.2/ 4.84 d (7.5)	103.3/ 4.79 d (8.0)	103.2/ 4.79 d (7.3)	104.4/ 4.25 d (8.0)
2'	74.9/ 3.43	79.1/ 3.61	77.2/ 3.50	75.0/ 3.44	74.9	75.1/ 3.18
3'	77.9/ 3.52	79.6/ 3.57	75.9/ 3.47	77.9/ 3.44	77.9	78.1/ 3.34
4'	71.5/ 3.34	72.5/ 3.34	70.4/ 3.12	71.5/ 3.35	71.6	71.8/ 3.26
5'	76.9/ 3.60	78.8/ 3.34	77.2/ 3.34	76.9/ 3.56	77.0	76.9/ 3.40
6'	68.2/ 3.63 d (10.0) and 4.06 d (10.0)	63.4/ 3.65 dd (12.2, 5.4) and 3.84 dd (12.2, 2.0)	60.8/ 3.74 m	68.3/ 3.63 dd (11.0, 2.0) and 4.06 dd (11.0, 6.0)	68.8	68.6/ 3.63 dd (10.0, 2.0)
1''	110.4/ 5.01 d (2.3)	111.3/ 5.50 s	108.6/ 5.42 s	110.5/ 5.01 d (2.0)	110.9/ 4.96 d (2.5)	110.8/ 5.05 d (2.0)
2''	78.7/ 3.94 d (2.3)	79.5/ 4.07 s	76.9/ 3.91 s	78.6/ 3.96 d (2.0)	77.9/ 3.87 d (2.5)	78.6/ 4.00 d (2.0)
3''	79.0	80.0	77.5	79.0	80.5	79.1
4''	75.0/ 3.85 m and 4.08 d (9.7)	76.1/ 3.90 m and 4.29 d (9.8)	73.9/ 3.85 d (9.4) and 4.11 d (9.4)	74.9/ 3.86 d (10.0) and 4.08 d (10.0)	74.9/ 3.73 d (9.8) and 3.94 d (9.8)	75.0/ 3.88 d (10.0) and 4.08 d (10.0)
5''	67.9/ 4.31 d (11.4) and 4.39 d (11.4)	68.9/ 4.26 d (11.5) and 4.42 d (11.5)	67.1/ 4.22 d (11.0) and 4.27 d (11.0)	67.6/ 4.31 d (11.5) and 4.36 d (11.5)	65.4/ 3.54 s	68.3/ 4.38 d (11.5) and 4.40 d (11.5)
1'''	120.6	121.8	119.1	123.3		126.4
2'',6'''	108.5/ 7.34 s	109.2/ 7.24 s	107.1/ 7.15 s	132.8		108.4/ 7.35 s
3'',5'''	149.1	149.6	147.4	114.9		154.5
4'''	143.1	142.9	140.9	165.3		143.9
C=O	167.9	168.5	165.3	167.6		167.4
3,5-	56.7/ 3.77	57.0/ 3.71	55.5/ 3.65	56.7/ 3.77	56.7/ 3.81	56.9
OCH <sub>3</sub>						
4-OCH <sub>3</sub>	61.2/ 3.68		60.0/ 3.53	61.2	61.2/ 3.70	61.2
3'',5''-	56.9/ 3.87	57.7/ 3.84	56.1/ 3.77			
OCH <sub>3</sub>						

**A** ( $\text{CD}_3\text{OD}$ ) and **B** ( $\text{DMSO}-d_6$ ): ref. 9 - Jung, M. J.; Kang, S. S.; Jung, Y. J.; Choi, J. S.; *Chem. Pharm. Bull.* **2004**, 52, 1501. **C, D** and **E** ( $\text{CD}_3\text{OD}$ ): ref. 10 - Warashina, T.; Nagatani, Y.; Noro, T. *Phytochemistry* **2004**, 65, 2003.

