

Electronic supplementary information for

**Bioassay-Guided Isolation of Bisepoxylignans from the Flower Buds of  
*Magnolia Biondii* Pamp and Their Antiallergic Effects†**

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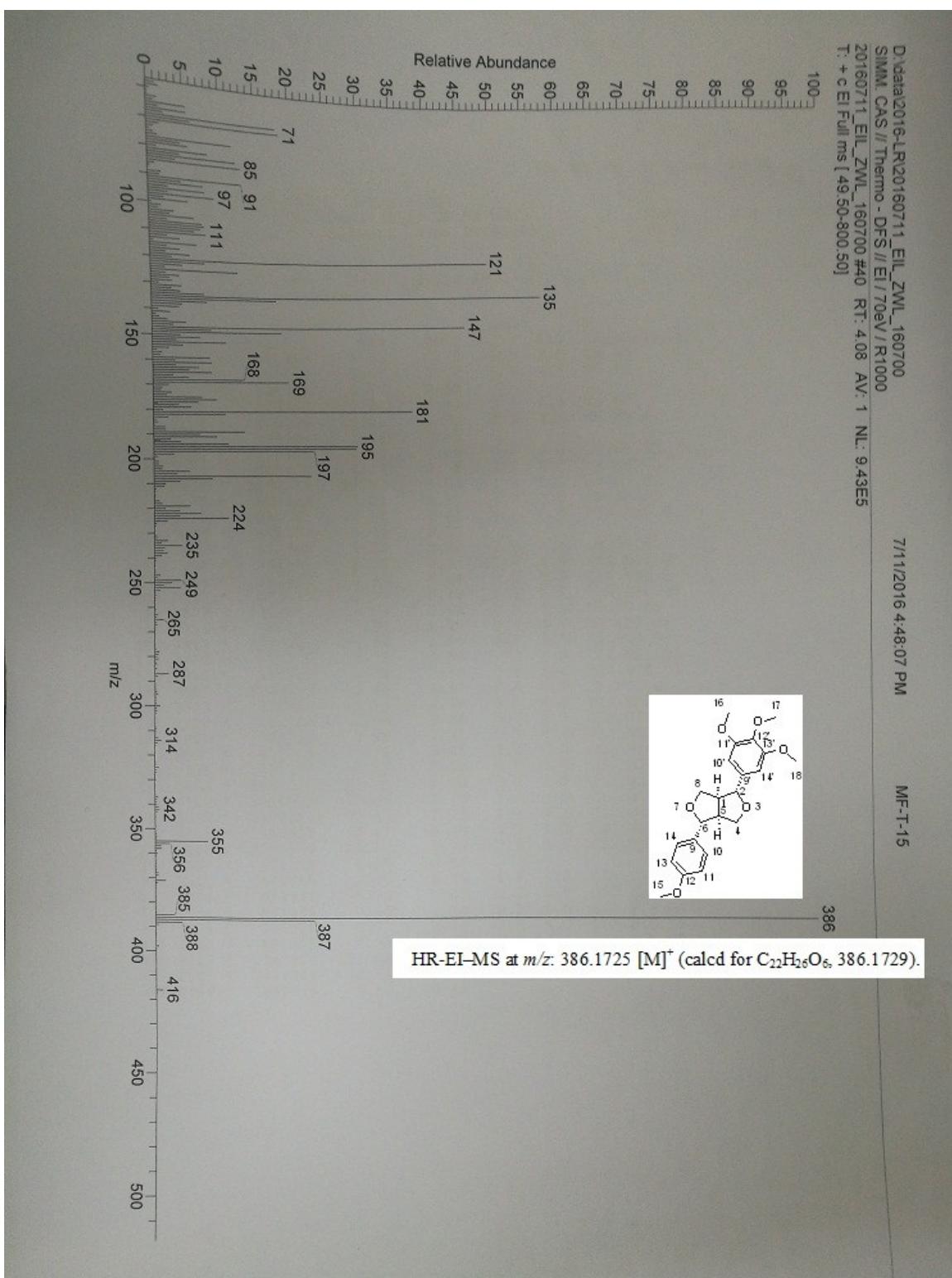
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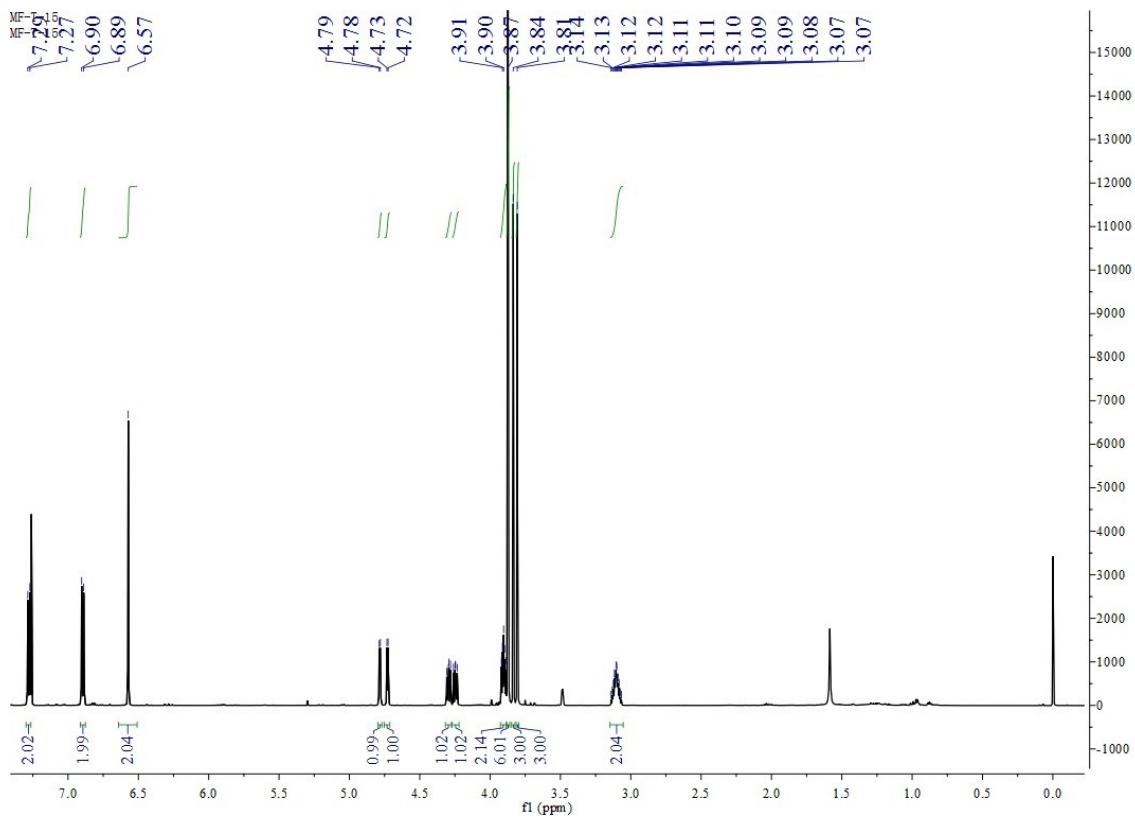
## S1. HR-EI-MS of 1



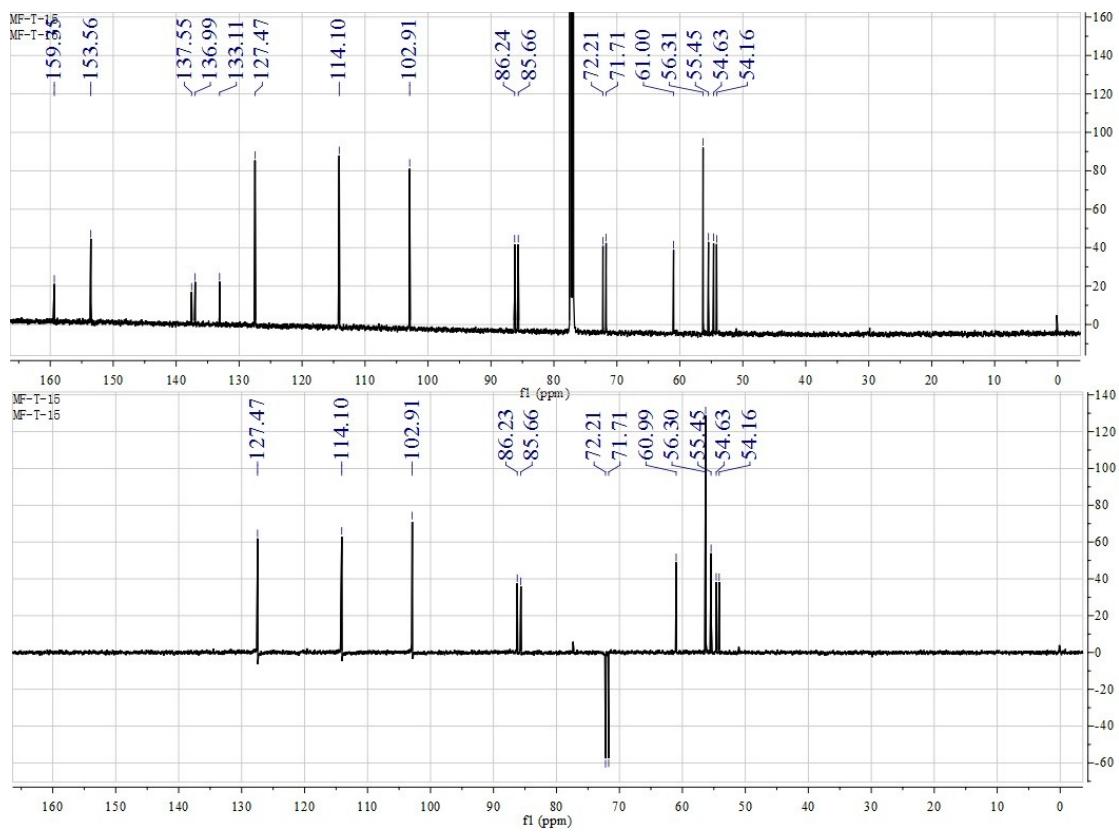
LIST: h16269-c2 13-Jul-16 Elapse: 06:58.3 33  
Samp: MF-T-15 Start : 11:12:59 34  
Comm: Finnigan/MAT95/70eV/R:10000 Study : S/N: PT200712-01-01  
Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM  
Oper: SIMM.CAS Client: S/N: PT001263 Inlet :  
Limit: ( 0 )  
: ( 485 ) C24.H100.06  
Peak: 1000.00 mmu R+D: -2.0 > 60.0  
Data: CMASS : converted

259313			(mmu)				
Mass	Intensity	%RA	%RIC	Delta	R+D	Composition	
77.04061	*	494498	5.72	0.76	-1.5	4.5	C6.H5
91.05448	*	468012	5.41	0.72	0.3	4.5	C7.H7
108.0543	*	308316	3.57	0.48			
115.0535	*	278705	3.22	0.43	1.2	6.5	C9.H7
121.0652	*	2940506	34.02	4.54	0.2	4.5	C8.H9.O
122.0697	*	298304	3.45	0.46			
125.0594	*	398851	4.61	0.62	0.8	3.5	C7.H9.02
134.0722	*	365406	4.23	0.56	1.0	5.0	C9.H10.O
135.0436	*	3252017	37.62	5.02	1.0	5.5	C8.H7.02
136.0496	*	808069	9.35	1.25	2.9	5.0	C8.H8.02
147.0810	*	2992342	34.62	4.61	0.0	5.5	C10.H11.O
148.0855	*	401123	4.64	0.62			
153.0567	*	478308	5.53	0.74	-1.6	4.5	C8.H9.03
159.0818	*	392389	4.54	0.61	-0.8	6.5	C11.H11.O
161.0966	*	282682	3.27	0.44	0.1	5.5	C11.H13.O
163.0757	*	282327	3.27	0.44	0.2	5.5	C10.H11.O2
165.0577	*	399561	4.62	0.62	-2.5	5.5	C9.H9.03
168.0786	*	783855	9.07	1.21	0.0	4.0	C9.H12.03
169.0863	*	1268981	14.68	1.96	0.2	3.5	C9.H13.03
175.0759	*	377974	4.37	0.58	0.0	6.5	C11.H11.O2
176.0833	*	585104	6.77	0.90	0.4	6.0	C11.H12.O2
181.0507	*	1080029	12.50	1.67	-0.6	5.5	C9.H9.04
181.0873	*	1420867	16.44	2.19	-0.8	4.5	C10.H13.03
182.0928	*	560820	6.49	0.86	1.4	4.0	C10.H14.03
189.0909	*	782790	9.06	1.21	0.7	6.5	C12.H13.02
190.0971	*	425124	4.92	0.66	2.3	6.0	C12.H14.02
194.0928	*	557553	6.45	0.86	1.5	5.0	C11.H14.03
195.0653	*	1891862	21.89	2.92	0.4	5.5	C10.H11.04
196.0719	*	1956408	22.63	3.02	1.7	5.0	C10.H12.04
197.0792	*	1770580	20.48	2.73	2.1	4.5	C10.H13.04
205.0848	*	299582	3.47	0.46	1.6	6.5	C12.H13.03
207.1015	*	1766036	20.43	2.72	0.6	5.5	C12.H15.03
208.1069	*	371513	4.30	0.57			
219.1031	*	292765	3.39	0.45	-1.0	6.5	C13.H15.03
222.0894	*	433929	5.02	0.67	-0.2	6.0	C12.H14.04
224.1044	*	869633	10.06	1.34	0.5	5.0	C12.H16.04
252.1003	*	325926	3.77	0.50	-0.5	6.0	C13.H16.05
355.1551	*	631969	7.31	0.97	-0.6	10.5	C21.H23.05
386.1725	*	8643584	100.00	13.33	0.5	10.0	C22.H26.06
387.1757	*	2034943	23.54	3.14			
388.1792	*	299014	3.46	0.46			

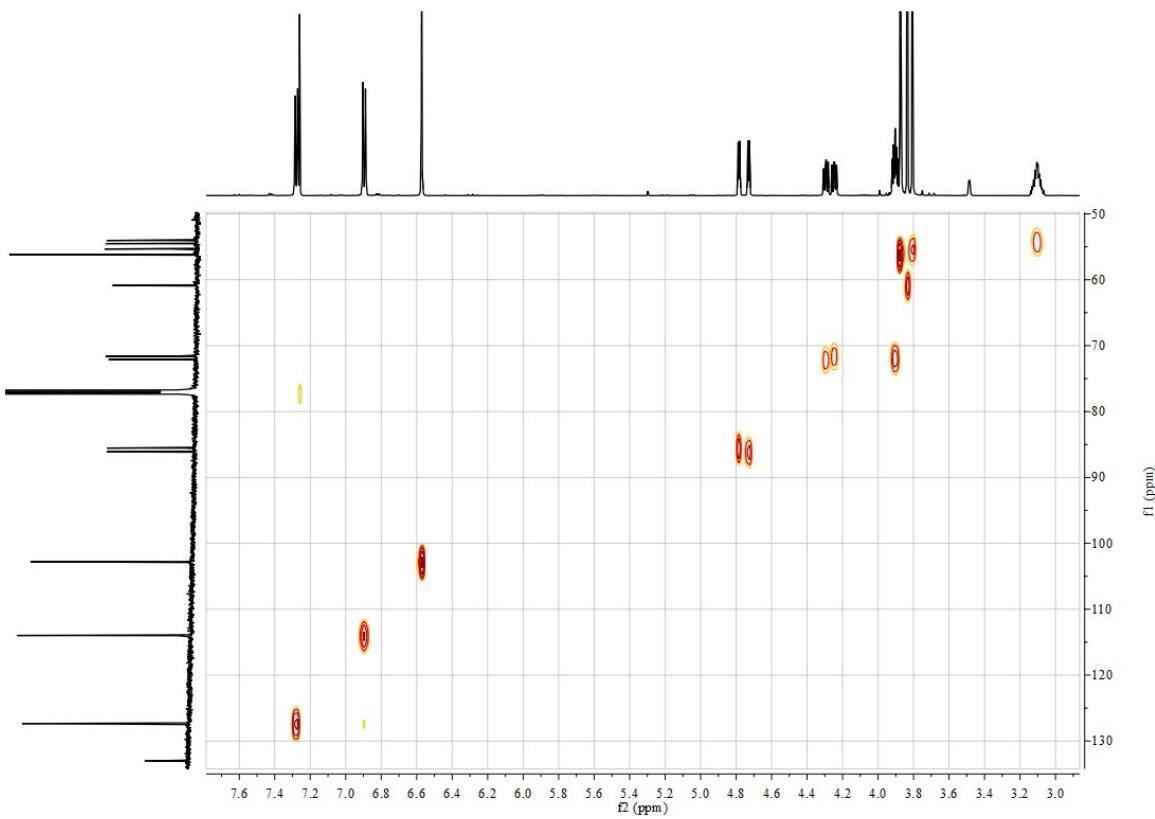
**S2.  $^1\text{H}$  NMR of 1 tested in  $\text{CDCl}_3$**



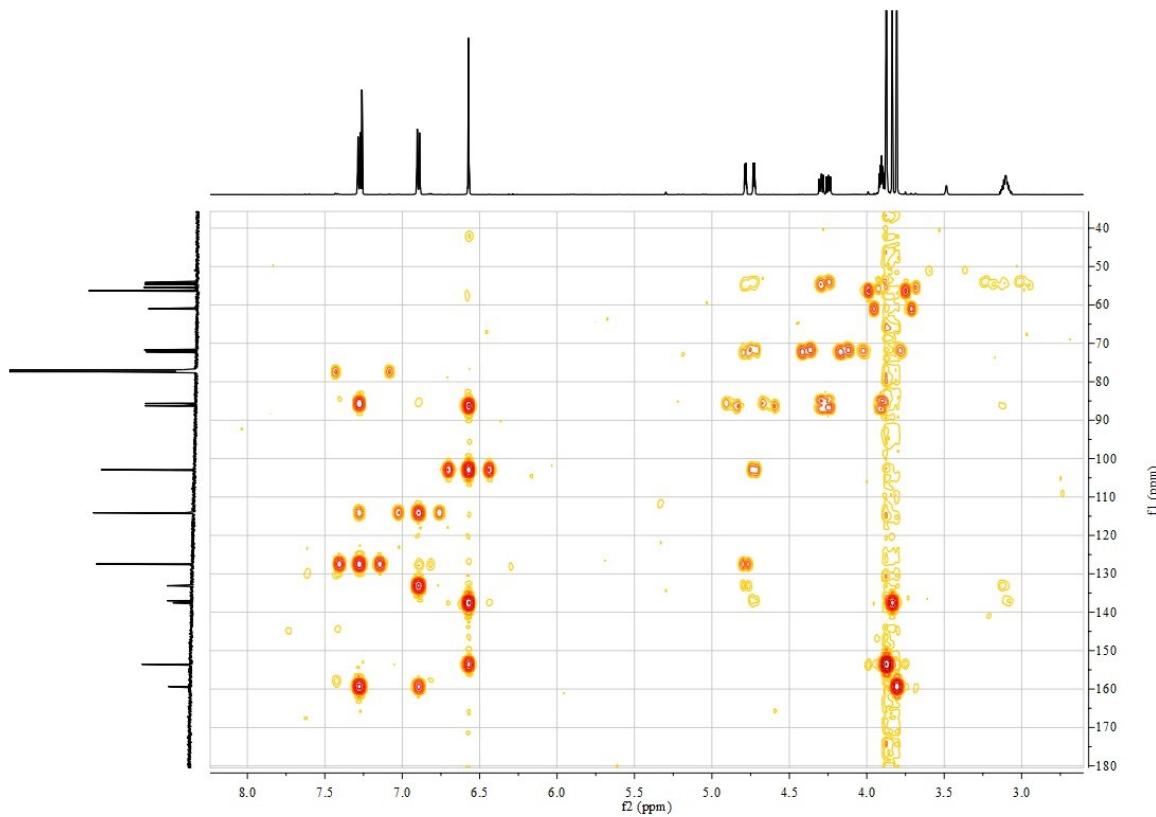
**S3.  $^{13}\text{C}$  NMR spectrum of 1 tested in  $\text{CDCl}_3$**



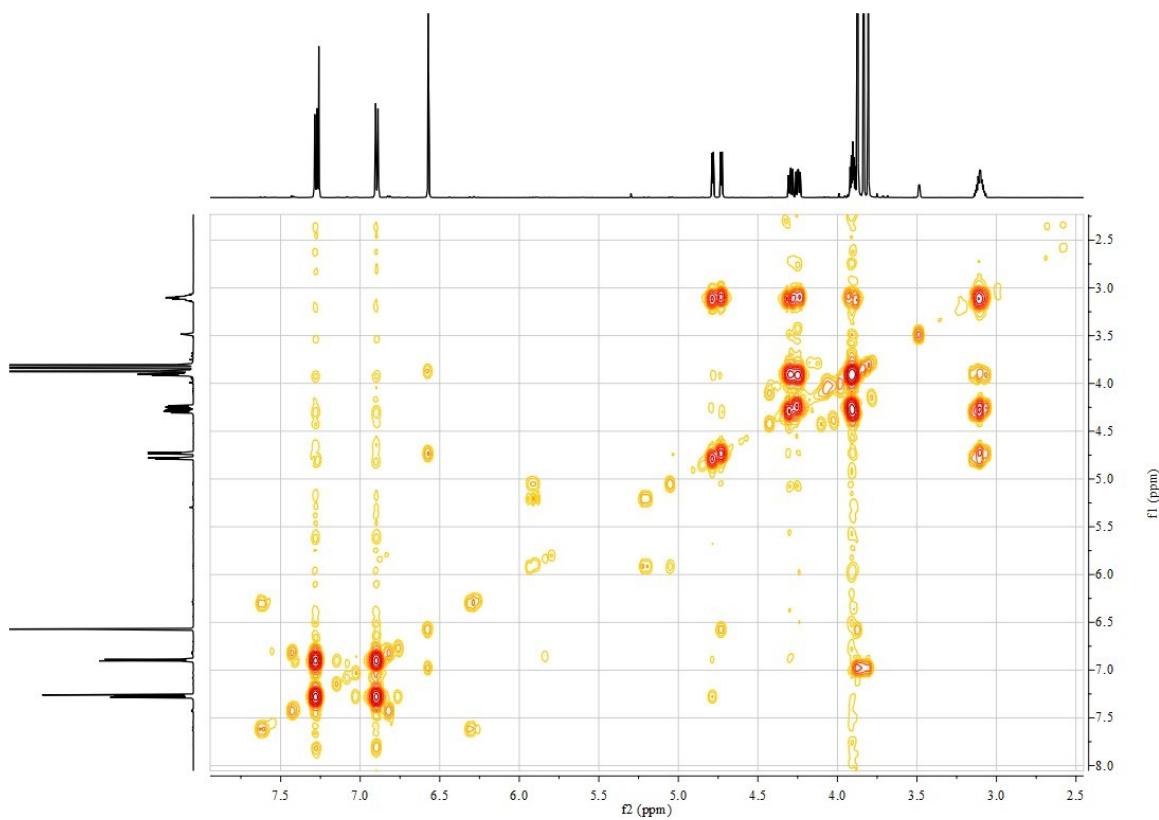
S4. HSQC spectrum of 1 tested in  $\text{CDCl}_3$



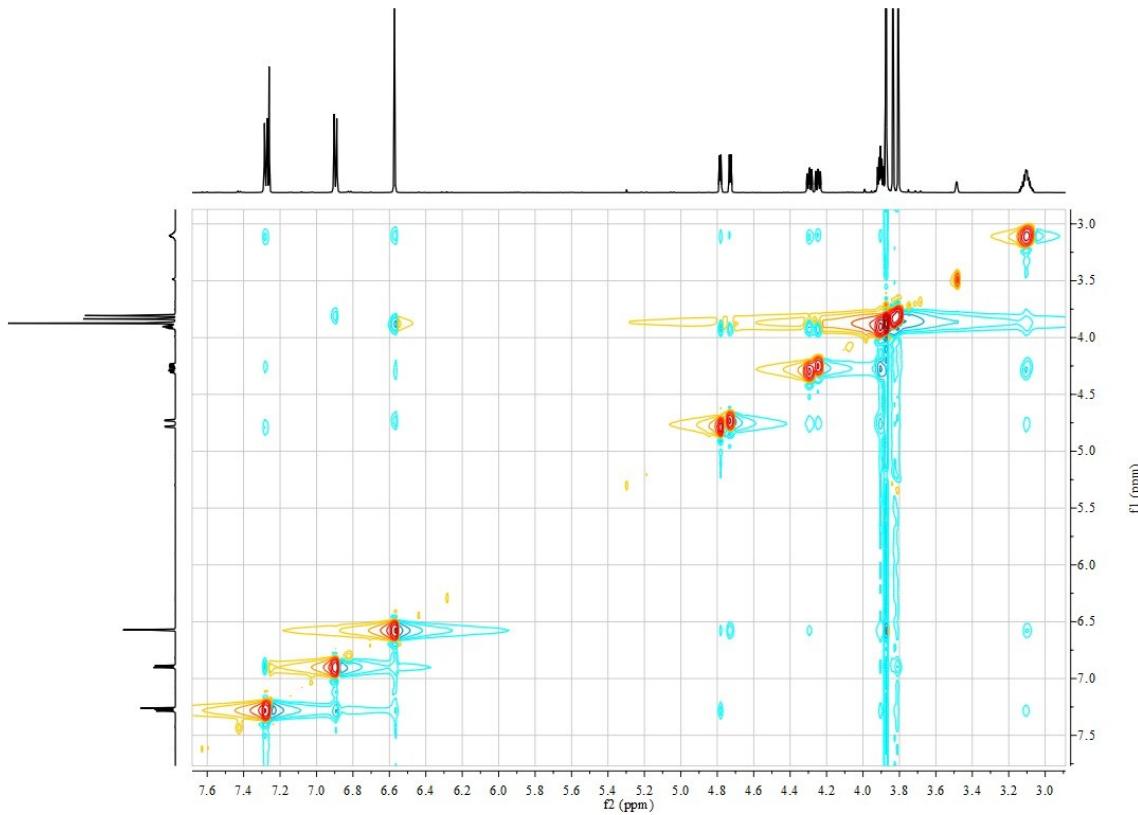
**S5. HMBC spectrum of 1 tested in  $\text{CDCl}_3$**



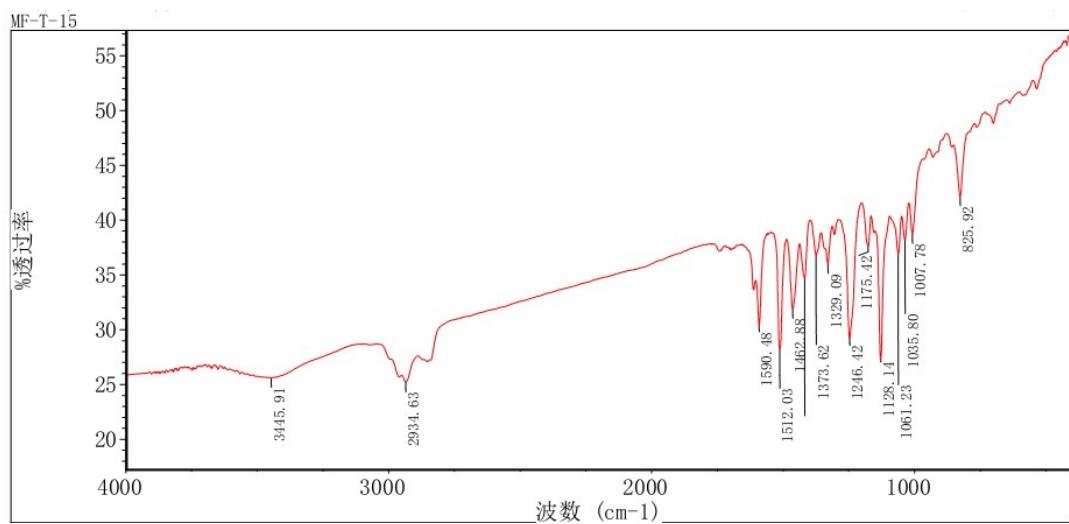
**S6.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 1 tested in  $\text{CDCl}_3$**



**S7. NOESY spectrum of 1 tested in  $\text{CDCl}_3$**



**S8. IR spectrum of 1**



## S9. CD data of 1

Rudolph Research Analytical

Wednesday, 08/24/2016

This sample was measured on an Autopol VI, serial number 90079,  
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

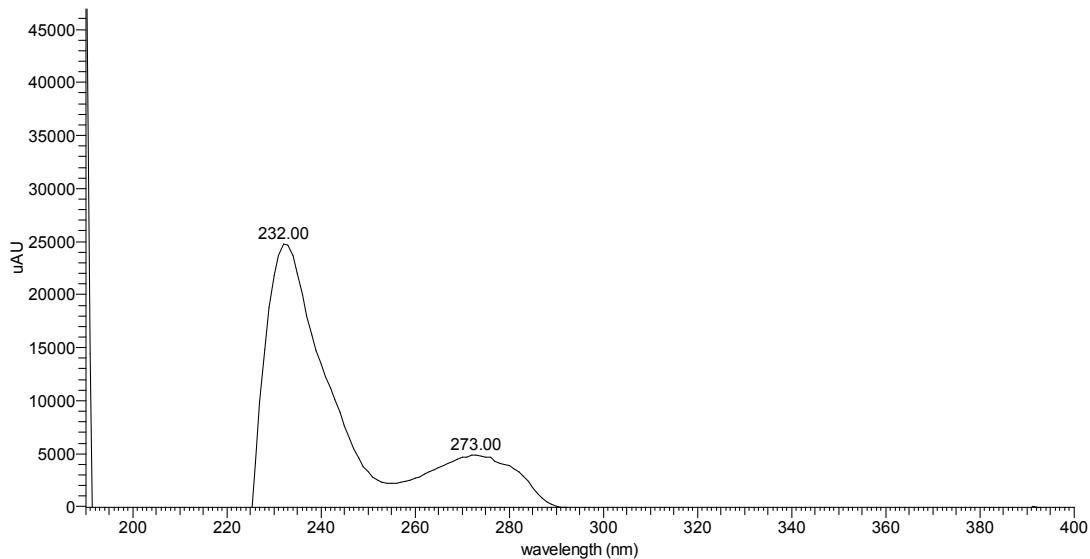
LotID : MF-T-15(25)  
Set Temperature : 25.0  
Temp Corr : OFF

n	Average	Std.Dev.	Maximum			Minimum		
6	70.000	0.0000	70.000			70.000		
S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.
1	MF-T-15(25)	04:26:52 PM	70.000	SR	0.070	589	100.00	0.100
2	MF-T-15(25)	04:26:58 PM	70.000	SR	0.070	589	100.00	0.100
3	MF-T-15(25)	04:27:03 PM	70.000	SR	0.070	589	100.00	0.100
4	MF-T-15(25)	04:27:09 PM	70.000	SR	0.070	589	100.00	0.100
5	MF-T-15(25)	04:27:15 PM	70.000	SR	0.070	589	100.00	0.100
6	MF-T-15(25)	04:27:20 PM	70.000	SR	0.070	589	100.00	0.100
								25.1
								25.2

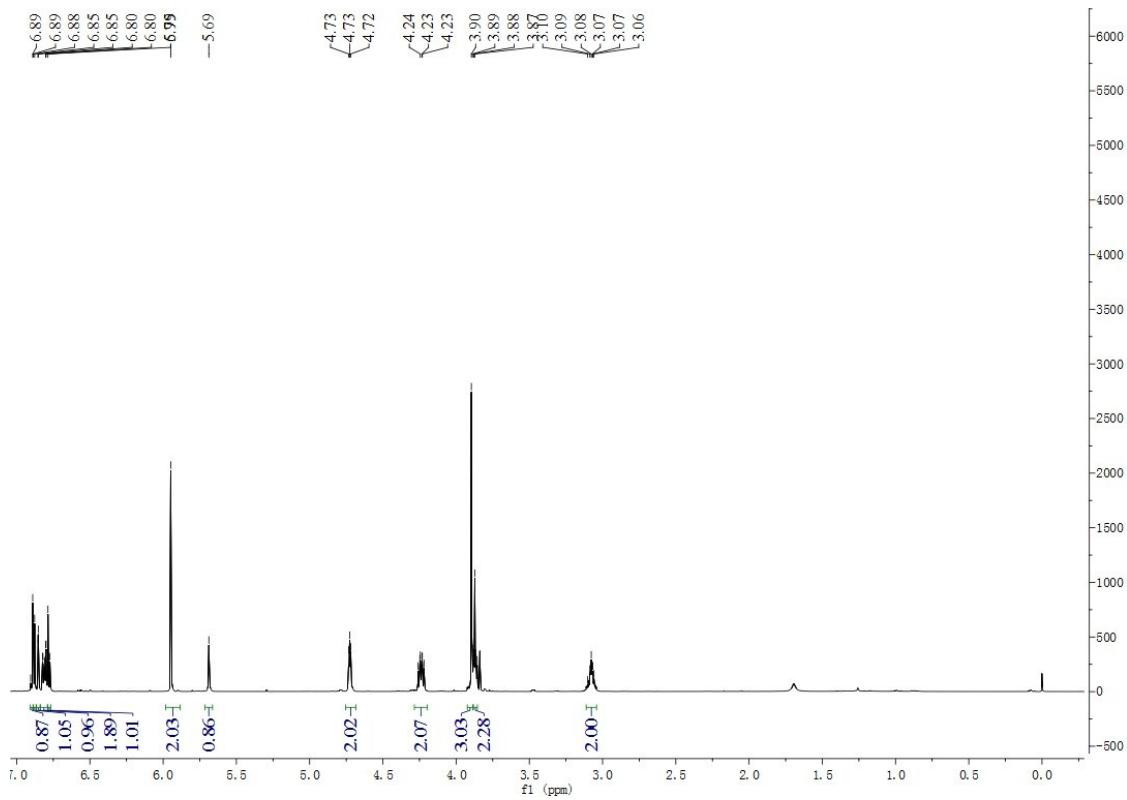
\_\_\_\_\_  
Signature

## S10. UV data of 1

T-15 #2407 RT: 9.63 AV: 1 NL: 9.37E4 microAU



**S11.  $^1\text{H}$  NMR of 2 tested in  $\text{CDCl}_3$**

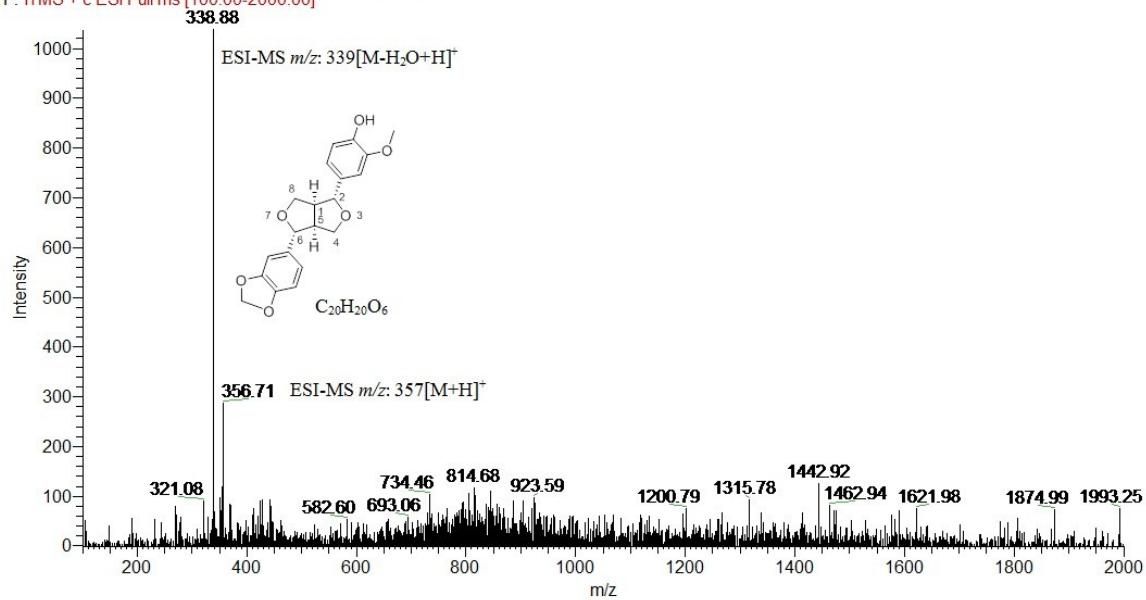


**Pluviatilol (2)**

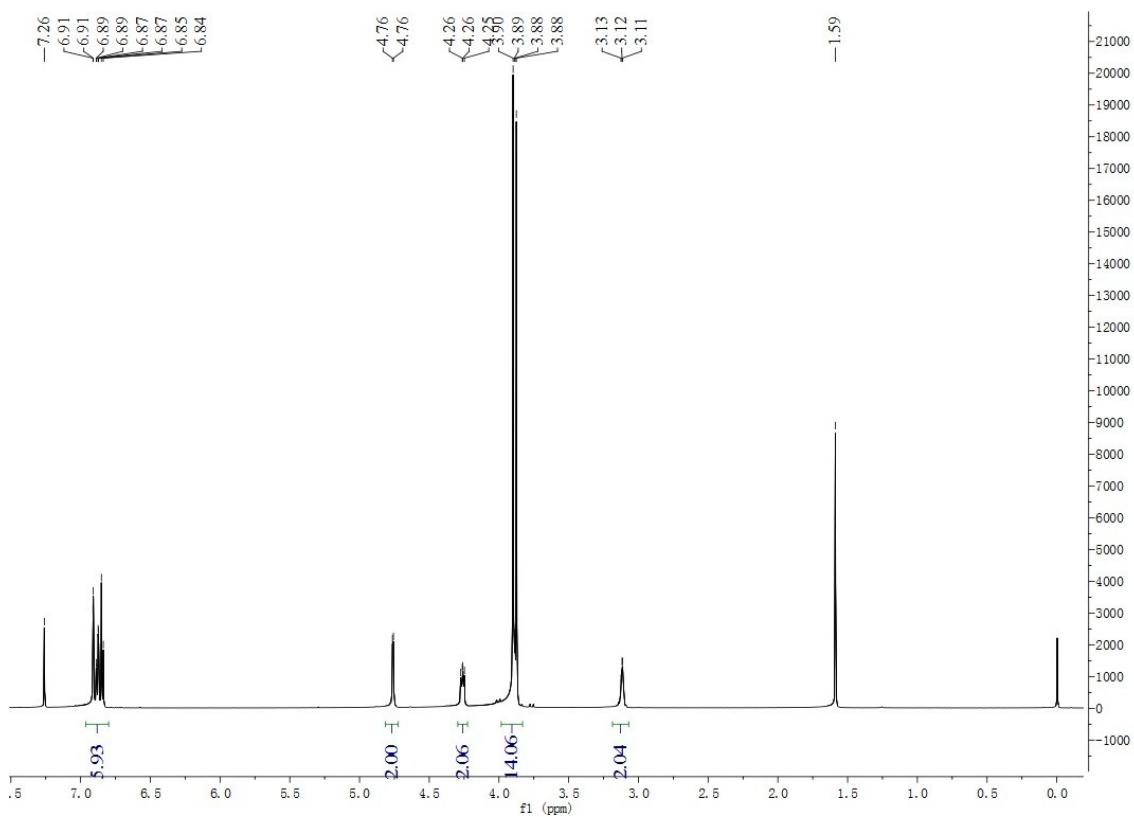
$^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.71~6.90 (6H, m, H-Ar), 5.95 (2H, s, H-OCH<sub>2</sub>O), 5.69 (1H, s, H-OH), 4.73 (2H, t,  $J$  = 3.7 Hz, H-2, 6), 4.24 (2H, m, H-8, 4), 3.90 (3H, s, H-OMe), 3.86~3.88 (2H, m, H-8, 4), 3.08 (2H, m, H-1, 5). C<sub>20</sub>H<sub>20</sub>O<sub>6</sub>, ESI-MS  $m/z$ : 357 [M+H]<sup>+</sup>, 339 [M-H<sub>2</sub>O+H]<sup>+</sup>.

## S12. LR-ESI-MS of 2

MF-T-5\_151112100654 #485 RT: 8.49 AV: 1 NL: 1.04E3  
F: ITMS + c ESI Full ms [100.00-2000.00]



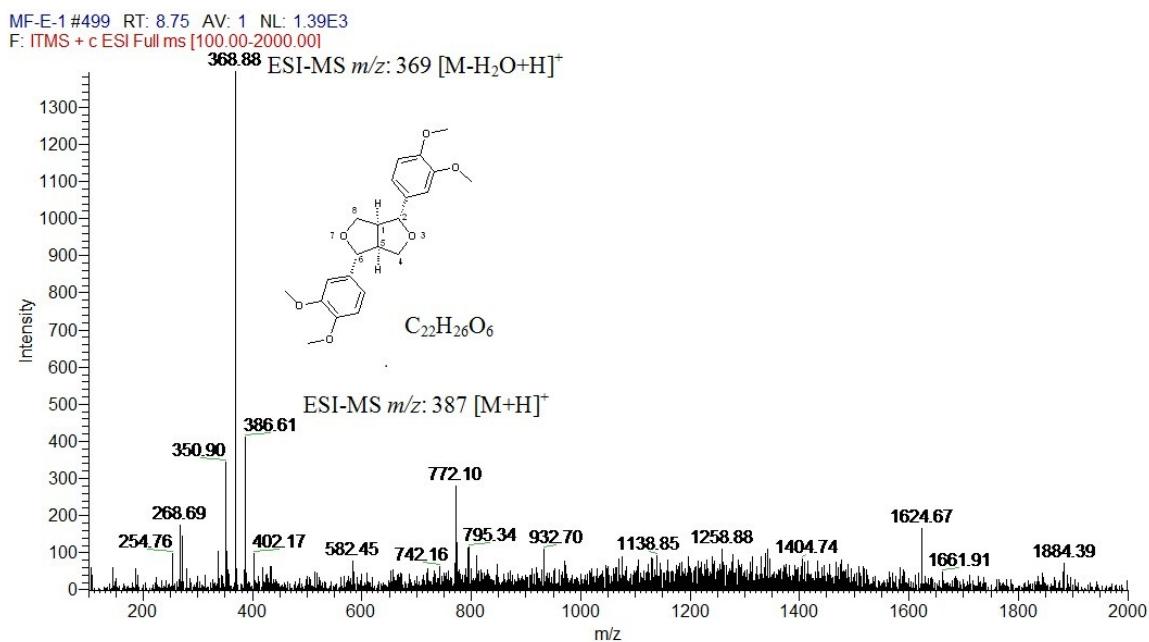
**S13.  $^1\text{H}$  NMR of 3 tested in  $\text{CDCl}_3$**



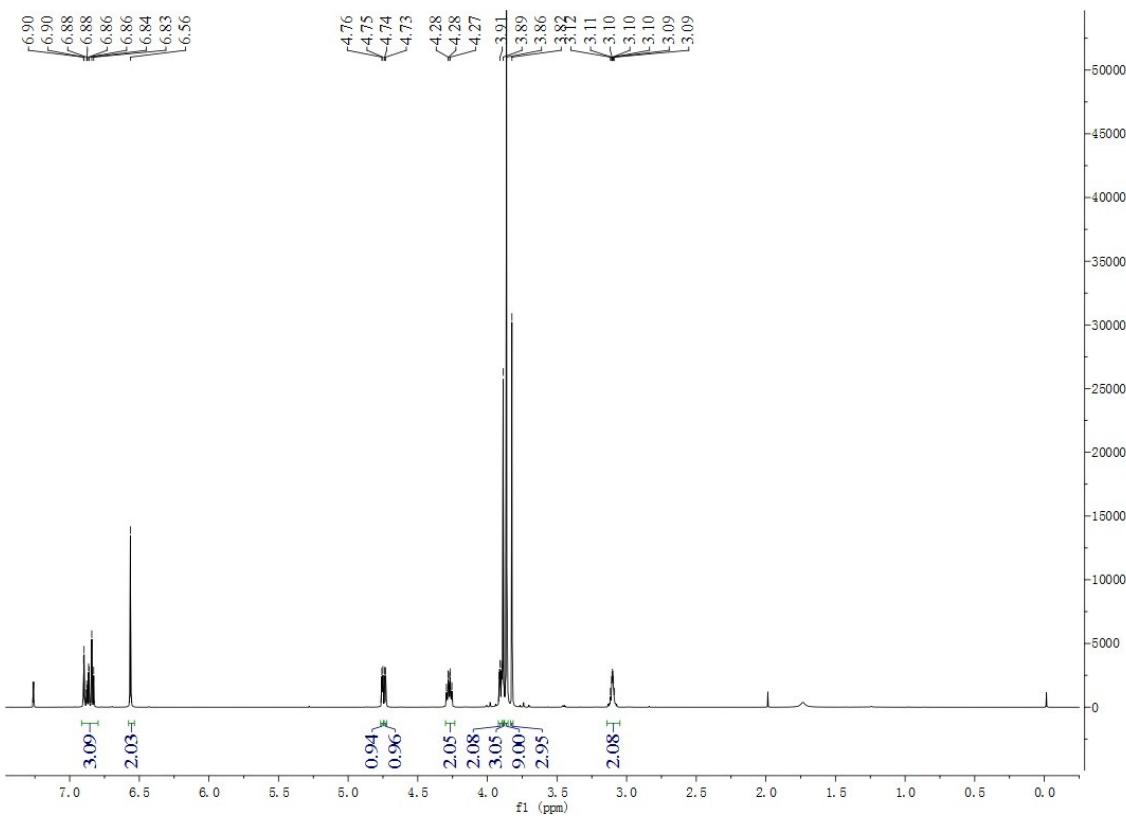
Pinoresinol dimethyl ether (**3**)

$^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.84-6.91 (6H, m, H-Ar), 4.76 (2H, d,  $J = 4.2$  Hz, H-2, 6), 4.26 (2H, dd,  $J = 6.8, 9.0$  Hz, H-4, 8), 3.88-3.90 (2H, m, H-4, 8), 3.90 (6H, s, H-OMe), 3.88 (6H, s, H-OMe), 3.12 (2H, m, H-1, 5).  $\text{C}_{22}\text{H}_{26}\text{O}_6$ , ESI-MS  $m/z$ : 387 [ $\text{M}+\text{H}]^+$ , 369 [ $\text{M}-\text{H}_2\text{O}+\text{H}]^+$ .

## S14. LR-ESI-MS of 3



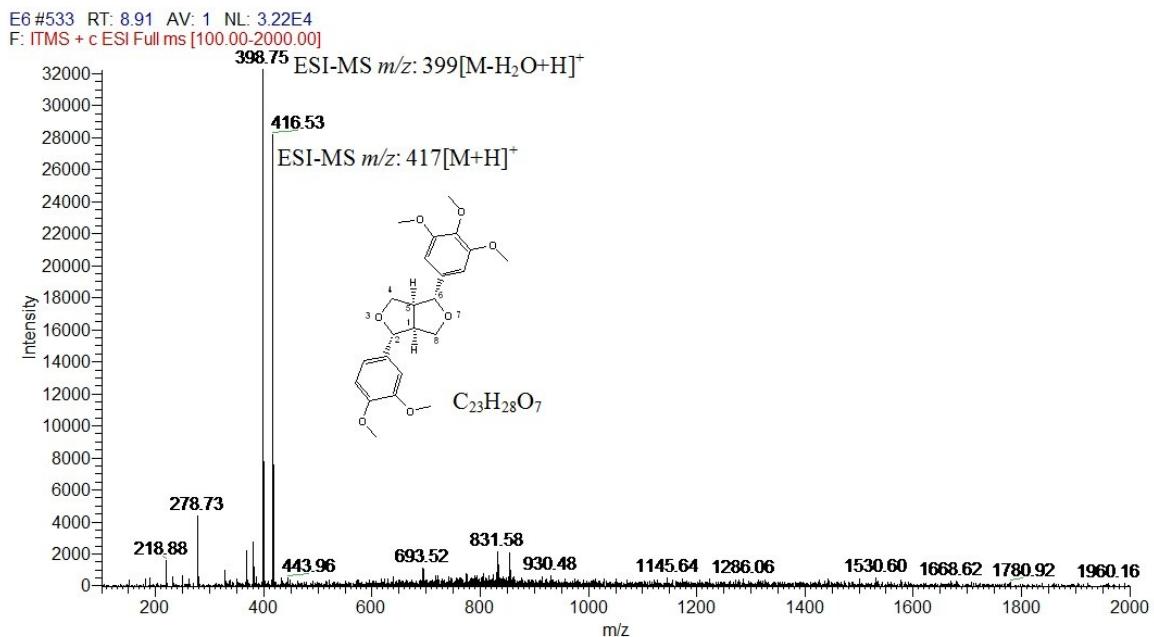
**S15.  $^1\text{H}$  NMR of 4 tested in  $\text{CDCl}_3$**



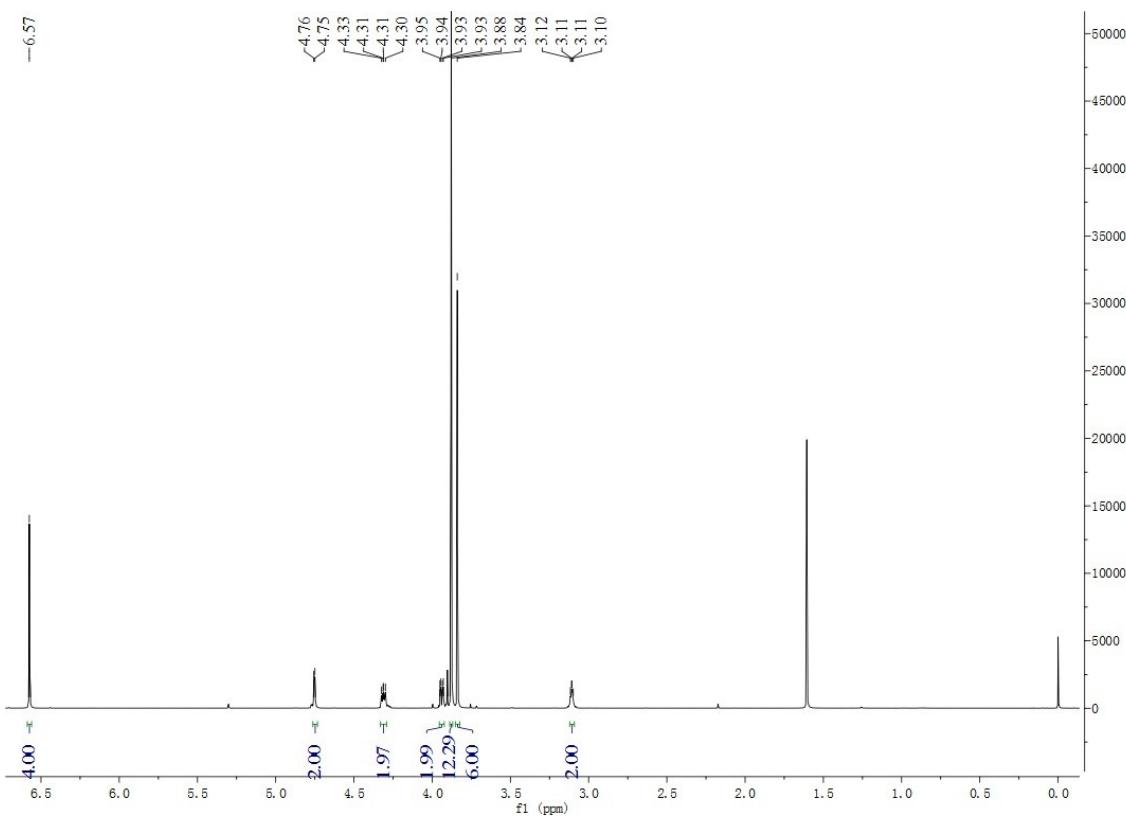
Magnolin (**4**)

$^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.83~6.90 (3H, m, H-Ar), 6.56 (2H, s, H-Ar), 4.75 (1H, d,  $J$  = 4.5 Hz, H-6), 4.73 (1H, d,  $J$  = 4.5 Hz, H-2), 4.27 (2H, m, H-4, 8), 3.91 (2H, m, H-4, 8), 3.89 (3H, s, H-OMe), 3.86 (9H, s, H-OMe), 3.82 (3H, s, H-OMe), 3.10 (2H, m, H-1, 5).  $\text{C}_{23}\text{H}_{28}\text{O}_7$ , ESI-MS  $m/z$ : 417 [ $\text{M}+\text{H}]^+$ , 399 [ $\text{M}-\text{H}_2\text{O}+\text{H}]^+$ .

## S16. LR-ESI-MS of 4



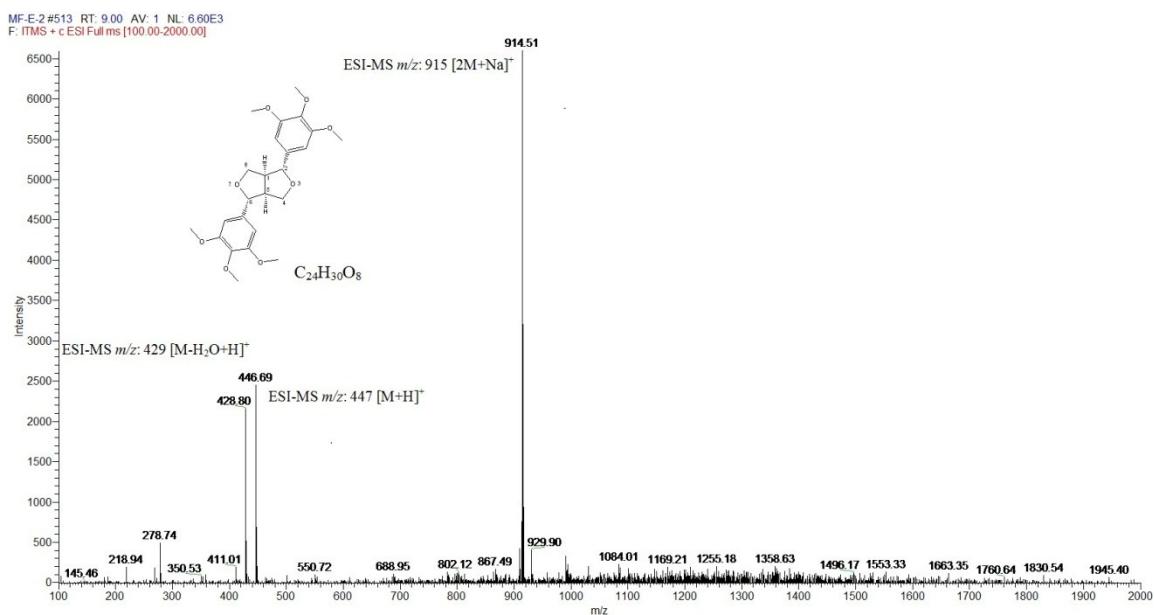
**S17.  $^1\text{H}$  NMR of 5 tested in  $\text{CDCl}_3$**



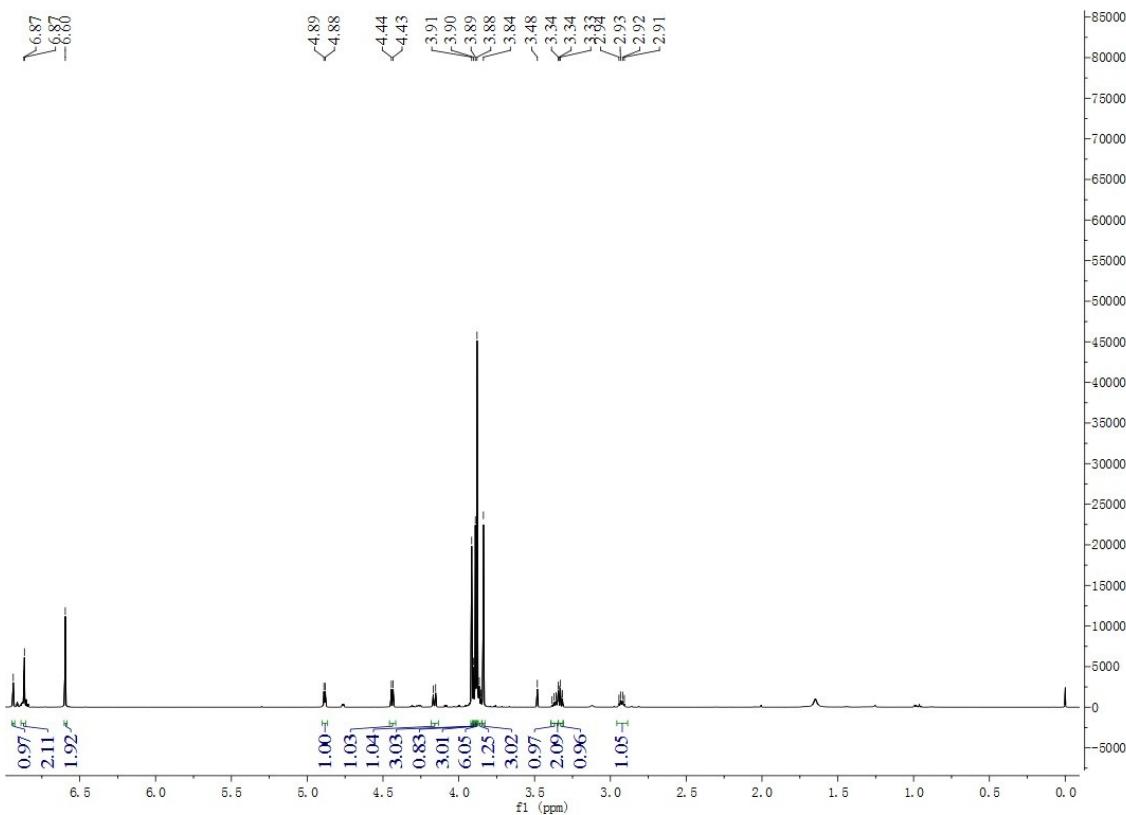
Lirioresinol-B dimethyl ether (**5**)

$^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.57 (4H, s, H-Ar), 4.75 (2H, d,  $J = 4.2$  Hz, H-2, 6), 4.31 (2H, dd,  $J = 6.9, 9.2$  Hz, H-4, 8), 3.94 (2H, m, H-4, 8), 3.88 (12H, s, H-OMe), 3.84 (6H, s, H-OMe), 3.11 (2H, m, H-1, 5).  $\text{C}_{24}\text{H}_{30}\text{O}_8$ , ESI-MS  $m/z$ : 447 [M+H] $^+$ , 429 [M-H<sub>2</sub>O+H] $^+$ .

## S18. LR-ESI-MS of 5



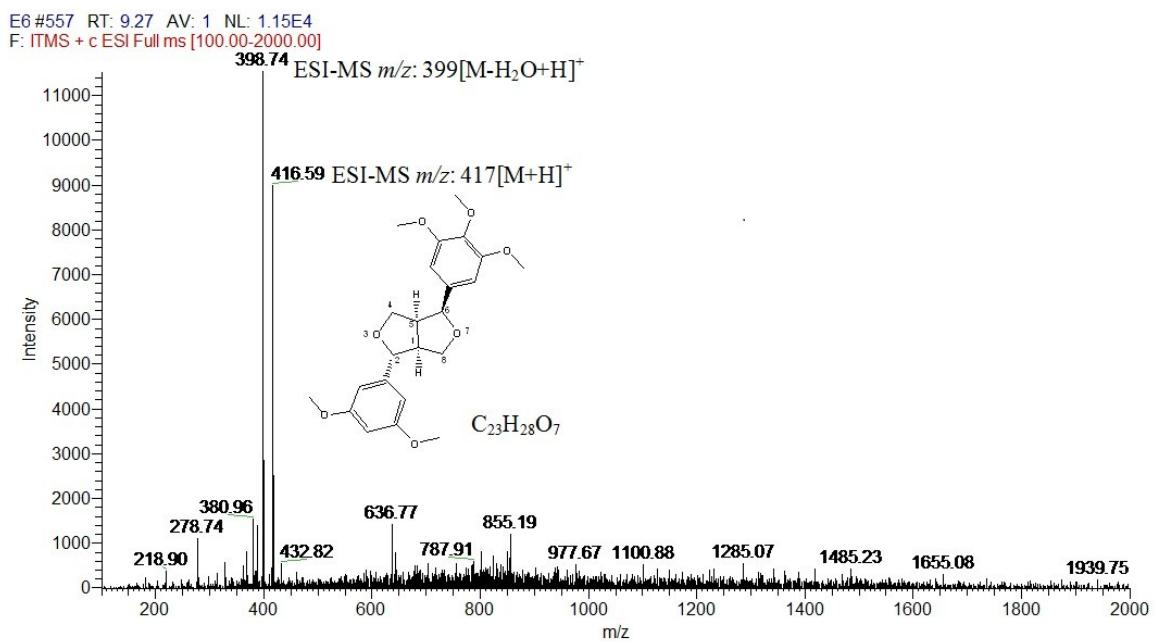
**S19.  $^1\text{H}$  NMR of 6 tested in  $\text{CDCl}_3$**



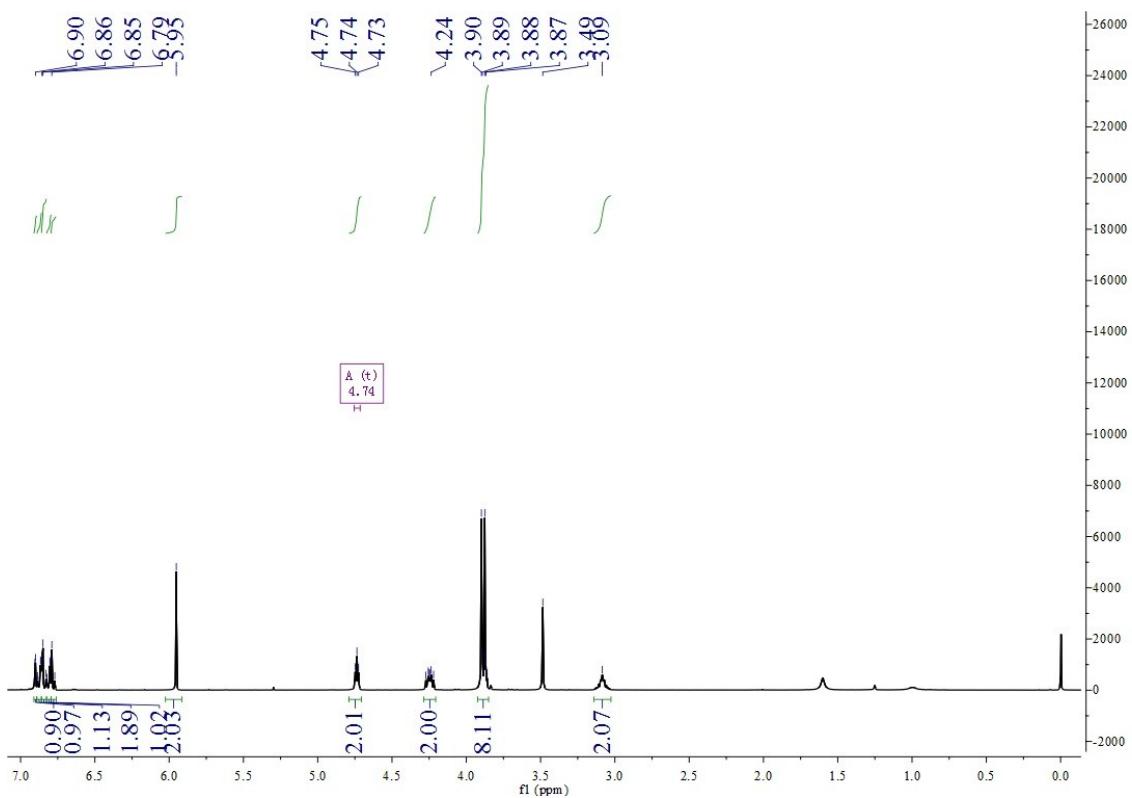
### Epimagnolin B (**6**)

<sup>1</sup>H-NMR (CDCl<sub>3</sub>, 600MHz) δH: 6.84~6.94 (3H, m, H-Ar), 6.60 (2H, s, H-Ar), 4.89 (1H, d, *J* = 5.6 Hz, H-6), 4.44 (1H, d, *J* = 7.0 Hz, H-2), 4.27 (1H, d, *J* = 9.7 Hz, H-8), 3.85~3.90 (2H, m, H-4, 8), 3.91 (3H, s, H-OMe), 3.89 (3H, s, H-OMe), 3.88 (6H, s, H-OMe), 3.84 (3H, s, H-OMe), 3.32~3.37 (2H, m, H-5, 4), 2.93 (1H, m, H-1). C<sub>23</sub>H<sub>28</sub>O<sub>7</sub>. ESI-MS *m/z*: 417 [M+H]<sup>+</sup>, 339 [M-H<sub>2</sub>O+H]<sup>+</sup>.

## S20. LR-ESI-MS of 6



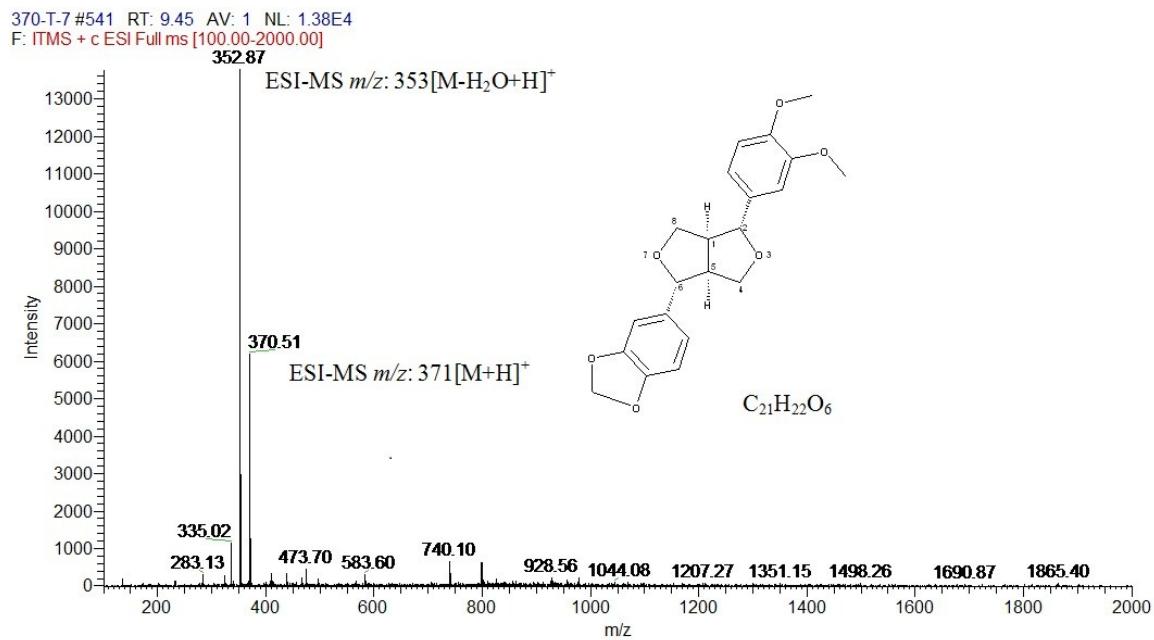
**S21.  $^1\text{H}$  NMR of 7 tested in  $\text{CDCl}_3$**



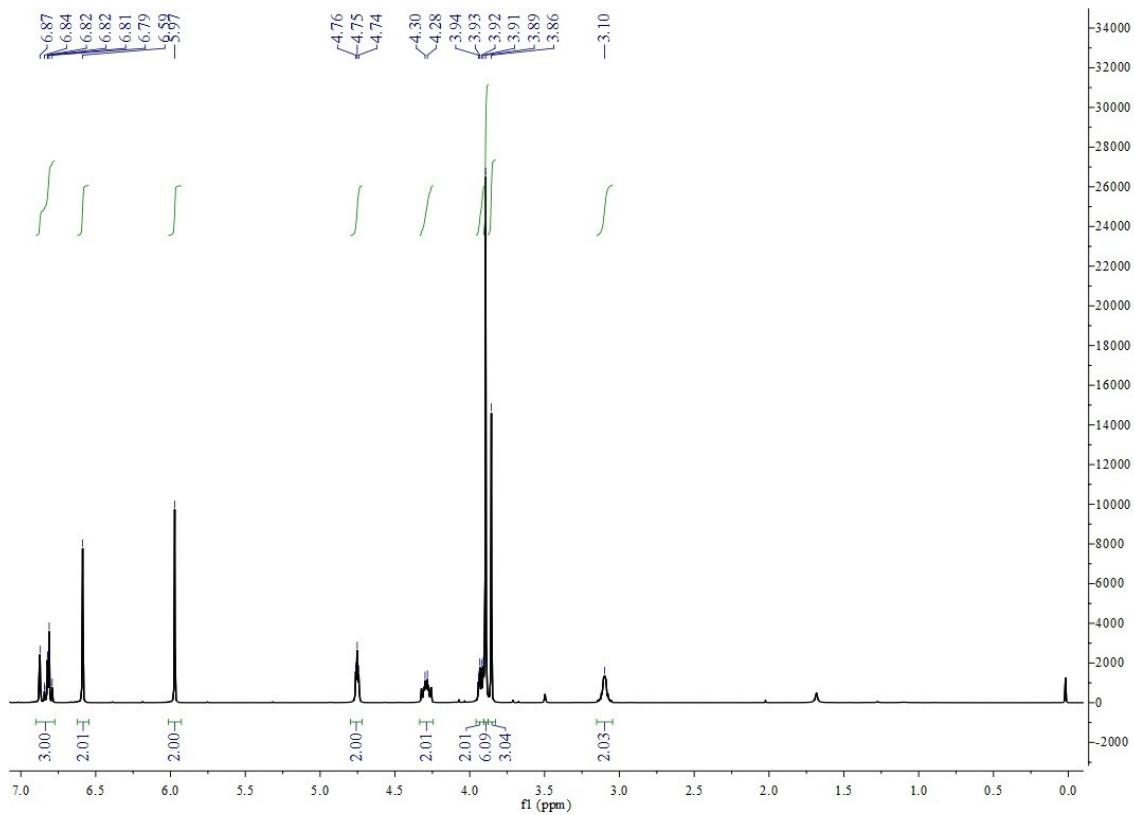
Kobusin (7)

$^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.77~6.90 (6H, m, H-Ar), 5.95 (2H, s, H-OCH<sub>2</sub>O), 4.74 (2H, t,  $J$  = 4.5 Hz, H-2, 6), 4.24 (2H, m, H-8, 4), 3.90 (3H, s, H-OMe), 3.88 (3H, s, H-OMe), 3.86~3.89 (2H, m, H-8, 4), 3.09 (2H, m, H-1, 5). C<sub>21</sub>H<sub>22</sub>O<sub>6</sub>, ESI-MS  $m/z$ : 371 [M+H]<sup>+</sup>, 353 [M-H<sub>2</sub>O+H]<sup>+</sup>.

## S22. LR-ESI-MS of 7



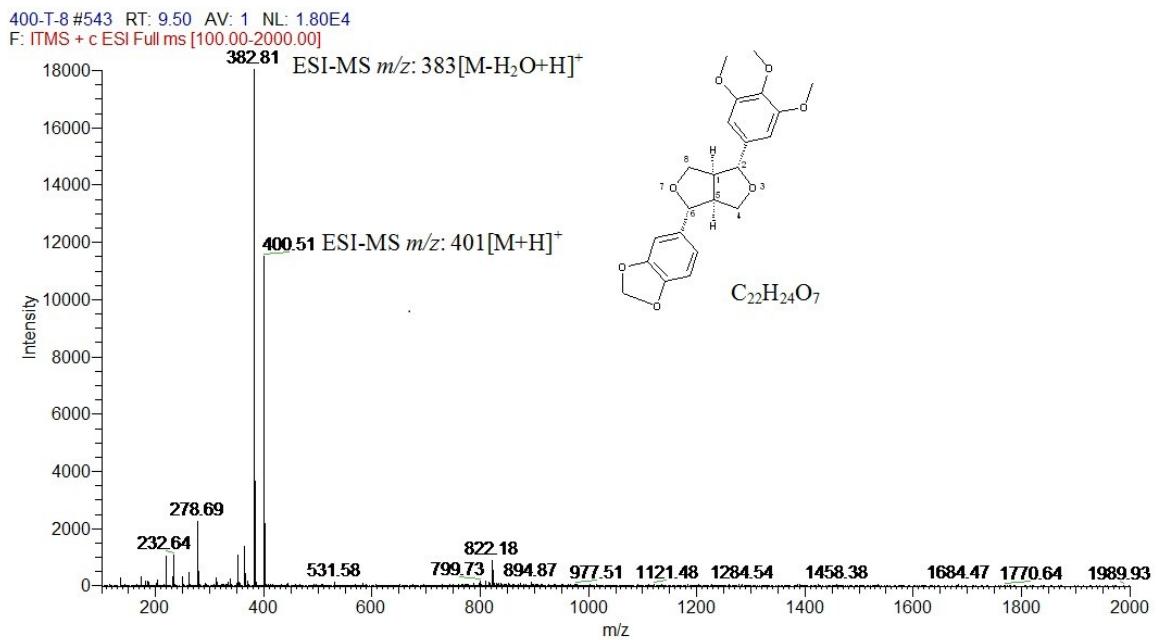
**S23.  $^1\text{H}$  NMR of **8** tested in  $\text{CDCl}_3$**



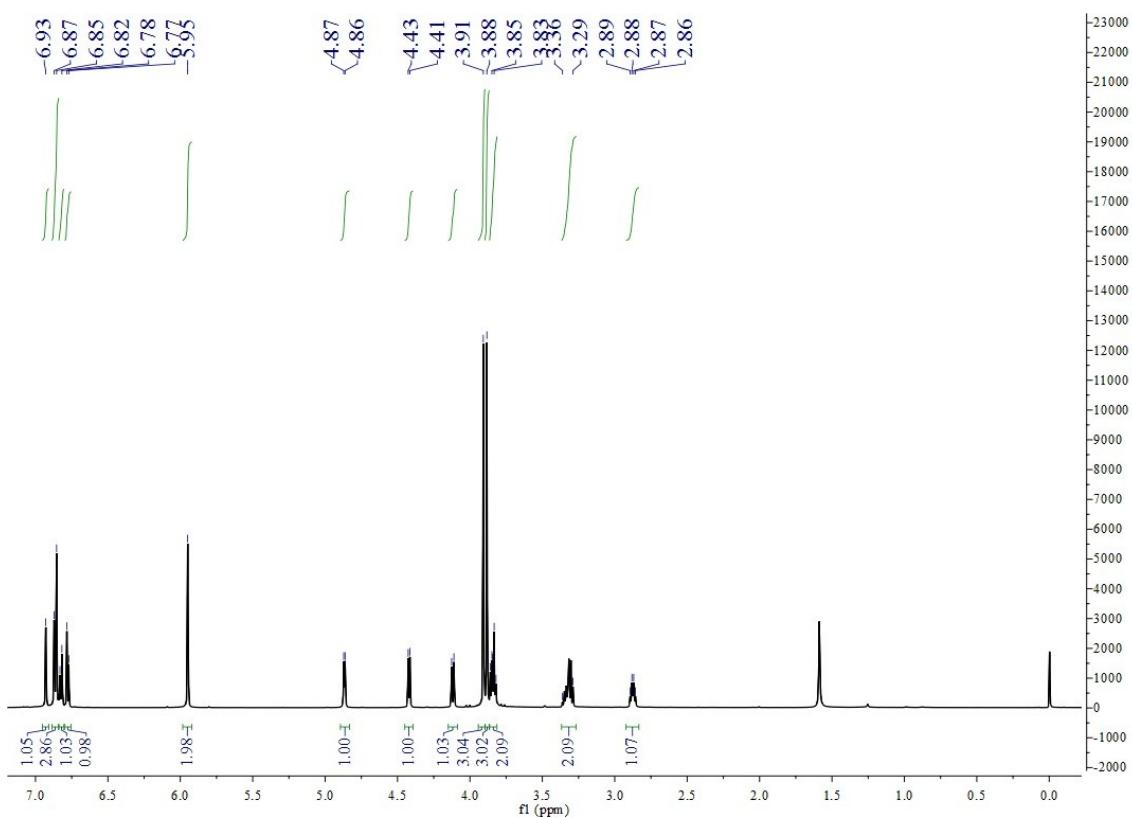
Aschantin(**8**)

$^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.79~6.87 (3H, m, H-Ar), 6.59 (2H, s, H-Ar), 5.97 (2H, s, H-OCH<sub>2</sub>O), 4.75 (2H, t,  $J$  = 4.0 Hz, H-2, 6), 4.29 (2H, m, H-8, 4), 3.91~3.94 (2H, m, H-8, 4), 3.89 (6H, s, H-OMe), 3.86 (3H, s, H-OMe), 3.10 (2H, m, H-1, 5). C<sub>22</sub>H<sub>24</sub>O<sub>7</sub>, ESI-MS  $m/z$ : 401 [M+H]<sup>+</sup>, 383 [M-H<sub>2</sub>O+H]<sup>+</sup>.

## S24. LR-ESI-MS of 8



**S25.  $^1\text{H}$  NMR of 9 tested in  $\text{CDCl}_3$**



Fargesin (**9**)

$^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.77~6.93(6H, m, H-Ar), 5.95(2H, s, H-OCH<sub>2</sub>O), 4.87(1H, d,  $J$  = 5.6 Hz, H-2), 4.42(1H, d,  $J$  = 7.0 Hz, H-6), 4.12(1H, d,  $J$  = 9.4 Hz, H-4e), 3.91 (3H, s, H-OMe), 3.88 (3H, s, H-OMe), 3.82~3.86 (2H, m, H-4a, 8e), 3.29~3.36 (2H, m, H-8a, 1), 2.88 (1H, m, H-5).  $\text{C}_{21}\text{H}_{22}\text{O}_6$ , ESI-MS  $m/z$ : 371 [M+H]<sup>+</sup>, 353 [M-H<sub>2</sub>O+H]<sup>+</sup>.

## S26. LR-ESI-MS of 9

T-14-370 #577 RT: 9.86 AV: 1 NL: 6.06E2  
F: ITMS + c ESI Full ms [100.00-2000.00]

