Supporting Information

***Rec. Nat. Prod.* X:X (2023) XX-XX**

Chemical Constituents from The Leaves and Twigs of *Magnolia Decidua*

Qi Zhou[1], Jiang Wan[1], Chun-Xiao Jiang[1,2], Ying-Peng Tong[1], Zhen-Da Xie [1], Ting Wang[1], Dao-An Xiao[3], Zhi-Yong Xiao[4] and Jin-Feng Hu[1,2]*

[1] Institute of Natural Medicine and Health Products, School of Pharmaceutical Sciences, Zhejiang Provincial Key Laboratory of Plant Evolutionary Ecology and Conservation, Taizhou University, Taizhou, Zhejiang 318000, P.R. China
[2] Department of Natural Medicine, School of Pharmacy, Fudan University, Shanghai 201203, P.R. China
[3] College of Chemistry and Bioengineer, Yichun University, Yichun, Jiangxi 336000, PR China
[4] Yichun Academy of Sciences, Yichun, Jiangxi 336000, PR China

Table of Contents	Page

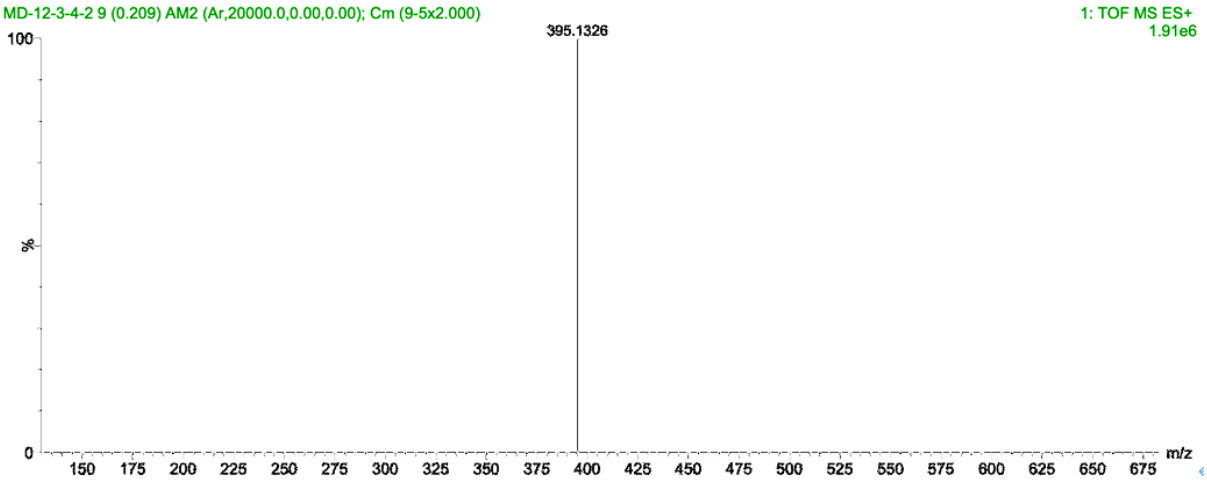


Figure S1: HR-ESI-MS spectrum of **1** (Manglycoside A)

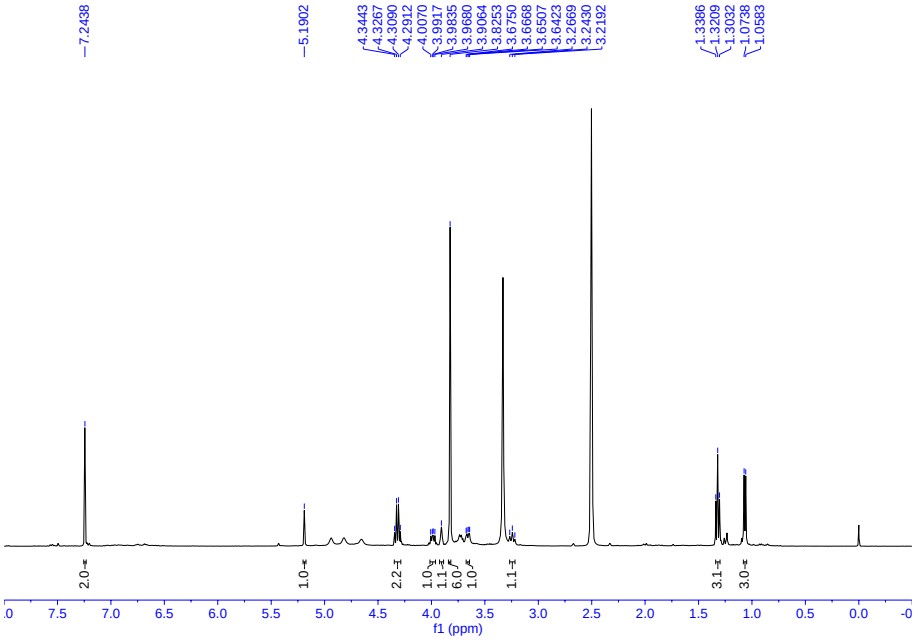


Figure S2: ^{1}H-NMR (400 MHz, DMSO) spectrum of **1** (Manglycoside A)

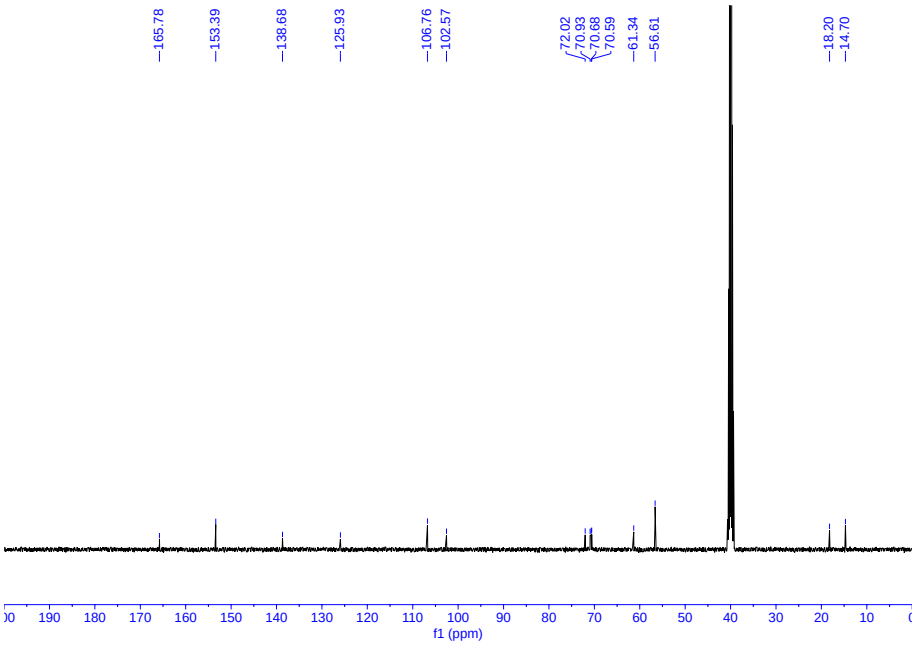


Figure S3: ^{13}C-NMR (100 MHz, DMSO) spectrum of **1** (Manglycoside A)

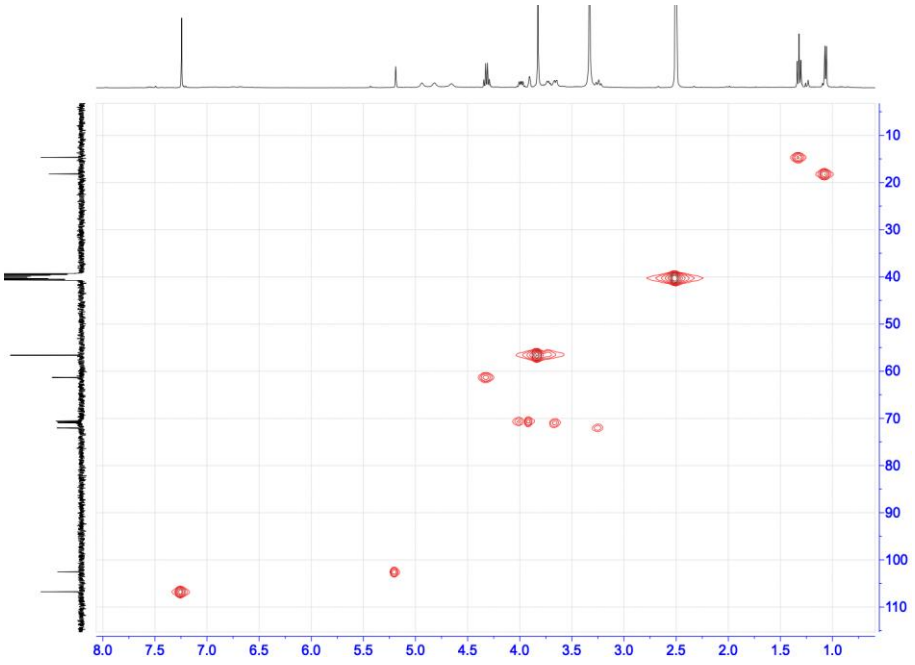


Figure S4: HSQC spectrum of **1** (Manglycoside A)

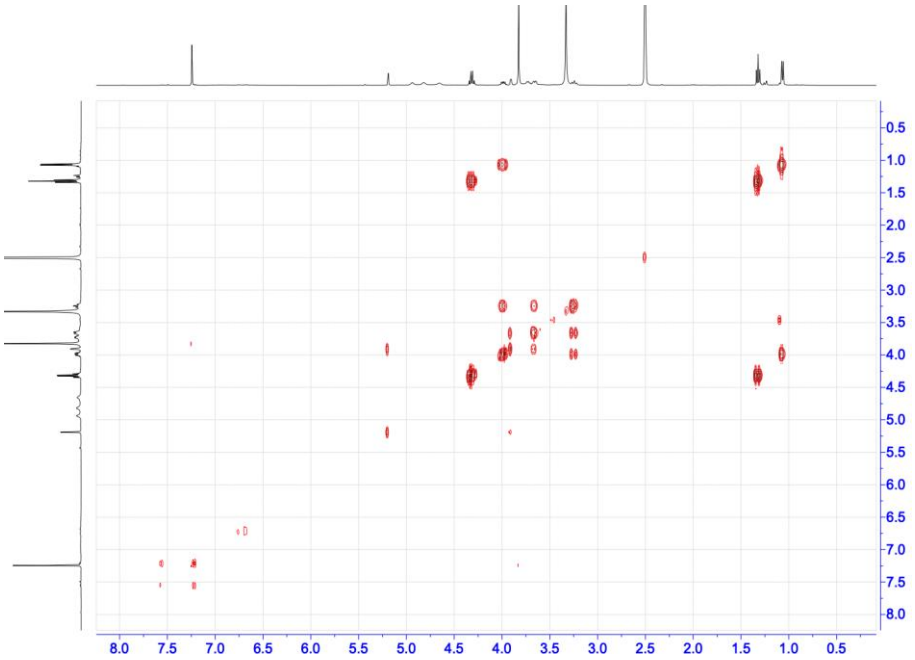


Figure S5: ^{1}H-^{1}H COSY spectrum of **1** (Manglycoside A)

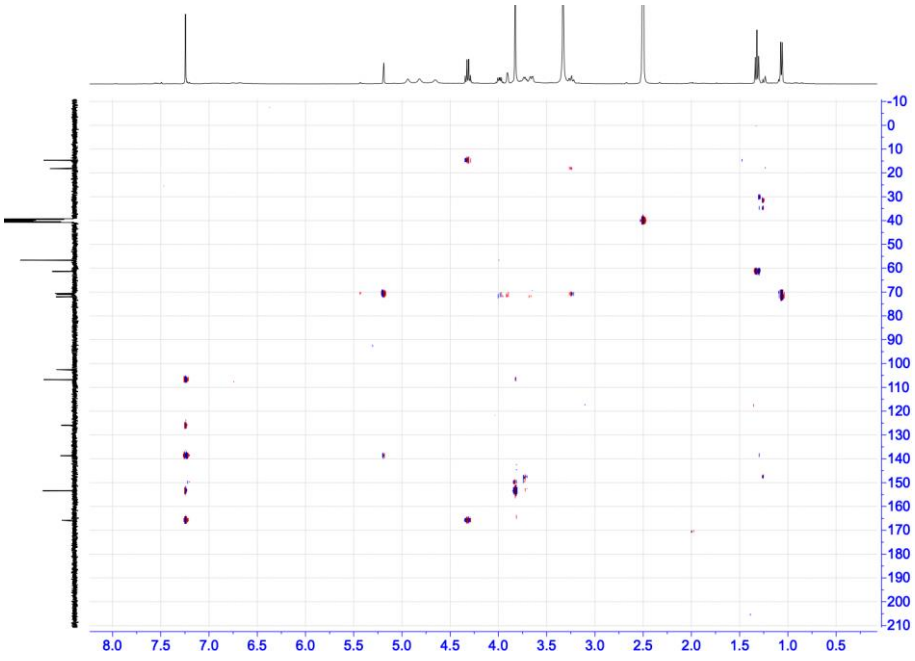


Figure S6: HMBC spectrum of **1** (Manglycoside A)

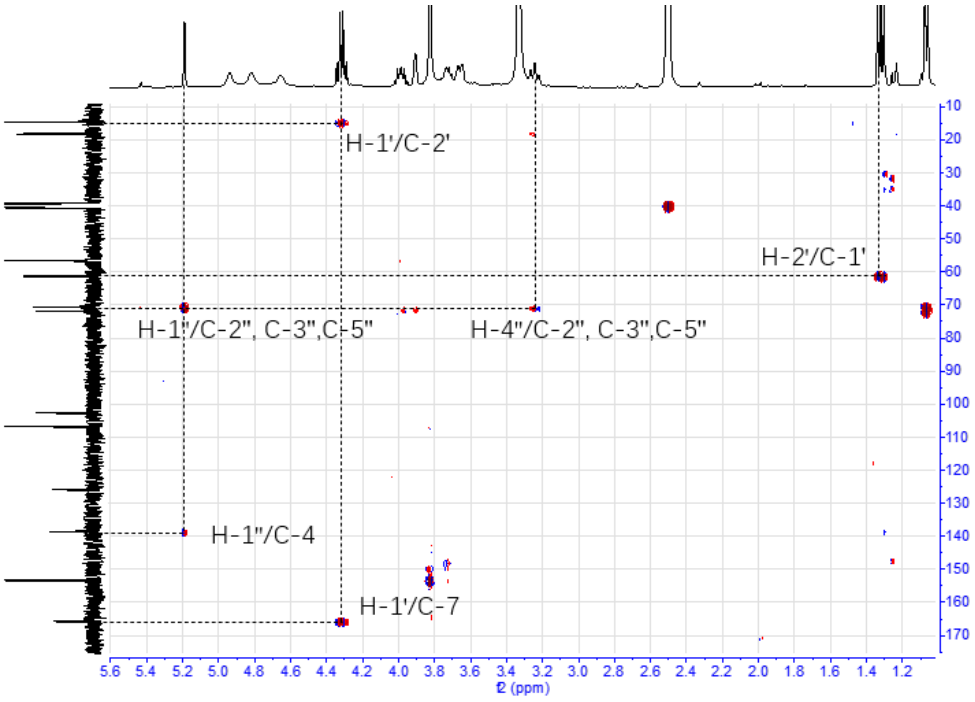


Figure S7: HMBC spectrum of **1** (Manglycoside A) (From δ_H1.0 ppm to δ_H 6.0 ppm)

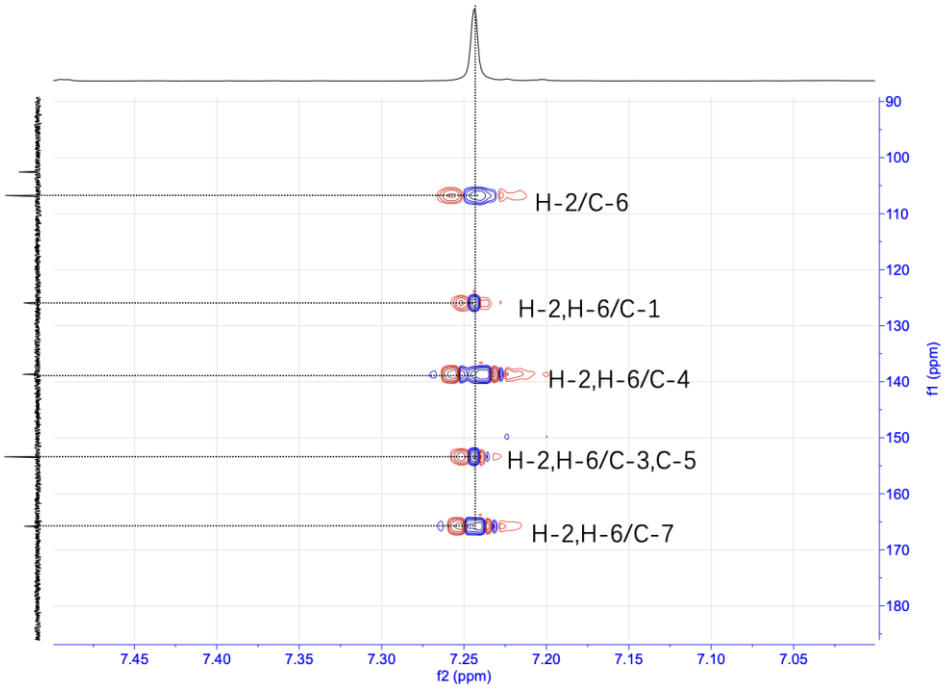


Figure S8: HMBC spectrum of **1** (Manglycoside A) (From δ_H7.0 ppm to δ_H 7.5 ppm)

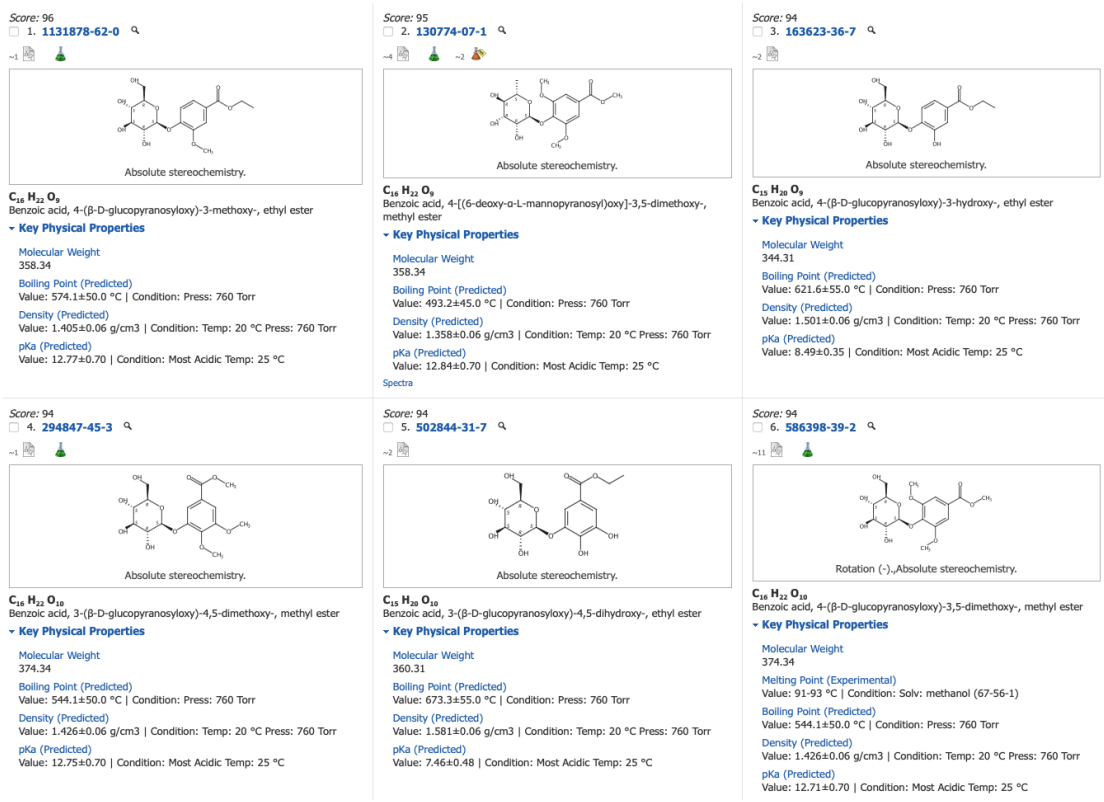


Figure S9: The Scifinder searching results of compound **1**

Table S1: The structural comparison of similar comounds with **1**

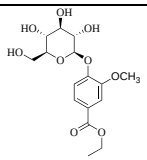
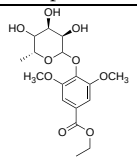
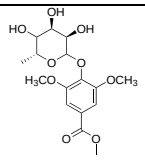
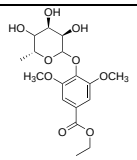
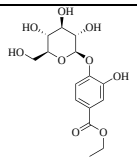
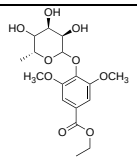
No.	Similarity score	Chemical structure and CAS Chemical structure of number	Chemical structure of compound **1**
1	96	 CAS NO. 1131878-62-0	
2	95	 CAS NO. 130774-07-1	
3	94	 CAS NO. 163623-36-7	

Table S2: The NMR data comparison of similar compounds with **1**

NO.	Compound **1**[a]		ethyl 4-β-D-glucopyranosyloxy-3-methoxybenzoate[b] (CAS NO. 1131878-62-0)	methyl syringate α-L-rhamnoside[c] (CAS NO. 130774-07-1)	
	δ_H	δ_C		δ_H	δ_C
1		125.93	NMR data is not available		127.9
2, 6	7.24 (2H, s)	106.76		7.31 (2H, s)	108.5
3, 5		153.39			155.3
4		138.68			140.8
7		165.78			168.9
1'	4.31 (2H, q, *J* = 7.2 Hz)	61.34		3.89 (3H, s)	53.6
2'	1.32 (3H, t, *J* = 7.2 Hz)	14.70			
1''	5.19 (1H, s)	102.57		5.34 (1H, d, *J* = 2Hz)	104.2
2''	3.90 (1H, br s)	70.93		4.14 (1H, dd, *J* =4, 2Hz)	73.0
3''	3.65 (1H, dd, *J* = 3.2, 9.6 Hz)	70.68		3.90 (1H, dd, *J* =10, 4Hz)	72.8
4''	3.24 (1H, t, *J* = 9.6 Hz)	72.02		3.44 (1H, t, *J* = 10Hz)	74.5
5''	3.99 (1H, dd, *J* = 6.4, 9.6 Hz)	70.59		4.24 (1H, dq, *J* = 10, 7Hz)	72.1
6''	1.06 (3H, d, *J* = 6.4 Hz)	18.20		1.21 (3H, d, *J* =7Hz)	18.7
3, 5-OCH$_3$	3.80 (6H, s)	56.61		3.87 (6H, s)	57.4

[a] in DMSO-d_6.

[b] H. T. Simonsen, M. S. Nielsen, N. J. Christensen, U. Christensen, T. V. La Cour, M. S. Motawia, B. P. A. Jespersen, S. B. Engelsen, B. L. Moller (2009). Molecular Interactions between Barley and Oat β--Glucans and Phenolic Derivatives, *J. Agric. Food Chem.* **57**, 2056-2064.

[c] R. C. Cambie, A. R. Lal, C. E. F. Rickard, and N. Tanaka (1990). Chemistry of Fijian plants. V.1) Constituents of Fagraea gracilipes A. Gray. *Chem Pharm Bull*. **38**, 1857-1861.

The spectra data of compounds 2-17

(-)-Syringaresinol (2) **:** colorless solid, $C_{22}H_{26}O_8$. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 3.05 (2H, m, H-8, 8′), 3.75 (12H, s, 3, 3′, 5, 5′-OMe), 3.79 (2H, m, H-9a, 9′a), 4.16 (2H, dd, *J* = 8.8, 6.8 Hz, H-9b, 9′b), 4.61 (2H, d, *J* = 3.6 Hz, H-7, 7′), 6.60 (4H, s, H-2, 2′, 6, 6′), 8.28 (2H, s, 4-OH′, 4′′-OH); ^{13}C-NMR (100 MHz, DMSO-d_6) δ: 53.7 (C-8, 8′), 56.0 (3, 3′, 5, 5′-OMe), 71.1 (C-9, 9′), 85.3 (C-7, 7′), 103.6 (C-2′, 2′′, 6′, 6′′), 131.4 (C-1, 1′), 134.8 (C-4, 4′), 147.9 (C-3, 3′, 5, 5′).

(+)-Pinoresinol (3) : White amorphous powder, $C_{20}H_{22}O_6$. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 3.02 (2H, m, H-1, 5), 3.74 (2H, dd, *J* = 8.0, 3.6 Hz, H-4a, 8a), 3.78 (6H, s, 3, 3′-OMe), 4.14 (2H, dd, *J* = 8.0, 7.2 Hz, H-4b, 8b), 4.60 (2H, d, *J* = 4 Hz, H-2, 6), 6.70 (2H, d, *J* = 8.0 Hz, H-5', 5''), 6.74 (2H, dd, *J* = 8.0, 1.2 Hz, H-6', 6''), 7.00 (2H, d, *J* = 1.2 Hz, H-2', 2''); ^{13}C-NMR (100 MHz, DMSO-d_6) δ: 54.1 (C-1, 5), 56.1 (OMe × 2), 71.4 (C-4, 8), 85.6 (C-2, 6), 110.9 (C-2', 2''), 115.6 (C-5', 5''), 119.1 (C-6', 6''), 132.7 (C-1', 1''), 146.4 (C-4', 4''), 148.0 (C-3', 3'').

Pharsyringaresinol (4) : White amorphous powder, $C_{30}H_{38}O_{14}$, ^{1}H NMR (400 MHz, DMSO-d_6) δ: 4.78 (1H, d, *J* = 4 Hz, H-2), 3.14 (1H, m, H-1), 4.30 (1H, dd, *J* = 16.0, 10.0 Hz, H-4a), 3.90 (1H, dd, *J* = 10.0, 4.0 Hz, H-4b), 3.16 (1H, m, H-5), 4.74 (1H, d, *J* = 4 Hz, H-6), 4.30 (1H, dd, *J* = 16.0, 10.0 Hz, H-8a), 3.90 (1H, dd, *J* = 10.0, 4.0 Hz, H-8b), 6.60 (1H, s, H-2′, 6′), 6.66 (1H, s, H-2′′, 6′′), 3.85 (1H, s, 3′/5′-OCH_3), 3.86 (1H, s, 3′′/5′′-OCH_3), 4.81 (1H, m, H-1′′), 3.36 (1H, m, H-2′′), 3.42 (1H, m, H-3′′), 3.35 (1H, m, H-4′′), 3.50 (1H, m, H-5′′), 4.28, (1H, m, H-6a′′) 4.24 (1H, m, H-6b′′), 1.94 (3H, s, H-OAc). ^{13}C-NMR (100 MHz, DMSO-d_6) δ: 131.8 (C-1), 104.1 (C-2, 6), 148.4 (C-3, 5), 135.3 (C-4), 85.8 (C-7), 54.2 (C-8), 71.7 (C-9), 170.5 (C-10), 21.0 (C-11), 133.8, (C-1′), 104.3 (C-2′, 6′), 153.3 (C-3′, 5′), 138.0 (C-4′), 85.5 (C-7′), 54.1 (C-8′), 71.6 (C-9′), 103.1 (C-1′′), 74.1 (C-2′′), 74.5 (C-3′′), 76.7 (C-4′′), 79.6 (C-5′′), 63.9 (C-6′′).

Syringaresinol-β-D-glucoside (5) **:** White amorphous powder, ^{1}H-NMR (DMSO-d_6, 400 MHz) δ: 6.67 (2H, s, H-2", H-6"), 6.61 (2H, s, H-2', H-6'), 4.89 (1H, d, *J* = 4.4 Hz, H-glc-1), 4.68 (1H, d, *J* = 4.4 Hz, H-2), 4.62 (1H, d, *J* = 4.2 Hz, H-6), 4.18 (2H, t, *J* = 6.4 Hz, H-8a, H-4a), 3.81 (1H, br. d, *J* = 3.6 Hz, H-4b), 3.77 (6H, s, 2×OCH_3), 3.76 (6H, s, 2 × OCH_3), 3.20-3.22 (2H, m, H-1, H-5). ^{13}C NMR (100 MHz, DMSO-d_6) δ 153.1 (C-3", C-5"), 148.4 (C-3', C-5'), 137.7 (C-4'), 135.3 (C-4"), 134.2 (C-1"), 131.8 (C-1'), 104.6 (C-2"), 104.6 (C-6"), 104.1 (C-2', C-6'), 103.2 (C-glc-1), 85.8 (C-2), 85.5 (C-6),

77.7 (C-glc-5), 77.0 (C-glc-3), 74.6 (C-glc-2), 71.7 (C-4, C-8), 70.4 (C-glc-4), 61.4 (C-glc-6), 56.9 (3",5"-OMe), 56.5 (3',5'-OMe), 54.1 (C-5), 54.0 (C-1).

Honokiol (6) **:** $C_{18}H_{18}O_2$, ^{1}H-NMR (400 MHz, $CDCl_3$) δ: 3.27, 3.36 (each 2H, br d, J = 7Hz, H-7, H,-7′), 5.15 (4H; m, H-9, H-9′), 5.99 (2H, m, H-8, H-8′), 6.90 (2H, d, J = 8 Hz), 7.03 (2H, dd, J = 8, 2Hz), 7.22 (2H, d, J = 2 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$) δ: 132.2 (C-1), 130.2 (C-2), 126.5 (C-3), 150.8 (C-4), 115.5 (C-5), 131.1 (C-6), 39.4 (C-7), 137.8 (C-8), 115.6 (C-9), 127.8 (C-1′), 128.5 (C-2′), 129.5 (C-3′), 128.8 (C-4′), 116.5 (C-5′), 154.0 (C-6′), 35.0 (C-7′), 136.1 (C-8′), 116.8 (C-9′),

Magnolol diacetate (7): colorless powder, $C_{22}H_{22}O_4$.^{1}H NMR (400 MHz, DMSO) δ: 6.96 (2H, d, J = 2.4 Hz, H-6, 6'), 6.80 (2H, dd, J = 2.4, 8 Hz, H-4, 4'), 6.52 (2H, d, J = 8 Hz, H-3, 3'), 4.22 (2H, t, J = 6.4 Hz, H-8, 8'), 3.24 (2H, d, J = 6.4 Hz, H-9, 9'), 1.74 (6H, s, 2-OAc, 2'-OAc), 1.63 (2H, m, H-7a,7'a), 1.35 (2H, m, H-7b,7'b)。^{13}C-NMR (100 MHz, DMSO) δ:130.3 (C-1, 1'), 129.2 (C-2, 2'), 118.6 (C-3, 3'), 127.7 (C-4, 4'), 132.0 (C-5, 5'), 129.1 (C-6, 6'), 30.5 (C-7, 7'), 65.5 (C-8, 8'), 39.6 (C-9, 9'), 174.6 (C=O), 24.1 (C-OAc)

Rel-(3R,3′S,4R,4′S)-3,3′,4,4′-tetrahydro-6,6′-dimethoxy[3,3′-bi-2H-benzopyran]-4,4′-diol (8) **:** colorless oil, $C_{20}H_{22}O_6$. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 6.89 (2H, d, J = 2.0 Hz, H-5, H-5'), 6.88 (1H, d, J = 7.8 Hz, H-8, H-8'), 6.82 (2H, dd, J = 1.8, 8.2 Hz, H-7, H-7'), 4.73 (2H, d, J = 4.0 Hz, H-4, H-4'), 4.24 (2H, dd, J = 6.8, 9.2 Hz, H-2a, H-2a'), 3.90 (6H, s, OCH_3), 3.87 (2H, dd, J = 3.8, 9.2 Hz, H-2e, H-2e'), 3.10 (2H, m, H-3, H-3'). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.7 (C-6, C-6'), 145.2 (C-9, C-9'), 132.9 (C-10, C-10'), 119.0 (C-7, C-7'), 114.3 (C-5, C-5'), 108.6 (C-8, C-8'), 85.9 (C-4, C-4'), 71.7 (C-2, C-2'), 56.0 (OCH_3), 54.2 (C-3, C-3').

Rhemaneolignan A (9) **:** colorless amorphous powder, $C_{21}H_{24}O_8$, ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.60 (1H, d, J = 16 Hz, H-7), 7.33 (1H, d, J = 2 Hz, H-3), 7.19 (1H, dd, J = 2.0, 8.0 Hz, H-5), 7.06 (1H, d, J = 8 Hz, H-6), 6.97 (1H, d, J = 2 Hz, H-3′), 6.75 (1H, dd, J = 2.0, 8.0 Hz, H-5′), 6.68 (1H, d, J = 8 Hz, H-6′), 6.53 (1H, d, J = 16 Hz, H-8), 4.71 (1H, t, J = 4 Hz, H-7′), 3.82 (1H, s, H- OCH_3), 3.73 (1H, s, H- OCH_3), 3.71 (1H, s, H- OCH_3), 4.40 (1H, m, H-8′), 3.56 (1H, m, H-9′a), 3.23 (2H, m, H-9′b). ^{13}C NMR (100 MHz, DMSO-d_6) δ:150.1 (C-1), 151.3 (C-2), 111.5 (C-3), 127.2 (C-4), 123.1 (C-5), 115.0 (C-6), 145.2 (C-7), 115.2 (C-8), 167.5 (C-9), 145.99 (C-1′), 147.51 (C-2′), 111.7 (C-3′), 133.3 (C-4′), 119.5 (C-5′), 115.6 (C-6′), 71.5 (C-7′), 84.3 (C-8′), 60.7 (C-9′), 51.7 (-OCH_3), 56.0 (-OCH_3′), 56.2 (-OCH_3″).

Melianoninol (10) **:** yellow oil, $C_{20}H_{20}O_6$,^{1}H-NMR (400 MHz, $CDCl_3$) δ: 7.60 (1H, s, H-6′), 7.04 (1H, s, H-3′), 6.90 (1H, d, J = 2.4 Hz, H-2), 6.88 (1H, dd, J = 7.2, 2.4 Hz, H-6), 6.87 (1H, d, J = 7.2 Hz, H-5), 4.97 (1H, d, J = 7.2 Hz, H-7′), 4.25 (1H, t, J = 7.2, 3.6, 4.0 Hz, H-8′), 3.70 (2H, m, J = 3.6, 4.0 Hz,

H-9′), 3.90 (6H, m, 7, H-13′)。 ^{13}C-NMR (100 MHz, $CDCl_3$) δ: 51.7 (C-8′), 56.0 (C-13′), 61.0 (C-7), 73.2 (C-9′), 86.2 (C-7′), 108.9 (C-5), 110.9 (C-6), 114.3 (C-2), 119.2 (C-6′), 120.0 (C-3′), 122.3 (C-11′), 127.8 (C-3), 129.8 (C-4′), 132.0 (C-1′), 145.3(C-2′), 146.7 (C-1), 149.1 (C-4), 151.2 (C-5′), 152.2 (C-10′), 193.6 (C-12′)。

9-Acetoxy syringin (11) **:** white amorphous powder, $C_{14}H_{16}O_8$, ^{1}H-NMR (400 MHz, $CDCl_3$) *δ*: 6.78 (2H, s, H-2, 6), 6.58 (1H, d, J = 16 Hz, H-7), 6.33 (1H, dt, J = 6.4, 12.4, 16 Hz, H-8), 4.67 (1H, d, J = 9.6 Hz, H-9), 2.06 (3H, s, H-11), 4.93 (1H, d, J = 7.2 Hz, H-1'), 3.20 (1H, m, H-2'), 3.03 (1H, m, H-3'), 3.12 (1H, m, H-4'), 3.20 (1H, m, H-5'), 3.60 (1H, m, H-6'a), 3.39 (1H, m, H-6'b), 3.78 (6H, s, H-3, 5-OCH_3); ^{13}C-NMR (100 MHz, $CDCl_3$) *δ*:132.04 (C-1),105.29 (C-2,6), 153.19 (C-3,5), 134.83 (C-4), 133.55 (C-7), 123.64 (C-8), 64.78 (C-9), 170.63 (C-10), 21.23 (C-11), 102.89 (C-1'), 74.64 (C-2'), 77.72 (C-3'), 70.39 (C-4'), 77.03 (C-5'), 61.34 (C-6'), 56.84 (3, 5-OCH_3)

4-Allylcatechol (12) **:** brown powder, $C_9H_{10}O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.74 (1H, d, *J* = 2 Hz, H-3), 5.68 (1H, dd, *J* = 8, 2 Hz, H-5), 5.55 (1H, d, *J* = 8 Hz, H-6), 4.95 (1H, m, H-8), 4.03 (2H, dd, *J* = 16, 8 Hz, H-9), 2.27 (2H, m, H-7). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.23 (C-1), 142.51 (C-2), 137.63 (C-3), 114.71 (C-4), 119.38 (C-5), 114.20 (C-6), 39.03 (C-7), 115.16 (C-8), 131.46 (C-9).

p-Hydroxybenzaldehyde (13) **:** white powder, $C_7H_6O_2$. ^{1}H-NMR (DMSO-d_6, 400 MHz) δ: 9.78 (1H, s, H-CHO), 7.75 (2H, d, *J* = 8.4 Hz, H-2, H-6), 6.92 (2H, d, *J* = 8.5 Hz, H-3, H-5). ^{13}C NMR (100 MHz, DMSO-d_6) δ: 191.4 (1-HO), 163.8 (C-4), 132.6 (C-1), 128.9 (C-2, C-6), 116.3 (C-3, C-5).

Liriodenine (14) **:** yellow amorphous powder, $C_{17}H_9NO_3$, ^{1}H-NMR (DMSO-d_6, 400 MHz) δ: 8.82 (1H, d, *J* = 7.6 Hz, H-5), 8.64 (1H, d, *J* = 7.2 Hz, H-11), 8.37 (1H, d, *J* = 7.2 Hz, H-8), 8.05 (1H, d, *J* = 6 Hz, H-4), 7.90 (1H, t, *J* = 8 Hz, H-9), 7.66 (1H, t, *J* = 8 Hz, H-10), 7.58 (1H, s, H-3), 6.52 (2H, s, -O-CH_2-O-).

N-Acetyldehydroanonaine (15) **:** $C_{18}H_{13}NO_3$, ^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 8.97 (1H, m, H-11), 7.71 (1H, m, H-8), 7.55 (2H, m, H-9, 10), 7.23 (1H, s, H-7), 7.18 (1H, br s, H-7), 7.05 (1H, s, H-3), 6.16 (2H, s, OCH_2O), 4.10 (2H, t, *J* = 7.2 Hz, H-5), 3.07 (2H, t, *J* = 7.2 Hz, H-4), 2.28 (3H, s, -CH_3)。 ^{13}C-NMR (100 MHz, $CDCl_3$) *δ*: 142.2 (C-1), 145.6, (C-2), 109.0 (C-3), 126.1 (C-3a), 30.7 (C-4),41.8 (C-5), (C-6a), 116.9 (C-7), 131.3 (C-7a), 127.8 (C-8), 126.8 (C-9), 127.0 (C-10), 127.2 (C-11), 127.4 (C-11a), 118.2 (C-11b), 120.0 (C-11c), 101.3 (-OCH_2O-), 169.9 (NC=O), 23.1 (-CH_3).

N-trans-feruloyltyramine (16) **:** $C_{18}H_{19}NO_4$, Colorless crystal, ^{1}H NMR (400 MHz, DMSO) δ 7.98 (1H, t, *J* = 5.5 Hz, NH), 7.32 (1H, d, *J* = 16 Hz, H-7), 7.11 (1H, d, *J* = 2 Hz, H-2), 7.01 (2H, d, *J* = 8 Hz, H-2′, 6′), 6.99 (2H, dd, *J* = 2, 8 Hz, H-6), 6.79 (1H, d, *J* = 8 Hz, H-5), 6.68 (2H, d, *J* = 8.4 Hz, H-3′, 5′), 6.44 (1H, d, *J* = 16 Hz, H-8), 3.80 (3H, s, OCH3), 3.34 (2H, q, *J* = 6.7 Hz, H-8′), 2.65(2H, t, *J* = 7.2 Hz, H-7′). ^{13}C NMR (100 MHz, DMSO) δ 129.9 (C-1), 111.2 (C-2), 148.3 (C-3), 148.7 (C-4),

115.6 (C-5), 122.0 (C-6), 139.3 (C-7), 119.5 (C-8), 165.8 (C-9), 56.0 (C-OCH3), 126.9 (C-1′), 130.0 (C-2′, 6′), 116.1 (C-3′, 5′), 156.1 (C-4′), 34.9 (C-7′), 41.1 (C-8′),

***N-trans-feruloyl-3-methoxytyrmine (17)* :** Colorless crystal, $C_{19}H_{21}NO_5$, ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 7.50 (1H, d, *J* = 16 Hz, H-7'), 7.31 (1H, d, *J* = 1.6 Hz, H-2'), 7.05 (1H, d, *J* = 1.6 Hz, H-2), 7.01 (1H, dd, *J* = 8.0, 1.6 Hz, H-6'), 6.85 (1H, d, *J* = 8.0 Hz, H-5'), 6.70 (1H, d, *J* = 8.0 Hz, H- 5), 6.68 (1H, dd, *J* = 8.0, 1.6 Hz, H-6), 6.25 (1H, d, *J* = 15.6 Hz, H- 8'), 3.59 (2H, m, H-8), 2.80 (2H, *J* = 8. 0 Hz, H-7). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.46 (C = O), 147.77 (C-4'), 147.30 (C-3'), 147.15(C-3), 144.43 (C-4), 140.84 (C-7'), 130.67 (C-1), 127.15 (C-1'), 122.04 (C-6), 121.25 (C-6'), 118.19 (C-5), 115.06 (C-2), 114.72 (C-8'), 111.60 (C-2'), 109.96 (C-5'), 56.38 (OMe), 55.90 (OMe), 41.00 (C-8), 35.26 (C-7).