

## Supporting Information

### **Structural modification of olibergin A, an isoflavonoid, from *Dalbergia stipulacea* Roxb. and their cytotoxicity**

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Yenjai).

- Figure S1** MS spectrum of olibergin A (1)
- Figure S2** IR spectrum of olibergin A (1)
- Figure S3** <sup>1</sup>H NMR spectrum of olibergin A (1)
- Figure S4** <sup>13</sup>C NMR spectrum of olibergin A (1)
- Figure S5** MS spectrum of 5-hydroxy-7,4'-dimesyl-2',5'-dimethoxyisoflavone (2)
- Figure S6** IR spectrum of 5-hydroxy-7,4'-dimesyl-2',5'-dimethoxyisoflavone (2)
- Figure S7** <sup>1</sup>H NMR spectrum 5-hydroxy-7,4'-dimesyl-2',5'-dimethoxyisoflavone (2)
- Figure S8** <sup>13</sup>C NMR spectrum of 5-hydroxy-7,4'-dimesyl-2',5'-dimethoxyisoflavone (2)
- Figure S9** MS spectrum of 7,4'-diacetoxy-5-hydroxy-2',5'-dimethoxyisoflavone (3)
- Figure S10** IR spectrum of 7,4'-diacetoxy-5-hydroxy-2',5'-dimethoxyisoflavone (3)
- Figure S11** <sup>1</sup>H NMR spectrum of 7,4'-diacetoxy-5-hydroxy-2',5'-dimethoxyisoflavone (3)
- Figure S12** <sup>13</sup>C NMR spectrum of 7,4'-diacetoxy-5-hydroxy-2',5'-dimethoxyisoflavone (3)
- Figure S13** MS spectrum of 7,4'-dibutoxy-5-hydroxy-2',5'-dimethoxyisoflavone (4)
- Figure S14** IR spectrum of 7,4'-dibutoxy-5-hydroxy-2',5'-dimethoxyisoflavone (4)
- Figure S15** <sup>1</sup>H NMR spectrum of 7,4'-dibutoxy-5-hydroxy-2',5'-dimethoxyisoflavone (4)
- Figure S16** <sup>13</sup>C NMR spectrum of 7,4'-dibutoxy-5-hydroxy-2',5'-dimethoxyisoflavone (4)
- Figure S17** MS spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavone (5)
- Figure S18** IR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavone (5)
- Figure S19** <sup>1</sup>H NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavone (5)
- Figure S20** <sup>13</sup>C NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavone (5)
- Figure S21** MS spectrum of 5,7,2',4',5'-pentamethoxyisoflavone (6)
- Figure S22** IR spectrum of 5,7,2',4',5'-pentamethoxyisoflavone (6)
- Figure S23** <sup>1</sup>H NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavone (6)
- Figure S24** <sup>13</sup>C NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavone (6)
- Figure S25** MS spectrum of 1-(5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-3-yl)-4-hydroxy-3-nitro-2,5-quinone (7)

- Figure S26** IR spectrum of 1-(5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-3-yl)-4-hydroxy-3-nitro-2,5-quinone (**7**)
- Figure S27** <sup>1</sup>H NMR spectrum of 1-(5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-3-yl)-4-hydroxy-3-nitro-2,5-quinone (**7**)
- Figure S28** <sup>13</sup>C NMR spectrum of 1-(5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-3-yl)-4-hydroxy-3-nitro-2,5-quinone (**7**)
- Figure S29** MS spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavanone (**8**)
- Figure S30** IR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavanone (**8**)
- Figure S31** <sup>1</sup>H NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavanone (**8**)
- Figure S32** <sup>13</sup>C NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavanone (**8**)
- Figure S33** MS spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone (**9**)
- Figure S34** IR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone (**9**)
- Figure S35** <sup>1</sup>H NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone (**9**)
- Figure S36** <sup>13</sup>C NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone (**9**)
- Figure S37** MS spectrum of 5,7,2',4',5'-pentamethoxyisoflavanone (**10**)
- Figure S38** IR spectrum of 5,7,2',4',5'-pentamethoxyisoflavanone (**10**)
- Figure S39** <sup>1</sup>H NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavanone (**10**)
- Figure S40** <sup>13</sup>C NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavanone (**10**)
- Figure S41** MS spectrum of 5,7,2',4',5'-pentamethoxyisoflavan (**11**)
- Figure S42** IR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan (**11**)
- Figure S43** <sup>1</sup>H NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan (**11**)
- Figure S44** <sup>13</sup>C NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan (**11**)
- Figure S45** MS spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan hydrazone (**12**)
- Figure S46** IR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan hydrazone (**12**)
- Figure S47** <sup>1</sup>H NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan hydrazone (**12**)
- Figure S48** <sup>13</sup>C NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan hydrazone (**12**)

- Figure S49** MS spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan oxime (**13**)
- Figure S50** IR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan oxime (**13**)
- Figure S51** <sup>1</sup>H NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan oxime (**13**)
- Figure S52** <sup>13</sup>C NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan oxime (**13**)
- Figure S53** MS spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone hydrazone (**14**)
- Figure S54** IR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone hydrazone (**14**)
- Figure S55** <sup>1</sup>H NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone hydrazone (**14**)
- Figure S56** <sup>13</sup>C NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone hydrazone (**14**)
- Figure S57** MS spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone oxime (**15**)
- Figure S58** IR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone oxime (**15**)
- Figure S59** <sup>1</sup>H NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone oxime (**15**)
- Figure S60** <sup>13</sup>C NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone oxime (**15**)
- Figure S61** MS spectrum of 5,7,2',4',5'-pentamethoxyisoflavan oxime (**16**)
- Figure S62** IR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan oxime (**16**)
- Figure S63** <sup>1</sup>H NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan oxime (**16**)
- Figure S64** <sup>13</sup>C NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan oxime (**16**)

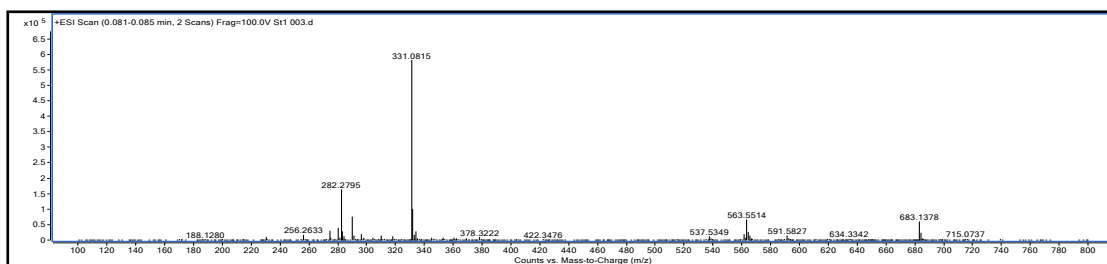


Figure S1 MS spectrum of olibergin A (1)

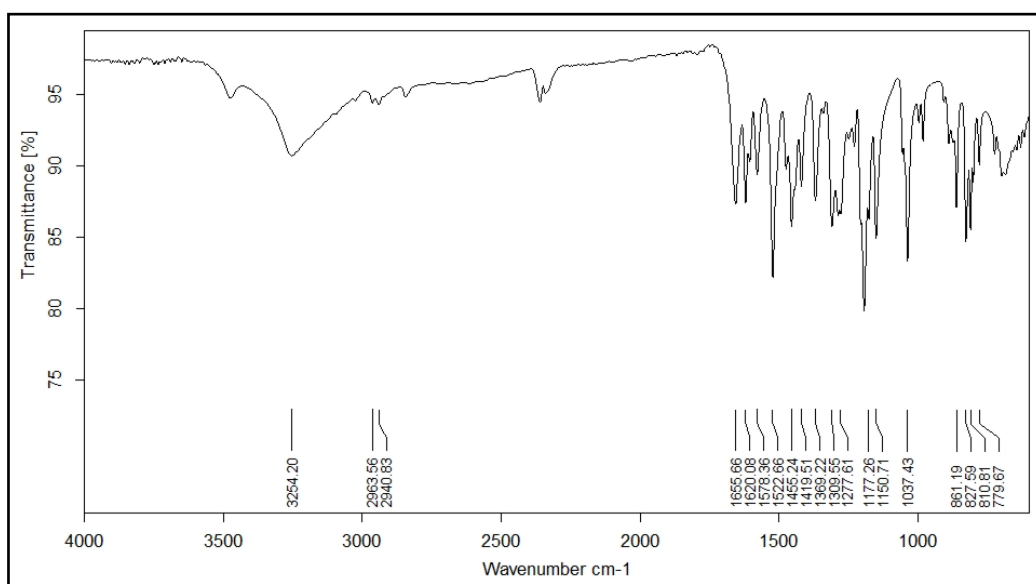


Figure S2 IR spectrum of olibergin A (1)

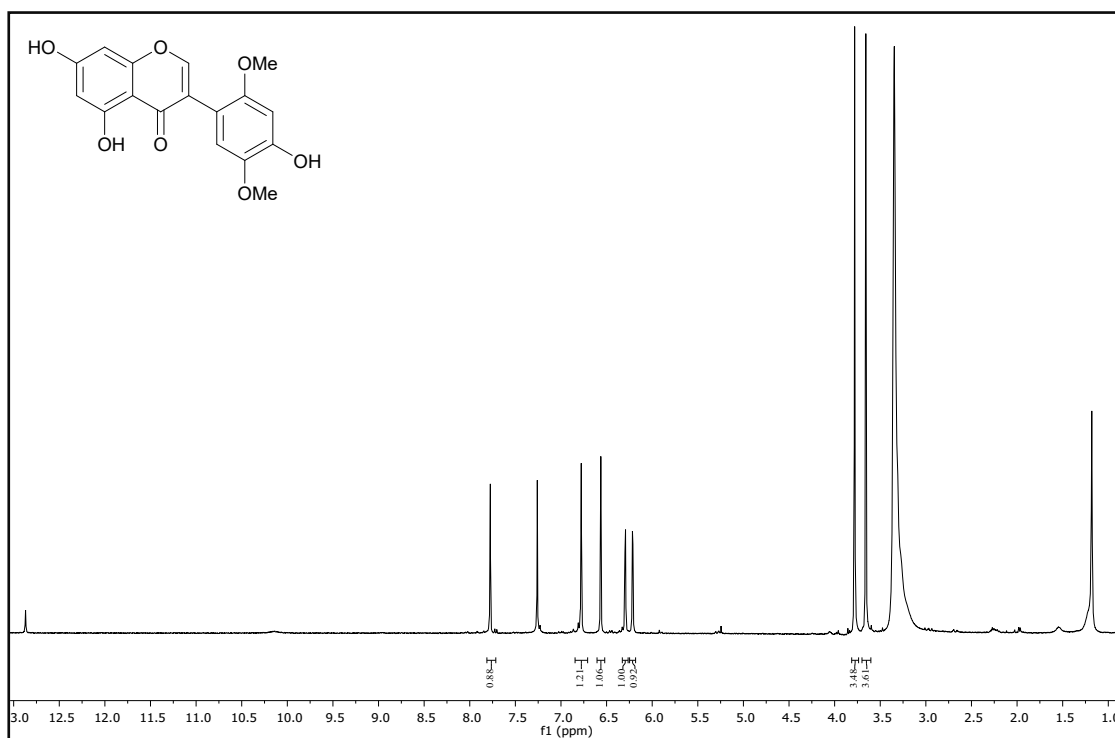


Figure S3 <sup>1</sup>H NMR spectrum of olibergin A (1)

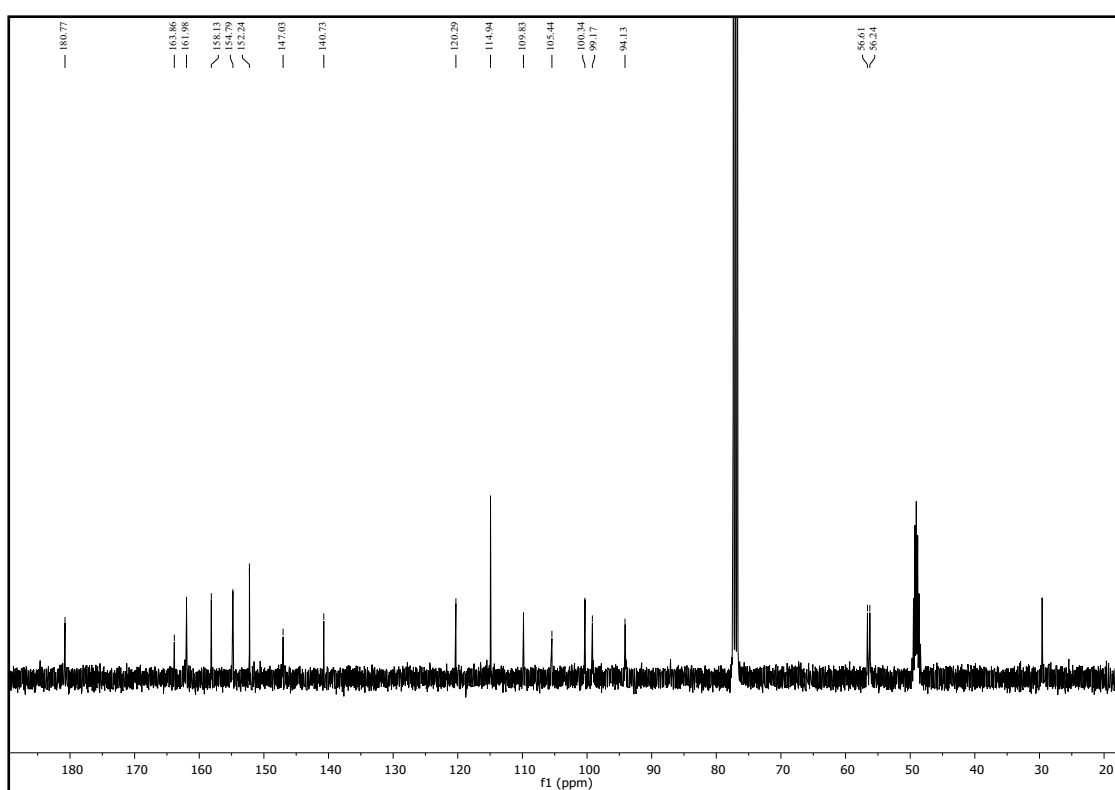
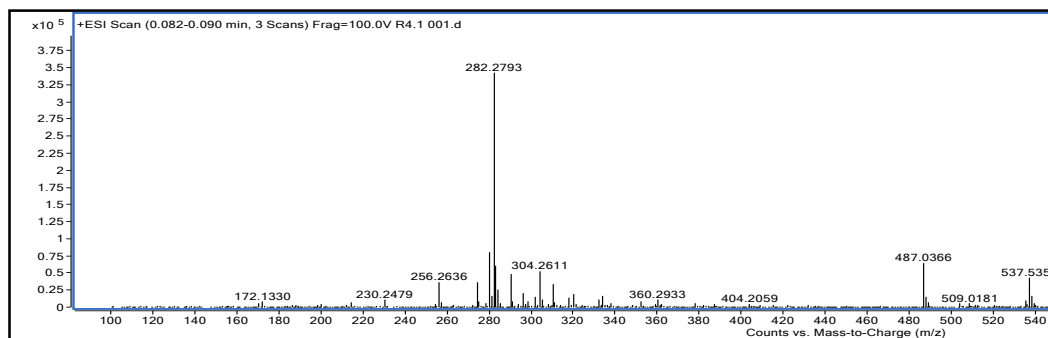
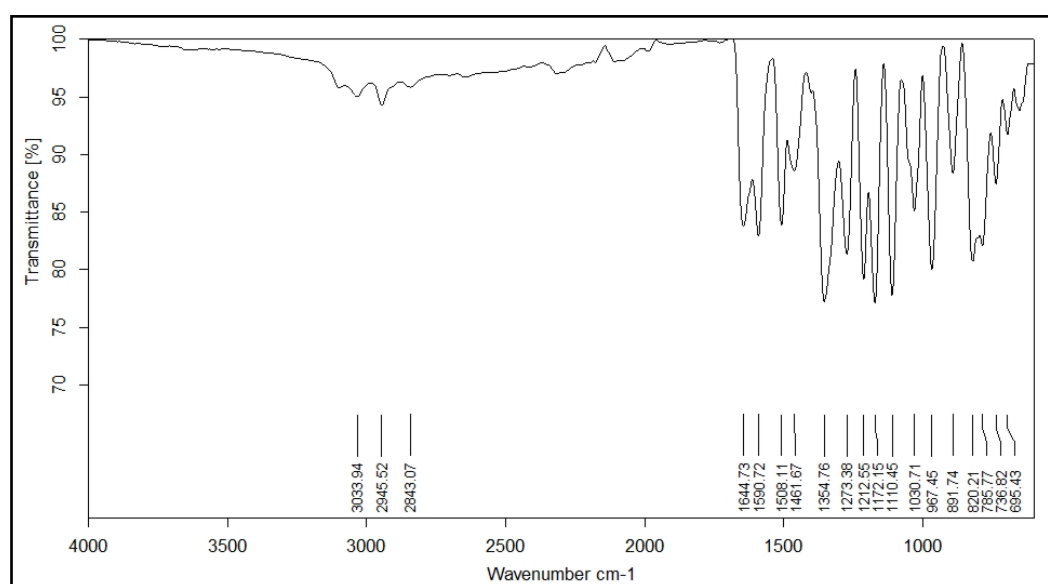


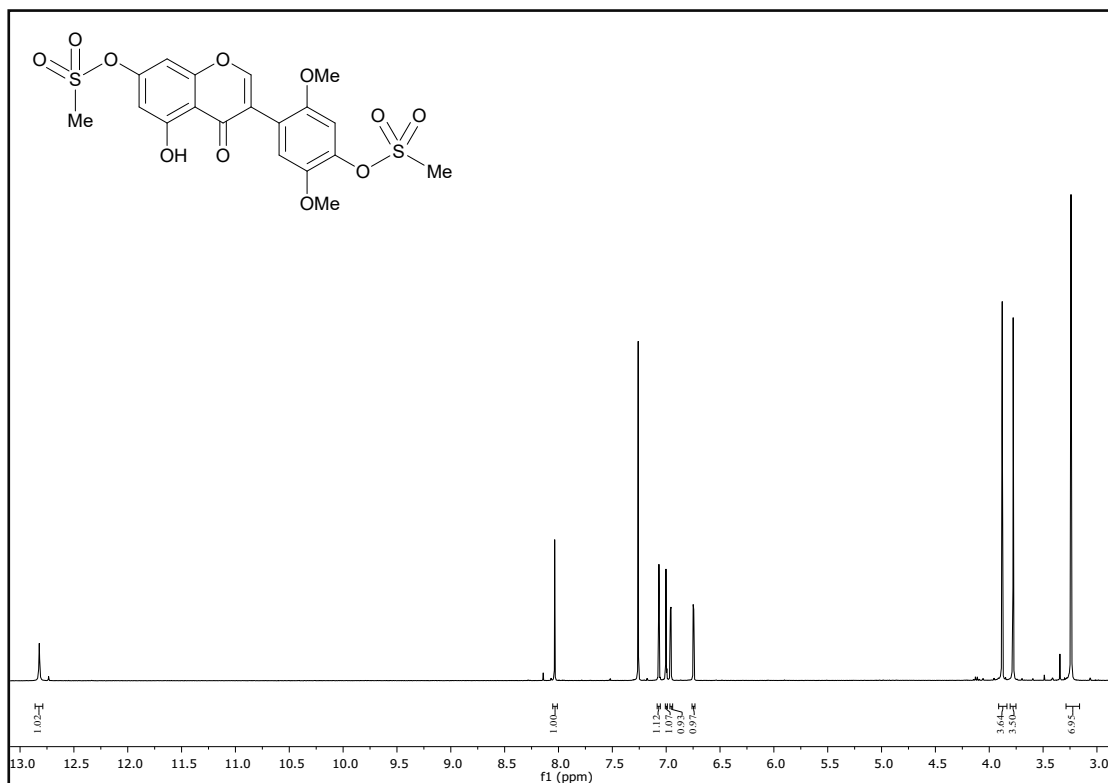
Figure S4 <sup>13</sup>C NMR spectrum of olibergin A (1)



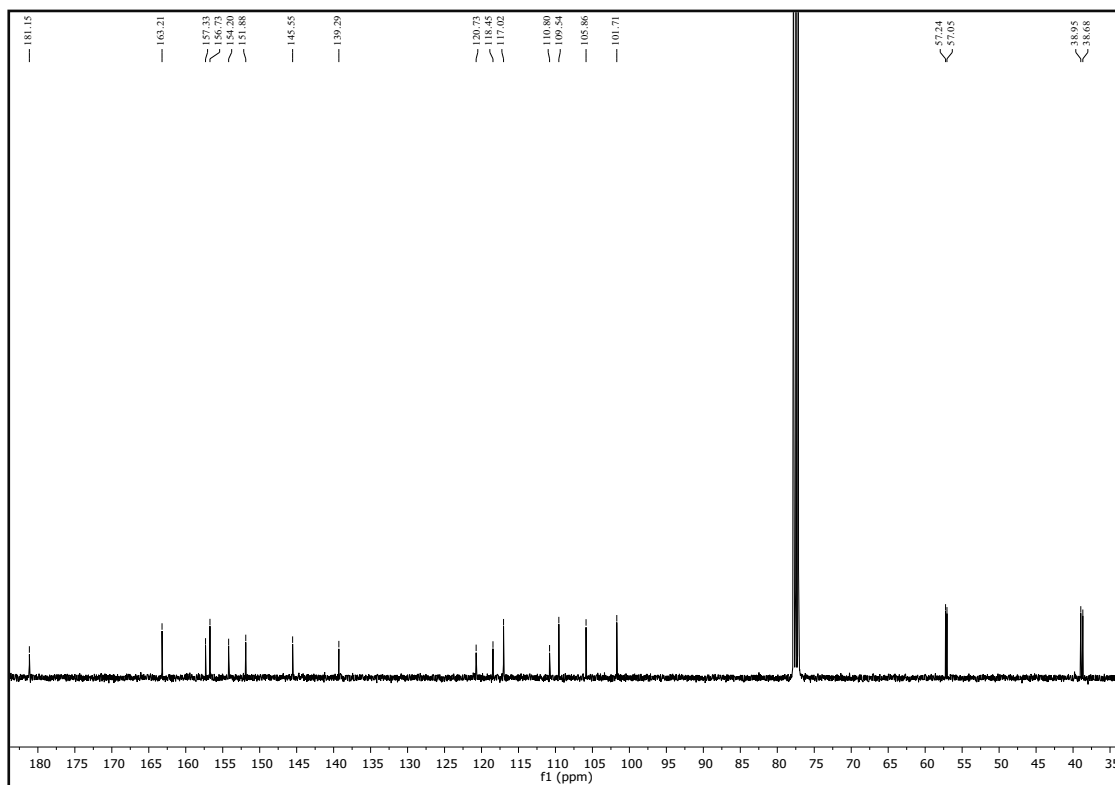
**Figure S5** MS spectrum of 5-hydroxy-7,4'-dimesyl-2',5'-dimethoxyisoflavone (**2**)



**Figure S6** IR spectrum of 5-hydroxy-7,4'-dimesyl-2',5'-dimethoxyisoflavone (**2**)



**Figure S7**  $^1\text{H}$  NMR spectrum of 5-hydroxy-7,4'-dimesyl-2',5'-dimethoxyisoflavone (**2**)



**Figure S8**  $^{13}\text{C}$  NMR spectrum of 5-hydroxy-7,4'-dimesyl-2',5'-dimethoxyisoflavone (**2**)



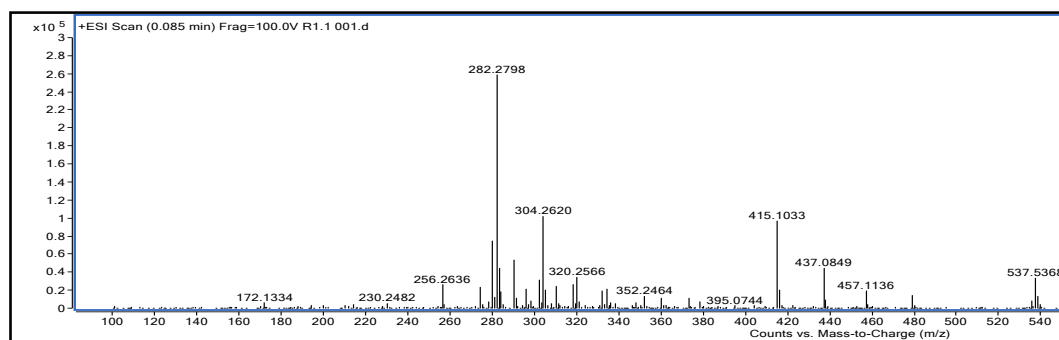


Figure S9 MS spectrum of 7,4'-diacetoxy-5-hydroxy-2',5'-dimethoxyisoflavone (3)

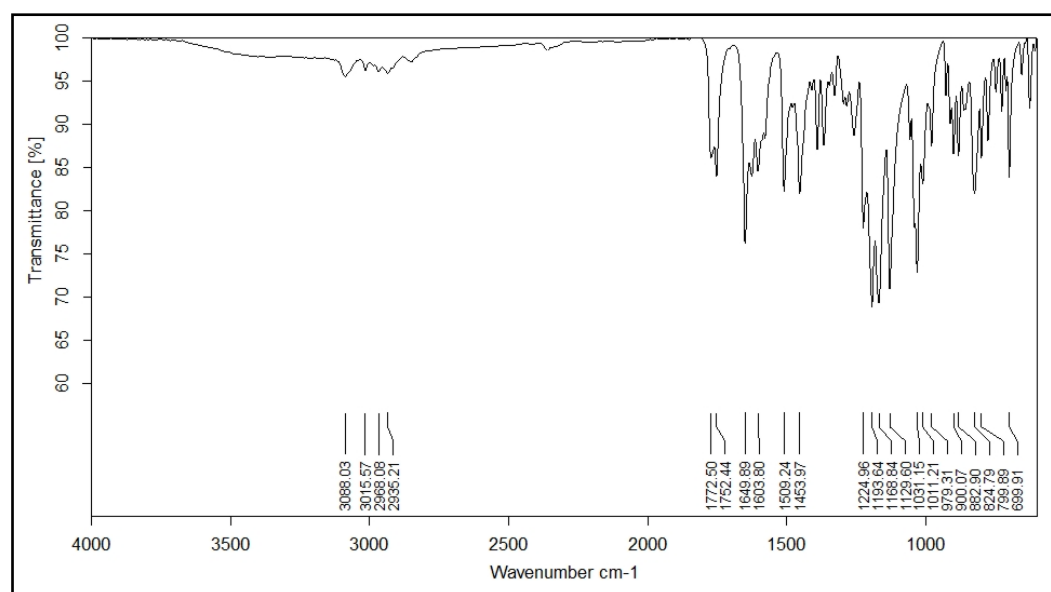


Figure S10 IR spectrum of 7,4'-diacetoxy-5-hydroxy-2',5'-dimethoxyisoflavone (3)

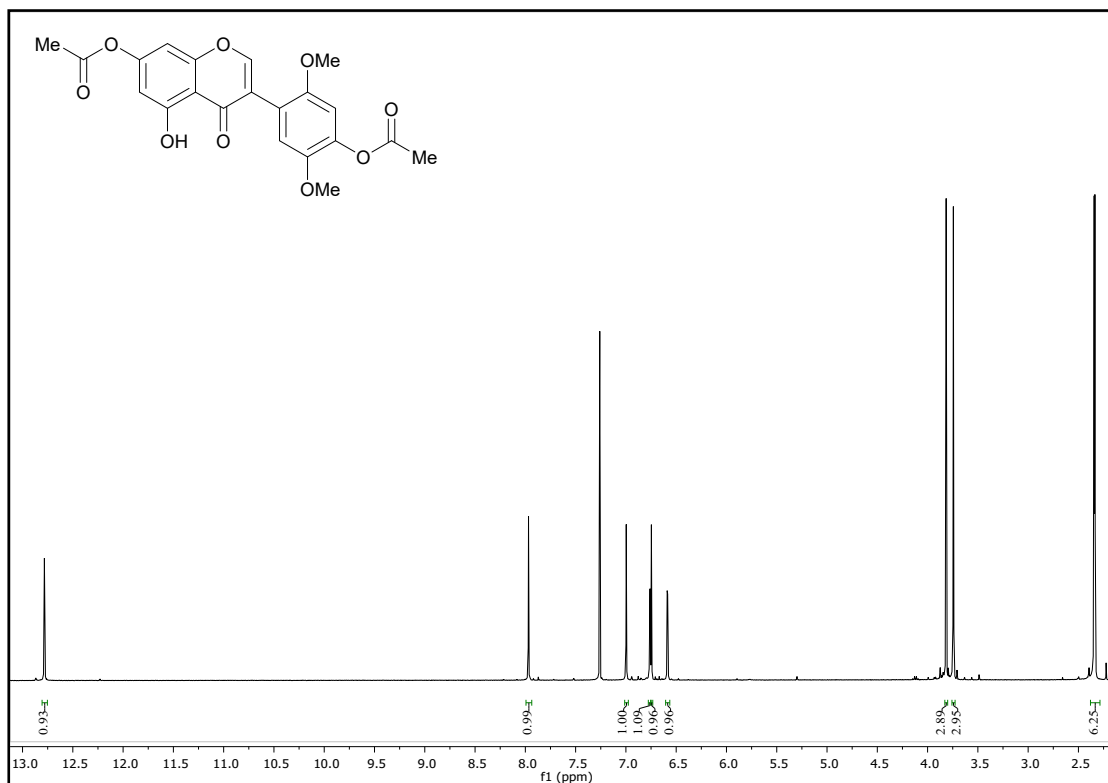


Figure S11  $^1\text{H}$  NMR spectrum of 7,4'-diacetoxy-5-hydroxy-2',5'-dimethoxyisoflavone (3)

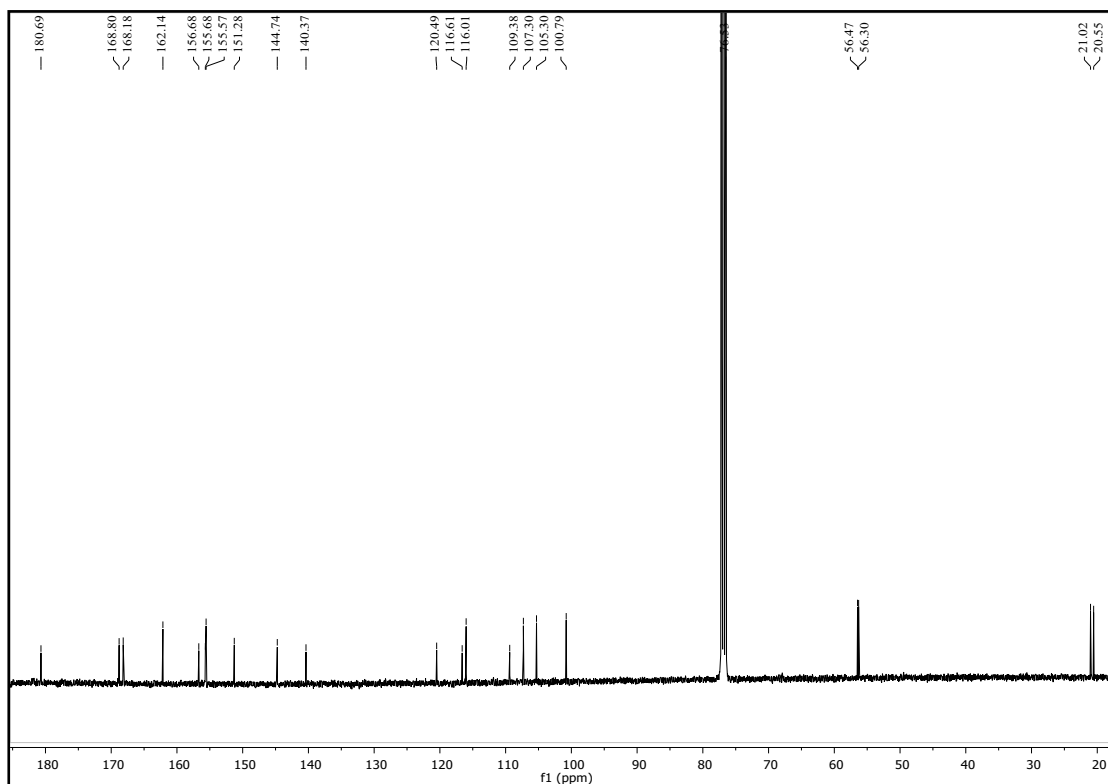


Figure S12  $^{13}\text{C}$  NMR spectrum of 7,4'-diacetoxy-5-hydroxy-2',5'-dimethoxyisoflavone (3)

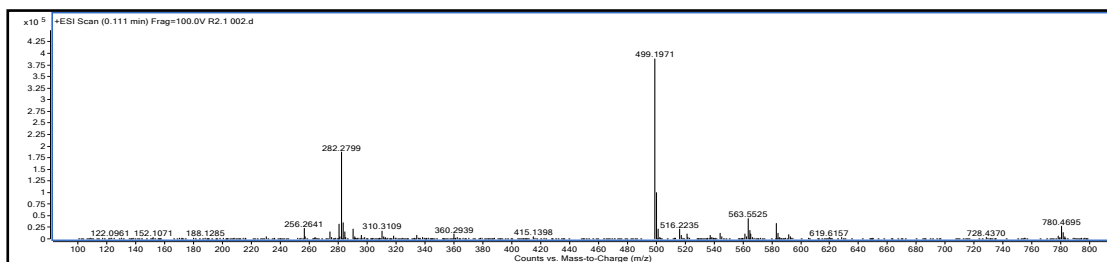


Figure S13 MS spectrum of 7,4'-dibutoxy-5-hydroxy-2',5'-dimethoxyisoflavone (**4**)

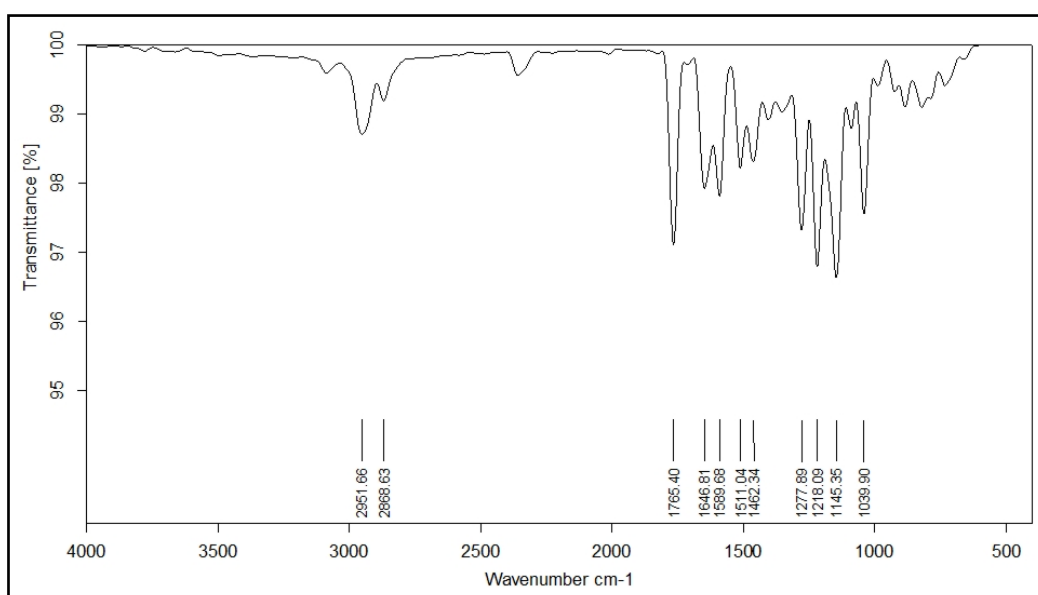


Figure S14 IR spectrum of 7,4'-dibutoxy-5-hydroxy-2',5'-dimethoxyisoflavone (**4**)

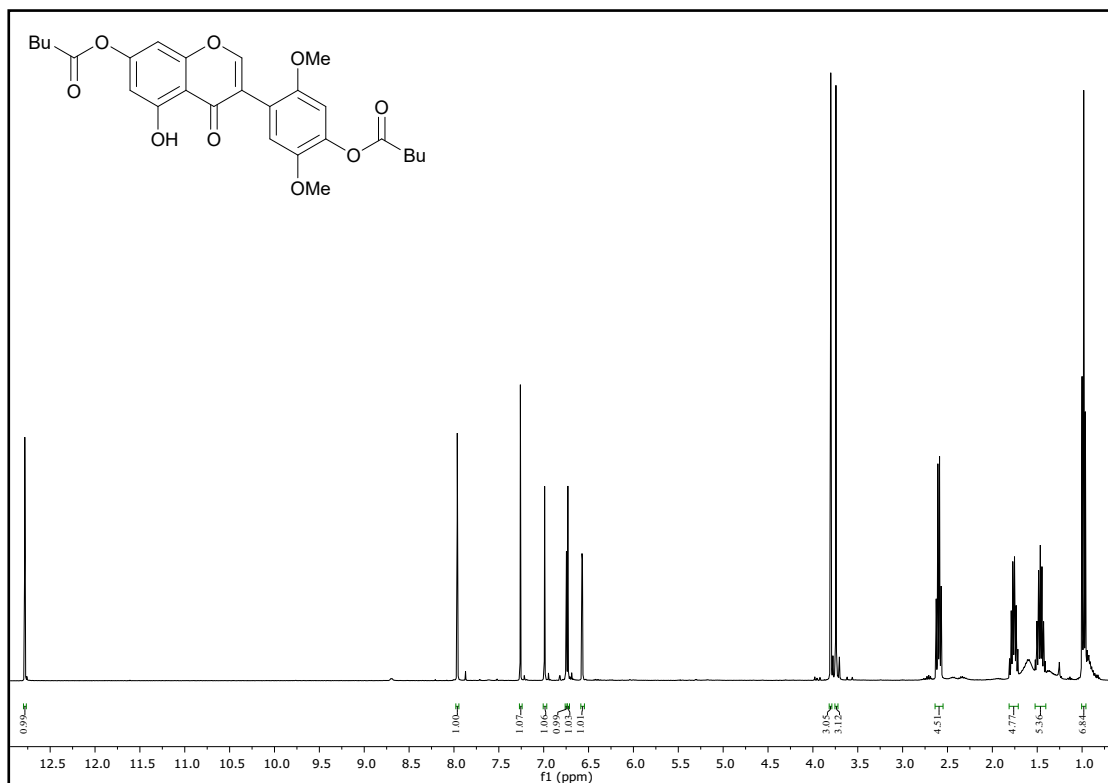


Figure S15 <sup>1</sup>H NMR spectrum of 7,4'-dibutoxy-5-hydroxy-2',5'-dimethoxyisoflavone (4)

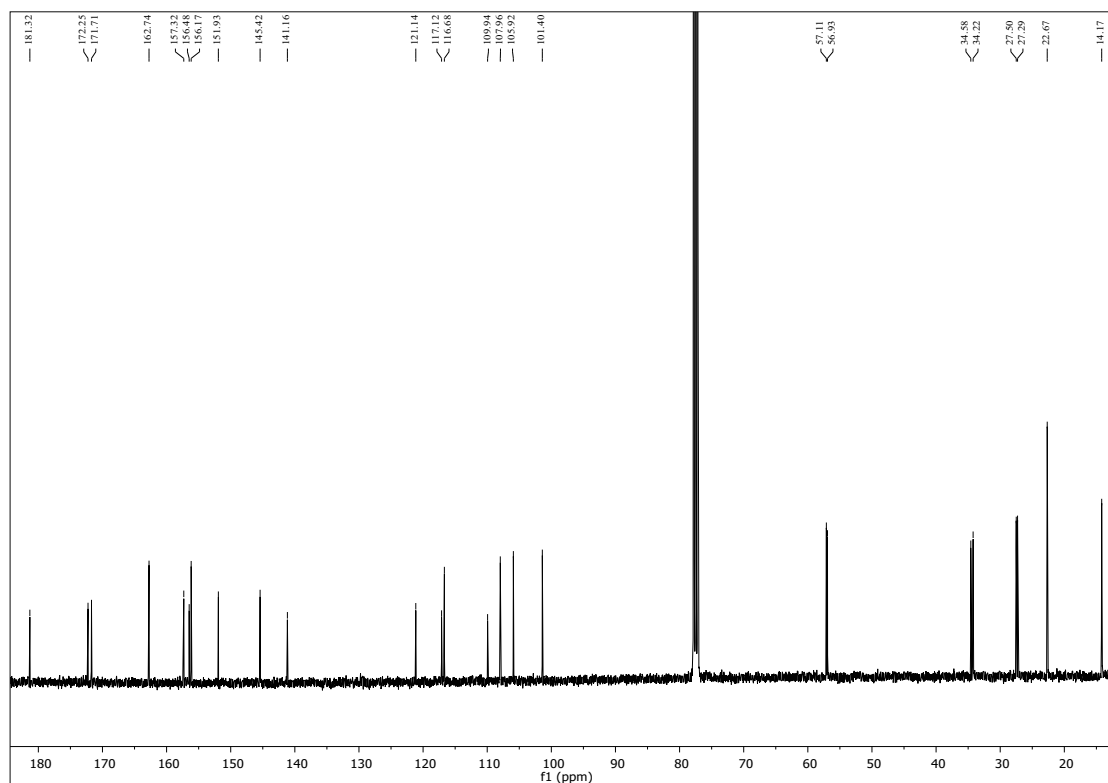
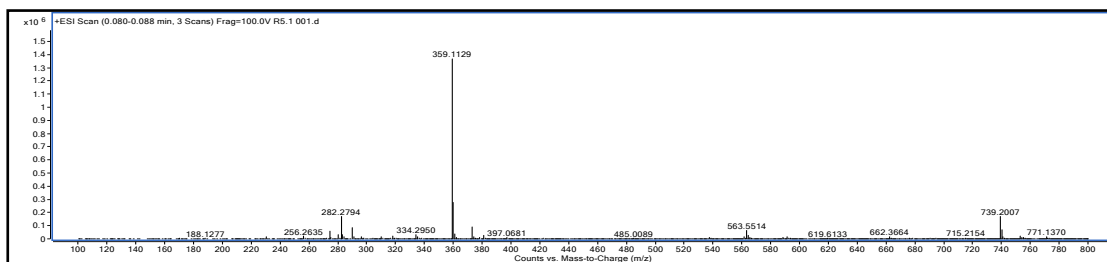
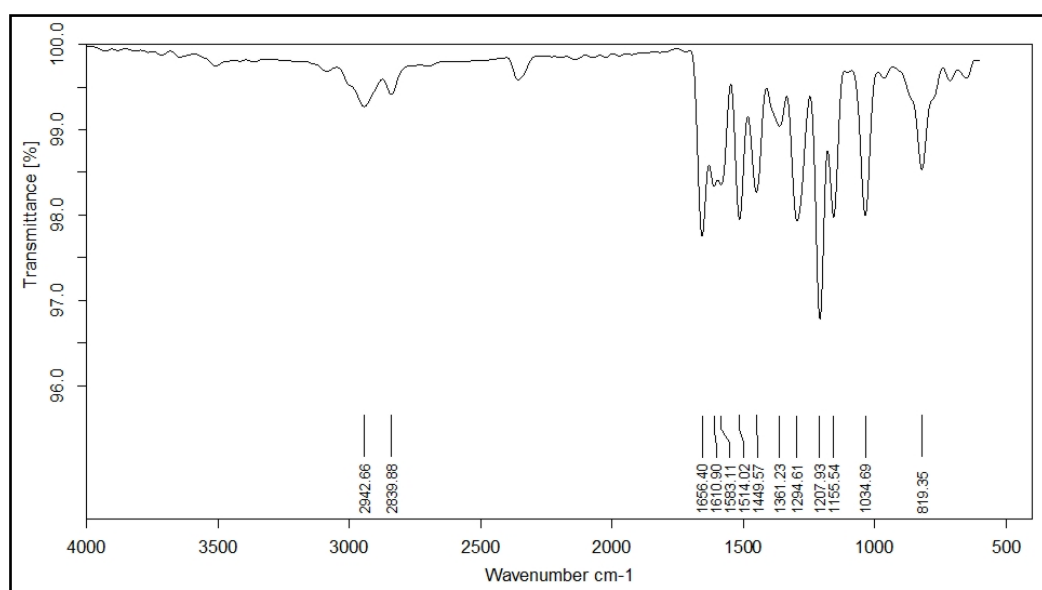


Figure S16 <sup>13</sup>C NMR spectrum of 7,4'-dibutoxy-5-hydroxy-2',5'-dimethoxyisoflavone (4)



**Figure S17** MS spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavone (**5**)



**Figure S18** IR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavone (**5**)

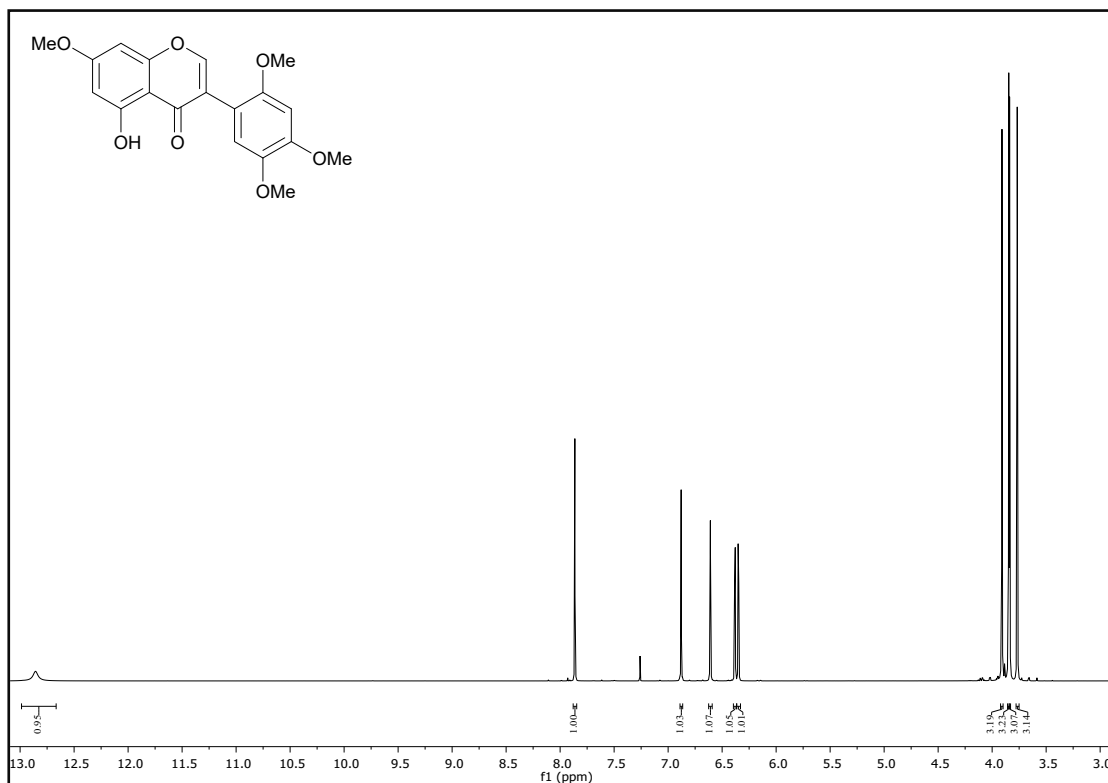


Figure S19 <sup>1</sup>H NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavone (5)

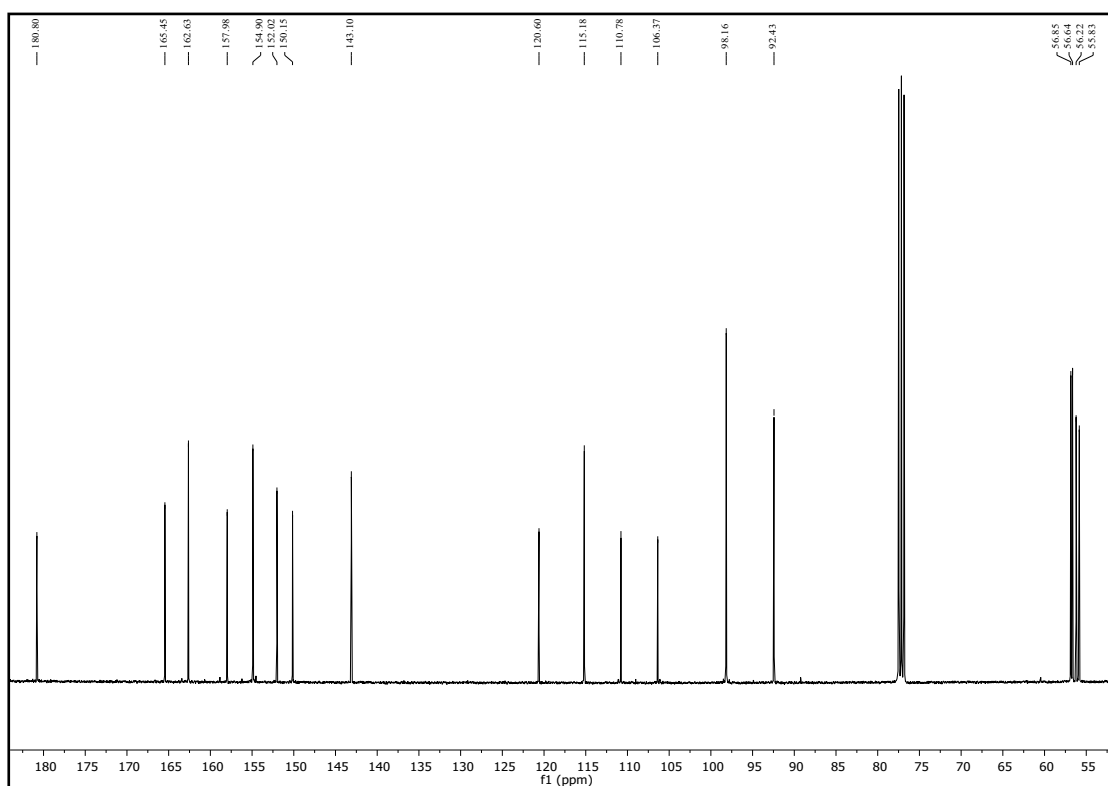


Figure S20 <sup>13</sup>C NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavone (5)

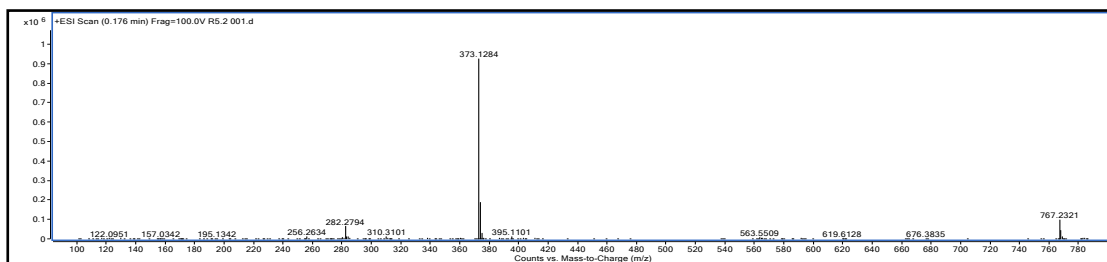


Figure S21 MS spectrum of 7,5,2',4',5'-pentamethoxyisoflavone (6)

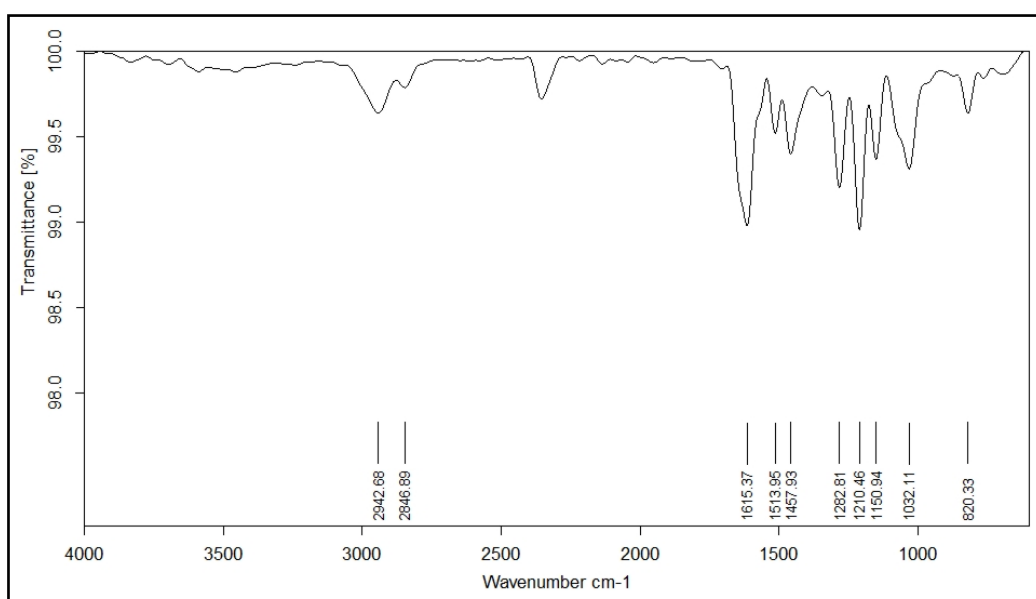


Figure S22 IR spectrum of 5,7,2',4',5'-pentamethoxyisoflavone (6)

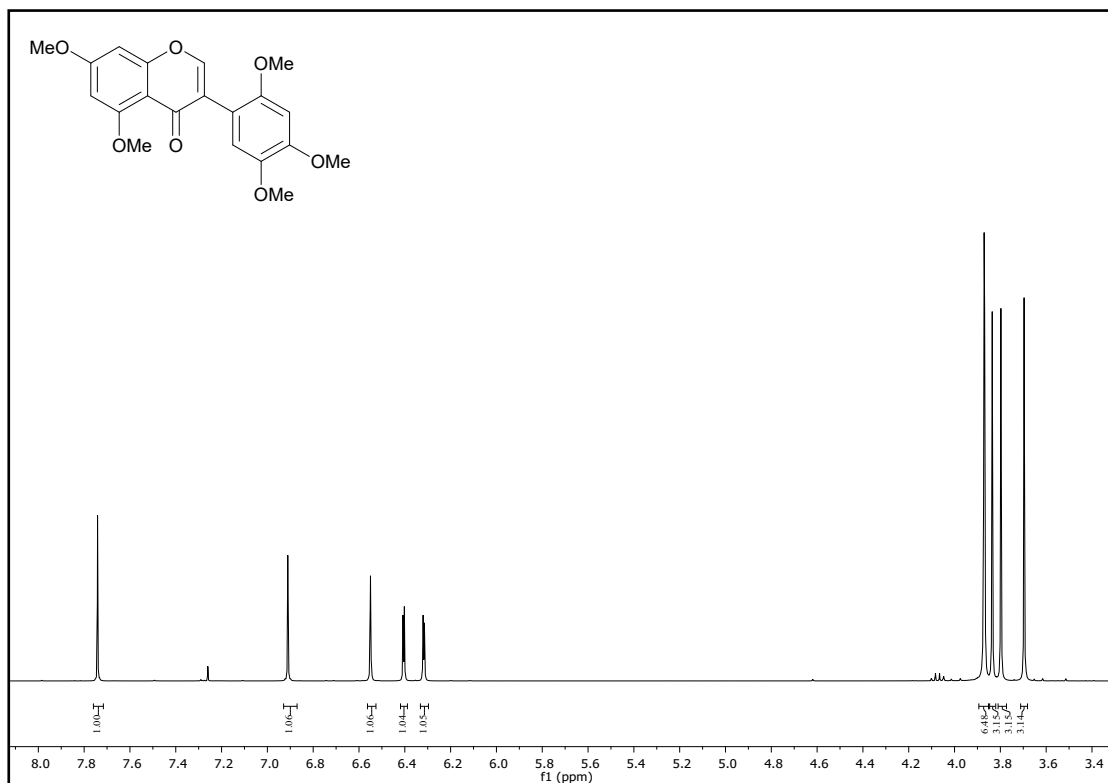


Figure S23 <sup>1</sup>H NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavone (6)

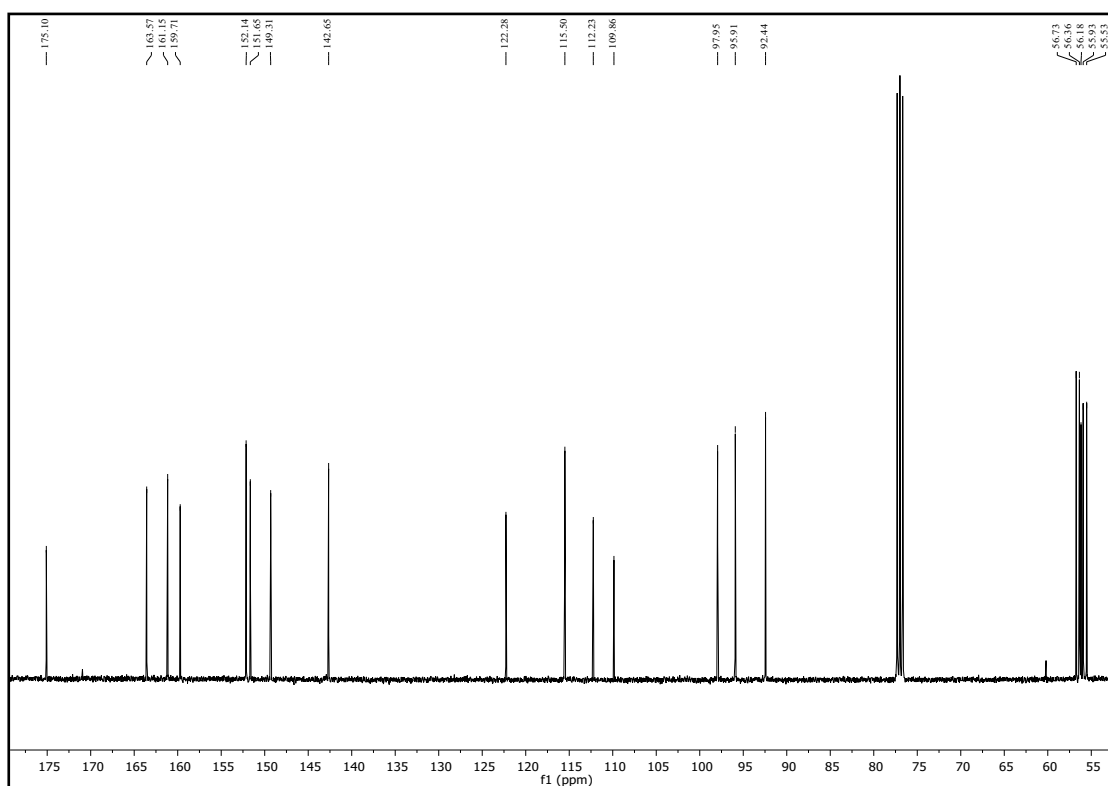
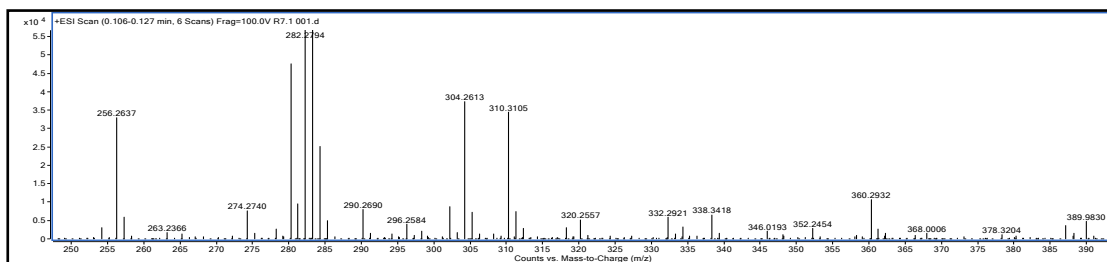
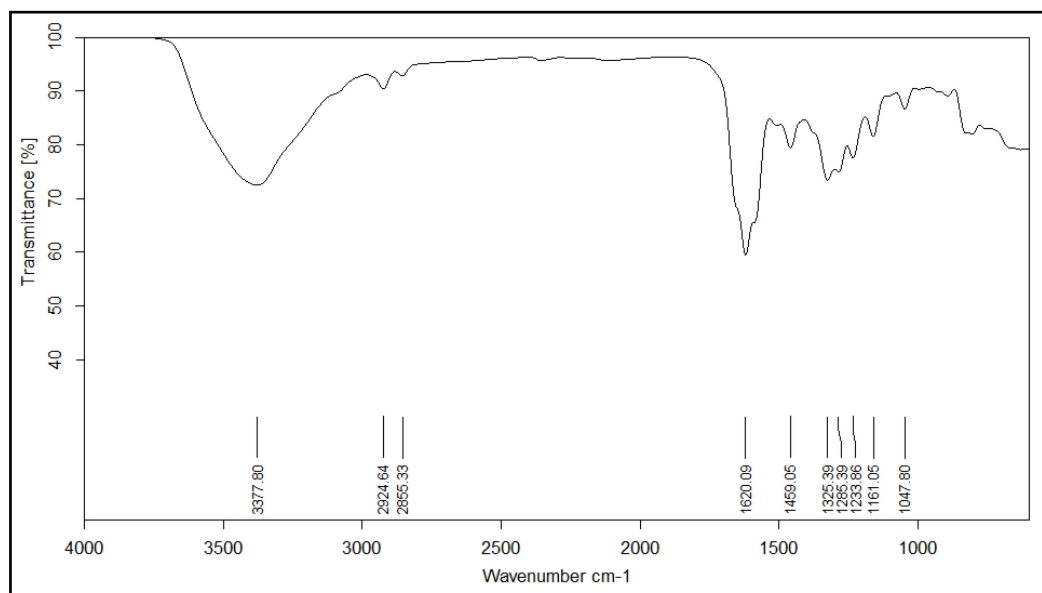


Figure S24 <sup>13</sup>C NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavone (6)

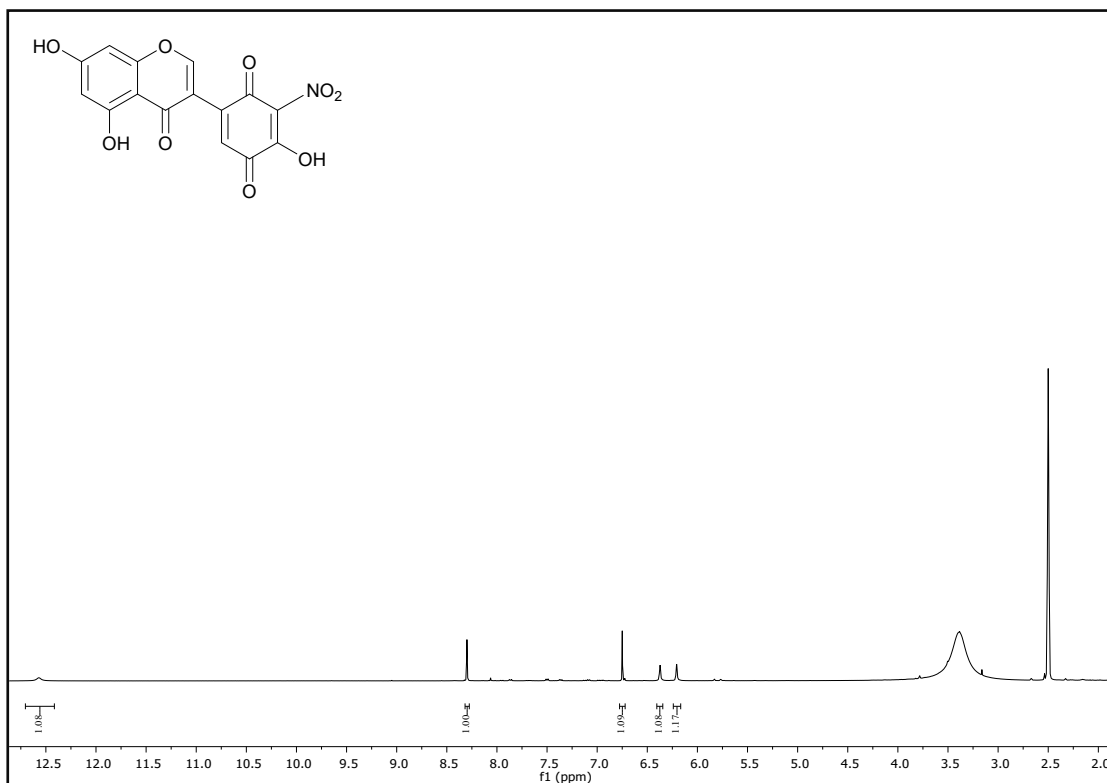




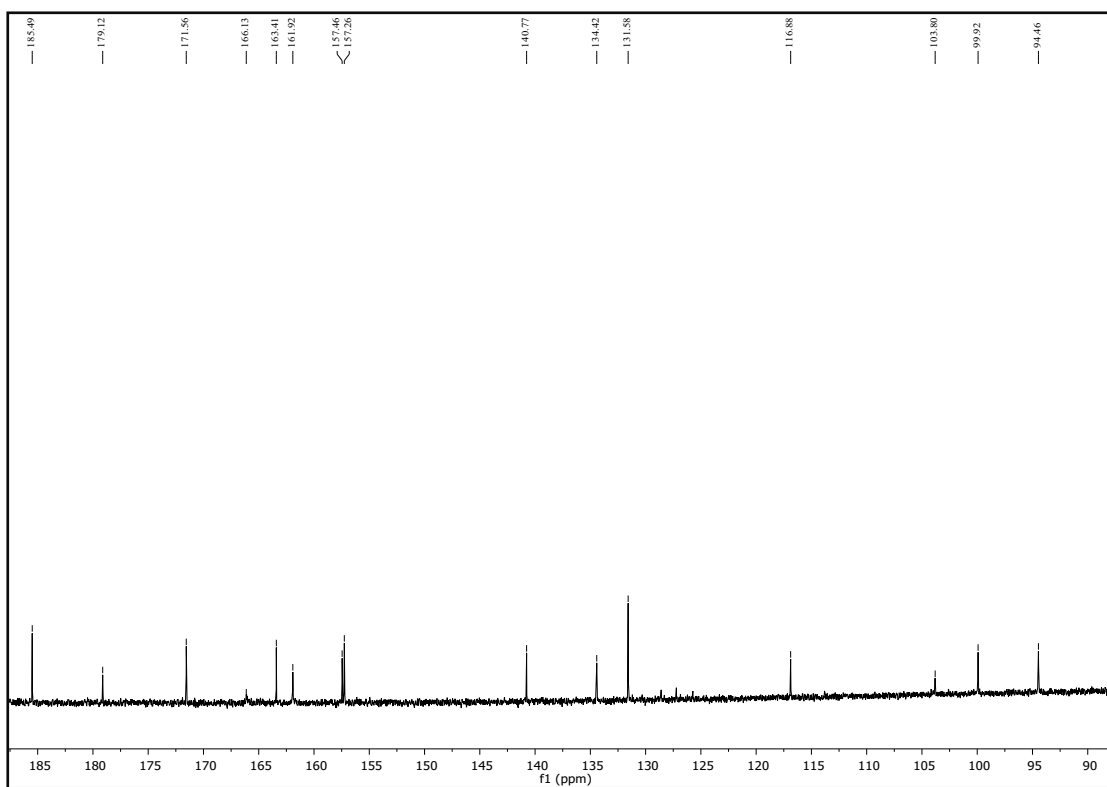
**Figure S25** MS spectrum of 1-(5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-3-yl)-4-hydroxy-3-nitro-2,5-quinone (**7**)



**Figure S26** IR spectrum of 1-(5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-3-yl)-4-hydroxy-3-nitro-2,5-quinone (**7**)



**Figure S27** <sup>1</sup>H NMR spectrum of 1-(5,7-dihydroxy-4-oxo-4H-1-benzopyran-3-yl)-4-hydroxy-3-nitro-2,5-quinone (**7**)



**Figure S28** <sup>13</sup>C NMR spectrum of 1-(5,7-dihydroxy-4-oxo-4H-1-benzopyran-3-yl)-4-hydroxy-3-nitro-2,5-quinone (**7**)

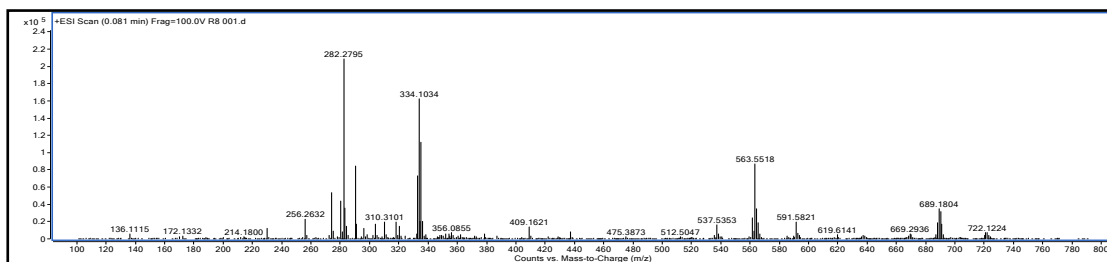


Figure S29 MS spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavanone (**8**)

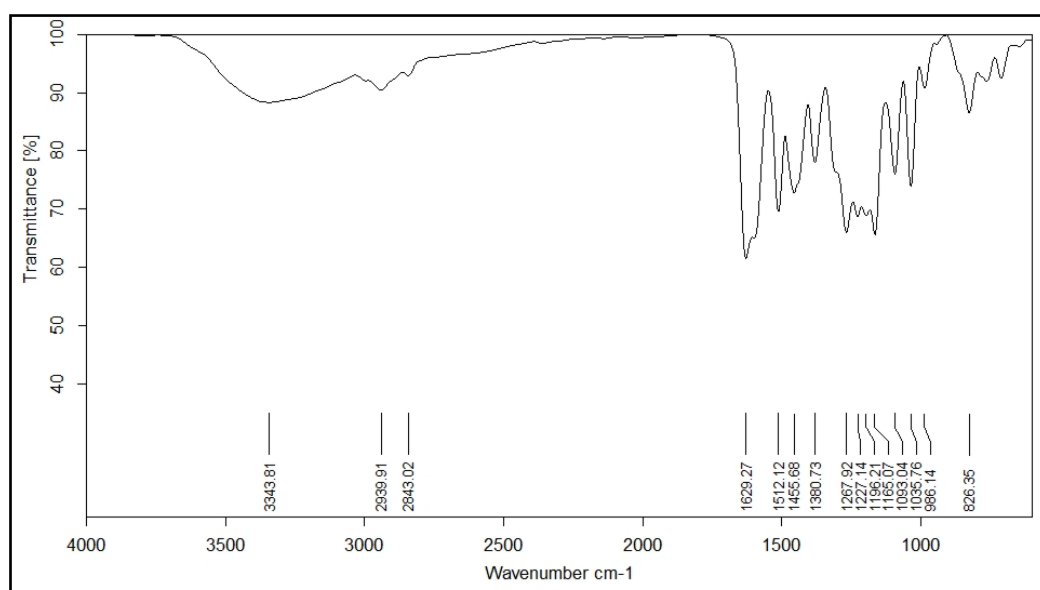


Figure S30 IR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavanone (**8**)

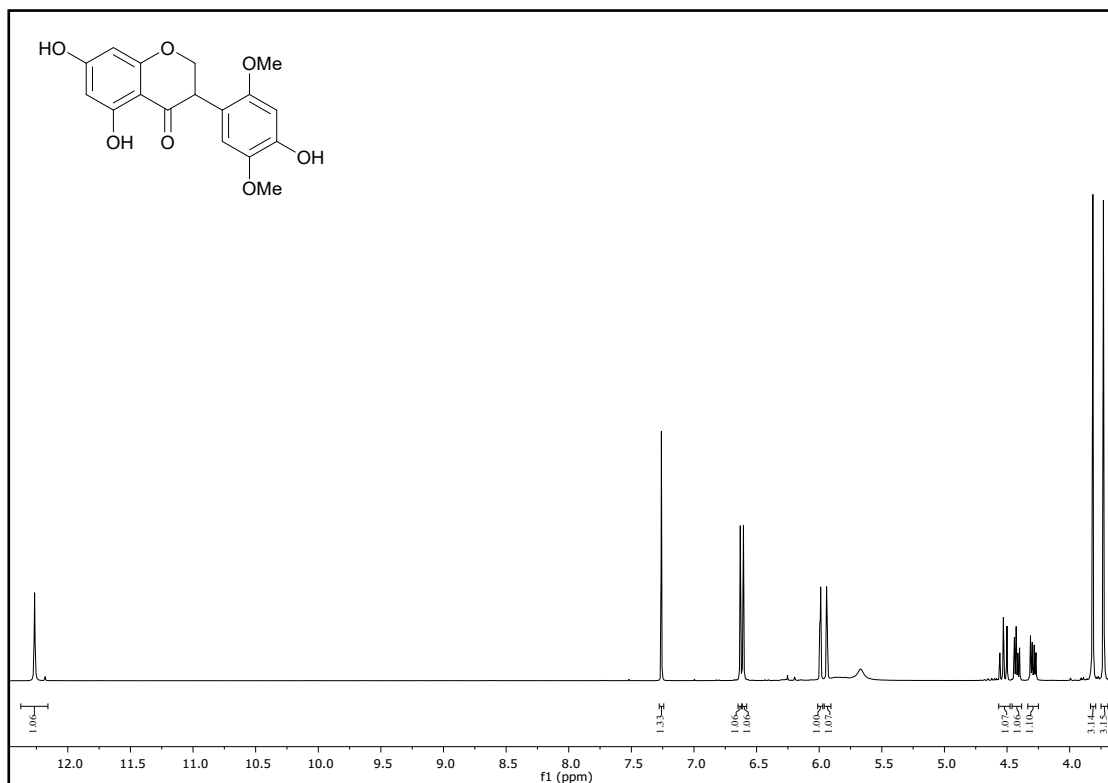


Figure S31 <sup>1</sup>H NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavanone (8)

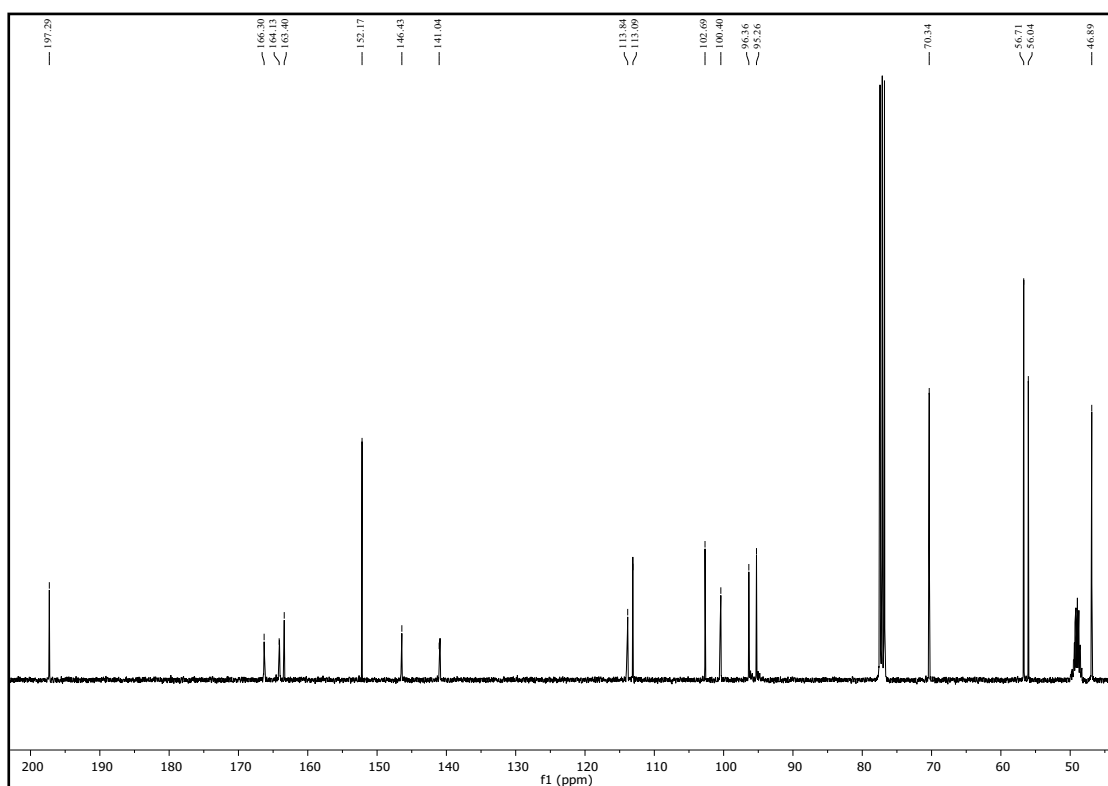


Figure S32 <sup>13</sup>C NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavanone (8)

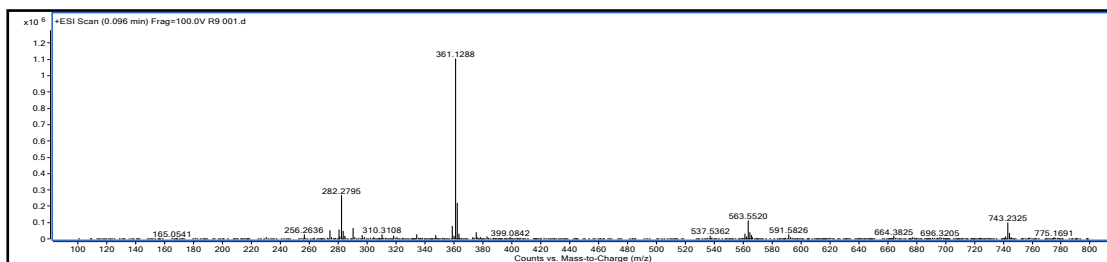


Figure S33 MS spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone (9)

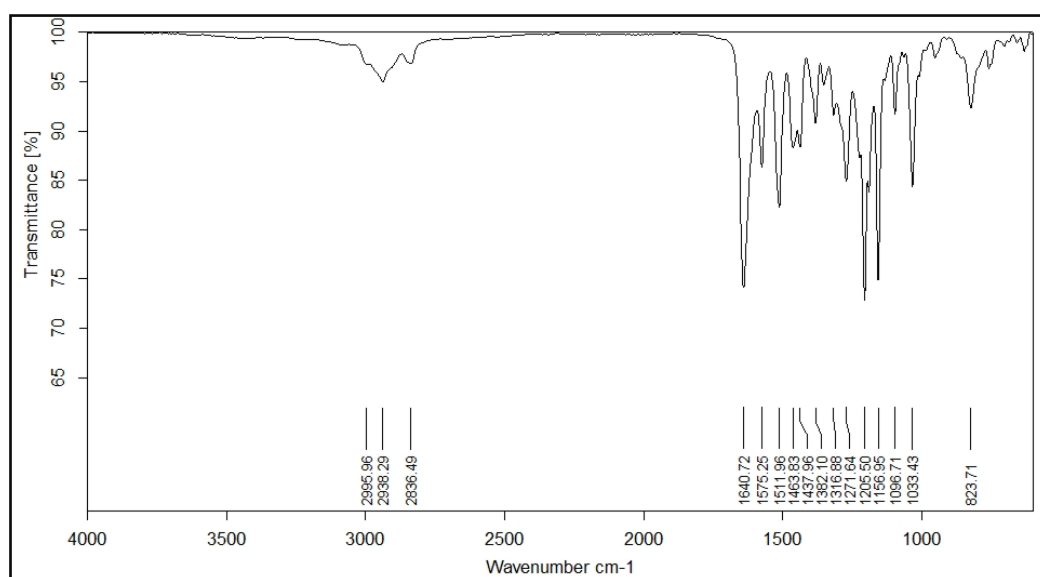


Figure S34 IR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone (9)

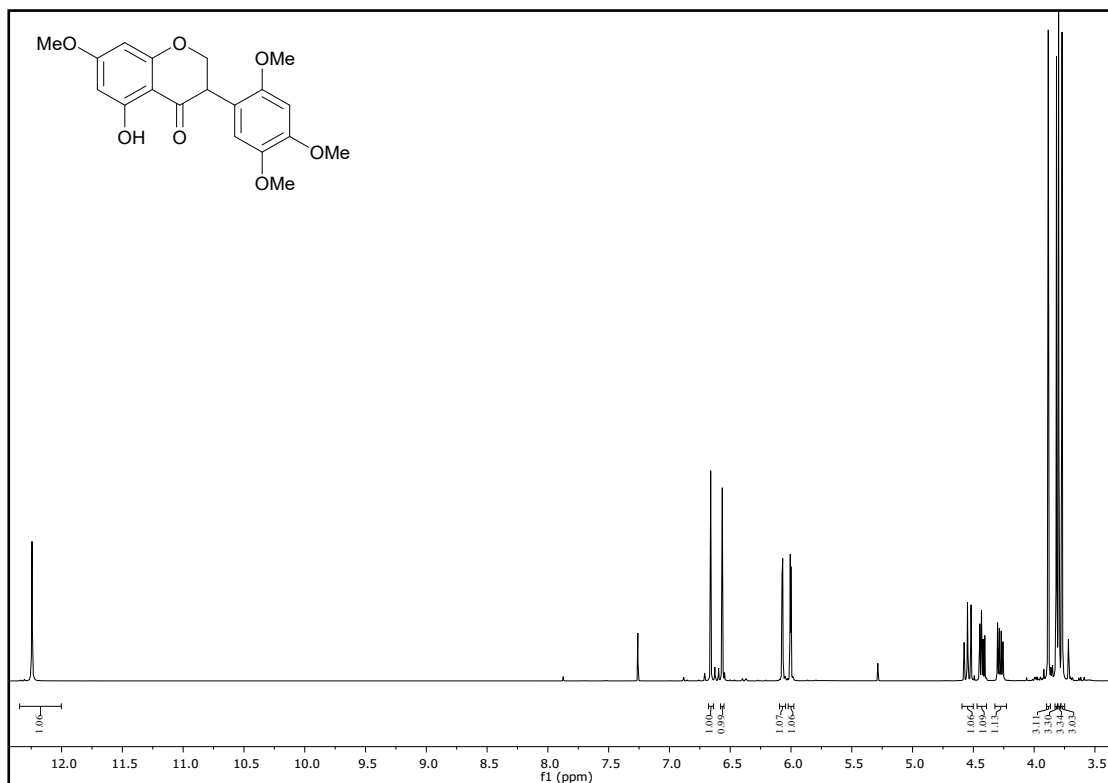


Figure S35 <sup>1</sup>H NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone (9)

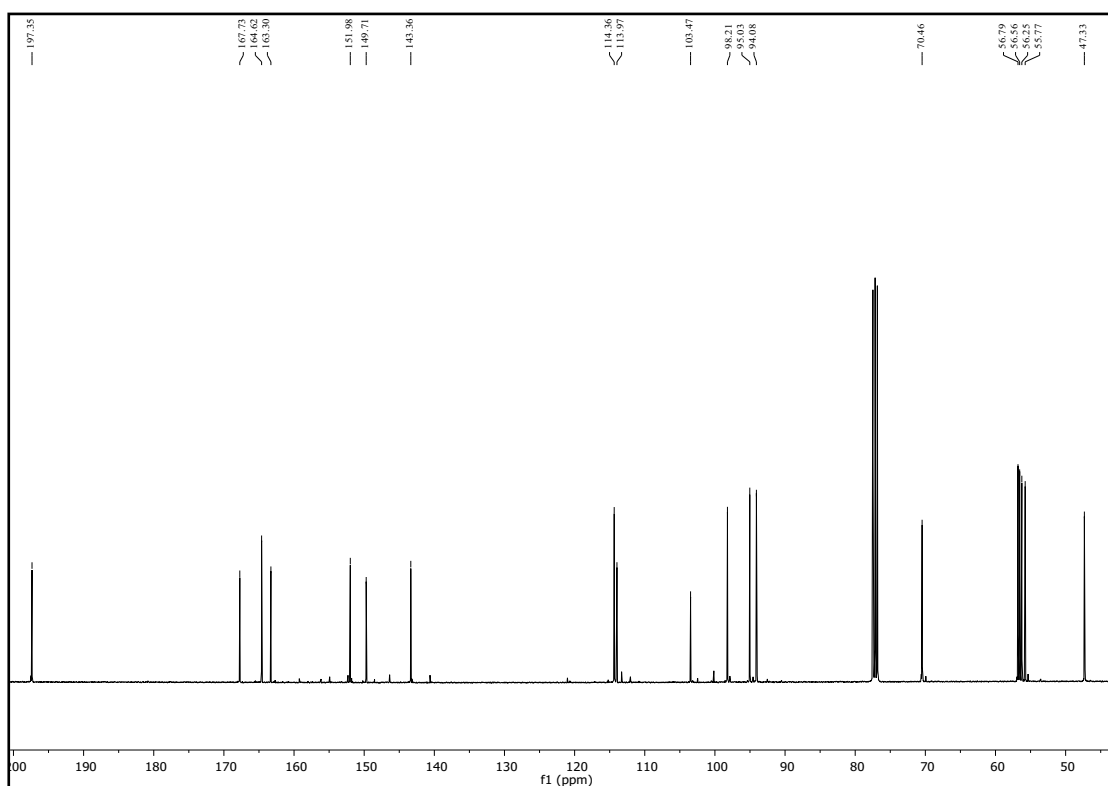


Figure S36 <sup>13</sup>C NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone (9)

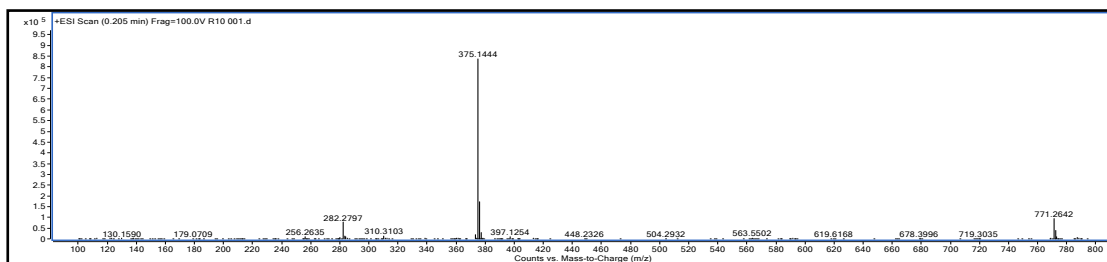


Figure S37 MS spectrum of 5,7,2',4',5'-pentamethoxyisoflavanone (10)

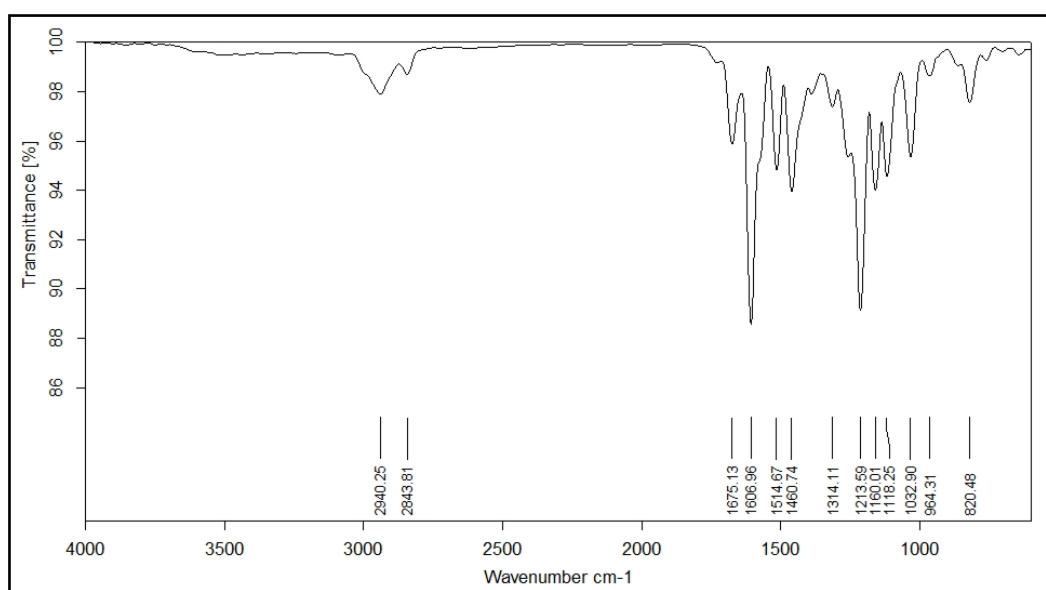


Figure S38 IR spectrum of 5,7,2',4',5'-pentamethoxyisoflavanone (10)

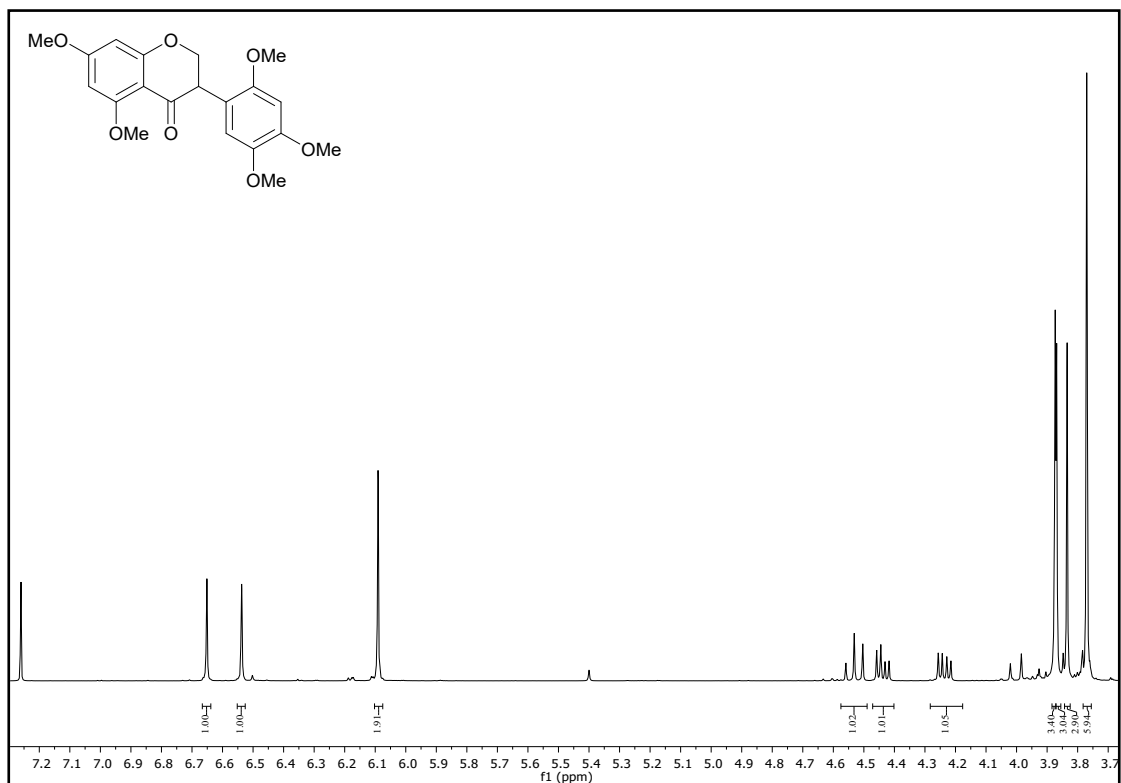


Figure S39  $^1\text{H}$  NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavanone (10)

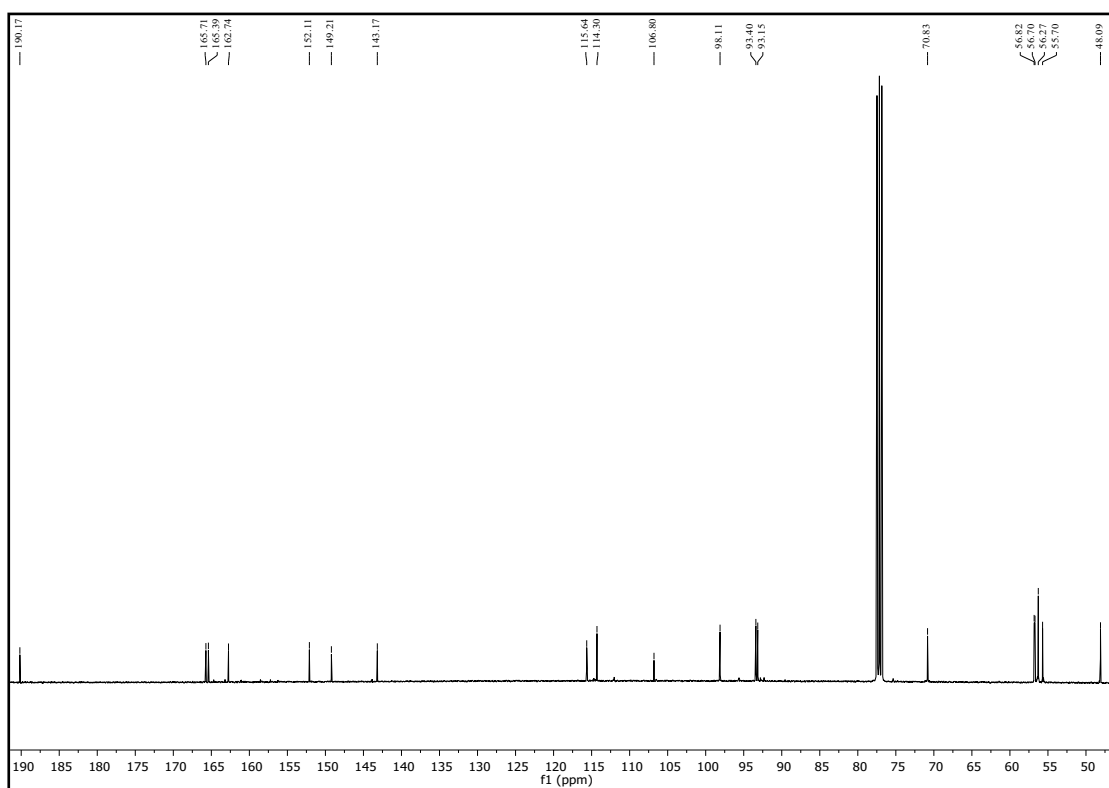


Figure S40  $^{13}\text{C}$  NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavanone (10)



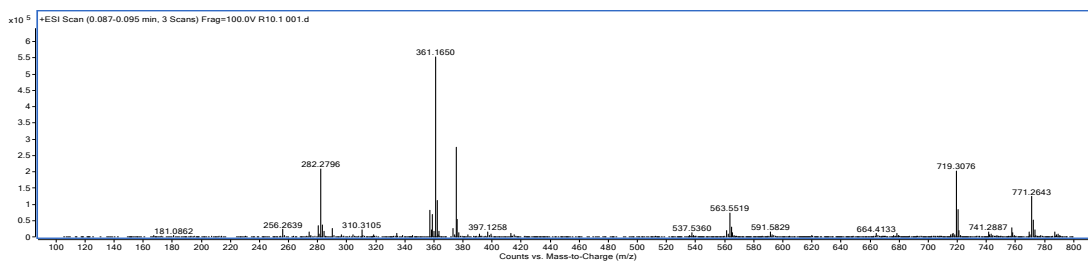


Figure S41 MS spectrum of 5,7,2',4',5'-pentamethoxyisoflavan (11)

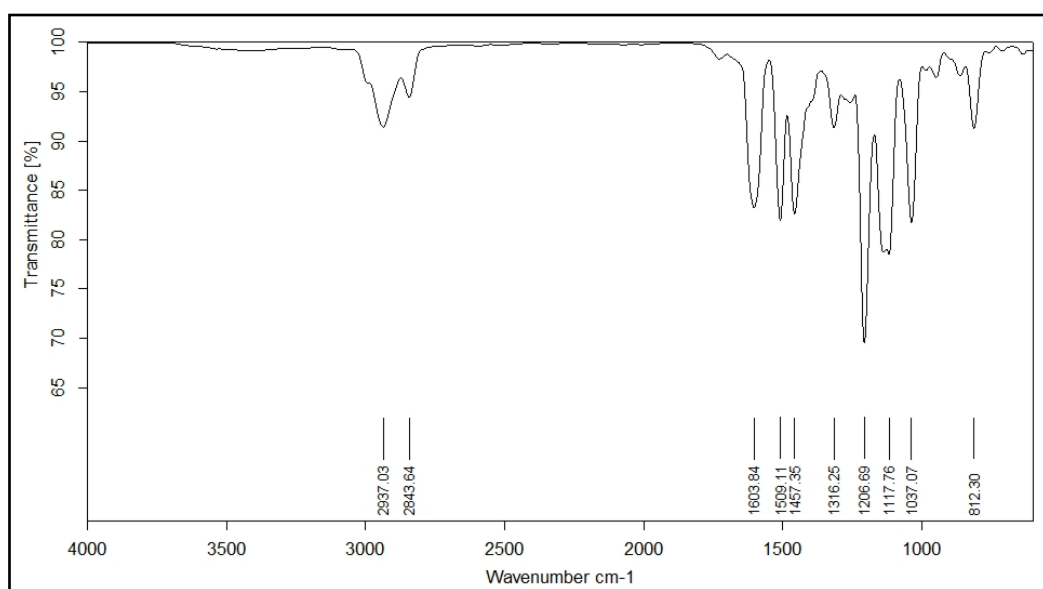


Figure S42 IR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan (11)

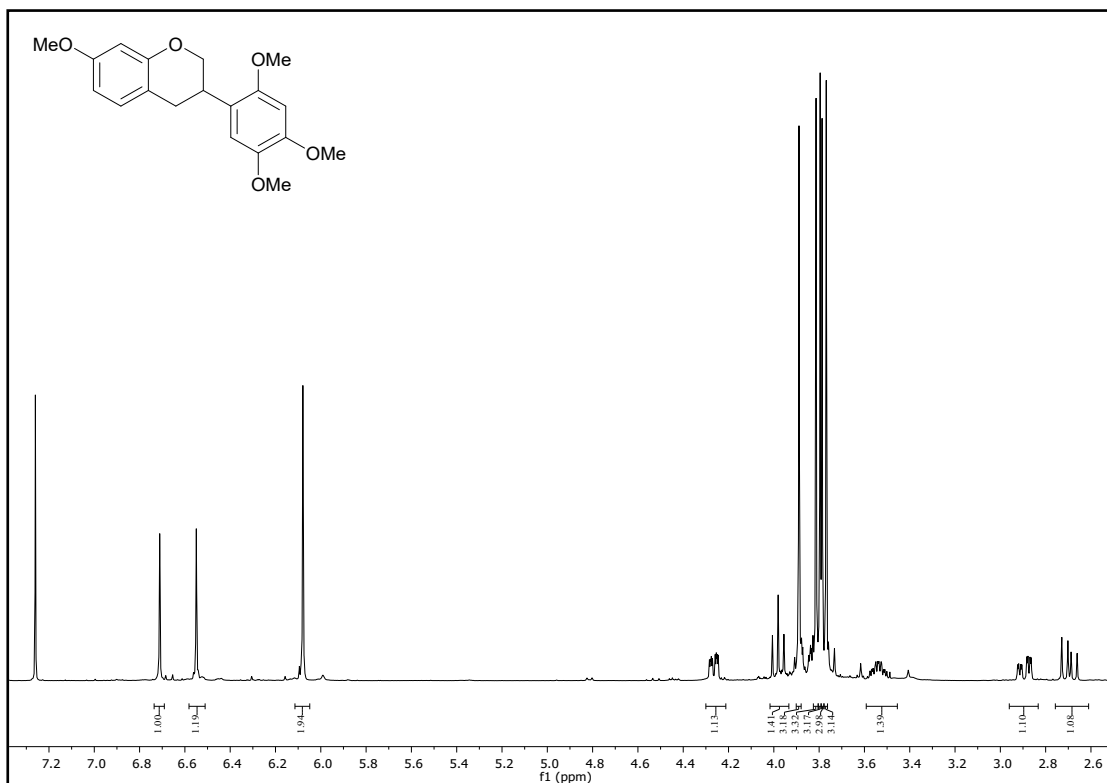


Figure S43  $^1\text{H}$  NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan (11)

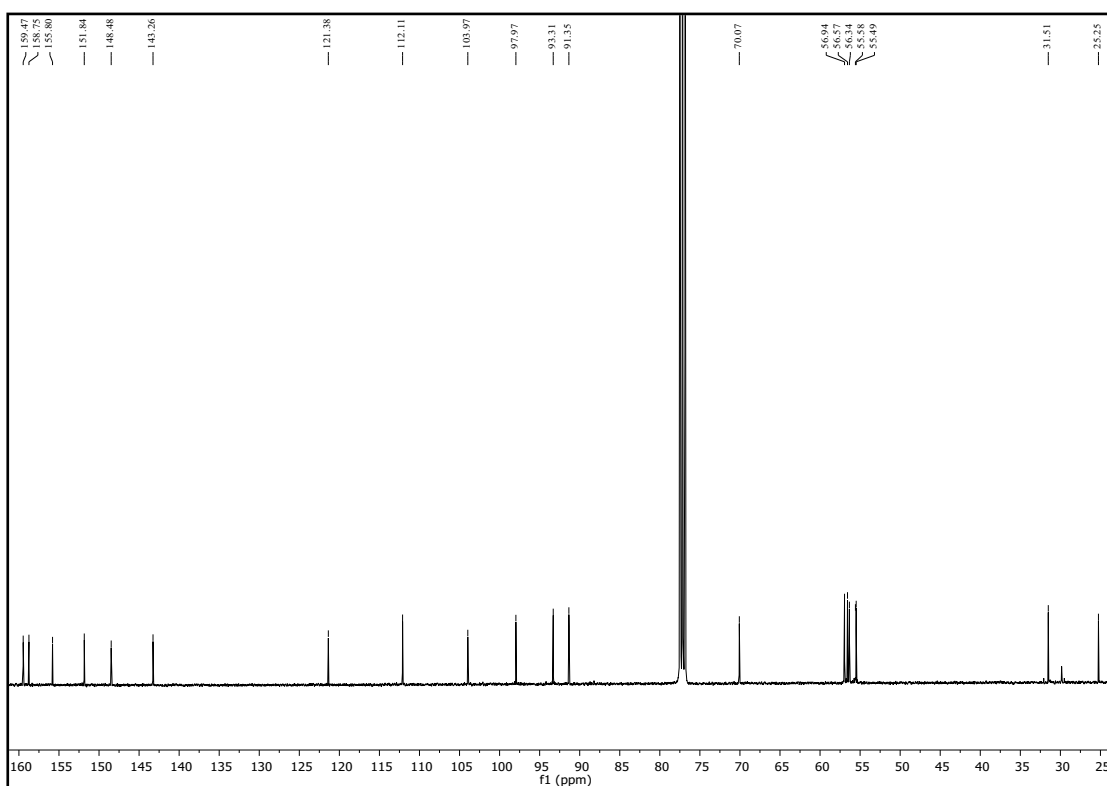
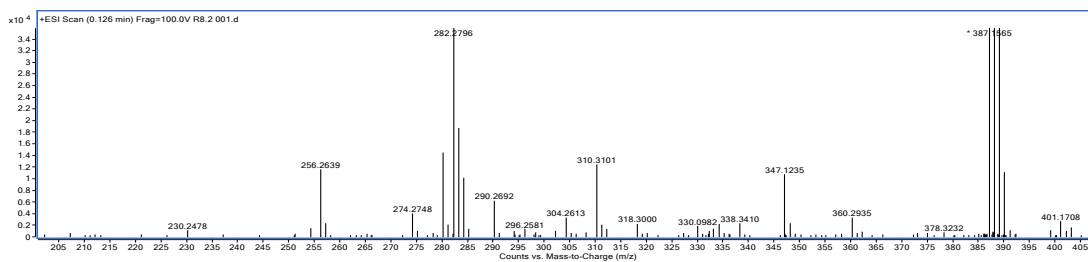
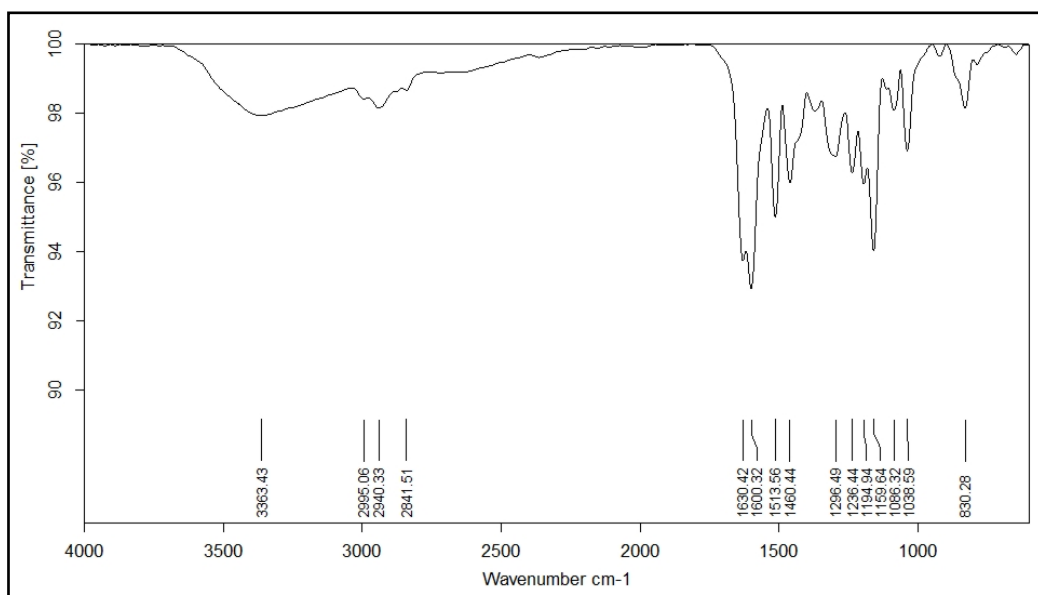


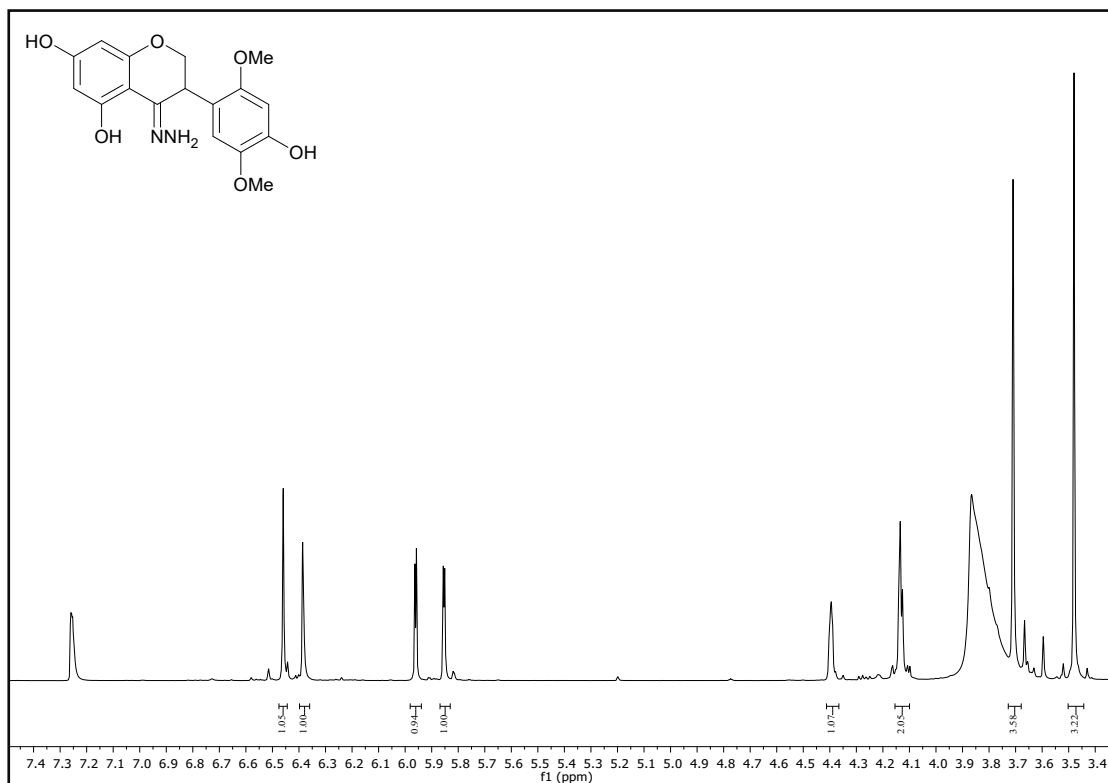
Figure S44  $^{13}\text{C}$  NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan (11)



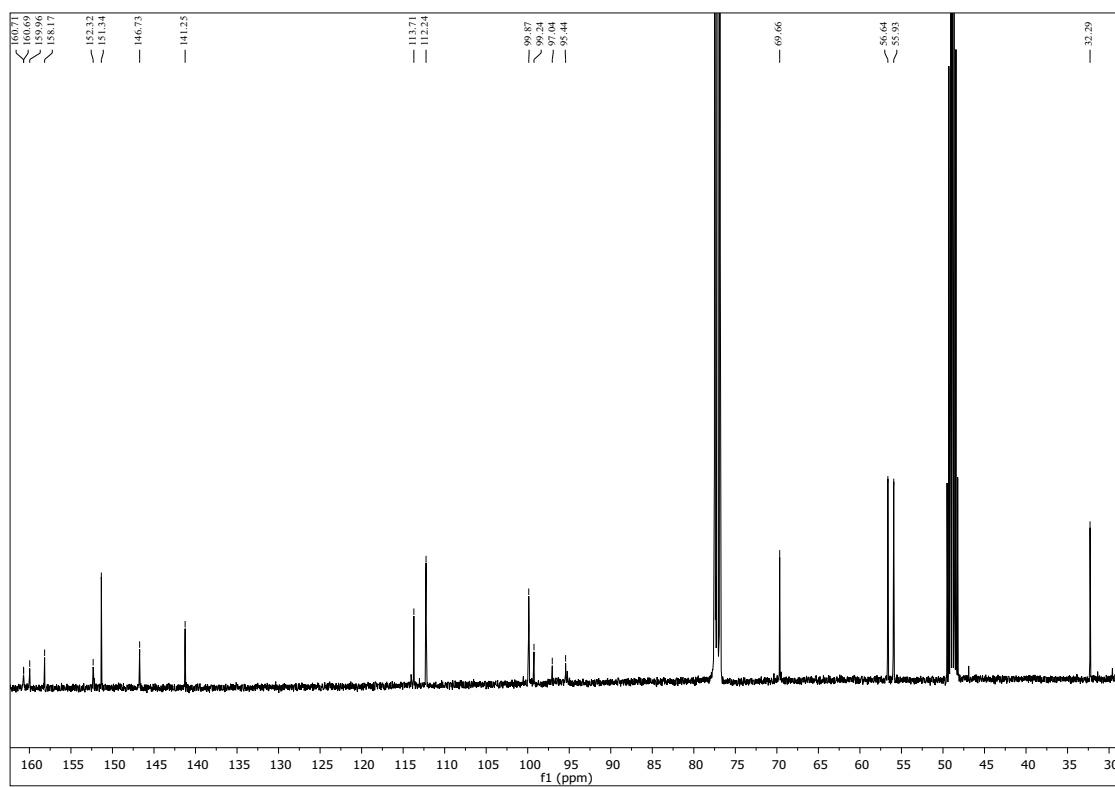
**Figure S45** MS spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan hydrazone  
(12)



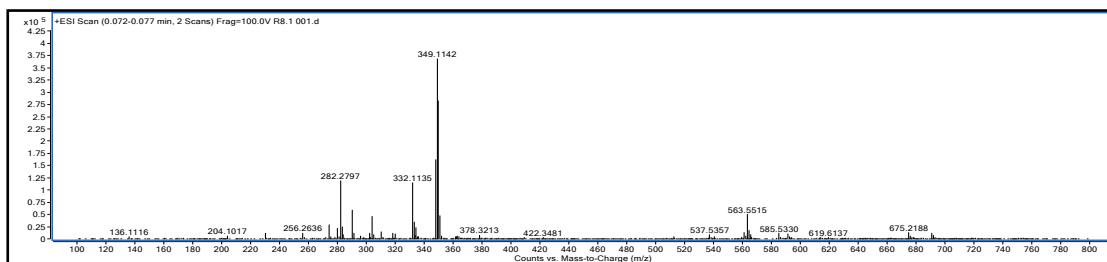
**Figure S46** IR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan hydrazone  
(12)



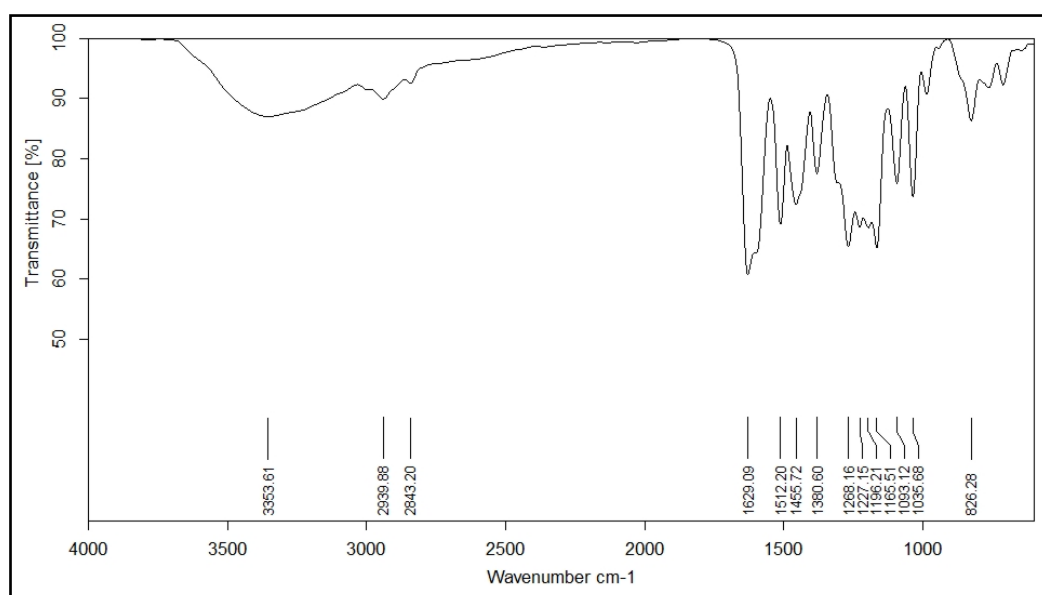
**Figure S47** <sup>1</sup>H NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan hydrazone (12)



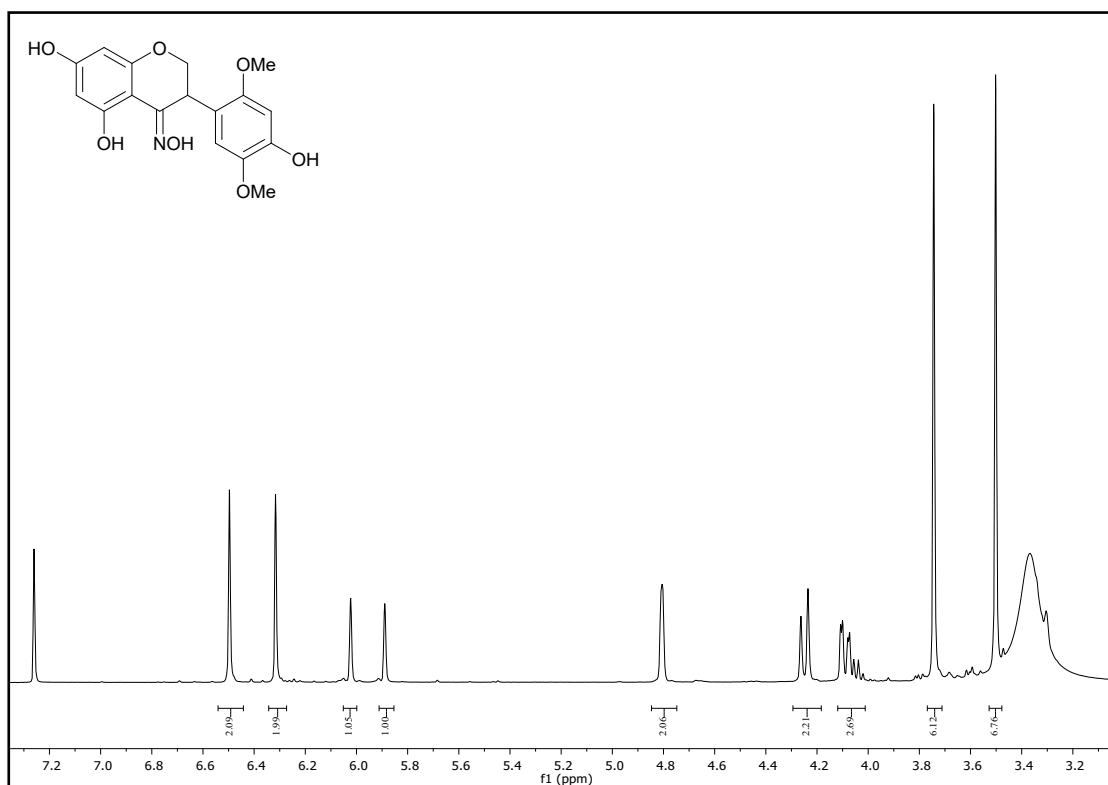
**Figure S48** <sup>13</sup>C NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan hydrazone (12)



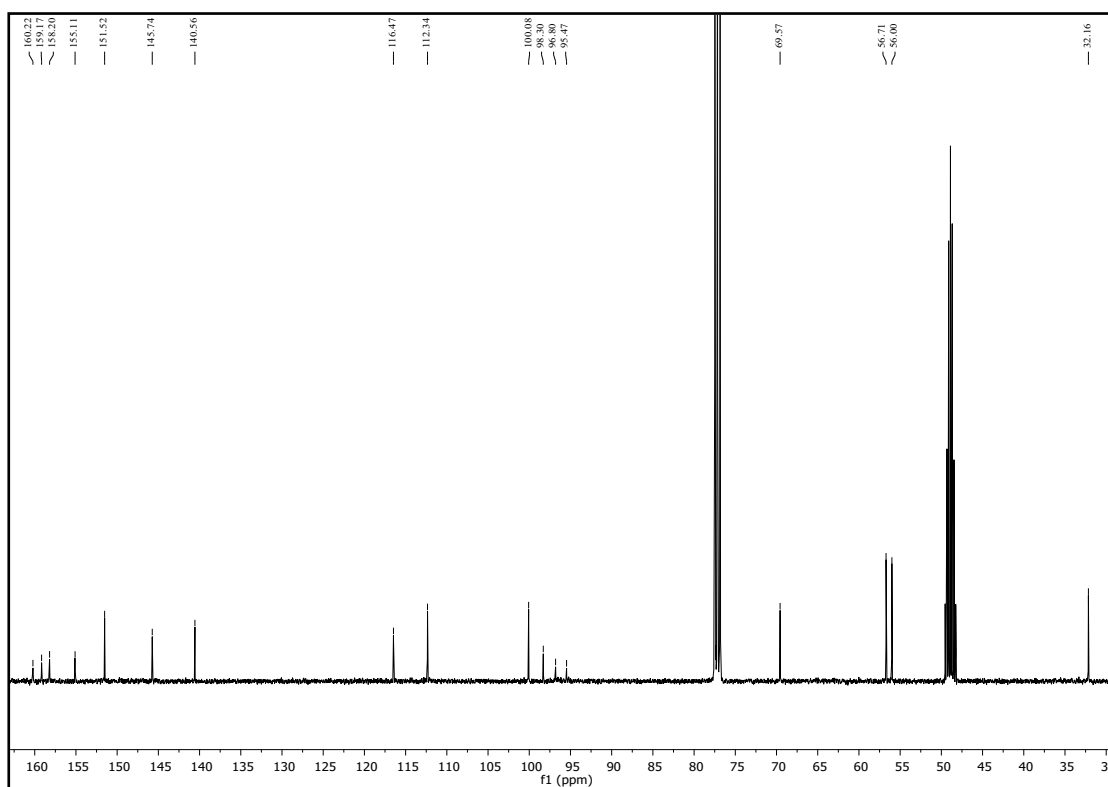
**Figure S49** MS spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan oxime (**13**)



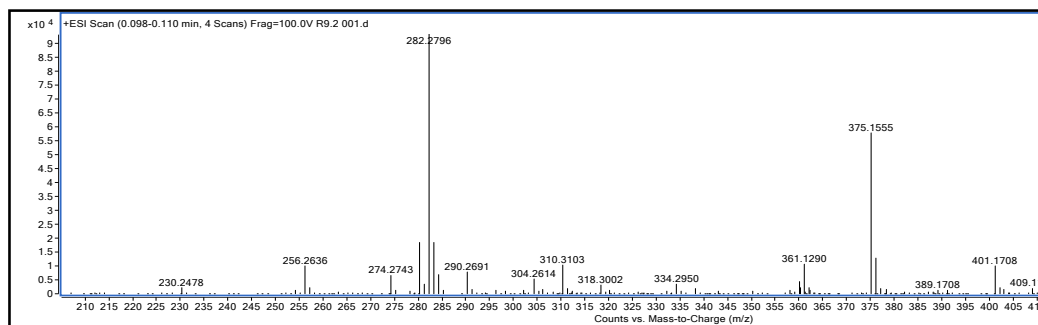
**Figure S50** IR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan oxime (**13**)



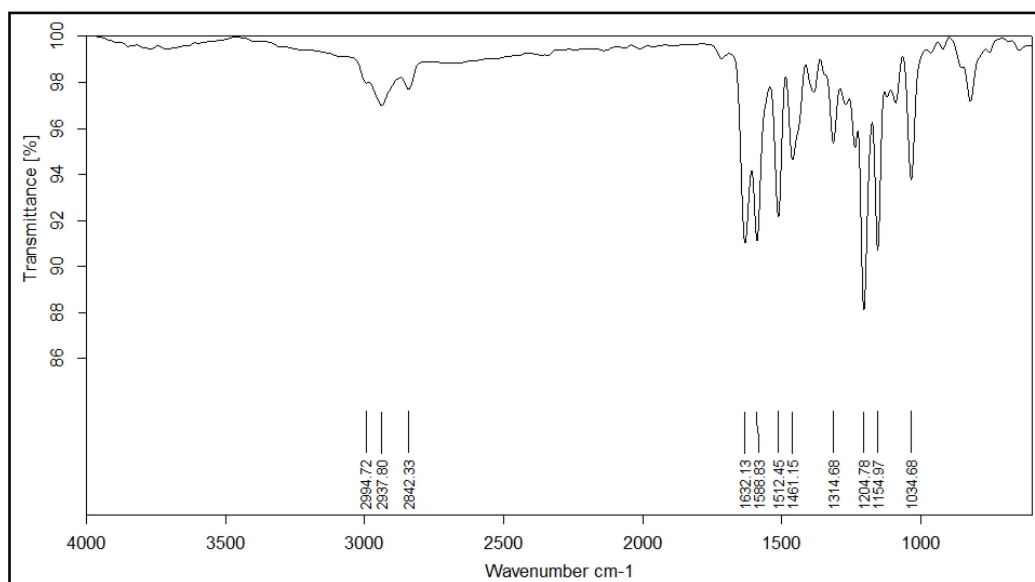
**Figure S51**  $^1\text{H}$  NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan oxime (**13**)



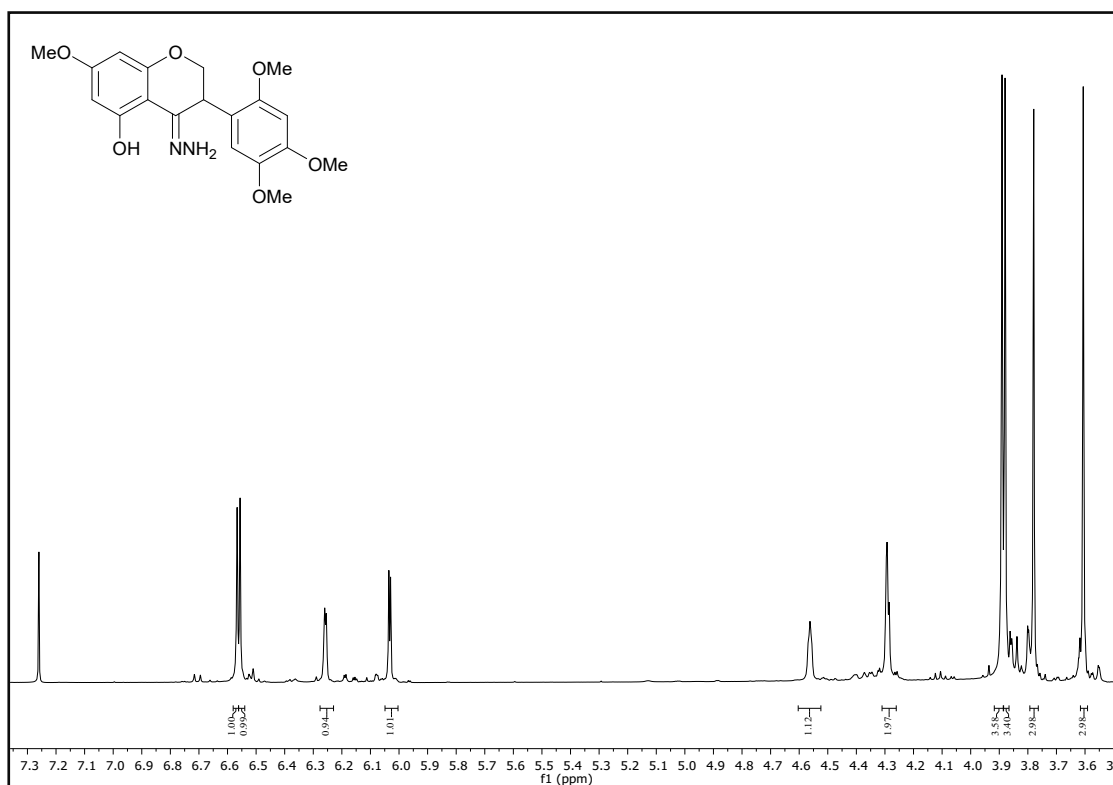
**Figure S52**  $^{13}\text{C}$  NMR spectrum of 5,7,4'-trihydroxy-2',5'-dimethoxyisoflavan oxime (**13**)



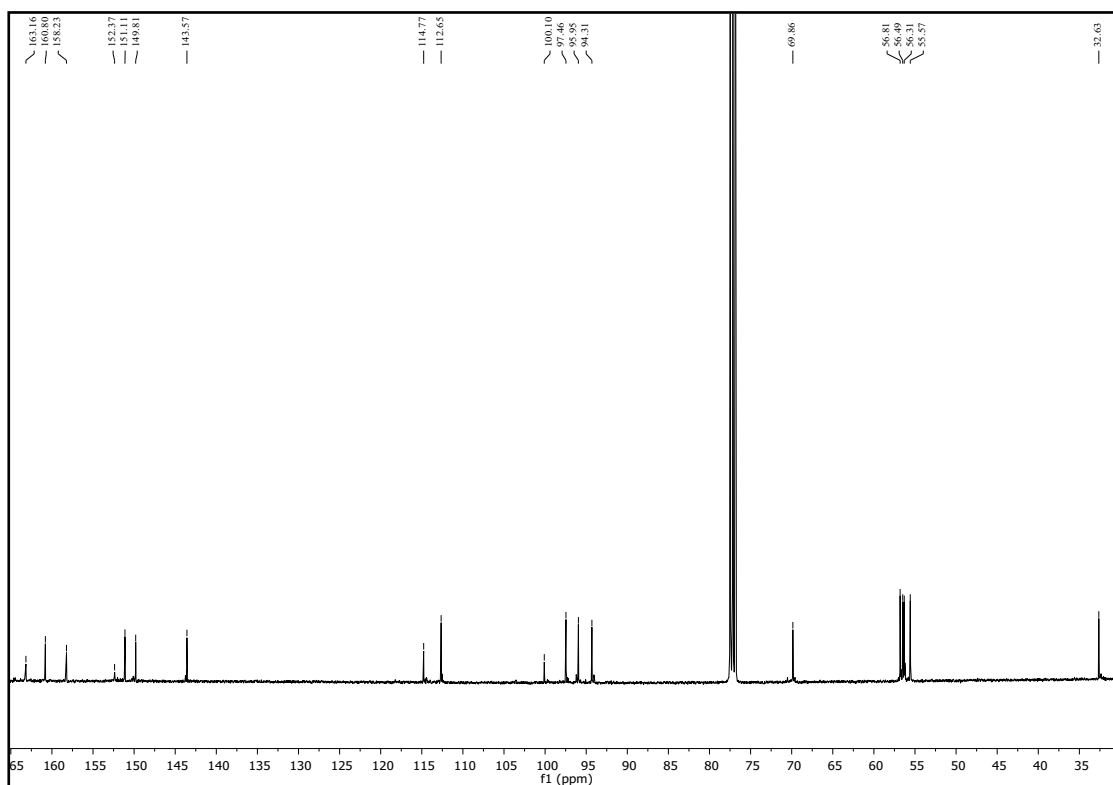
**Figure S53** MS spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone hydrazone (**14**)



**Figure S54** IR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone hydrazone (**14**)

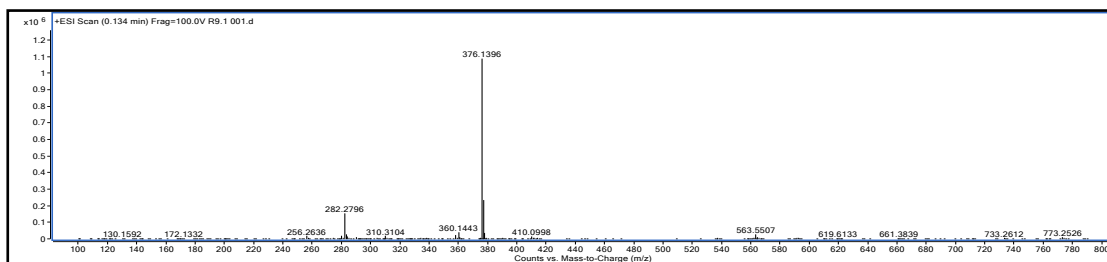


**Figure S55** <sup>1</sup>H NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone hydrazone (14)

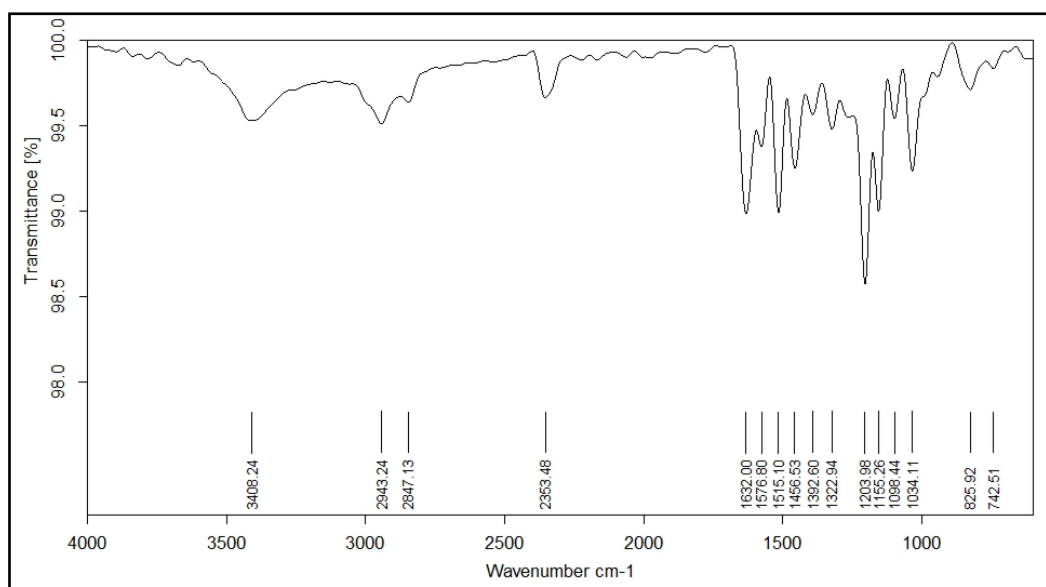


**Figure S56** <sup>13</sup>C NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone hydrazone (14)

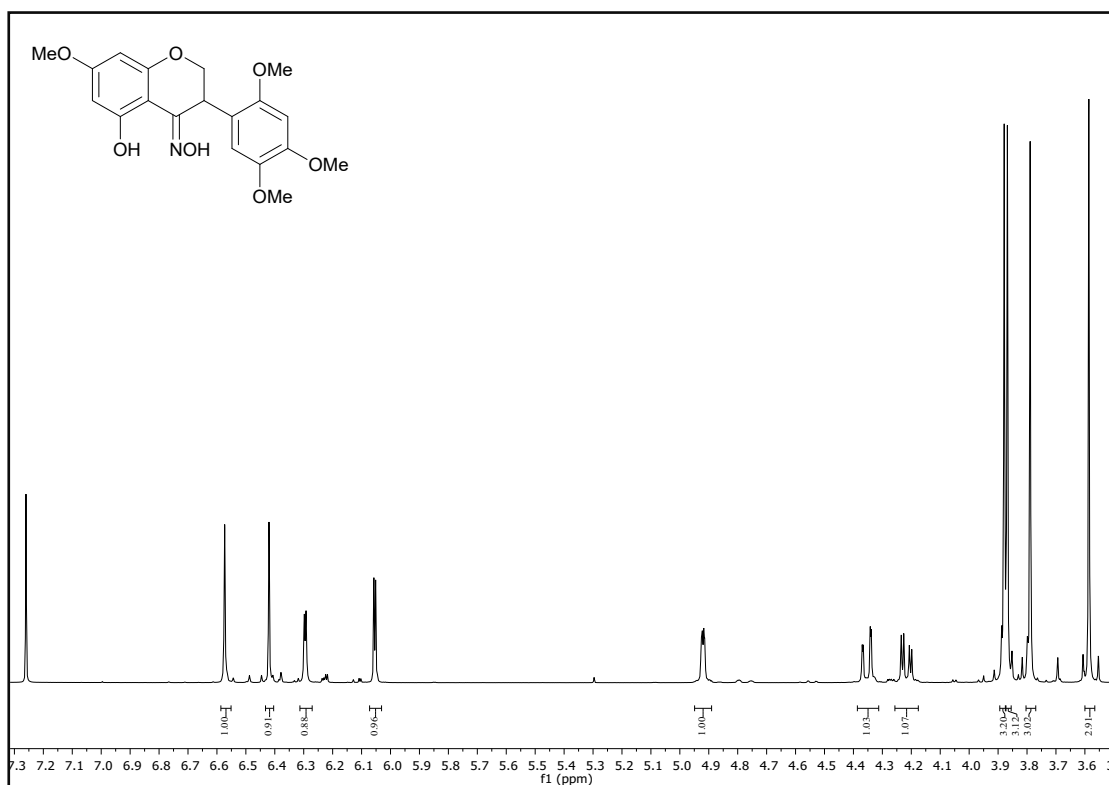




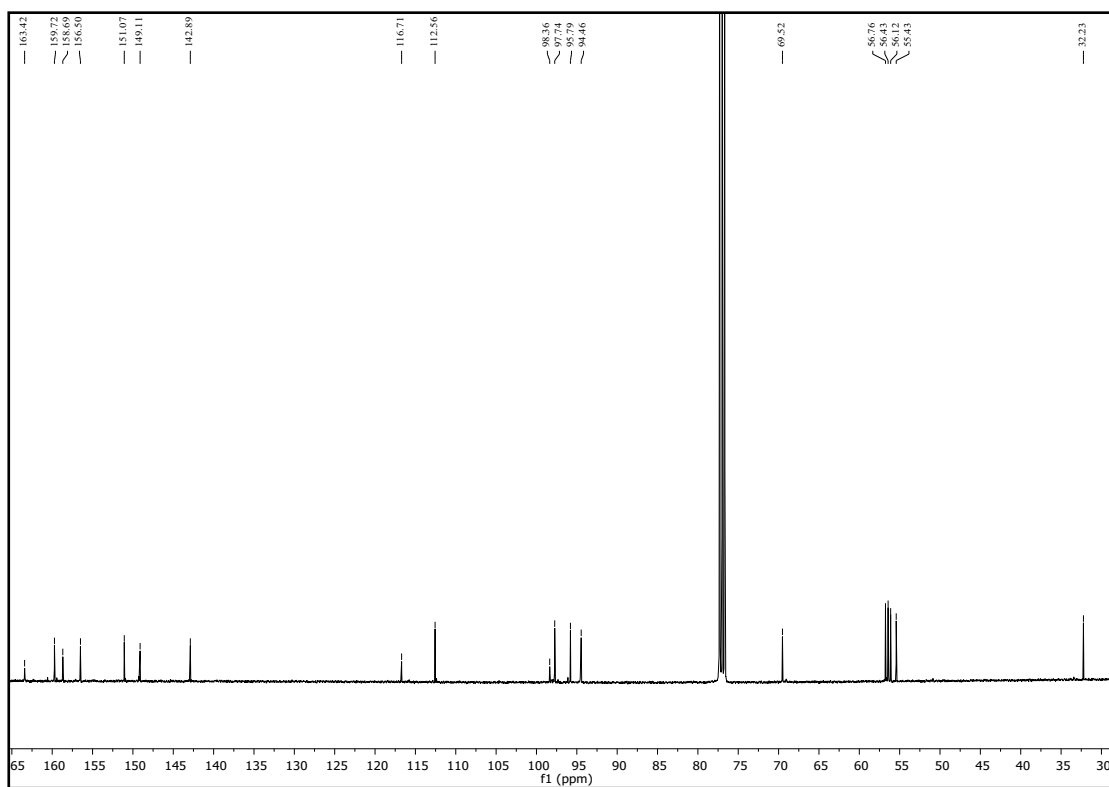
**Figure S57** MS spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone oxime (**15**)



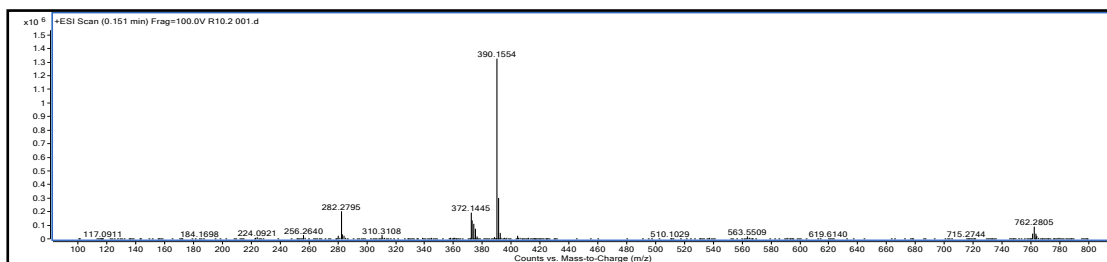
**Figure S58** IR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone oxime (**15**)



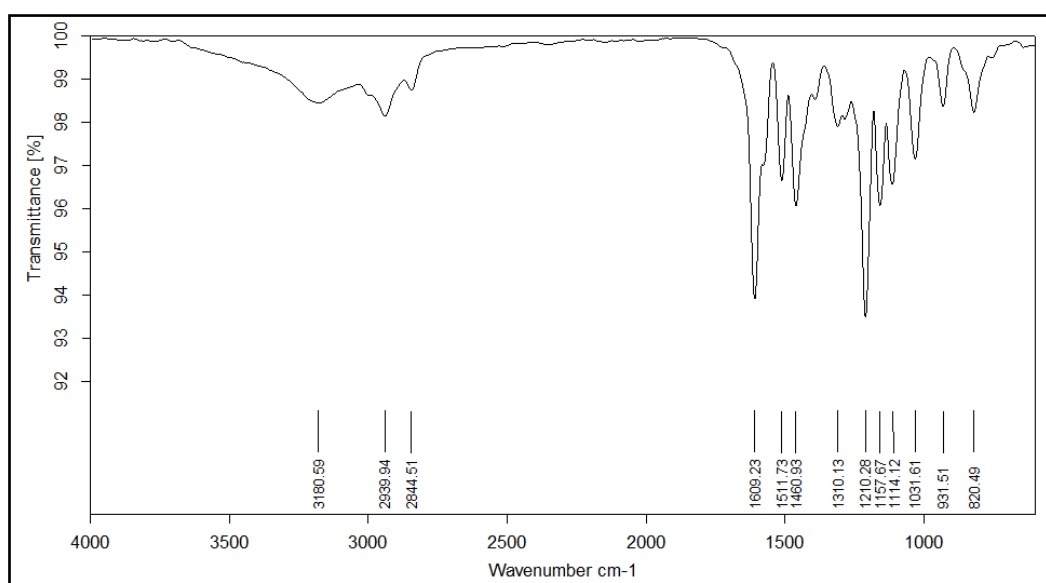
**Figure S59** <sup>1</sup>H NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone oxime (15)



**Figure S60** <sup>13</sup>C NMR spectrum of 5-hydroxy-7,2',4',5'-tetramethoxyisoflavanone oxime (15)



**Figure S61** MS spectrum of 5,7,2',4',5'-pentamethoxyisoflavan oxime (**16**)



**Figure S62** IR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan oxime (**16**)

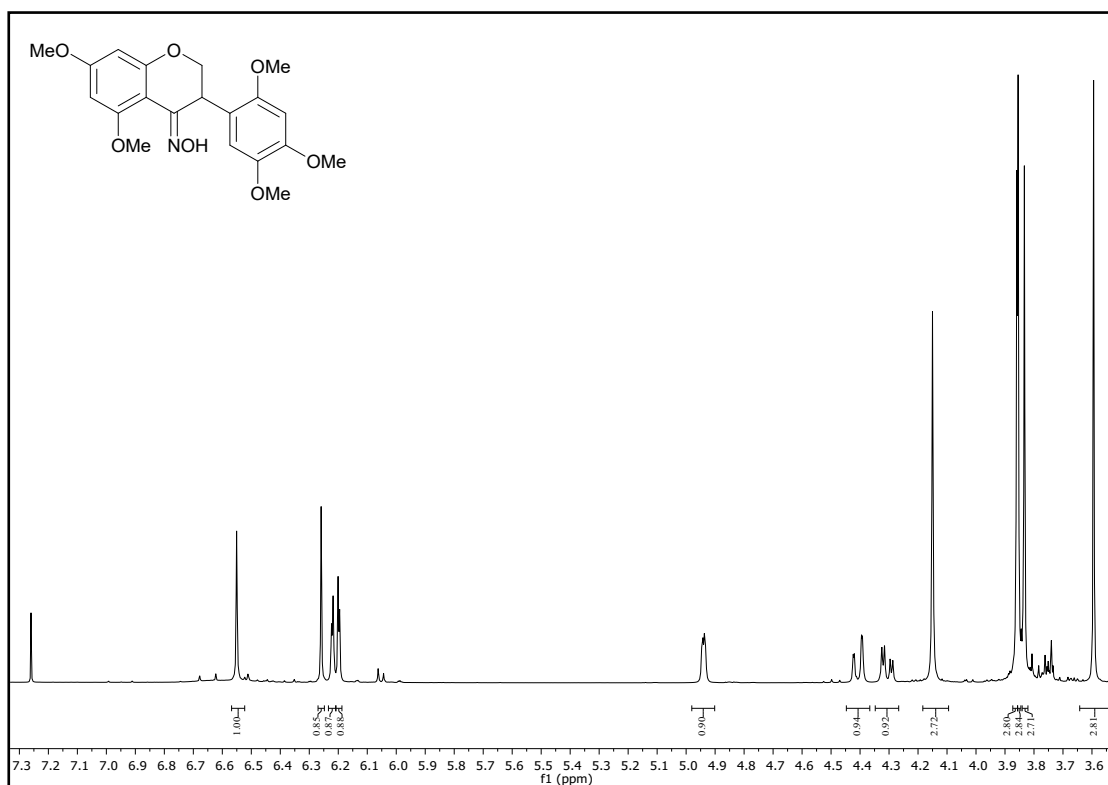


Figure S63 <sup>1</sup>H NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan oxime (16)

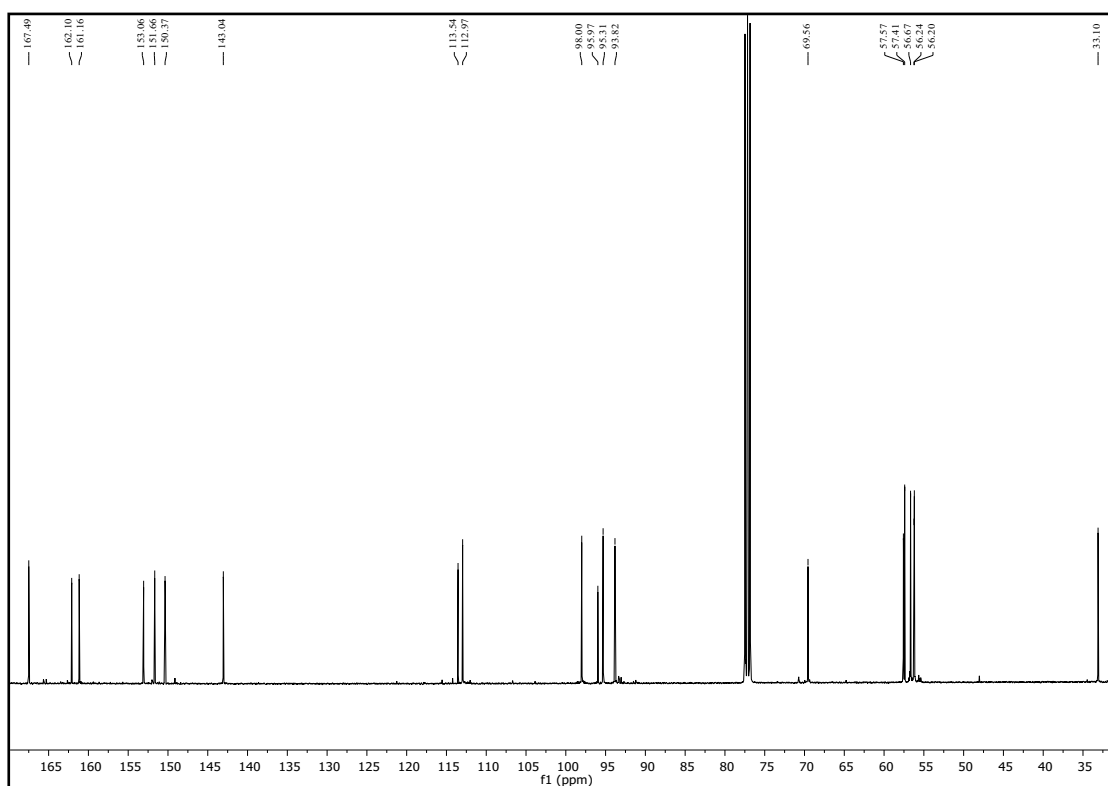


Figure S64 <sup>13</sup>C NMR spectrum of 5,7,2',4',5'-pentamethoxyisoflavan oxime (16)