

Electronic supplementary information for

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

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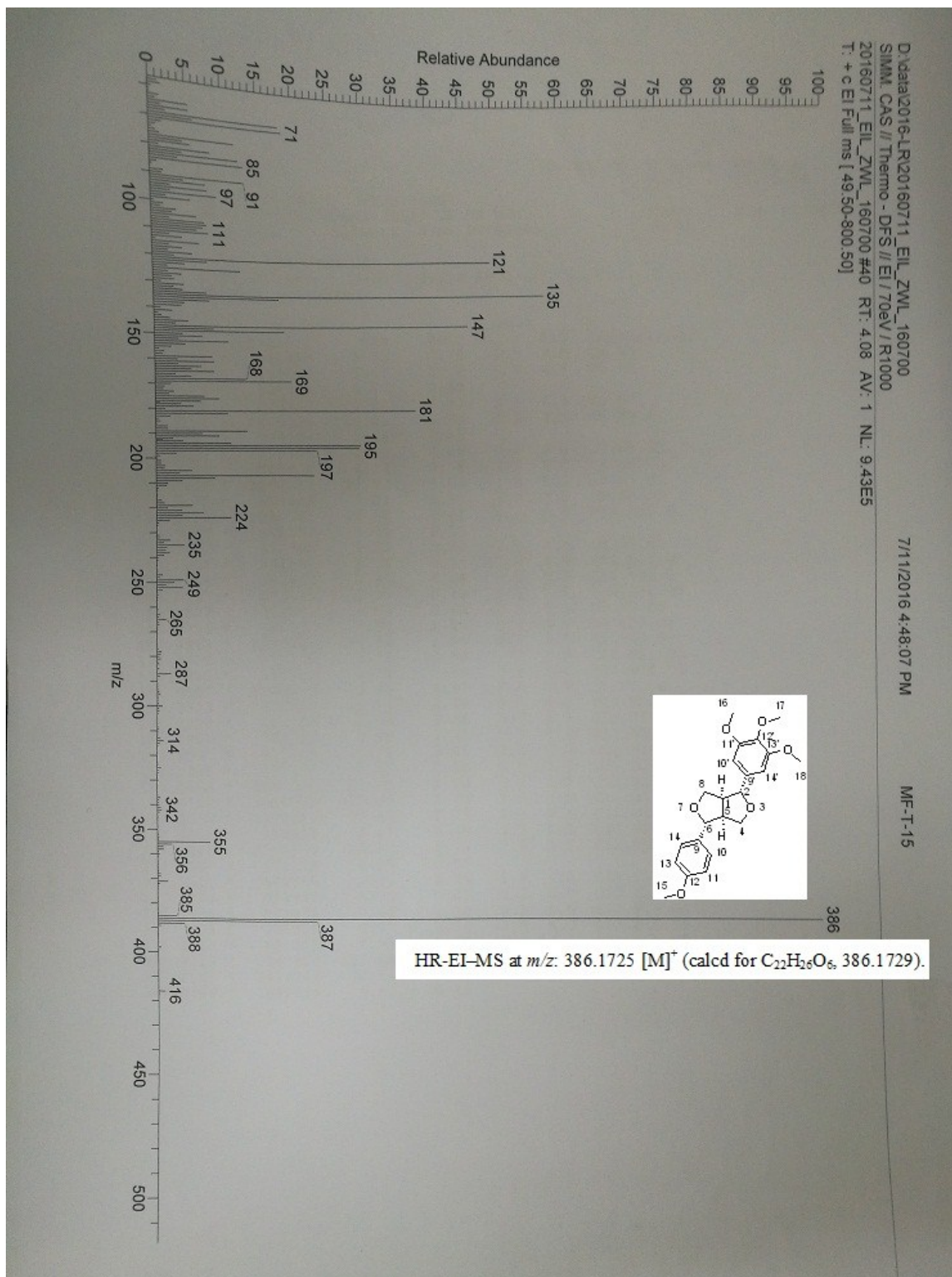
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# S1. HR-EI-MS of 1

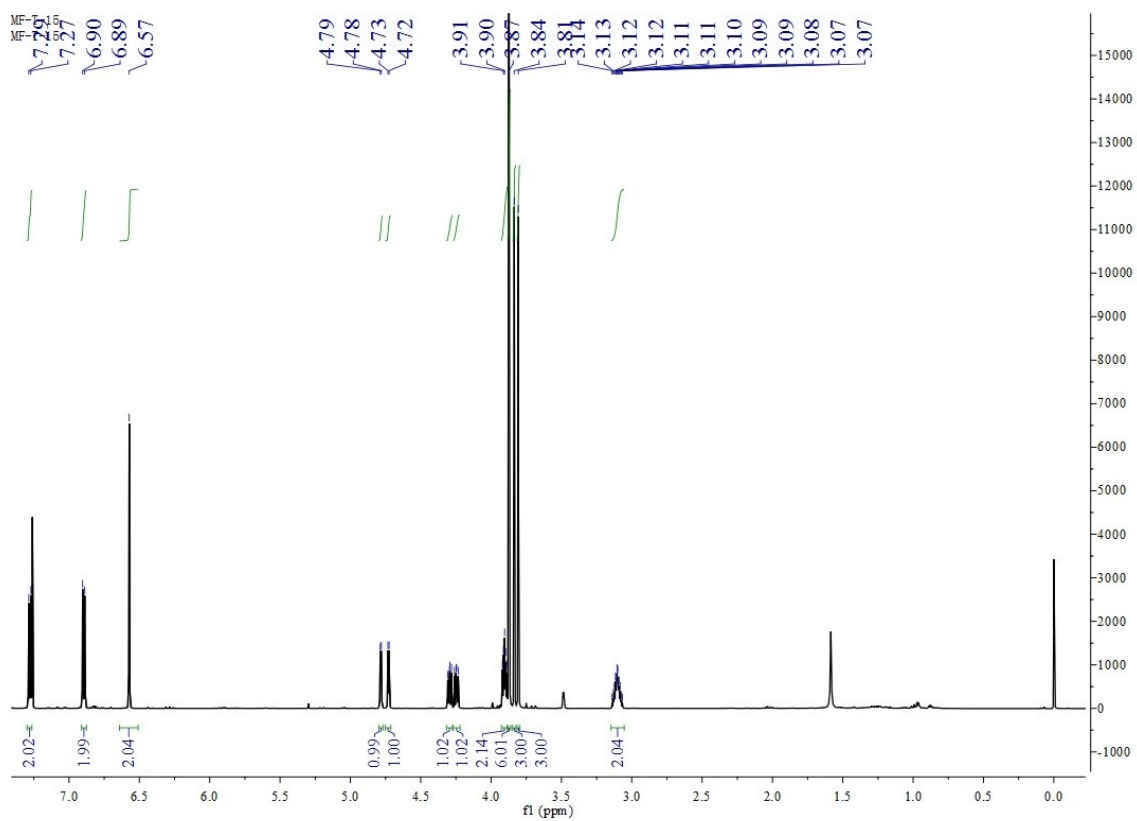


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 Comm: Finnigan/MAT95/70eV/R:10000  
 Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM  
 Oper: SIMM.CAS Client: S/N: PT001263  
 Limt: ( 0 )  
 : ( 485 ) C24.H100.O6  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: CMASS : converted

13-Jul-16 Elapse: 06:58.3 33  
 Start : 11:12:59 34  
 Study : S/N: PT200712-01-01  
 Inlet :

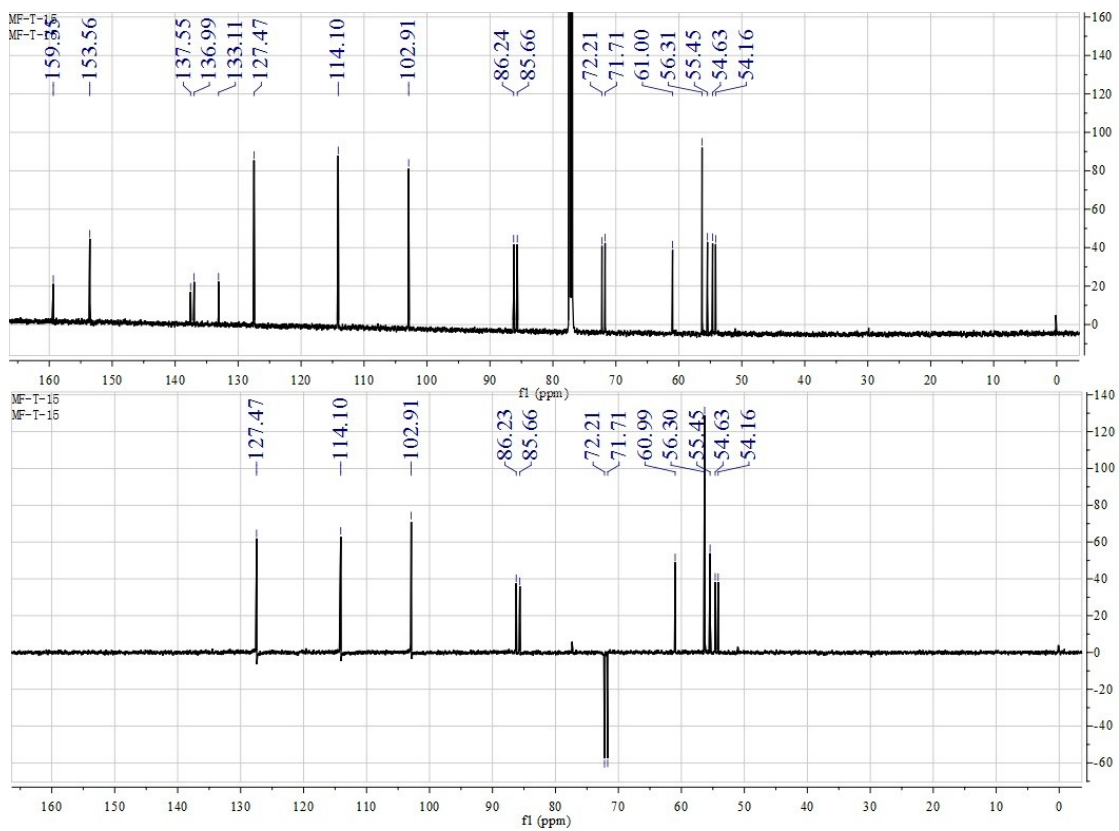
| 259313   |           | (mmu)  |       |       |      |             |
|----------|-----------|--------|-------|-------|------|-------------|
| Mass     | Intensity | %RA    | %RIC  | Delta | R+D  | Composition |
| 77.04061 | * 494498  | 5.72   | 0.76  | -1.5  | 4.5  | C6.H5       |
| 91.05448 | * 468012  | 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.O2    |
| 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.O2    |
| 136.0496 | * 808069  | 9.35   | 1.25  | 2.9   | 5.0  | C8.H8.O2    |
| 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.O3    |
| 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.O3    |
| 168.0786 | * 783855  | 9.07   | 1.21  | 0.0   | 4.0  | C9.H12.O3   |
| 169.0863 | * 1268981 | 14.68  | 1.96  | 0.2   | 3.5  | C9.H13.O3   |
| 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.O4    |
| 181.0873 | * 1420867 | 16.44  | 2.19  | -0.8  | 4.5  | C10.H13.O3  |
| 182.0928 | * 560820  | 6.49   | 0.86  | 1.4   | 4.0  | C10.H14.O3  |
| 189.0909 | * 782790  | 9.06   | 1.21  | 0.7   | 6.5  | C12.H13.O2  |
| 190.0971 | * 425124  | 4.92   | 0.66  | 2.3   | 6.0  | C12.H14.O2  |
| 194.0928 | * 557553  | 6.45   | 0.86  | 1.5   | 5.0  | C11.H14.O3  |
| 195.0653 | * 1891862 | 21.89  | 2.92  | 0.4   | 5.5  | C10.H11.O4  |
| 196.0719 | * 1956408 | 22.63  | 3.02  | 1.7   | 5.0  | C10.H12.O4  |
| 197.0792 | * 1770580 | 20.48  | 2.73  | 2.1   | 4.5  | C10.H13.O4  |
| 205.0848 | * 299582  | 3.47   | 0.46  | 1.6   | 6.5  | C12.H13.O3  |
| 207.1015 | * 1766036 | 20.43  | 2.72  | 0.6   | 5.5  | C12.H15.O3  |
| 208.1069 | * 371513  | 4.30   | 0.57  |       |      |             |
| 219.1031 | * 292765  | 3.39   | 0.45  | -1.0  | 6.5  | C13.H15.O3  |
| 222.0894 | * 433929  | 5.02   | 0.67  | -0.2  | 6.0  | C12.H14.O4  |
| 224.1044 | * 869633  | 10.06  | 1.34  | 0.5   | 5.0  | C12.H16.O4  |
| 252.1003 | * 325926  | 3.77   | 0.50  | -0.5  | 6.0  | C13.H16.O5  |
| 355.1551 | * 631969  | 7.31   | 0.97  | -0.6  | 10.5 | C21.H23.O5  |
| 386.1725 | * 8643584 | 100.00 | 13.33 | 0.5   | 10.0 | C22.H26.O6  |
| 387.1757 | * 2034943 | 23.54  | 3.14  |       |      |             |
| 388.1792 | * 299014  | 3.46   | 0.46  |       |      |             |

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

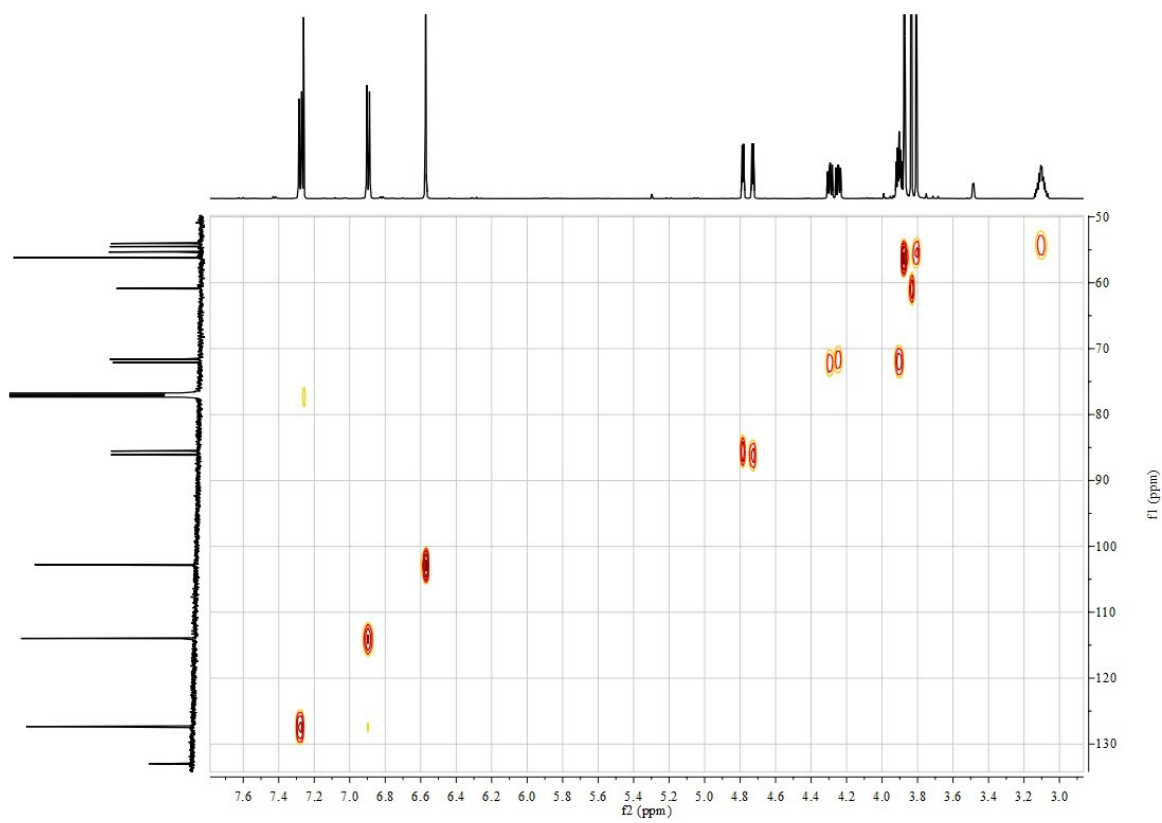




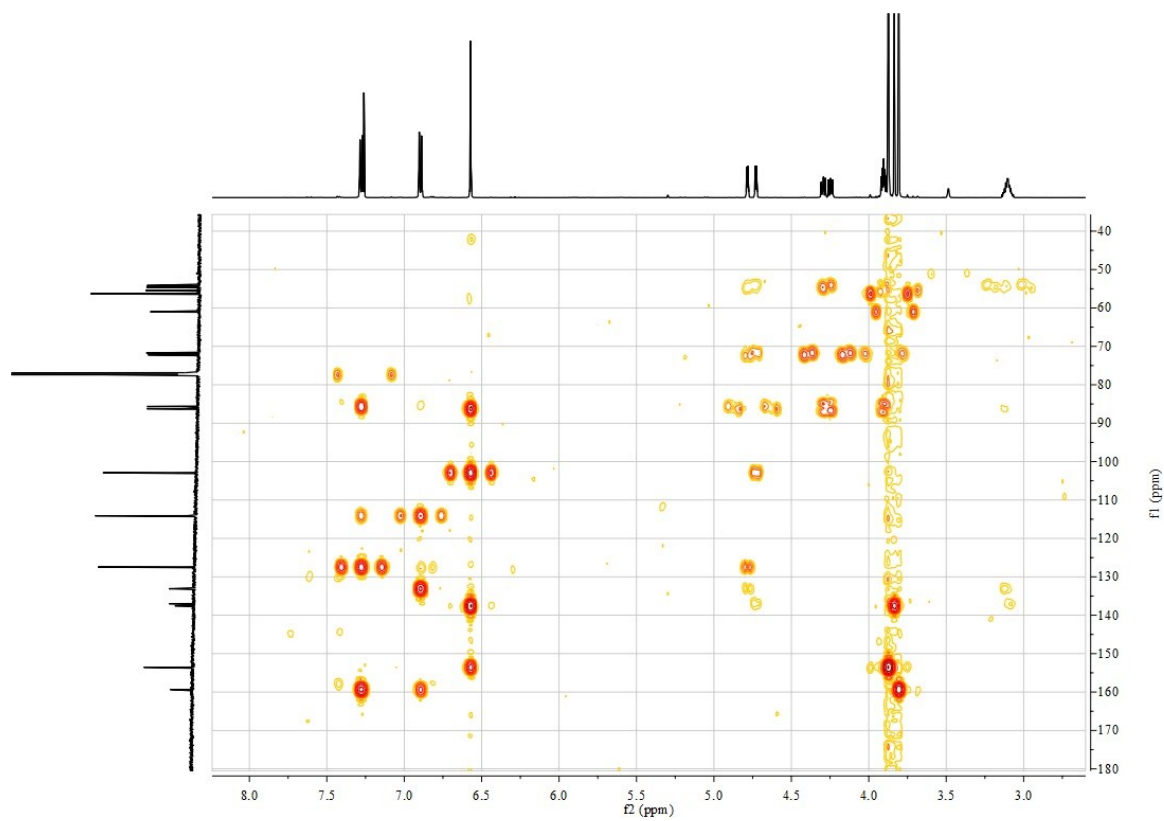
S3.  $^{13}\text{C}$  NMR spectrum of 1 tested in  $\text{CDCl}_3$



**S4. HSQC spectrum of 1 tested in CDCl<sub>3</sub>**

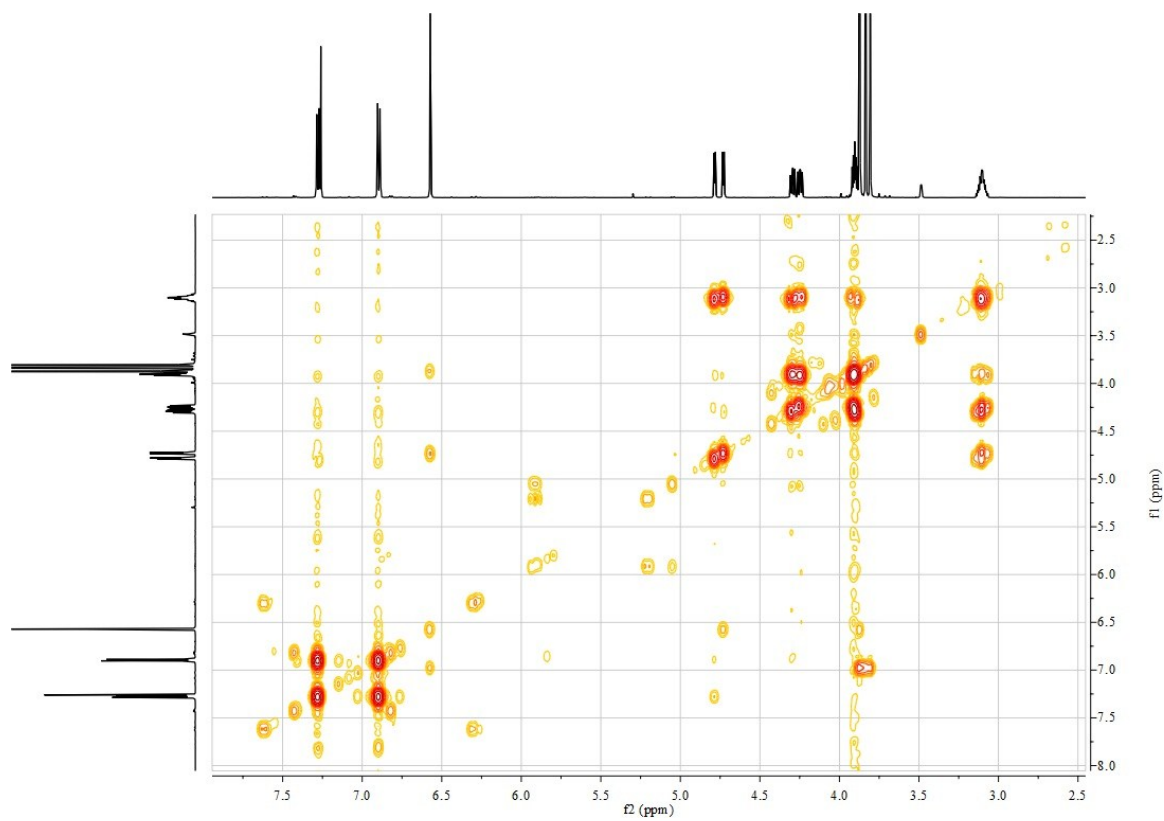


S5. HMBC spectrum of 1 tested in CDCl<sub>3</sub>

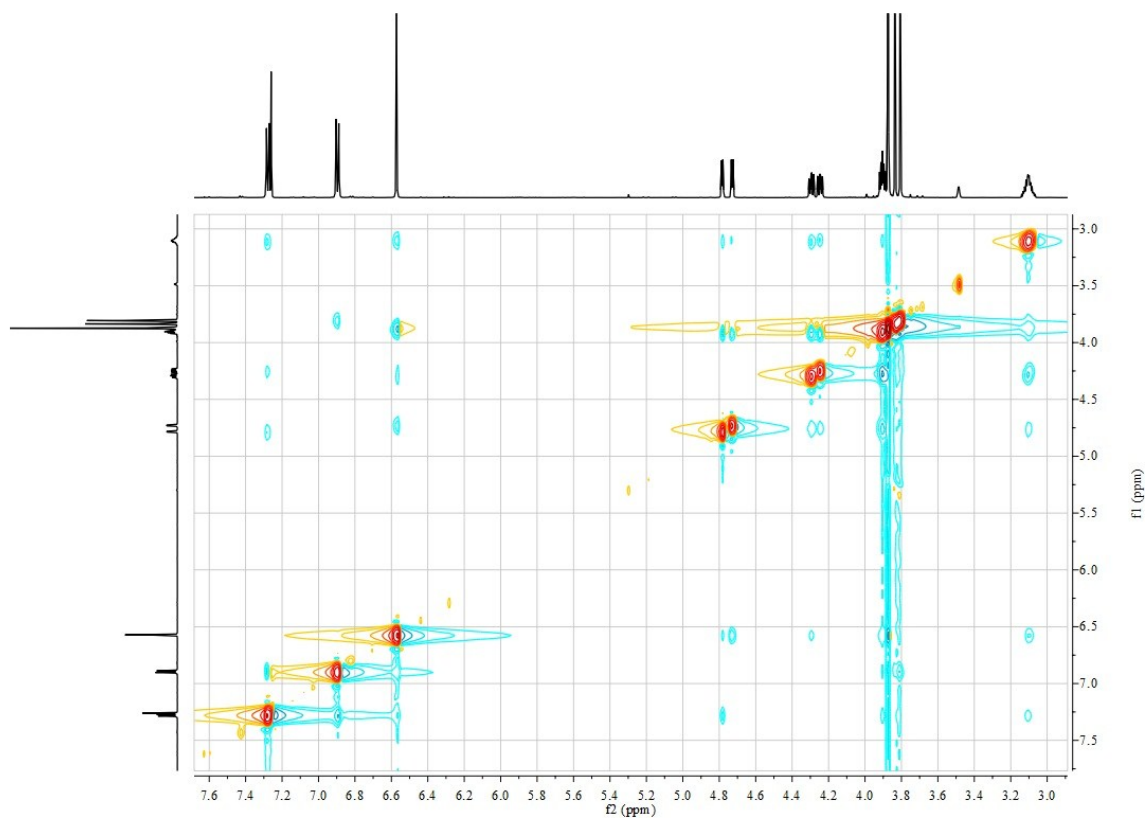




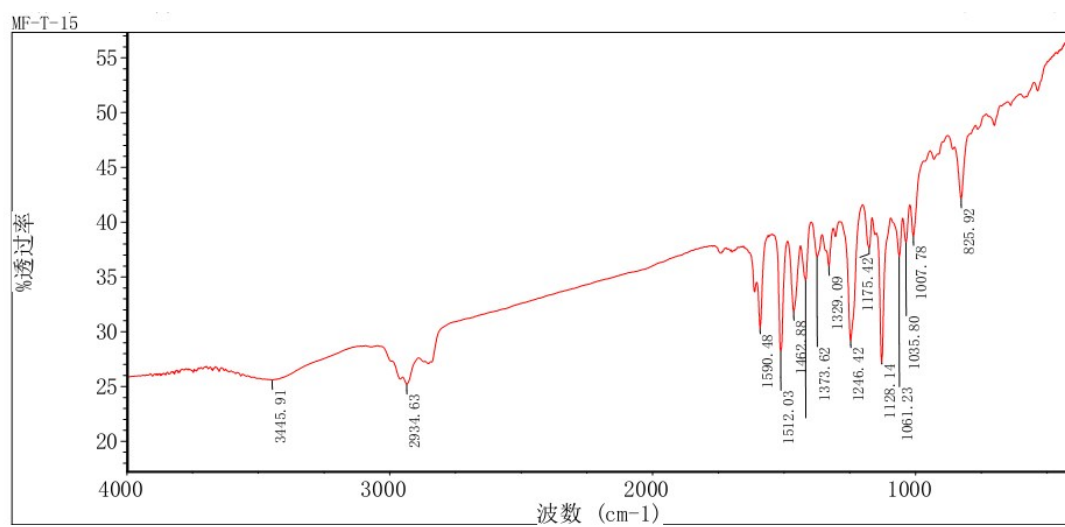
S6.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 1 tested in  $\text{CDCl}_3$



### S7. NOESY spectrum of 1 tested in CDCl<sub>3</sub>



### 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.

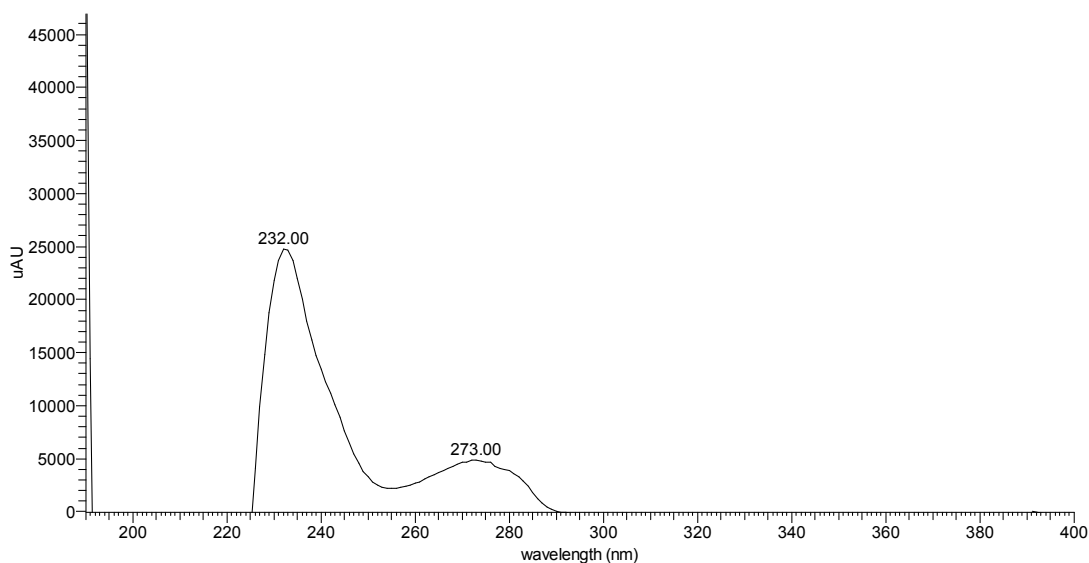
LotID : MF-T-15(25)  
Set Temperature : 25.0  
Temp Corr : OFF

| 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. | Temp. | Comment |
| 1    | MF-T-15(25) | 04:26:52 PM | 70.000  | SR      | 0.070   | 589 | 100.00 | 0.100 | 25.1  |         |
| 2    | MF-T-15(25) | 04:26:58 PM | 70.000  | SR      | 0.070   | 589 | 100.00 | 0.100 | 25.1  |         |
| 3    | MF-T-15(25) | 04:27:03 PM | 70.000  | SR      | 0.070   | 589 | 100.00 | 0.100 | 25.1  |         |
| 4    | MF-T-15(25) | 04:27:09 PM | 70.000  | SR      | 0.070   | 589 | 100.00 | 0.100 | 25.1  |         |
| 5    | MF-T-15(25) | 04:27:15 PM | 70.000  | SR      | 0.070   | 589 | 100.00 | 0.100 | 25.1  |         |
| 6    | MF-T-15(25) | 04:27:20 PM | 70.000  | SR      | 0.070   | 589 | 100.00 | 0.100 | 25.2  |         |

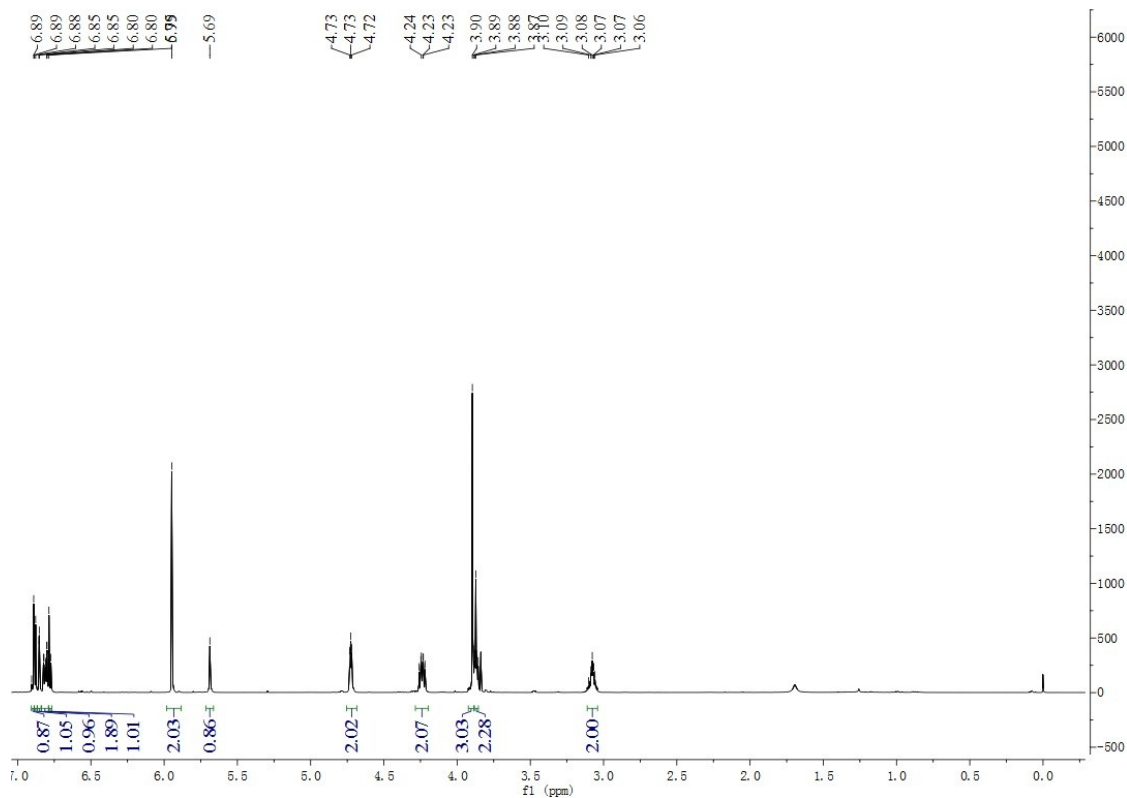
Signature

## 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  $\text{CDCl}_3$**

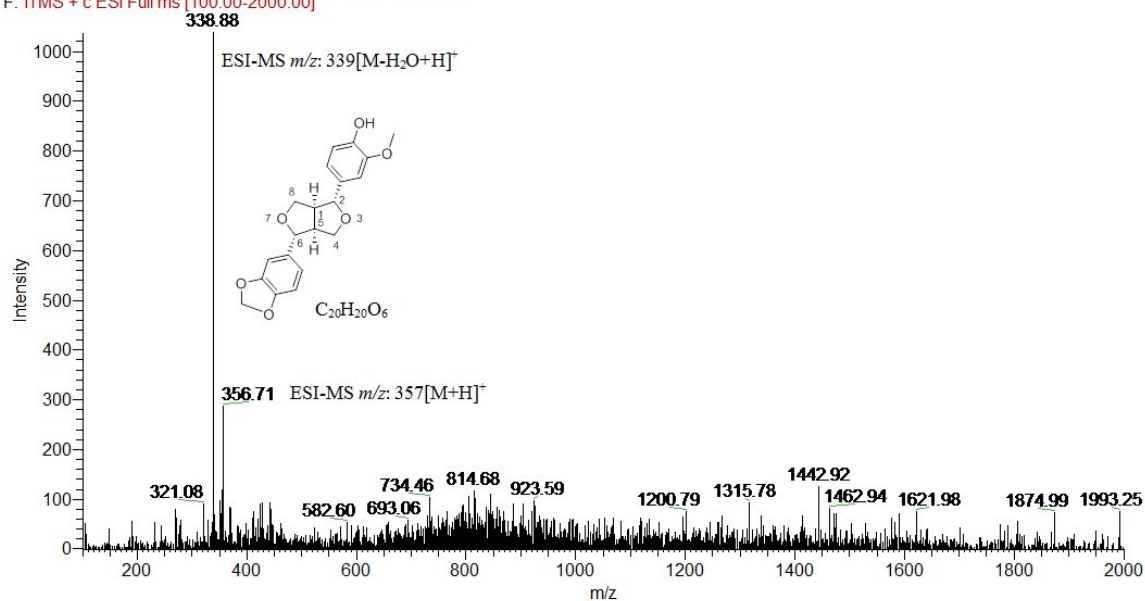


**Pluviatilol (2)**

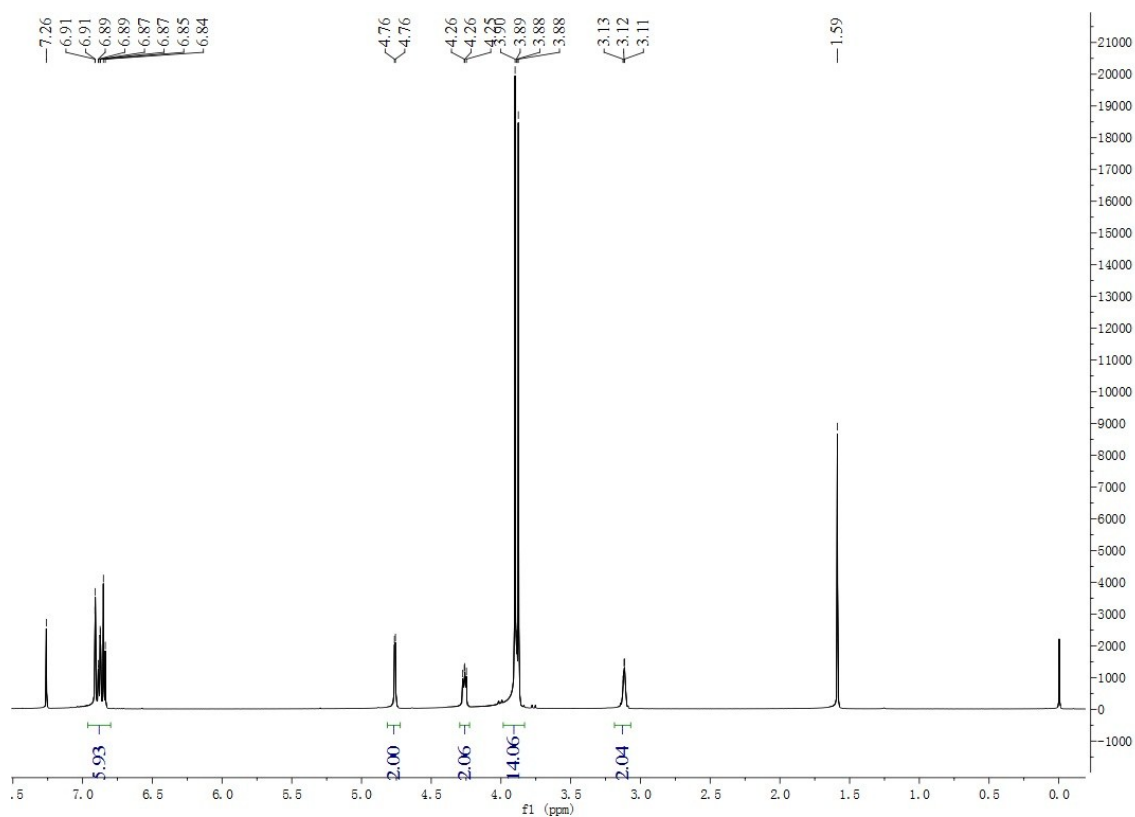
$^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.71~6.90 (6H, m, H-Ar), 5.95 (2H, s, H- $\text{OCH}_2\text{O}$ ), 5.69 (1H, s, H-OH), 4.73 (2H, t,  $J = 3.7$  Hz, H-2, 6), 4.24 (2H, m, H-8, 4), 3.90 (3H, s, H-OMe), 3.86~3.88 (2H, m, H-8, 4), 3.08 (2H, m, H-1, 5).  $\text{C}_{20}\text{H}_{20}\text{O}_6$ , ESI-MS  $m/z$ : 357  $[\text{M}+\text{H}]^+$ , 339  $[\text{M}-\text{H}_2\text{O}+\text{H}]^+$ .

## 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  $\text{CDCl}_3$**

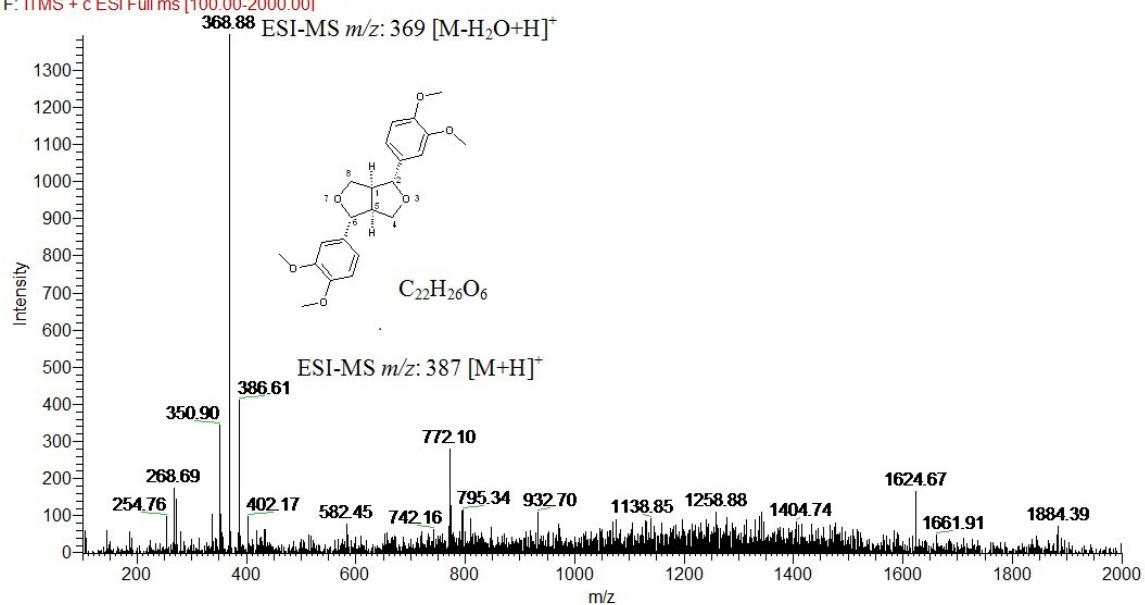


**Pinoresinol dimethyl ether (**3**)**

$^1\text{H}$ -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  $[\text{M}-\text{H}_2\text{O}+\text{H}]^+$ .

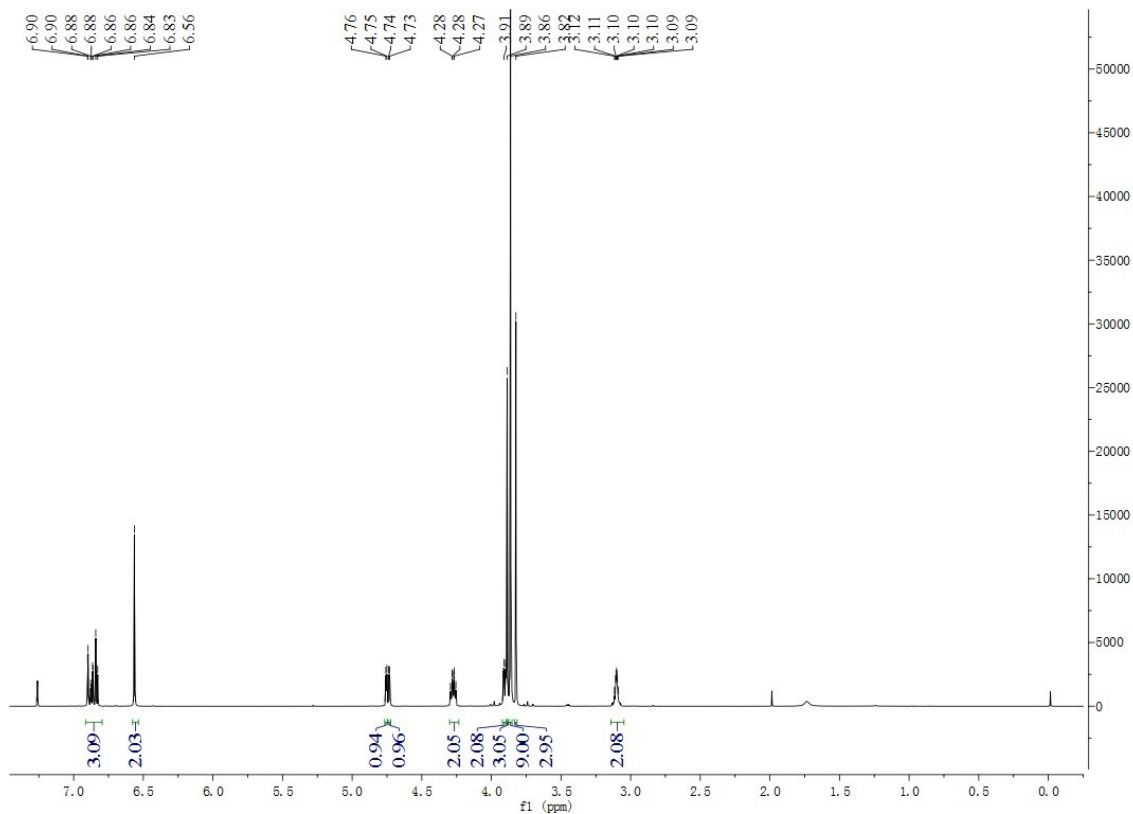
# S14. LR-ESI-MS of 3

MF-E-1 #499 RT: 8.75 AV: 1 NL: 1.39E3  
F: ITMS + c ESI Full ms [100.00-2000.00]





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

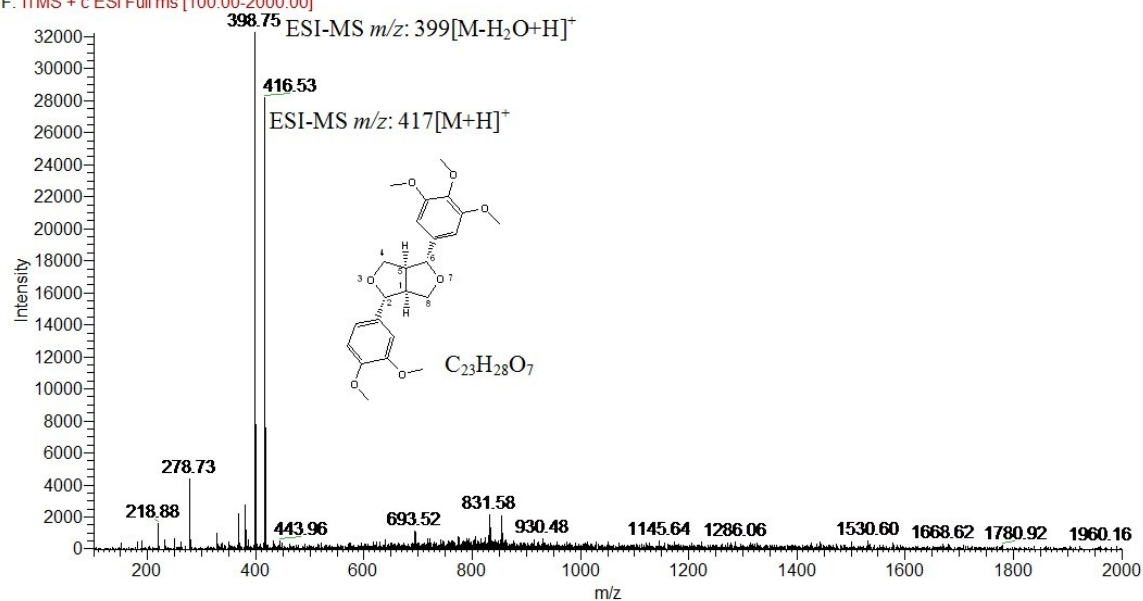


**Magnolol (4)**

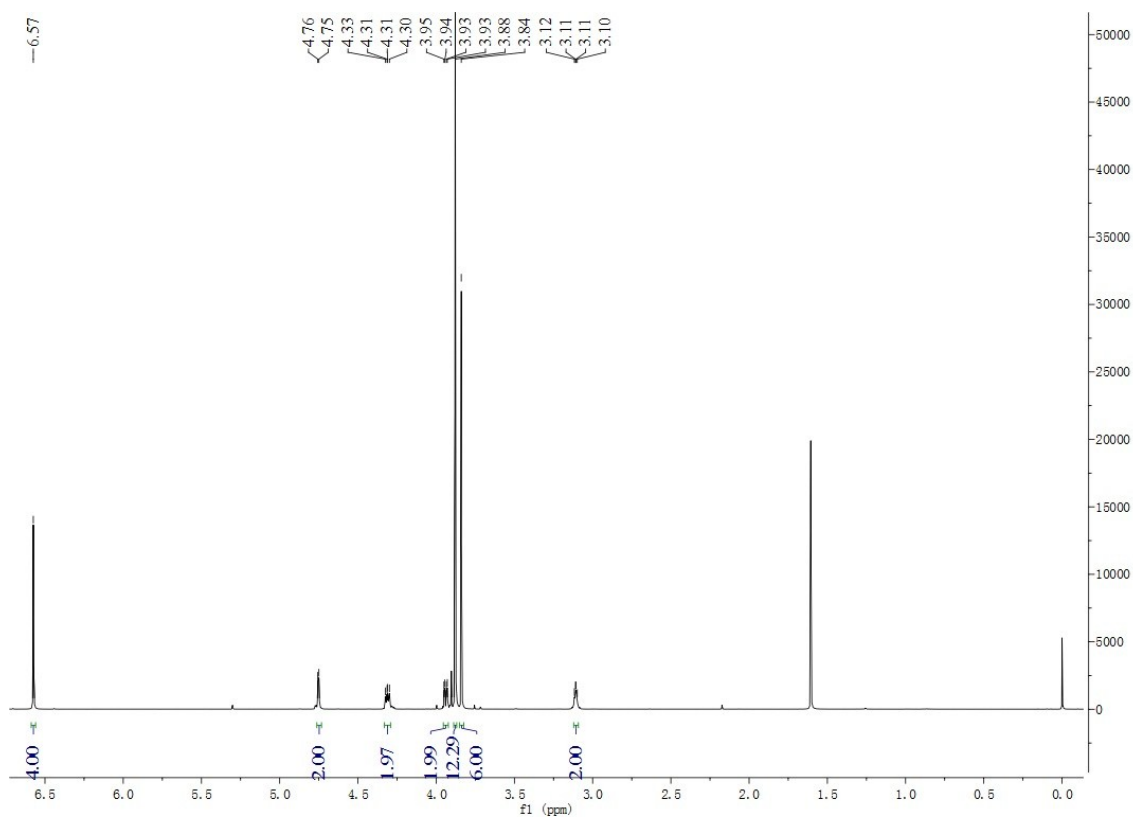
$^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.83~6.90 (3H, m, H-Ar), 6.56 (2H, s, H-Ar), 4.75 (1H, d,  $J = 4.5$  Hz, H-6), 4.73 (1H, d,  $J = 4.5$  Hz, H-2), 4.27 (2H, m, H-4, 8), 3.91 (2H, m, H-4, 8), 3.89 (3H, s, H-OMe), 3.86 (9H, s, H-OMe), 3.82 (3H, s, H-OMe), 3.10 (2H, m, 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

E6 #533 RT: 8.91 AV: 1 NL: 3.22E4  
F: ITMS + c ESI Full ms [100.00-2000.00]



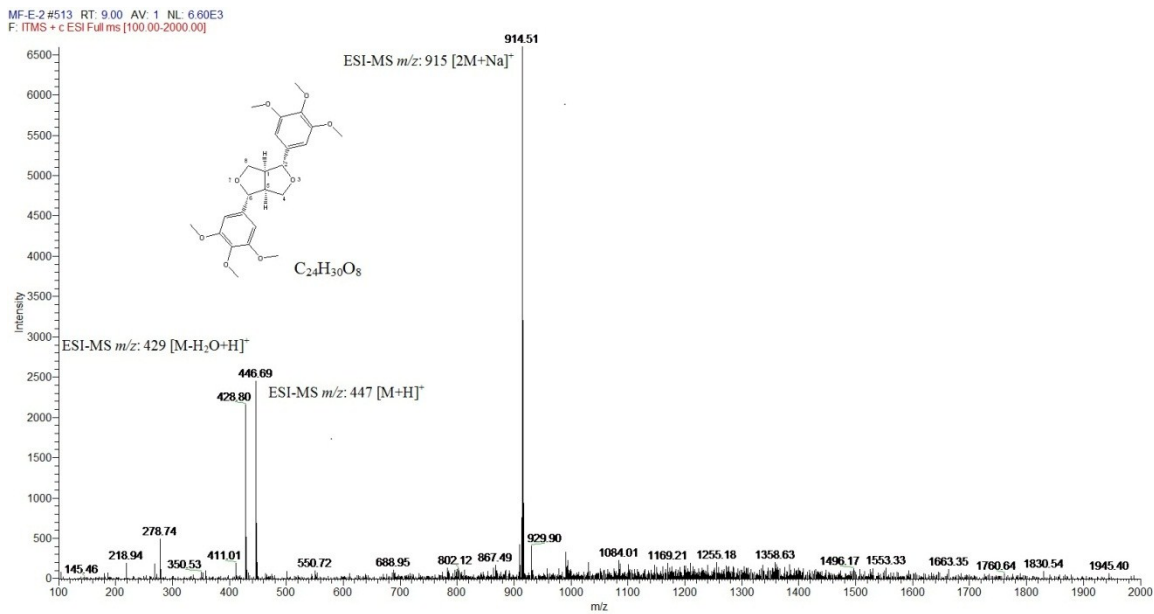
**S17.  $^1\text{H}$  NMR of **5** tested in  $\text{CDCl}_3$**



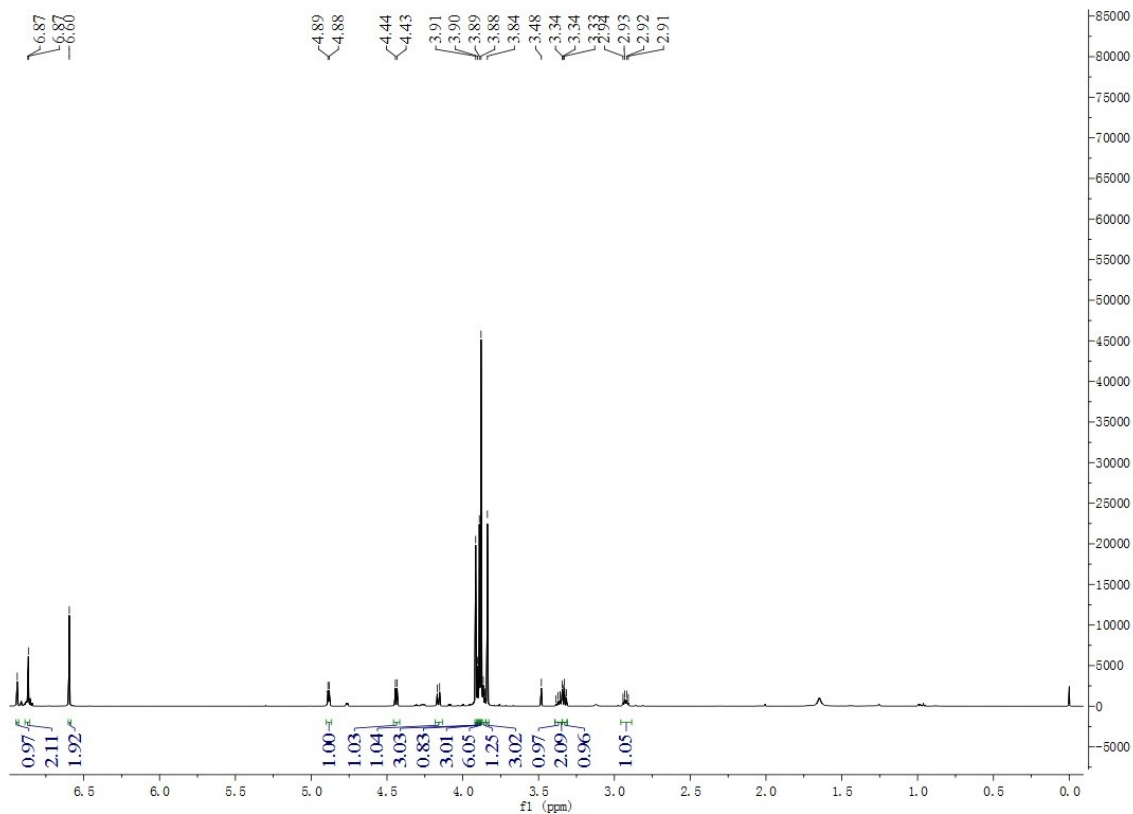
Lirioresinol-B dimethyl ether (**5**)

$^1\text{H}$ -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  $[\text{M}+\text{H}]^+$ , 429  $[\text{M}-\text{H}_2\text{O}+\text{H}]^+$ .

## S18. LR-ESI-MS of 5



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

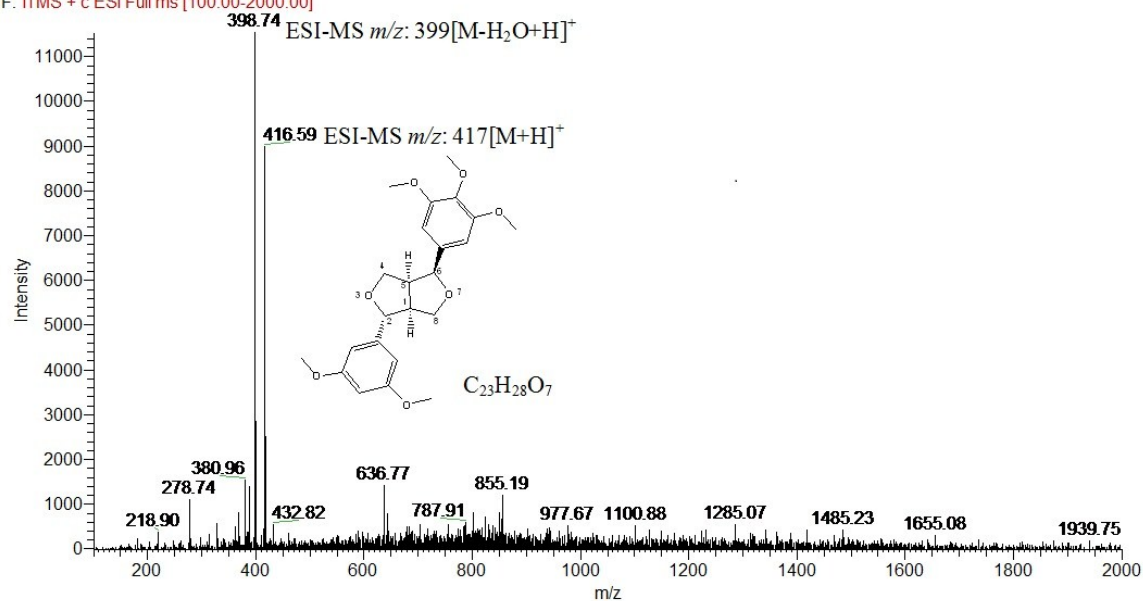


**Epimagnolin B (6)**

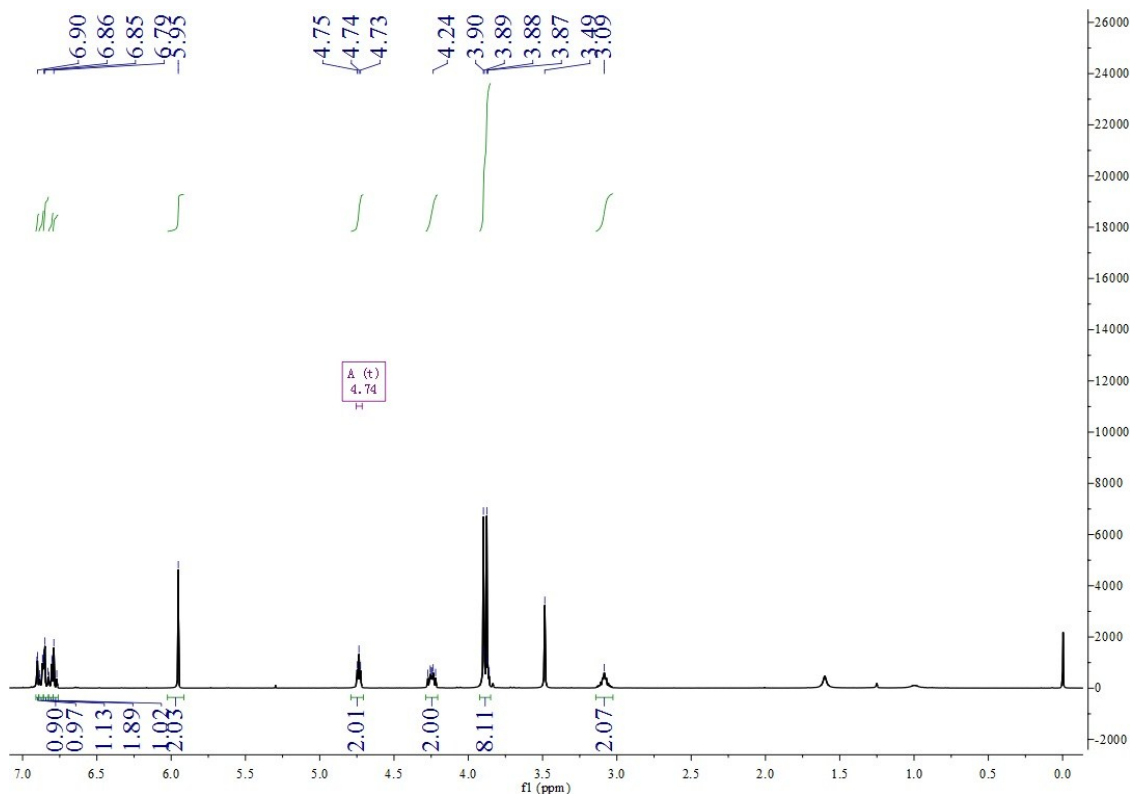
$^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.84~6.94 (3H, m, H-Ar), 6.60 (2H, s, H-Ar), 4.89 (1H, d,  $J = 5.6$  Hz, H-6), 4.44 (1H, d,  $J = 7.0$  Hz, H-2), 4.27 (1H, d,  $J = 9.7$  Hz, H-8), 3.85~3.90 (2H, m, H-4, 8), 3.91 (3H, s, H-OMe), 3.89 (3H, s, H-OMe), 3.88 (6H, s, H-OMe), 3.84 (3H, s, H-OMe), 3.32~3.37 (2H, m, H-5, 4), 2.93 (1H, m, H-1).  $\text{C}_{23}\text{H}_{28}\text{O}_7$ , ESI-MS  $m/z$ : 417  $[\text{M}+\text{H}]^+$ , 339  $[\text{M}-\text{H}_2\text{O}+\text{H}]^+$ .

## S20. LR-ESI-MS of 6

E6 #557 RT: 9.27 AV: 1 NL: 1.15E4  
F: ITMS + c ESI Full ms [100.00-2000.00]



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

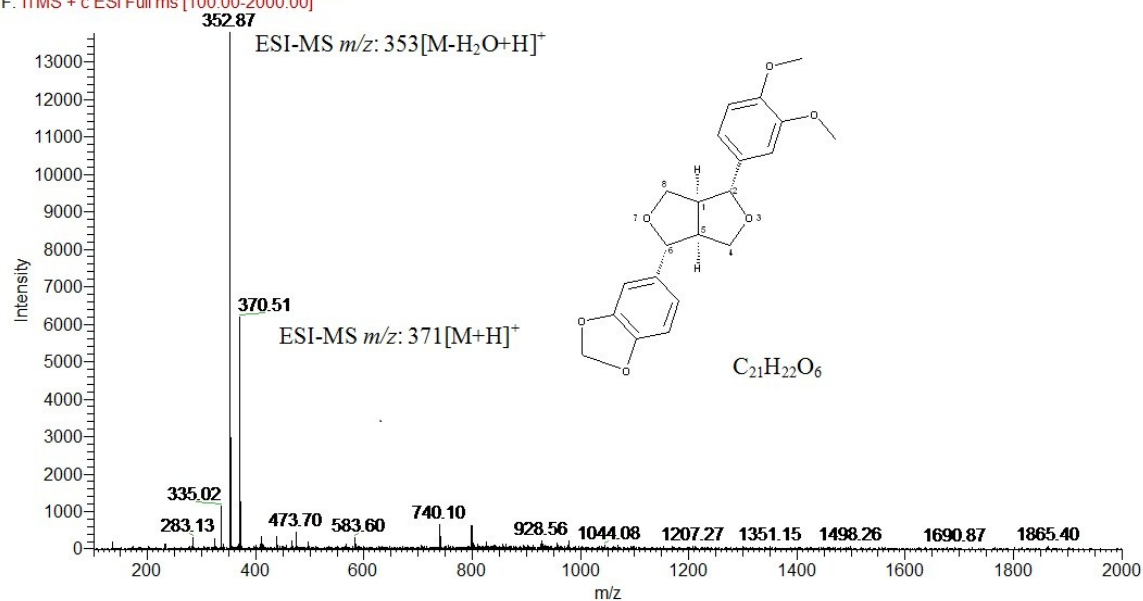


**Kobusin (7)**

$^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.77~6.90 (6H, m, H-Ar), 5.95 (2H, s, H- $\text{OCH}_2\text{O}$ ), 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).  $\text{C}_{21}\text{H}_{22}\text{O}_6$ , ESI-MS  $m/z$ : 371  $[\text{M}+\text{H}]^+$ , 353  $[\text{M}-\text{H}_2\text{O}+\text{H}]^+$ .

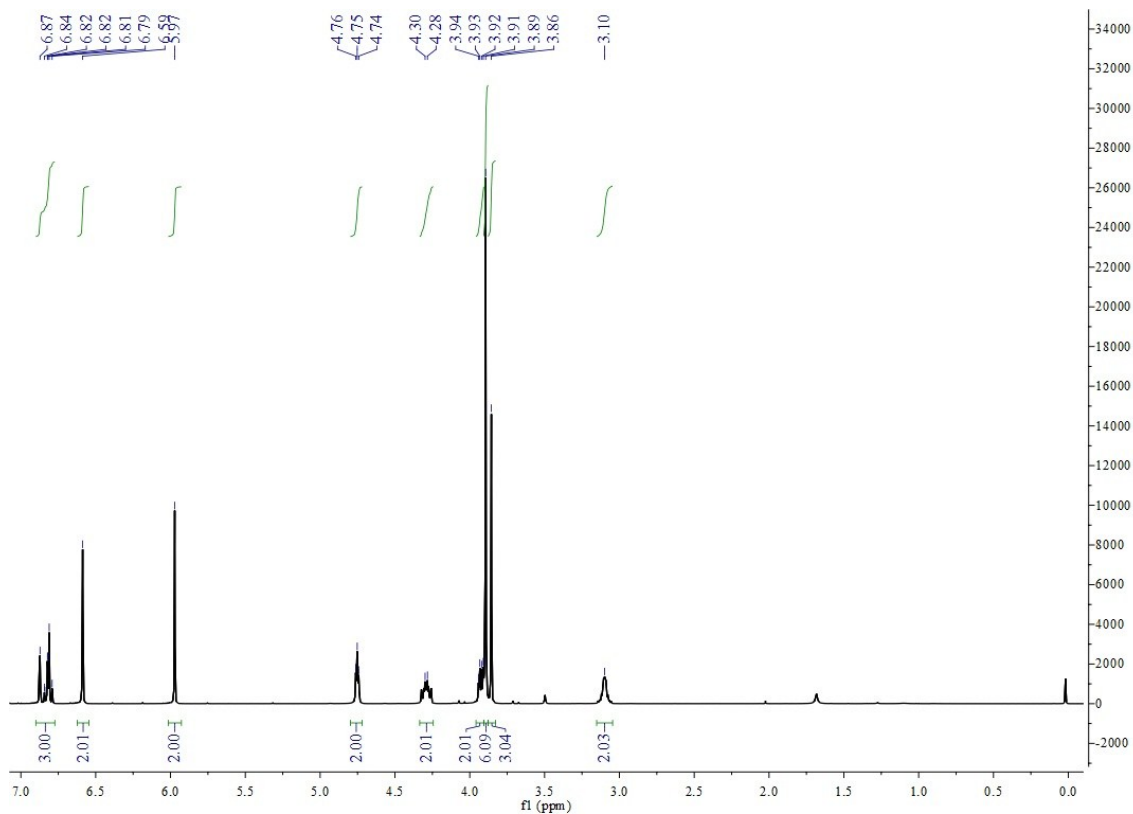
## S22. LR-ESI-MS of 7

370-T-7 #541 RT: 9.45 AV: 1 NL: 1.38E4  
F: ITMS + c ESI Full ms [100.00-2000.00]





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

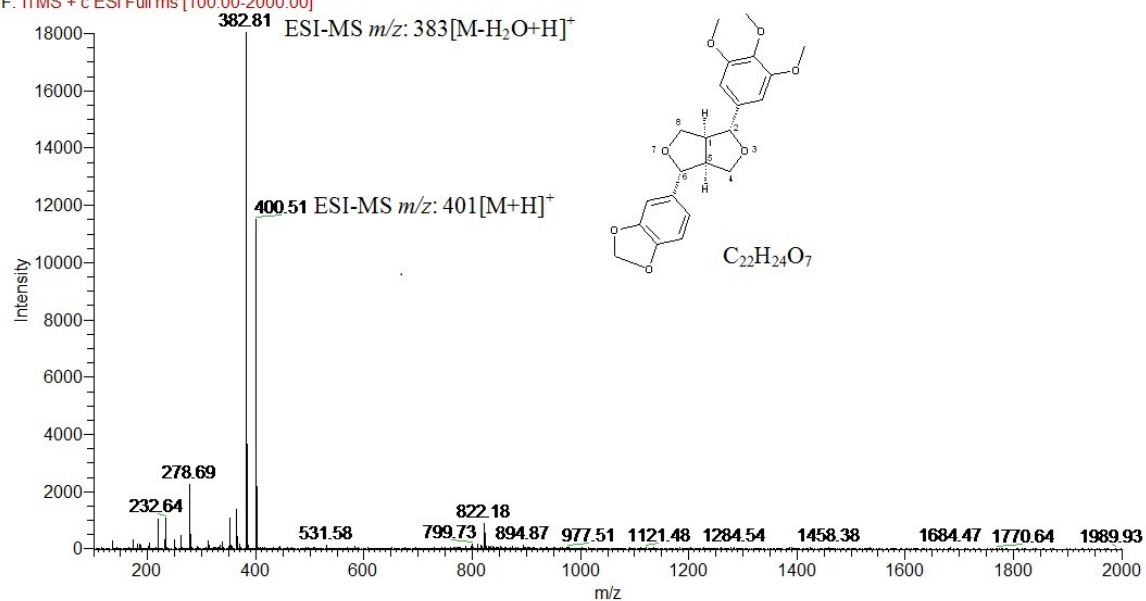


**Aschantin(8)**

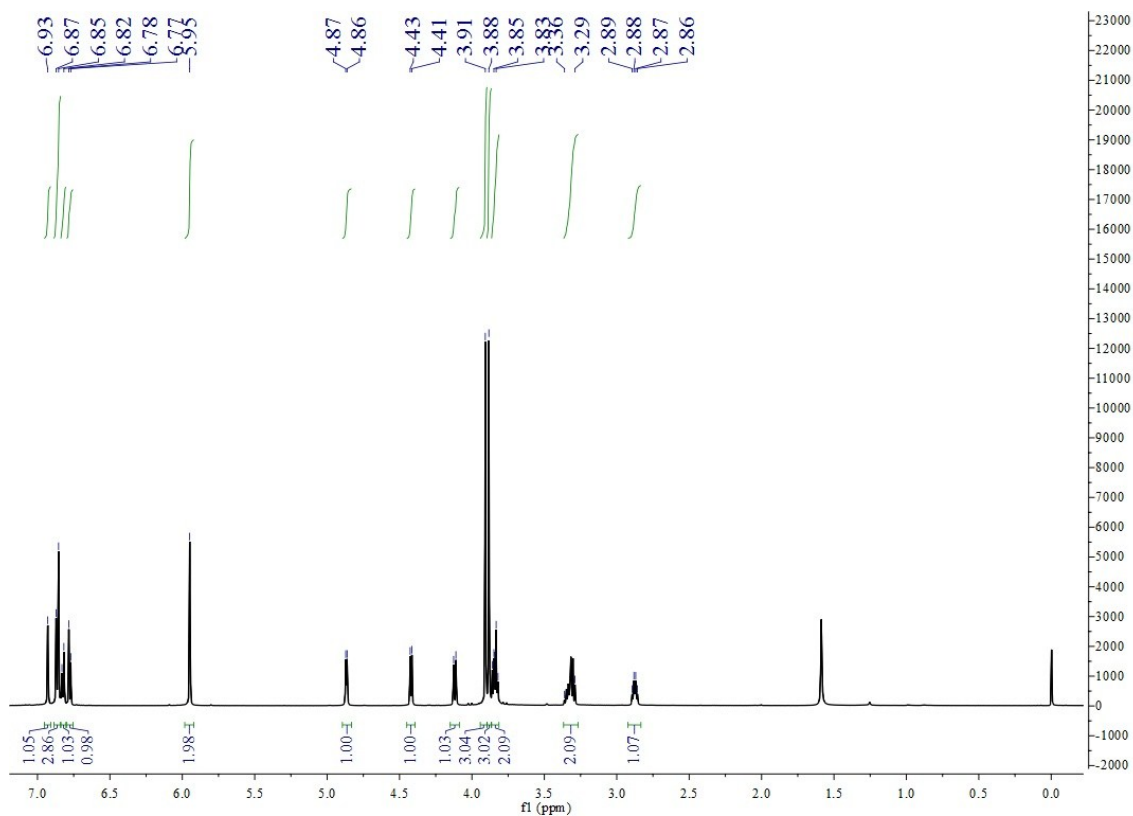
$^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 600MHz)  $\delta\text{H}$ : 6.79~6.87 (3H, m, H-Ar), 6.59 (2H, s, H-Ar), 5.97 (2H, s, H- $\text{OCH}_2\text{O}$ ), 4.75 (2H, t,  $J = 4.0$  Hz, H-2, 6), 4.29 (2H, m, H-8, 4), 3.91~3.94 (2H, m, H-8, 4), 3.89 (6H, s, H-OMe), 3.86 (3H, s, H-OMe), 3.10 (2H, m, H-1, 5).  $\text{C}_{22}\text{H}_{24}\text{O}_7$ , ESI-MS  $m/z$ : 401  $[\text{M}+\text{H}]^+$ , 383  $[\text{M}-\text{H}_2\text{O}+\text{H}]^+$ .

## S24. LR-ESI-MS of 8

400-T-8 #543 RT: 9.50 AV: 1 NL: 1.80E4  
F: ITMS + c ESI Full ms [100.00-2000.00]



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  $[\text{M}+\text{H}]^+$ , 353  $[\text{M}-\text{H}_2\text{O}+\text{H}]^+$ .

## 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]

