

# Supplementary Data

## Biotransformation of methoxyflavone by selected entomopathogenic filamentous fungi

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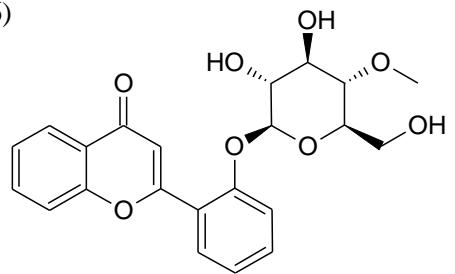
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Fig.S1. MS analysis flavone 2'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**6**)

Molecular Formula = C<sub>22</sub>H<sub>22</sub>O<sub>8</sub>  
 Formula Weight = 414.40528  
 Precursor: = 415.4000  
 CE (collision energy): -15.0



CE:-35.0



CE:-45.0



Fig.S2.  $^1\text{H}$  NMR spectral of flavone 2'- $O$ - $\beta$ -D-(4"- $O$ -methyl)-glucopyranoside (**6**) (DMSO- $d_6$ , 600 MHz)

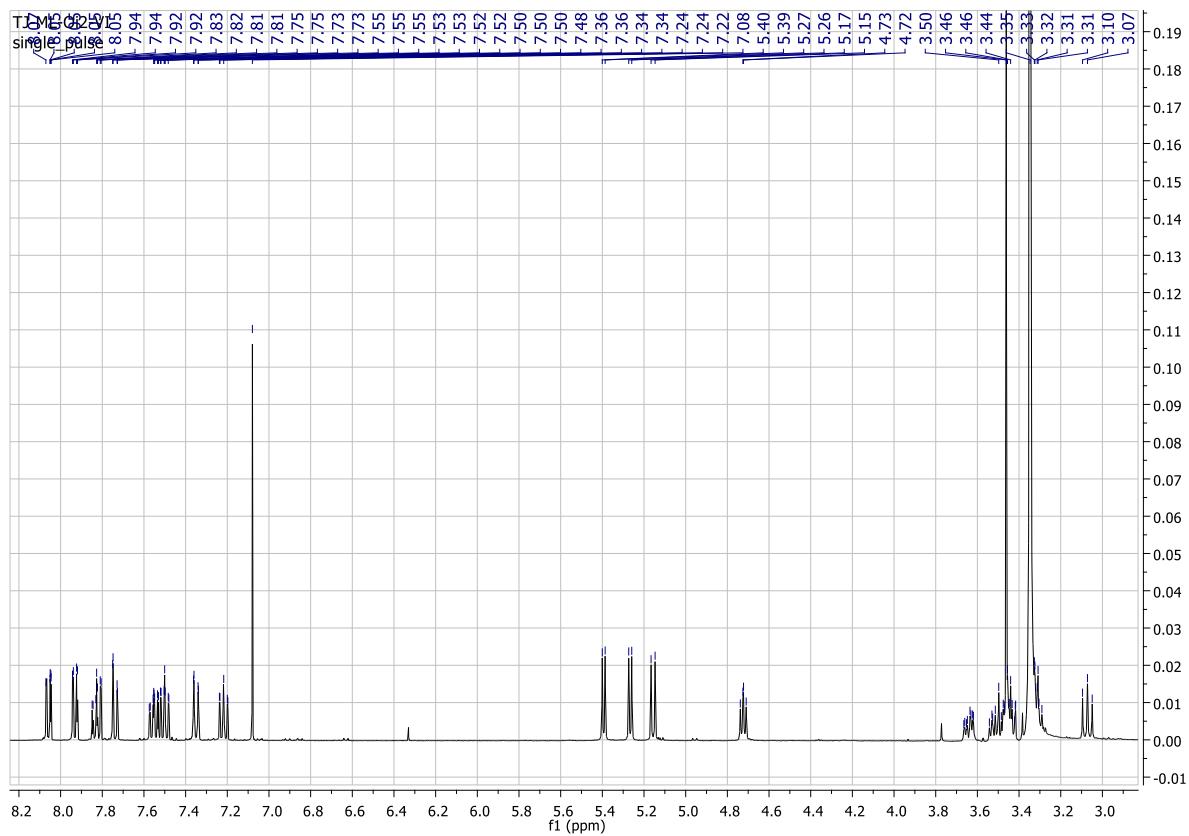


Fig.S3. Flavone part of the  $^1\text{H}$  NMR spectral flavone 2'- $O$ - $\beta$ -D-(4"- $O$ -methyl)-glucopyranoside (**6**) (DMSO- $d_6$ , 600 MHz)

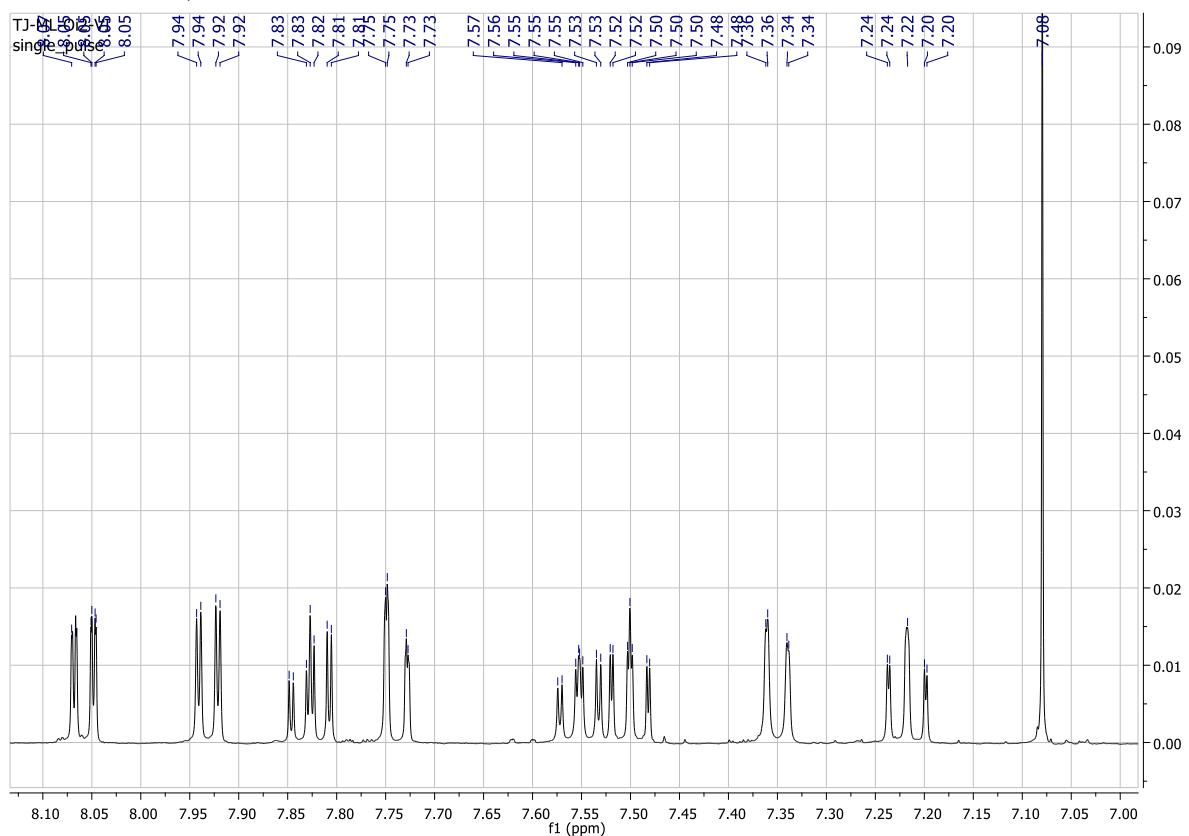


Fig.S4. Glucopyranoside part of the  $^1\text{H}$  NMR spectral flavone 2'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**6**) (DMSO- $d_6$ , 600 MHz)

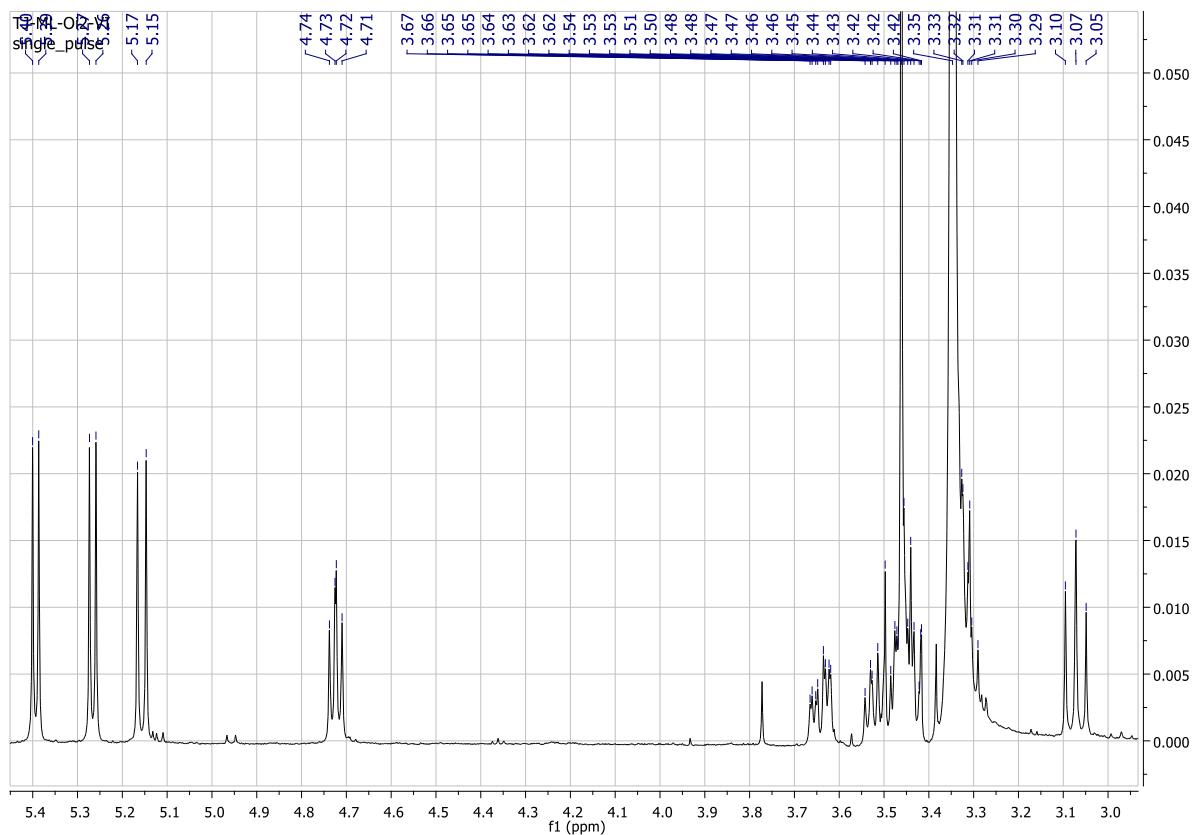


Fig.S5.  $^{13}\text{C}$  NMR spectral of flavone 2'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**6**) (DMSO- $d_6$ , 151 MHz)

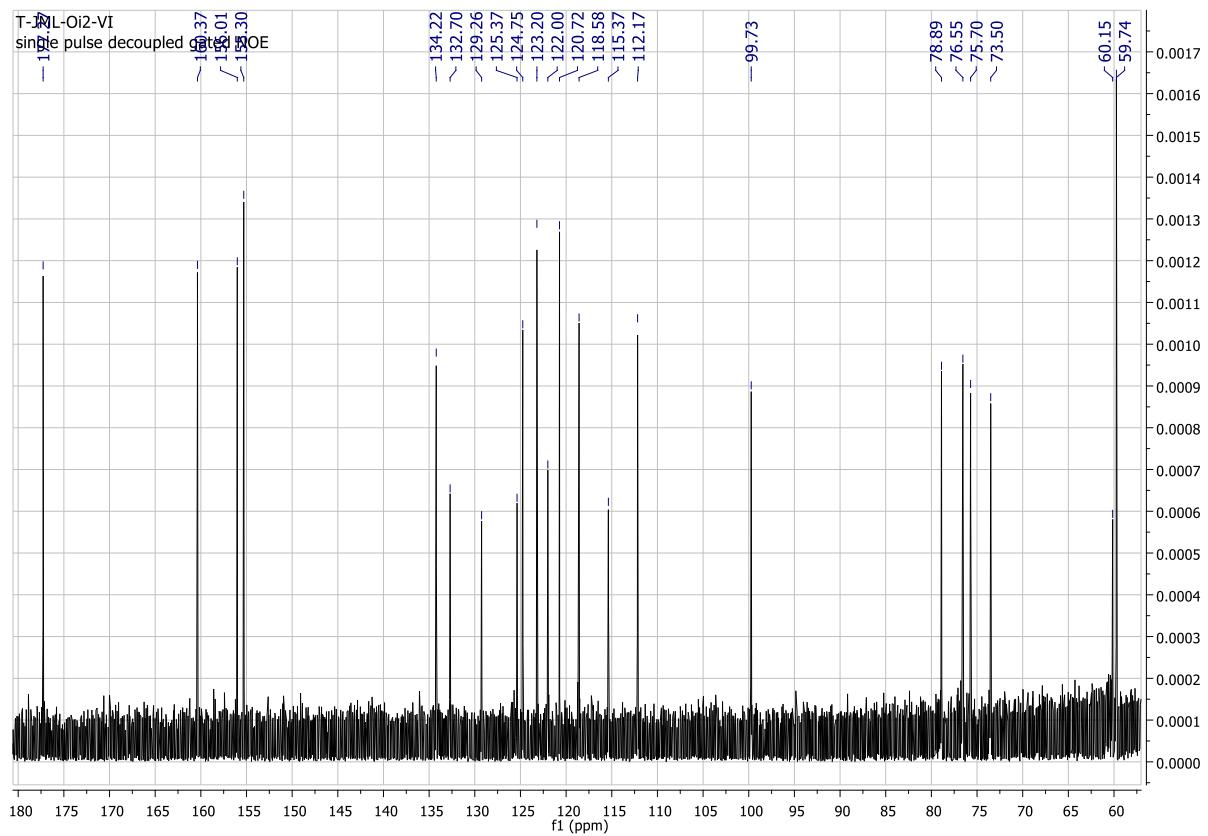


Fig.S6. COSY spectral of flavone 2'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**6**) (DMSO-*d*<sub>6</sub>, 151 MHz)

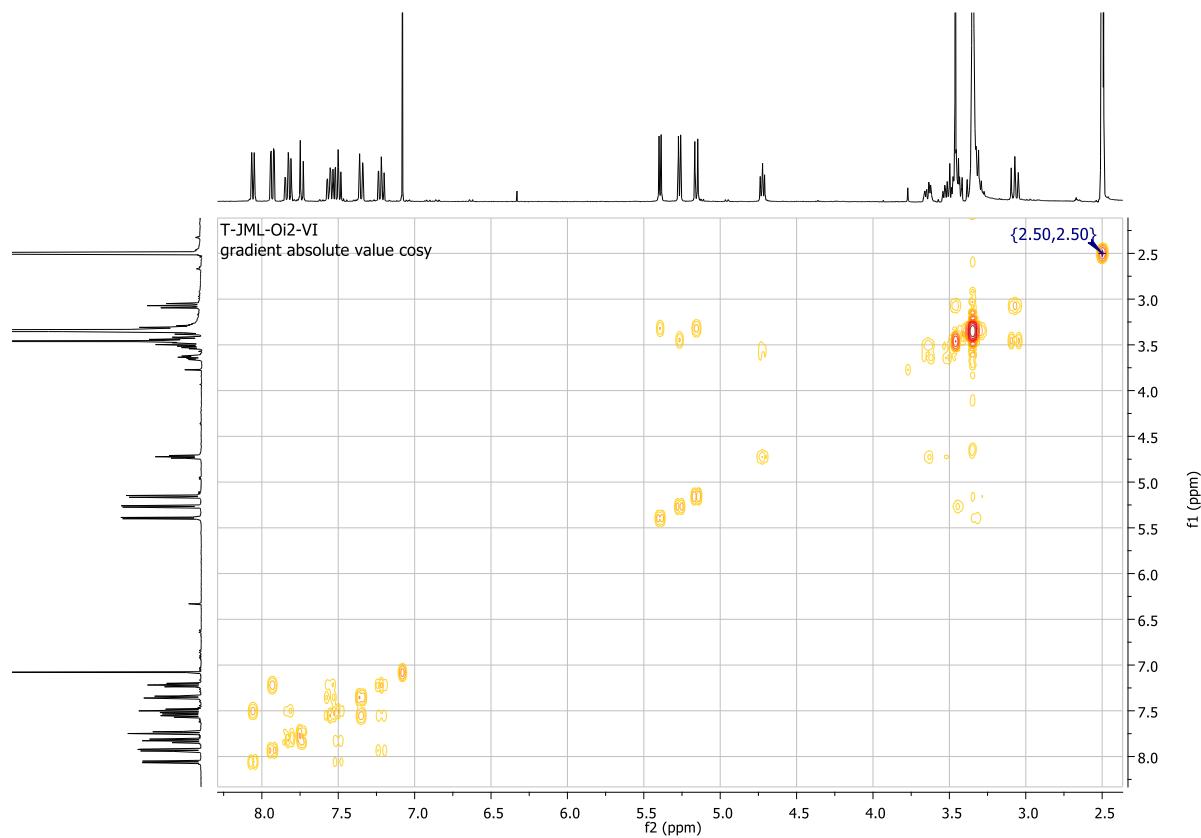


Fig.S7. HMQC spectral of flavone 2'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**6**) (DMSO-*d*<sub>6</sub>, 151 MHz)

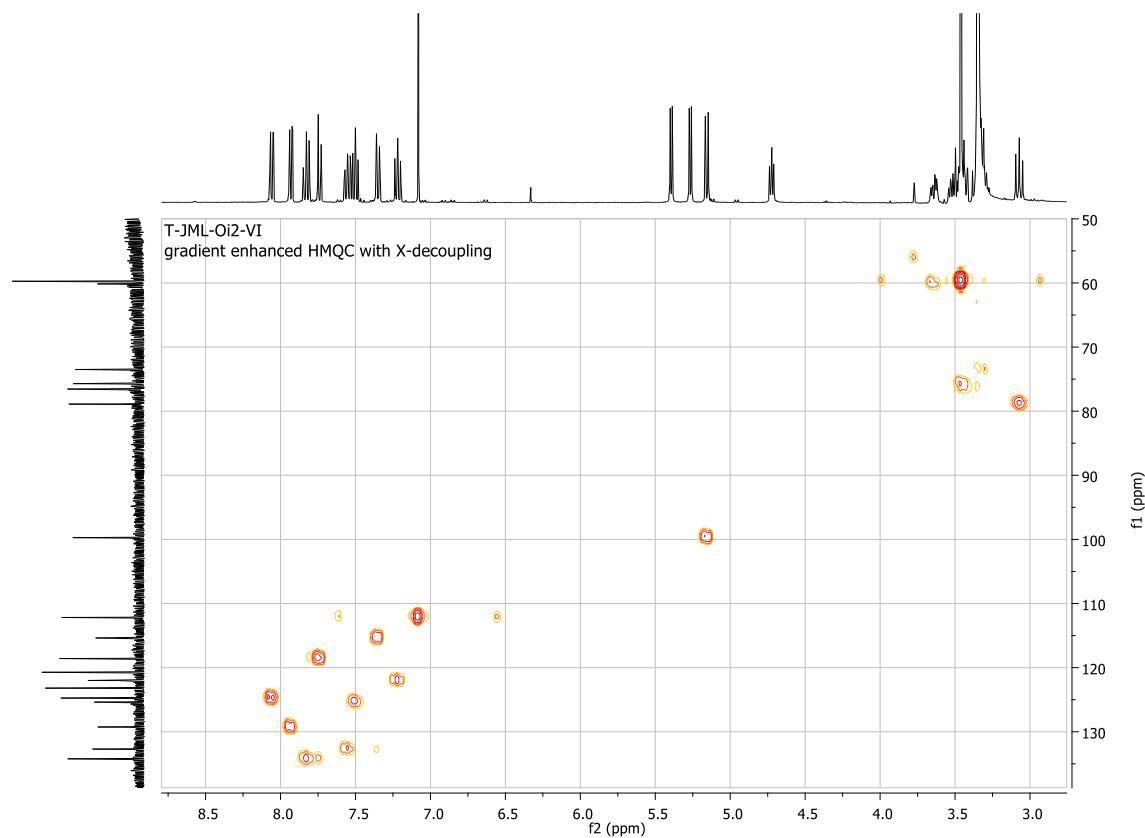


Fig.S8. HMBC spectral of flavone 2'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**6**) (DMSO- $d_6$ , 151 MHz)

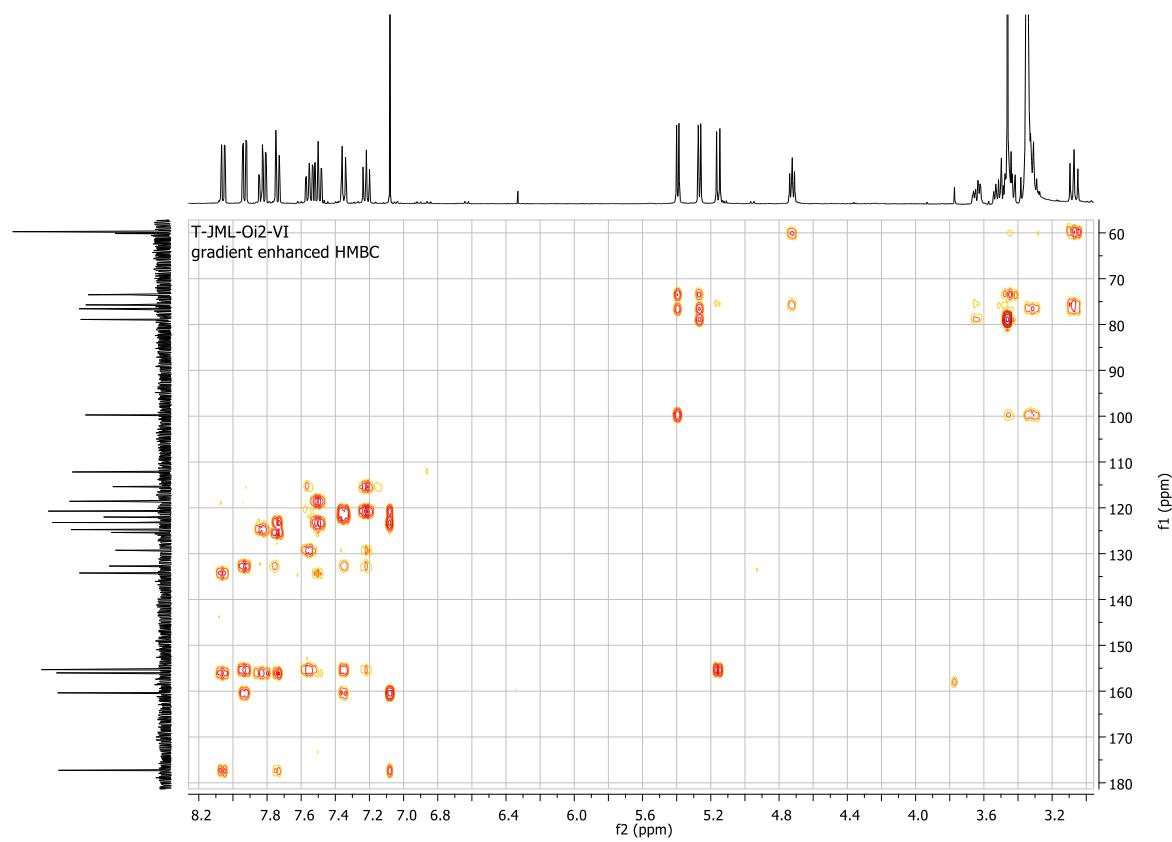
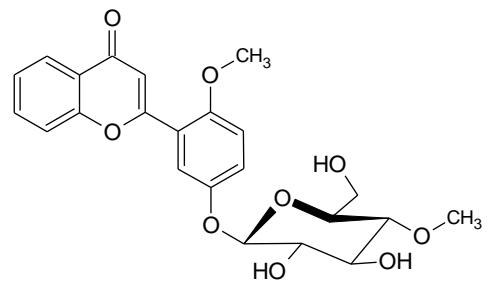


Fig.S9. MS analysis 2'-methoxyflavone 5'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**8**)

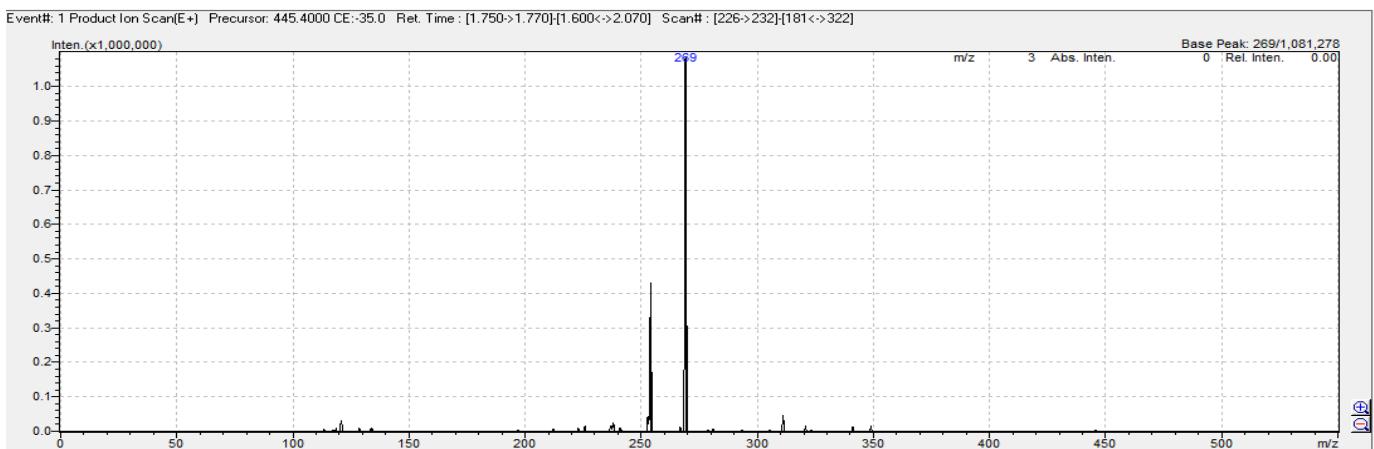
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CE: -15.0



CE:-35.0



CE:-45.0

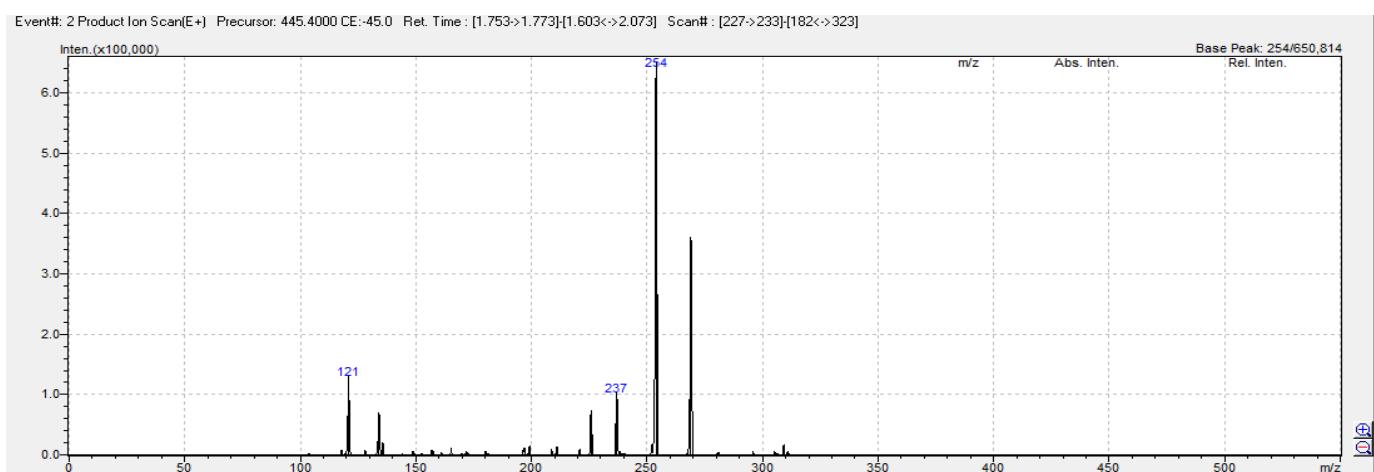


Fig.S10.  $^1\text{H}$  NMR spectral of 2'-methoxyflavone 5'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**8**) (Acetone- $d_6$ , 600 MHz)

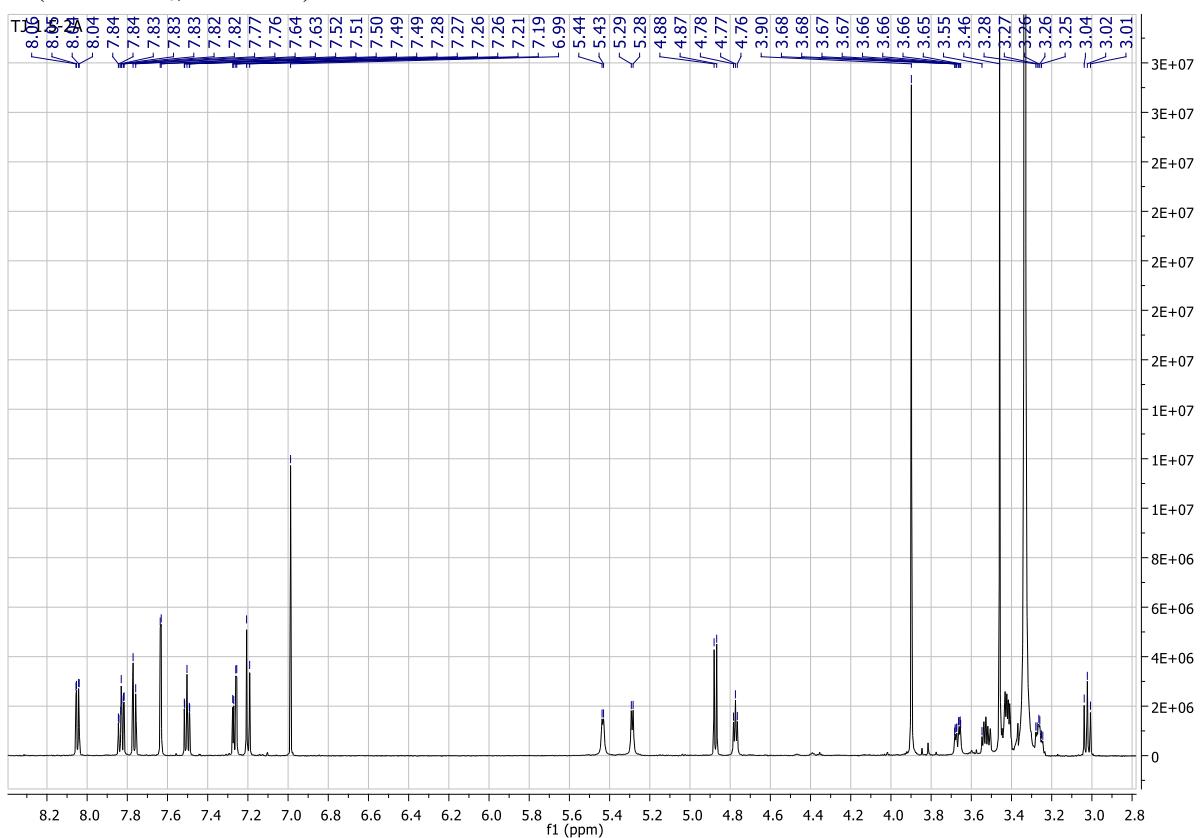


Fig.S11. Flavone part of the  $^1\text{H}$  NMR spectral 2'-methoxyflavone 5'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**8**) (Acetone- $d_6$ , 600 MHz)

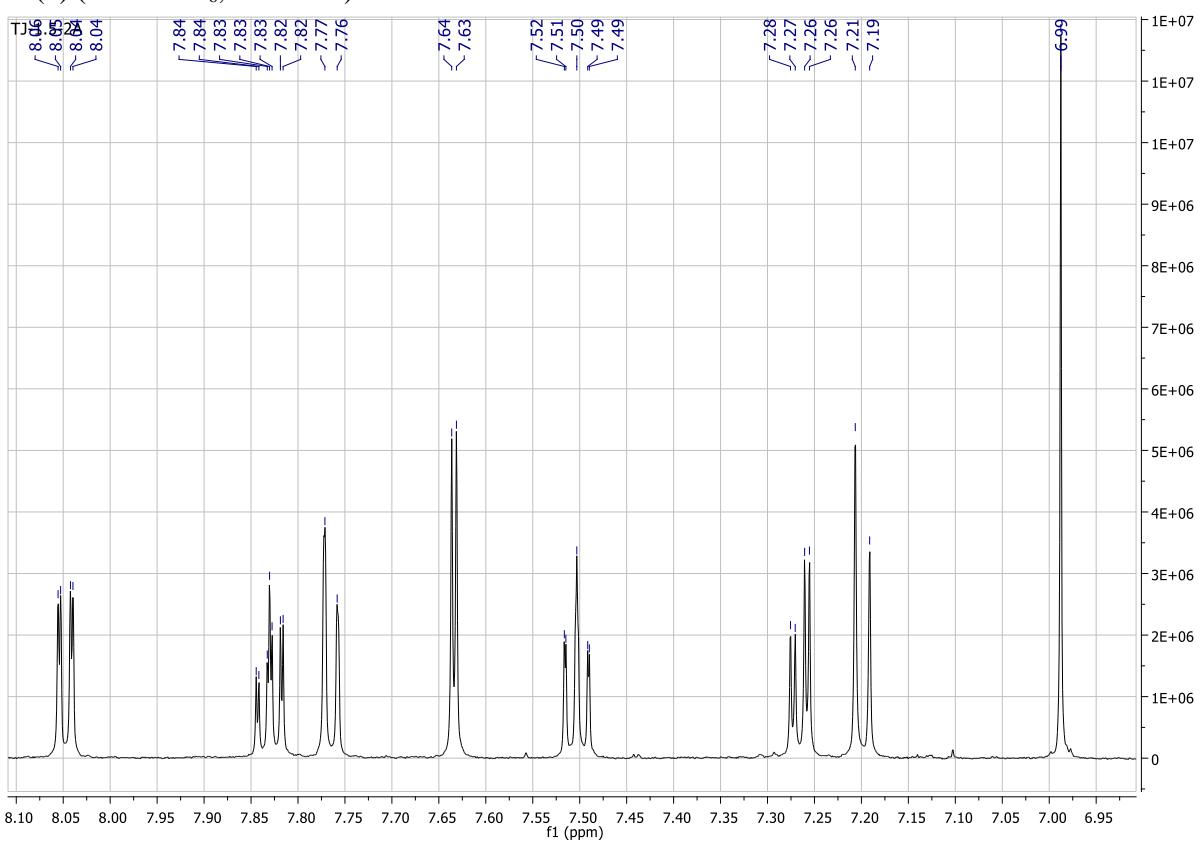


Fig.S12. Glucopyranoside part of the  $^1\text{H}$  NMR spectral 2'-methoxyflavone 5'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**8**) (Acetone- $d_6$ , 600 MHz)

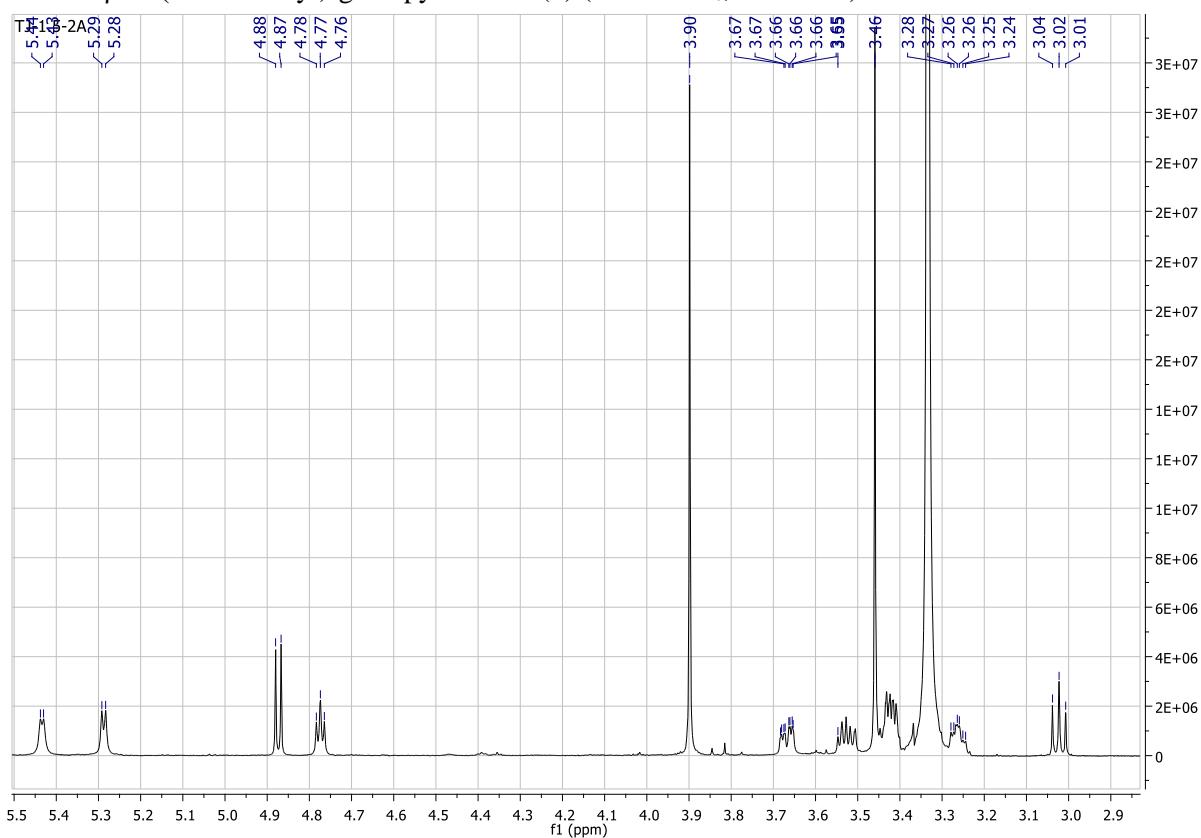


Fig.S13.  $^{13}\text{C}$  NMR spectral of 2'-methoxyflavone 5'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**8**) (Acetone- $d_6$ , 151 MHz)

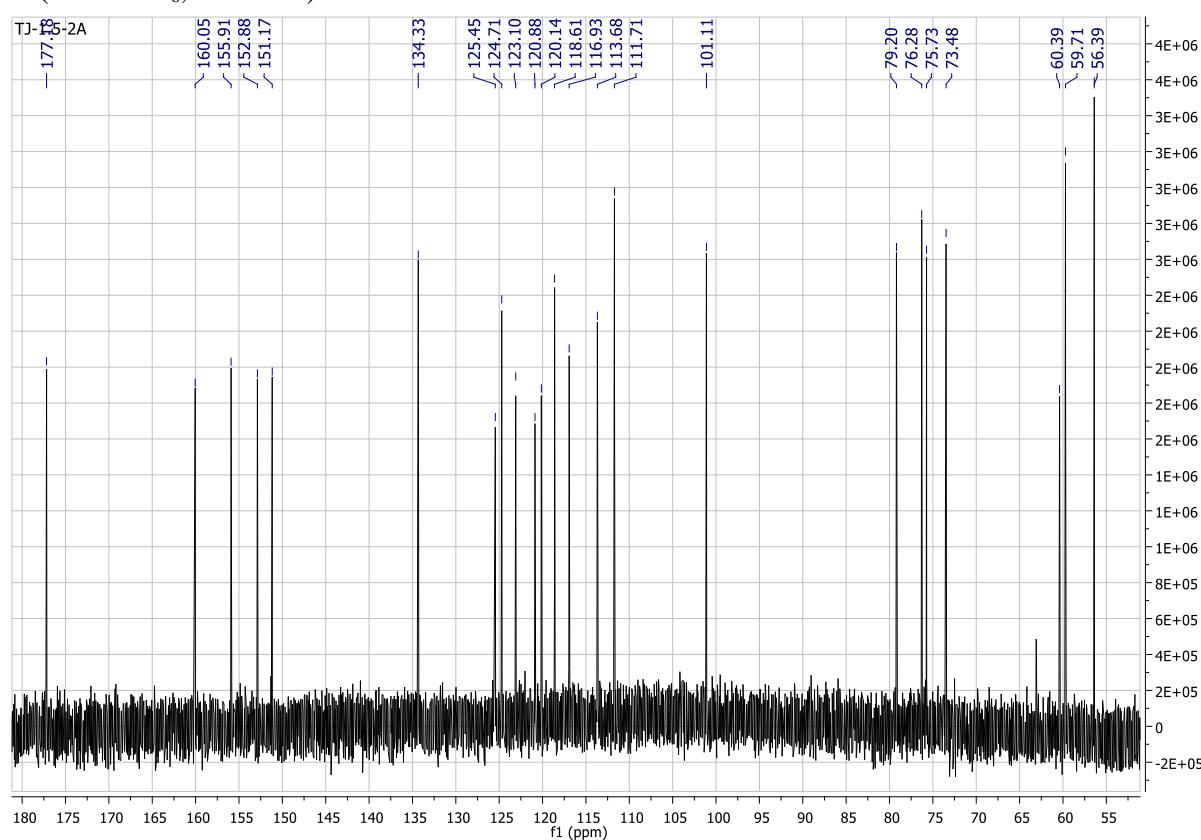


Fig.S14. COSY spectral of 2'-methoxyflavone 5'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**8**)  
(Acetone- $d_6$ , 151 MHz)

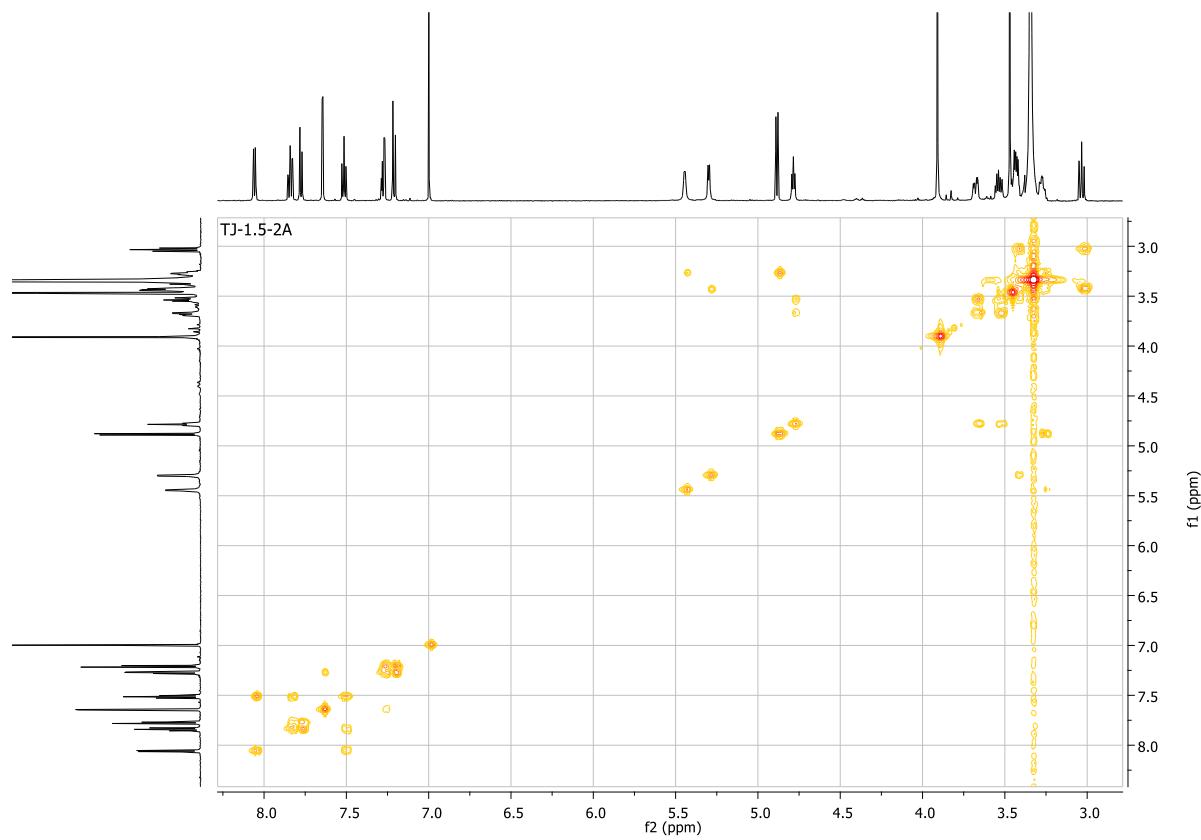


Fig.S15. HMQC spectral of 2'-methoxyflavone 5'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**8**)  
(Acetone- $d_6$ , 151 MHz)

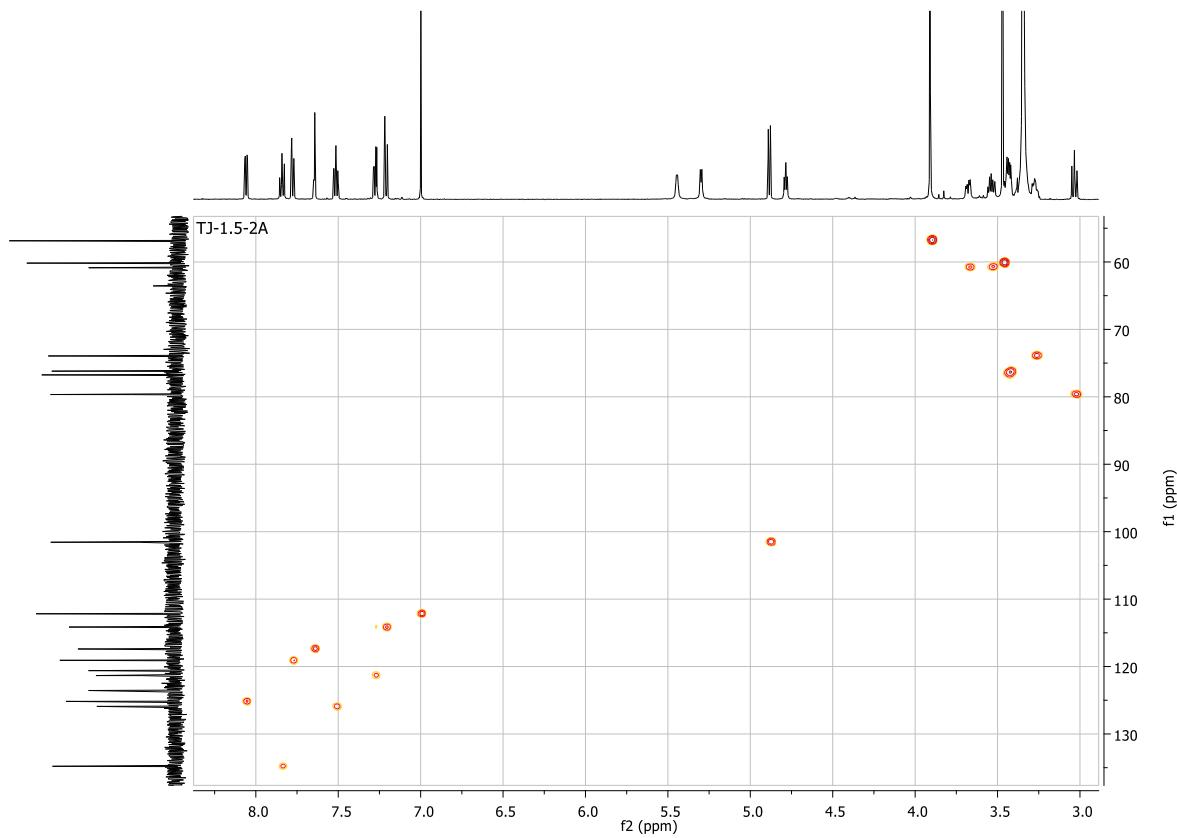


Fig.S16. HMBC spectral of 2'-methoxyflavone 5'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside flavone (**8**)  
(Acetone- $d_6$ , 151 MHz)

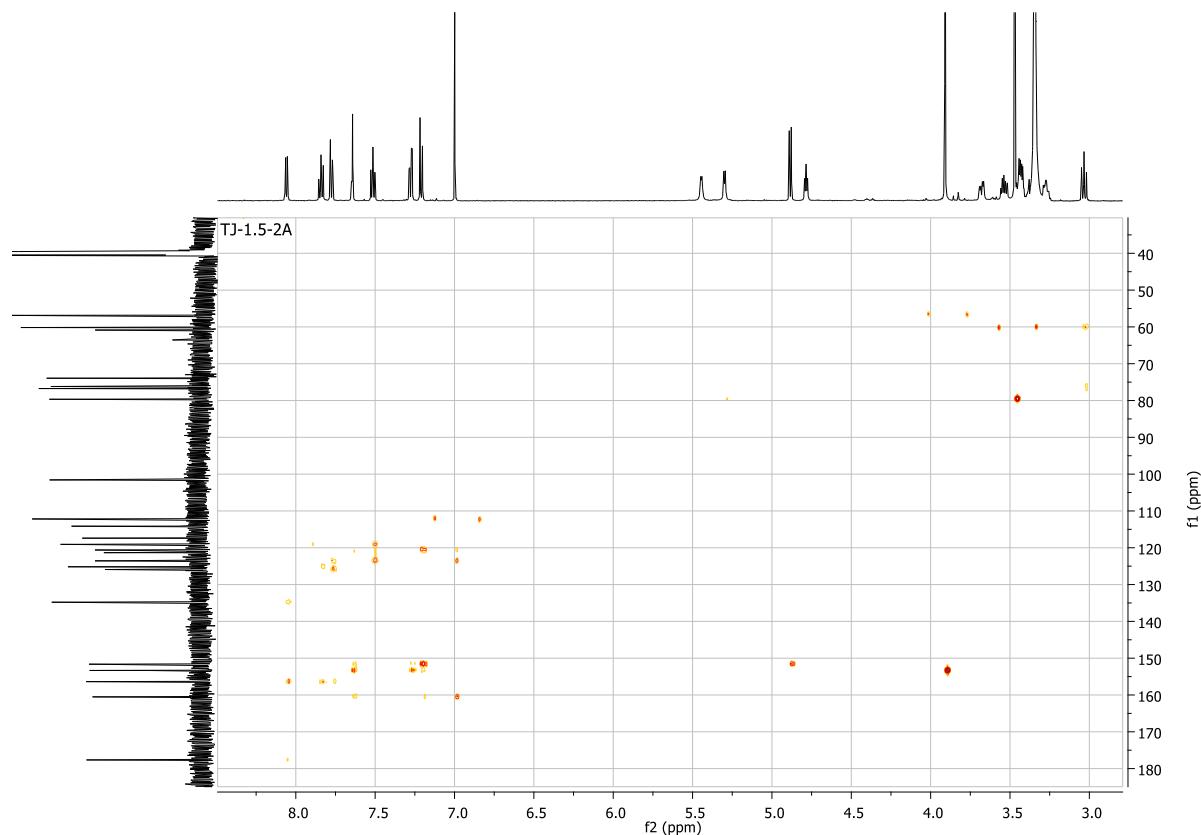
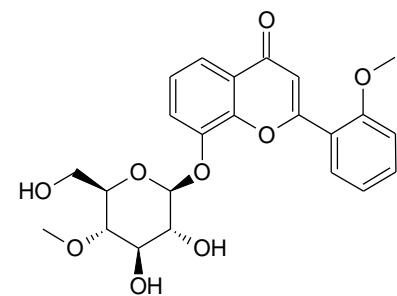


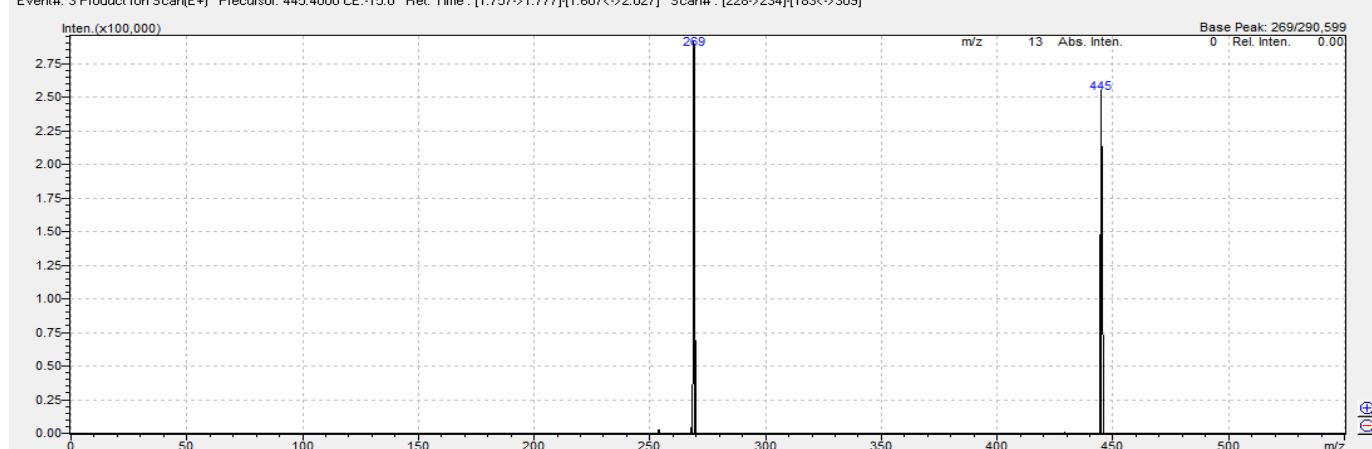
Fig.S17. MS analysis 2'-methoxyflavone 8-O- $\beta$ -D-(4''-O-metyloglukopiranozylo)-2'-metoksyflawon (7)



Molecular Formula = C<sub>23</sub>H<sub>24</sub>O<sub>9</sub>  
 Formula Weight = 444.43126  
 Precursor = 445.4000

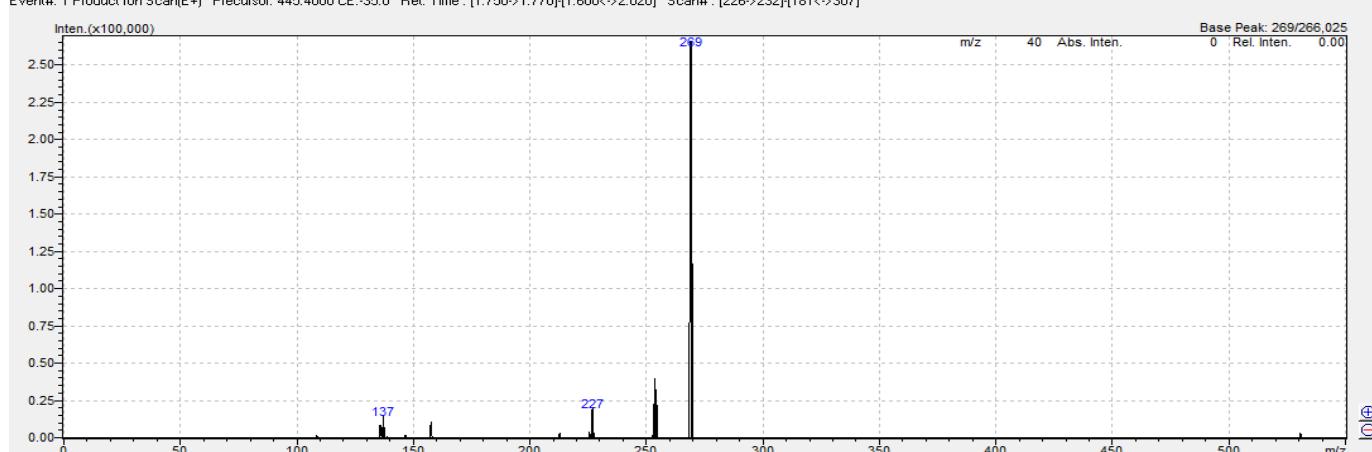
CE: -15.0

Event#: 3 Product Ion Scan(E+) Precursor: 445.4000 CE:-15.0 Ret. Time : [1.757->1.777][1.607<->2.027] Scan#: [228->234][183<->309]



CE:-35.0

Event#: 1 Product Ion Scan(E+) Precursor: 445.4000 CE:-35.0 Ret. Time : [1.750->1.770][1.600<->2.020] Scan#: [226->232][181<->307]



CE:-45.0

Event#: 2 Product Ion Scan(E+) Precursor: 445.4000 CE:-45.0 Ret. Time : [1.753->1.773][1.603<->2.023] Scan#: [227->233][182<->308]

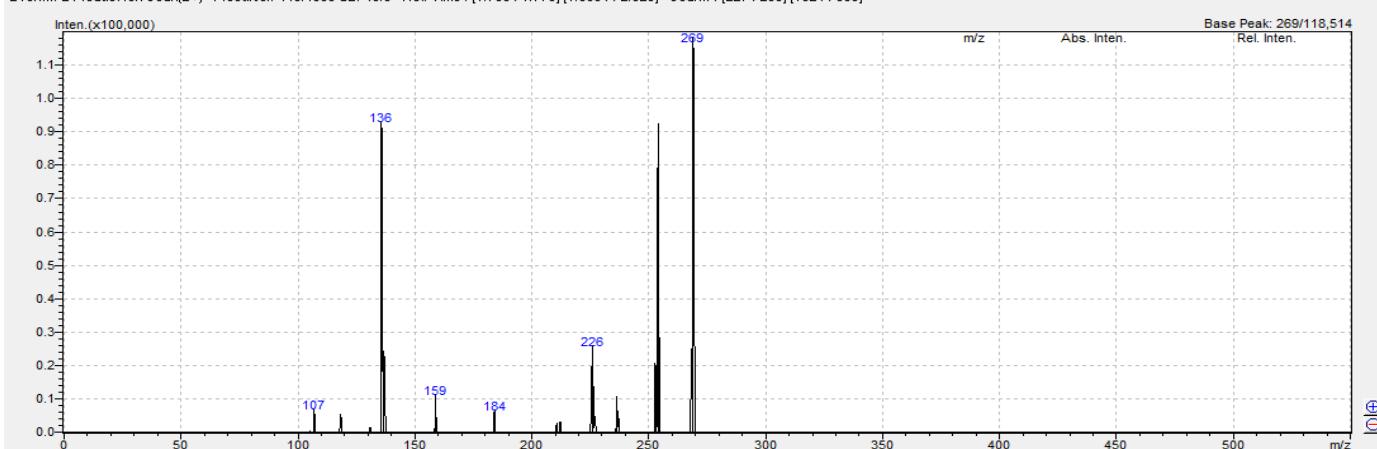


Fig.S18.  $^1\text{H}$  NMR spectral of 2'-methoxyflavone 8-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**7**) (Acetone- $d_6$ , 600 MHz)

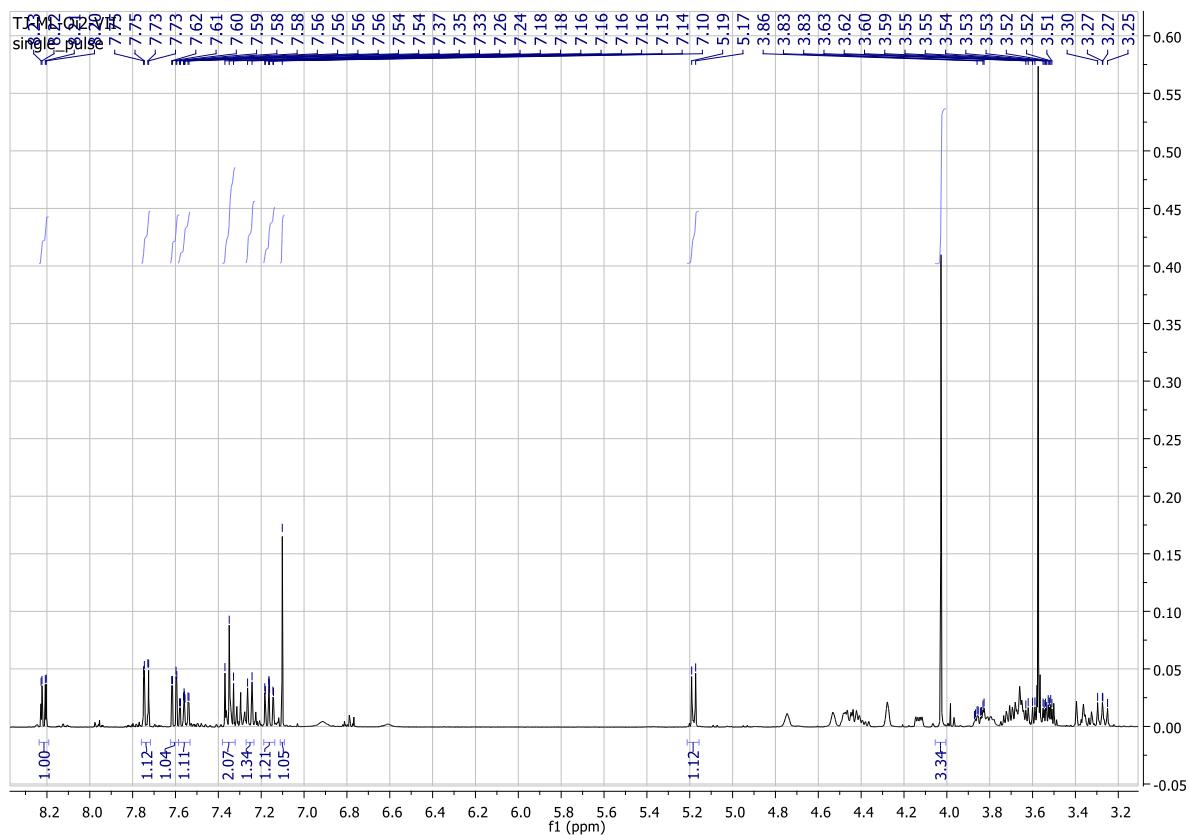


Fig.S19. Flavone part of the  $^1\text{H}$  NMR spectral 2'-methoxyflavone 8-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**7**) (Acetone- $d_6$ , 600 MHz)

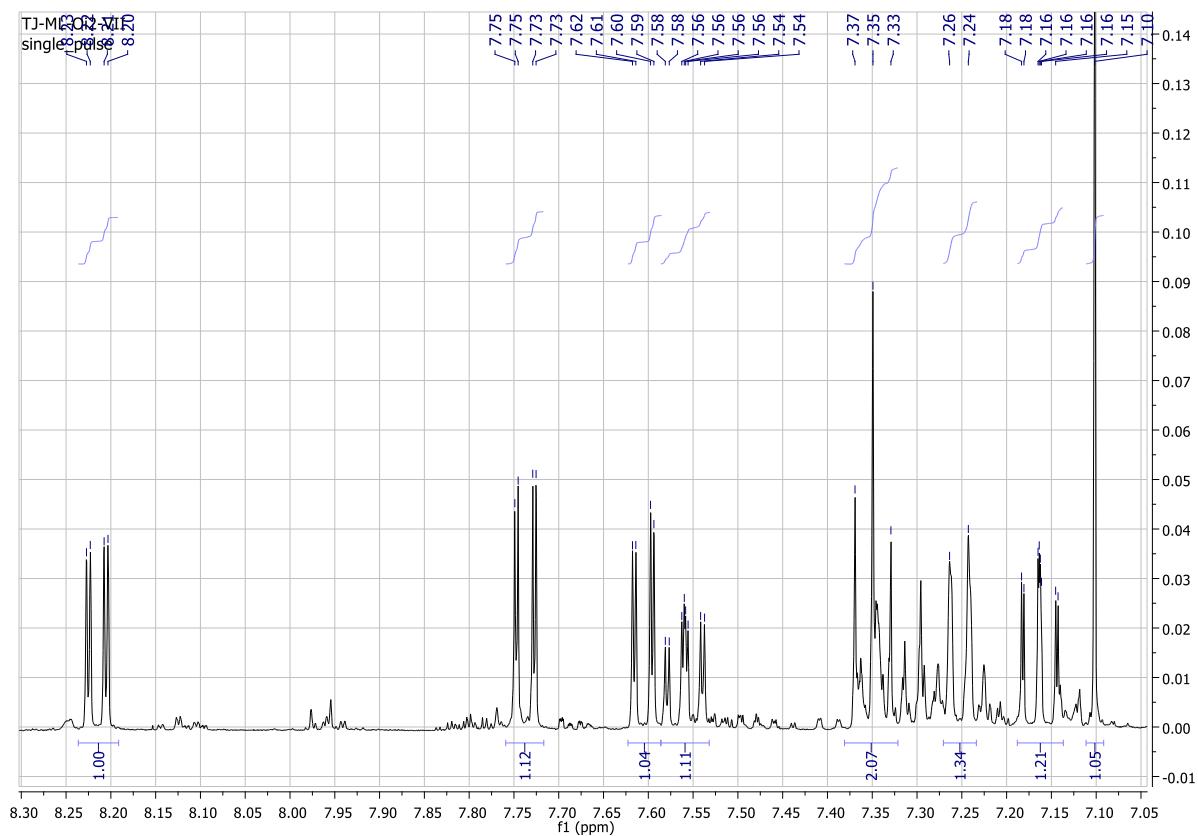


Fig.S20.  $^{13}\text{C}$  NMR spectral of 2'-methoxyflavone 8-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**7**)  
(Acetone- $d_6$ , 151 MHz)

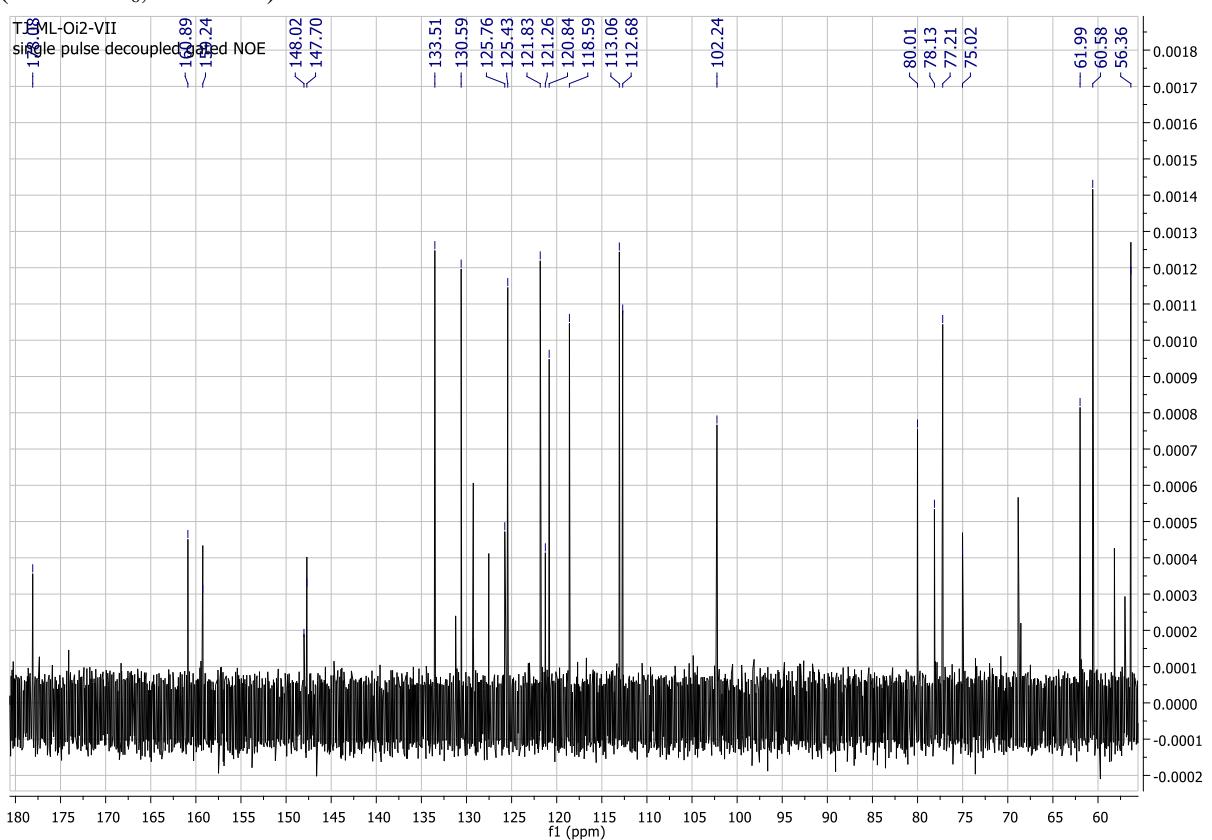


Fig.S21. COSY spectral of 2'-methoxyflavone 8-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**1**)  
(Acetone- $d_6$ , 151 MHz)

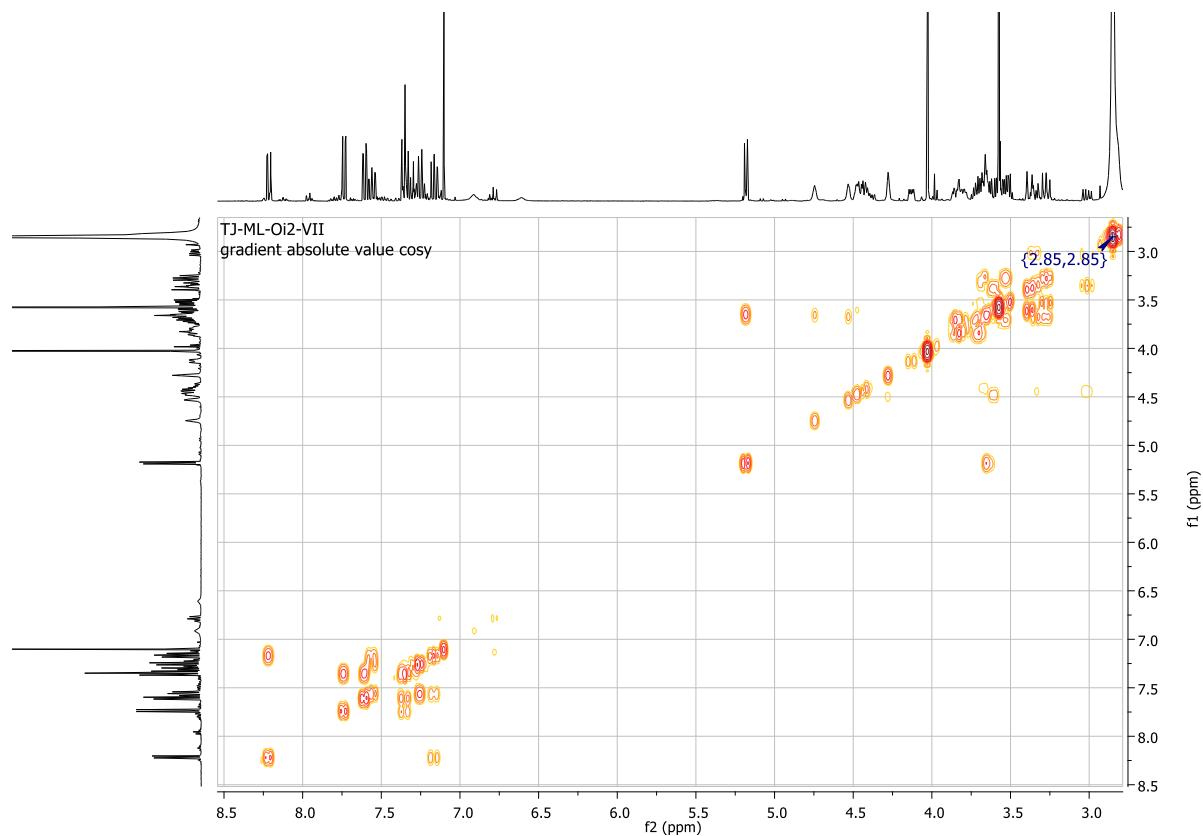


Fig.S22. HMQC spectral of 2'-methoxyflavone 8-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**7**)  
(Acetone- $d_6$ , 151 MHz)

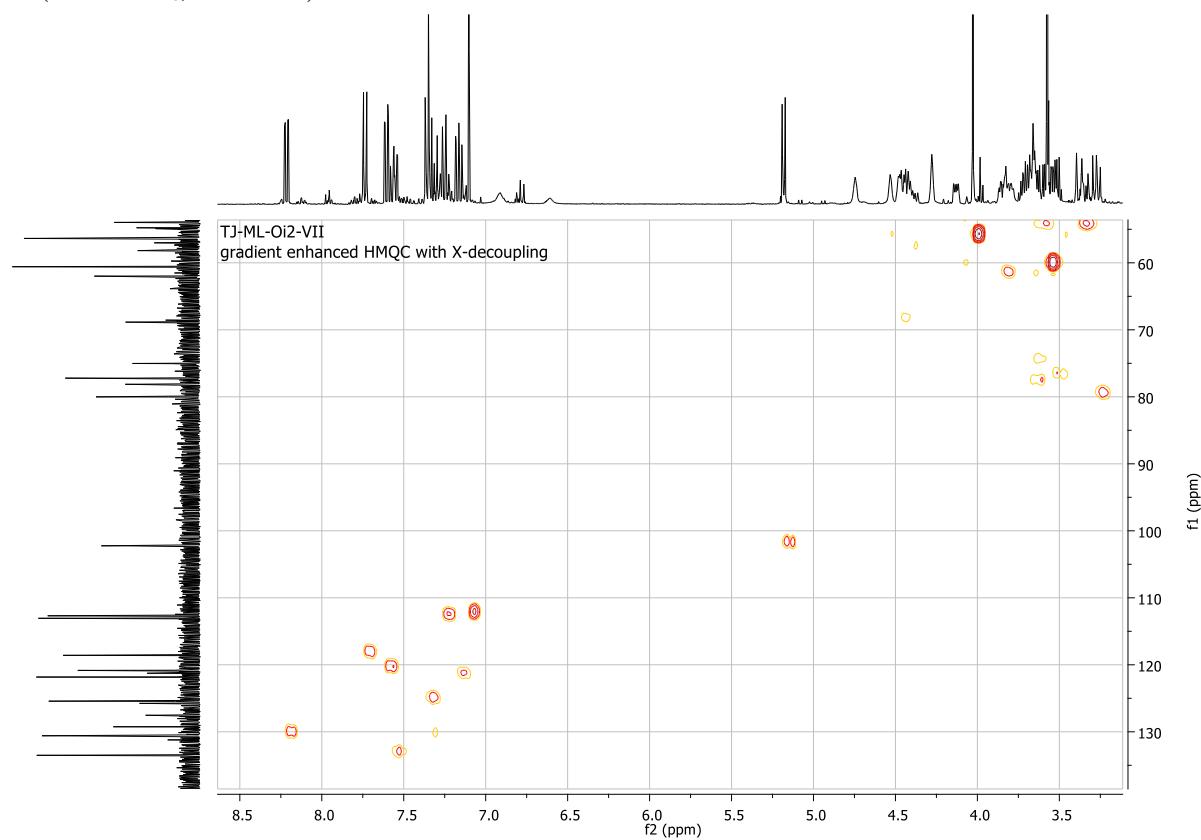


Fig.S23. HMBC spectral of 2'-methoxyflavone 8-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside flavone (**7**)  
(Acetone- $d_6$ , 151 MHz)

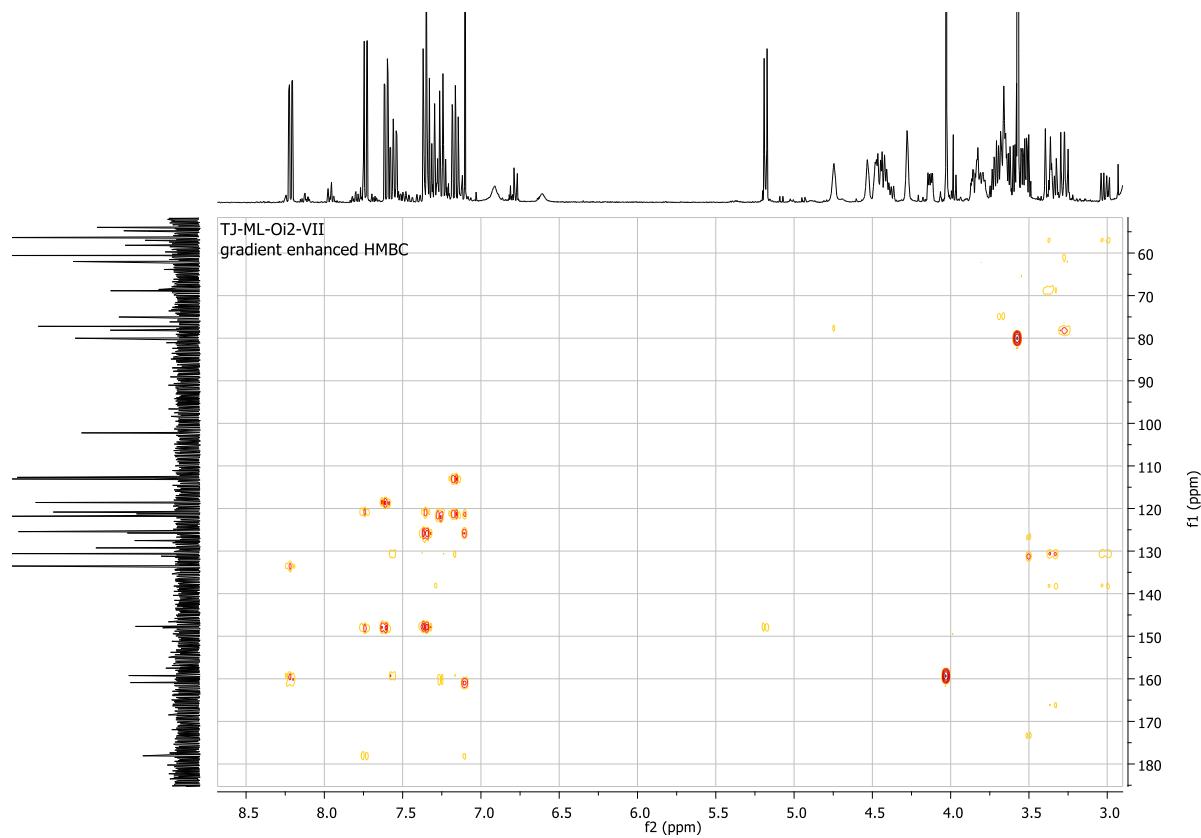
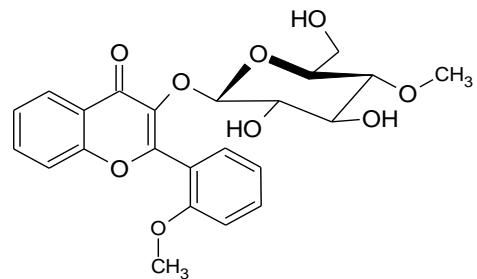


Fig.S24. MS analysis 3-O- $\beta$ -D-(4''-O-metyloglukopiranoylo)-2'-metoksyflawon (**9**)



Molecular Formula = C<sub>23</sub>H<sub>24</sub>O<sub>9</sub>  
 Formula Weight = 444.43126  
 Precursor = 445.4000

CE: -15.0



CE:-35.0



CE:-45.0

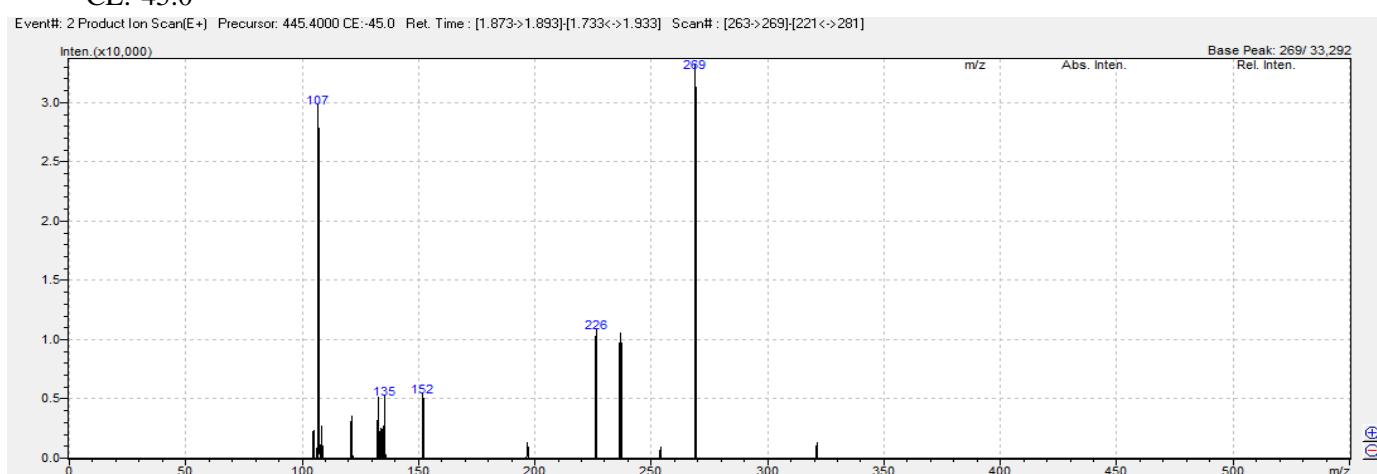


Fig.S25.  $^1\text{H}$  NMR spectral of 2'-methoxyflavone 3- $O$ - $\beta$ -D-(4"- $O$ -methyl)-glucopyranoside (**9**) (DMSO- $d_6$ , 600 MHz)

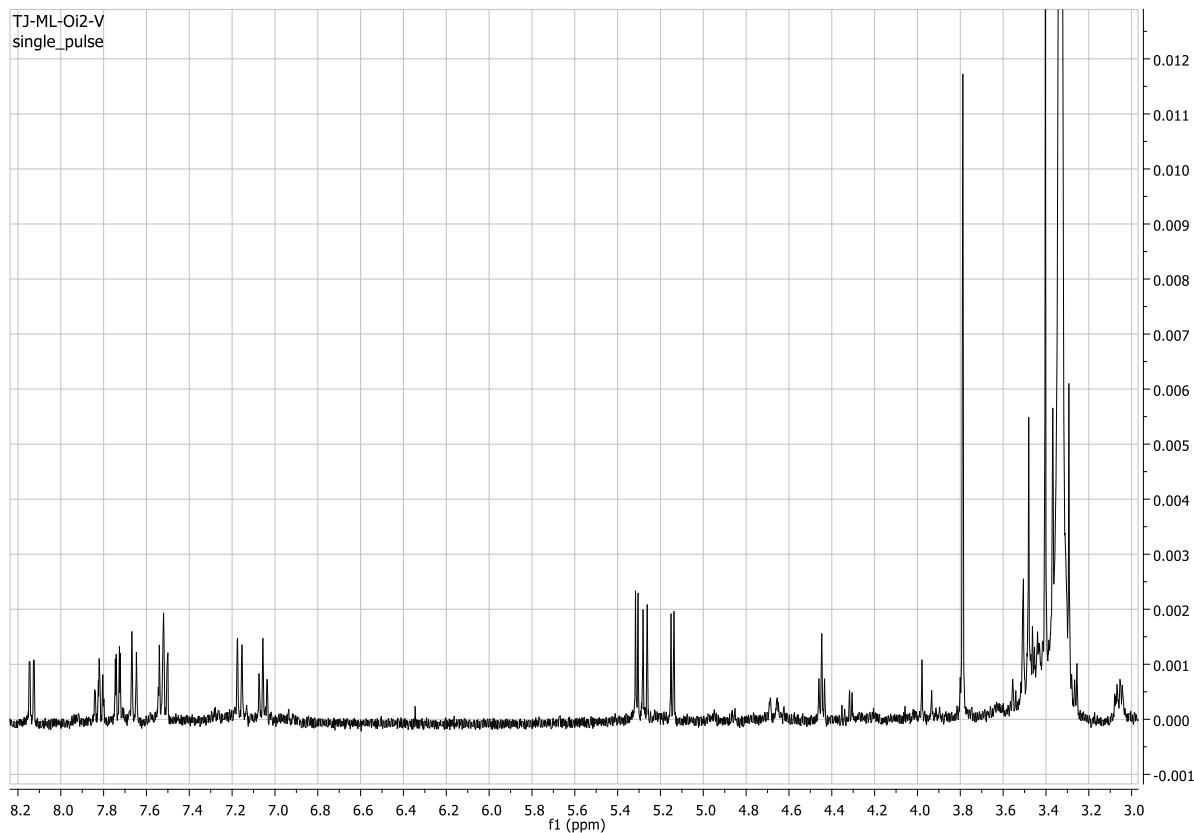


Fig.S26. Flavone part of the  $^1\text{H}$  NMR spectral 2'-methoxyflavone 3- $O$ - $\beta$ -D-(4"- $O$ -methyl)-glucopyranoside (**9**) (DMSO- $d_6$ , 600 MHz)

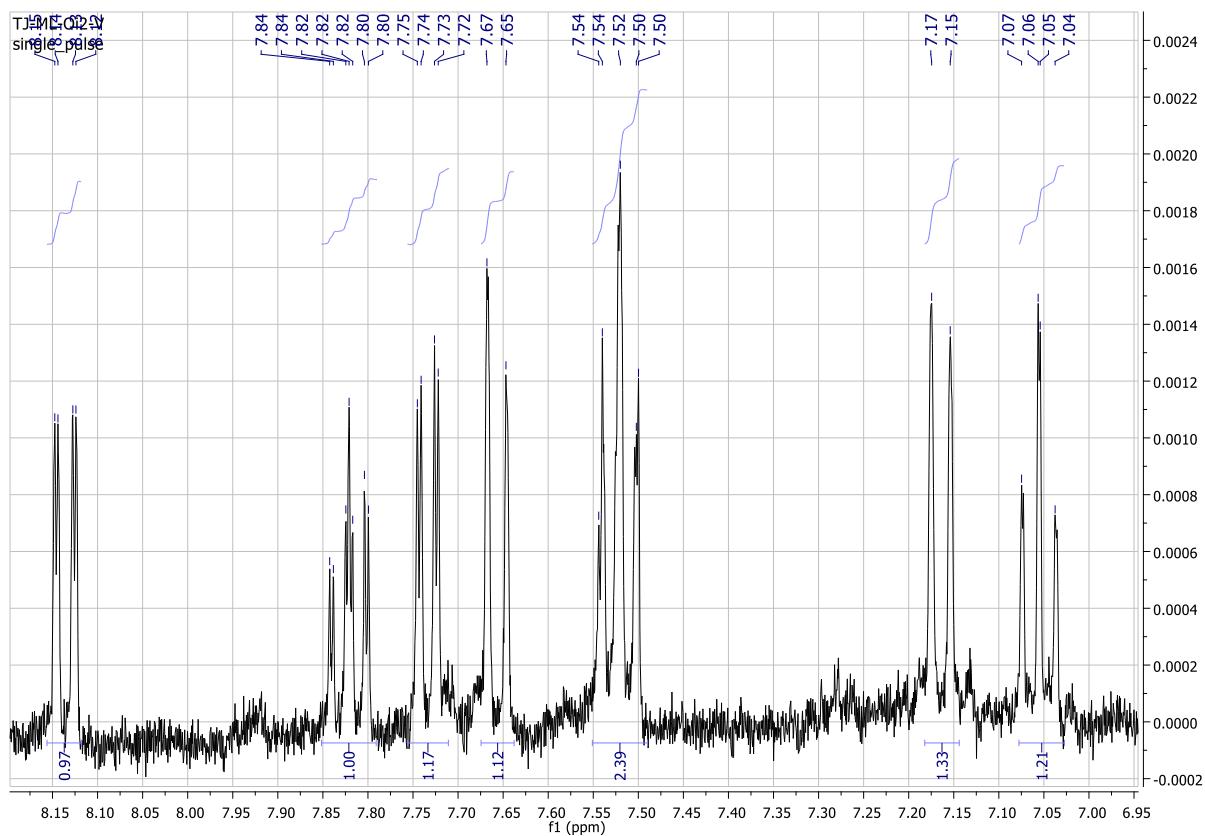


Fig.S27. Glucopyranoside part of the  $^1\text{H}$  NMR spectral 2'-methoxyflavone 3-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**9**) (DMSO- $d_6$ , 600 MHz)

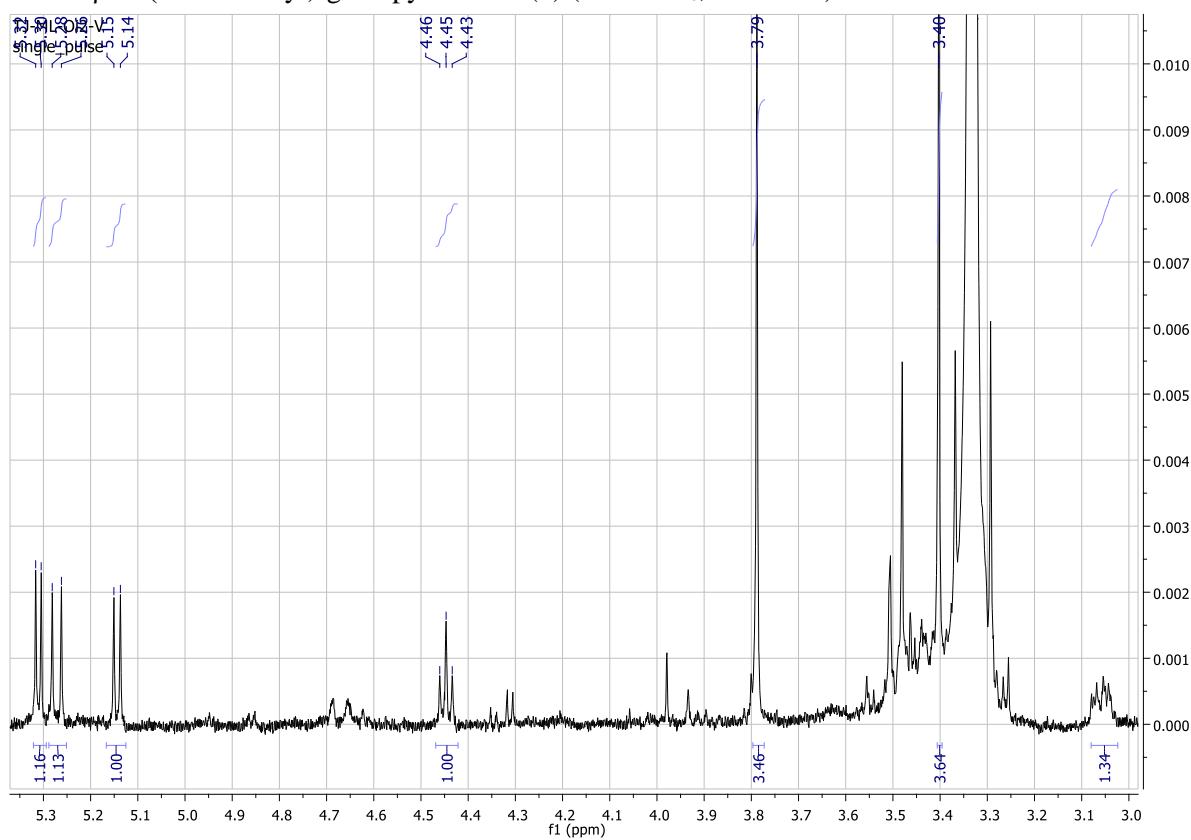
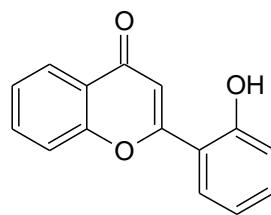


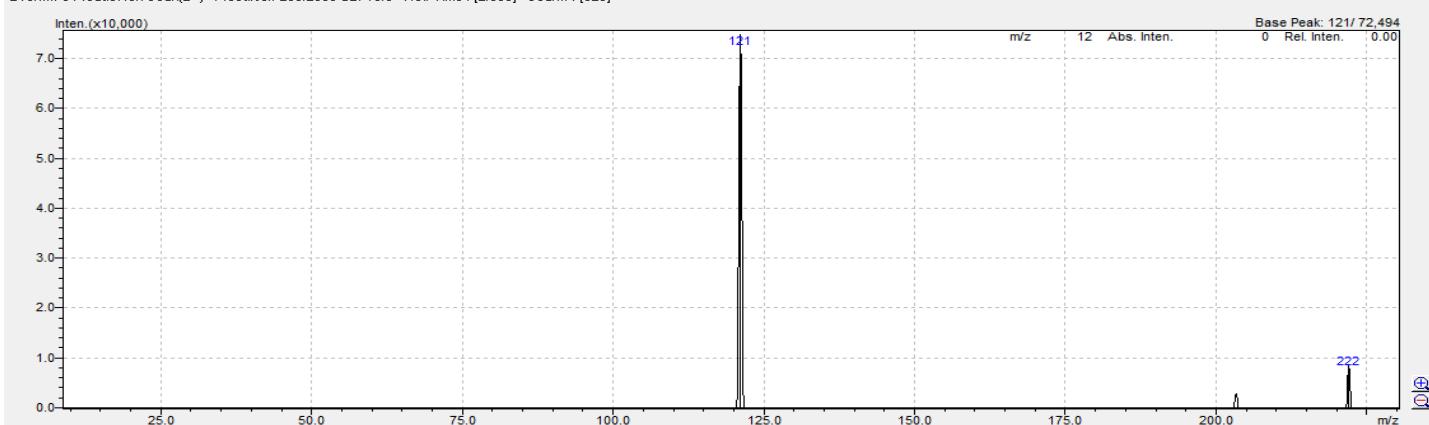
Fig.S28. MS analysis 2'-hydroxyflavone (**10**)

Molecular Formula: C<sub>15</sub>H<sub>10</sub>O<sub>3</sub>  
 Formula Weight: 238.2381  
 Precursor: 239.2000



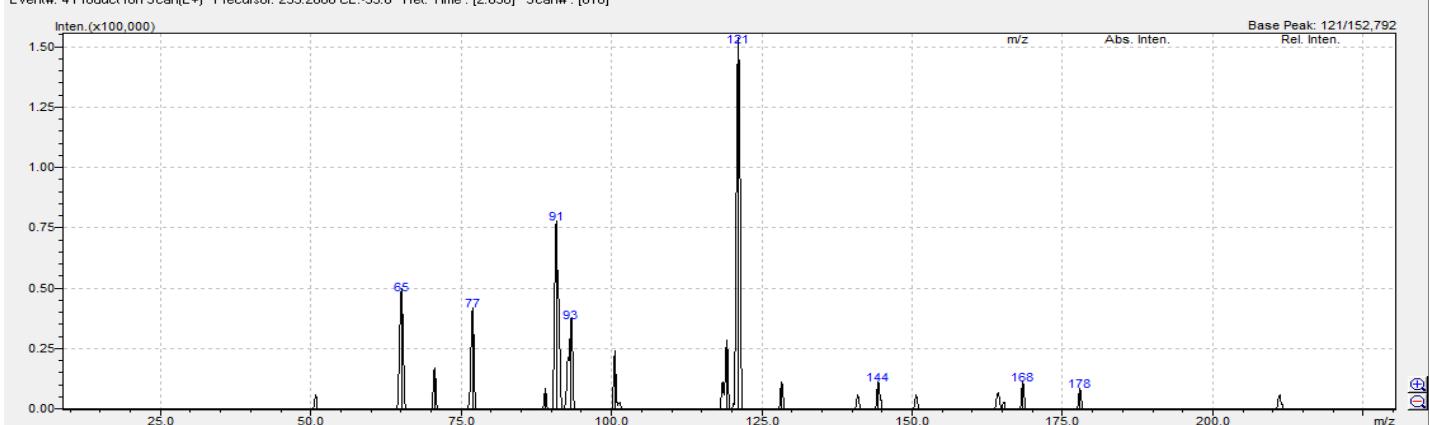
CE: -15.0

Event#: 8 Product Ion Scan(E+) Precursor: 239.2000 CE:-15.0 Ret. Time : [2.063] Scan#: [620]



CE:-35.0

Event#: 4 Product Ion Scan(E+) Precursor: 239.2000 CE:-35.0 Ret. Time : [2.050] Scan#: [616]



CE:-45.0

Event#: 2 Product Ion Scan(E+) Precursor: 239.2000 CE:-45.0 Ret. Time : [2.043] Scan#: [614]

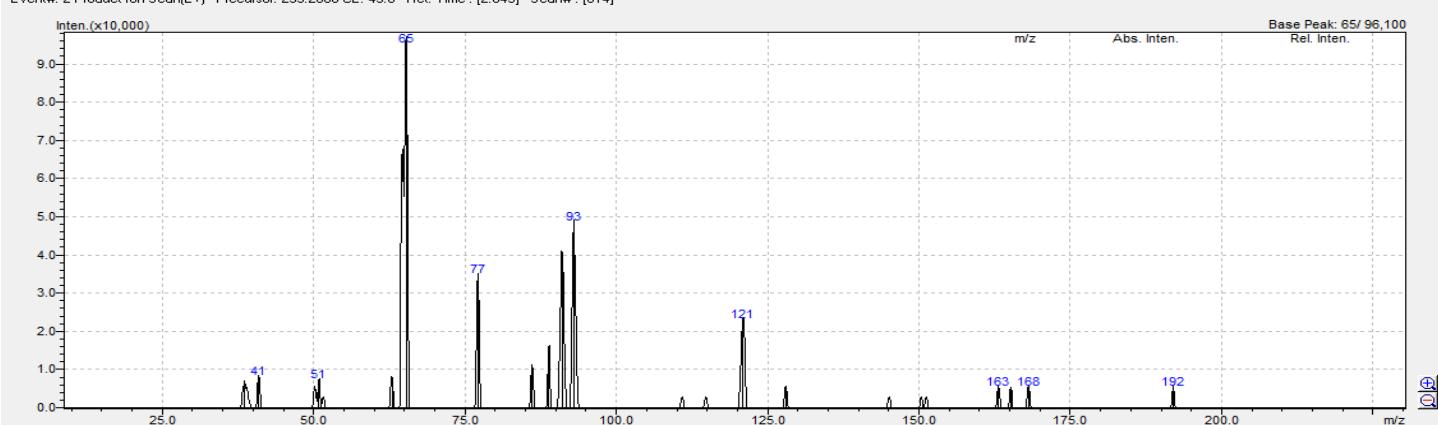


Fig.S29.  $^1\text{H}$  NMR spectral of 2'-hydroxyflavone (**10**) (Acetone- $d_6$ , 600 MHz)

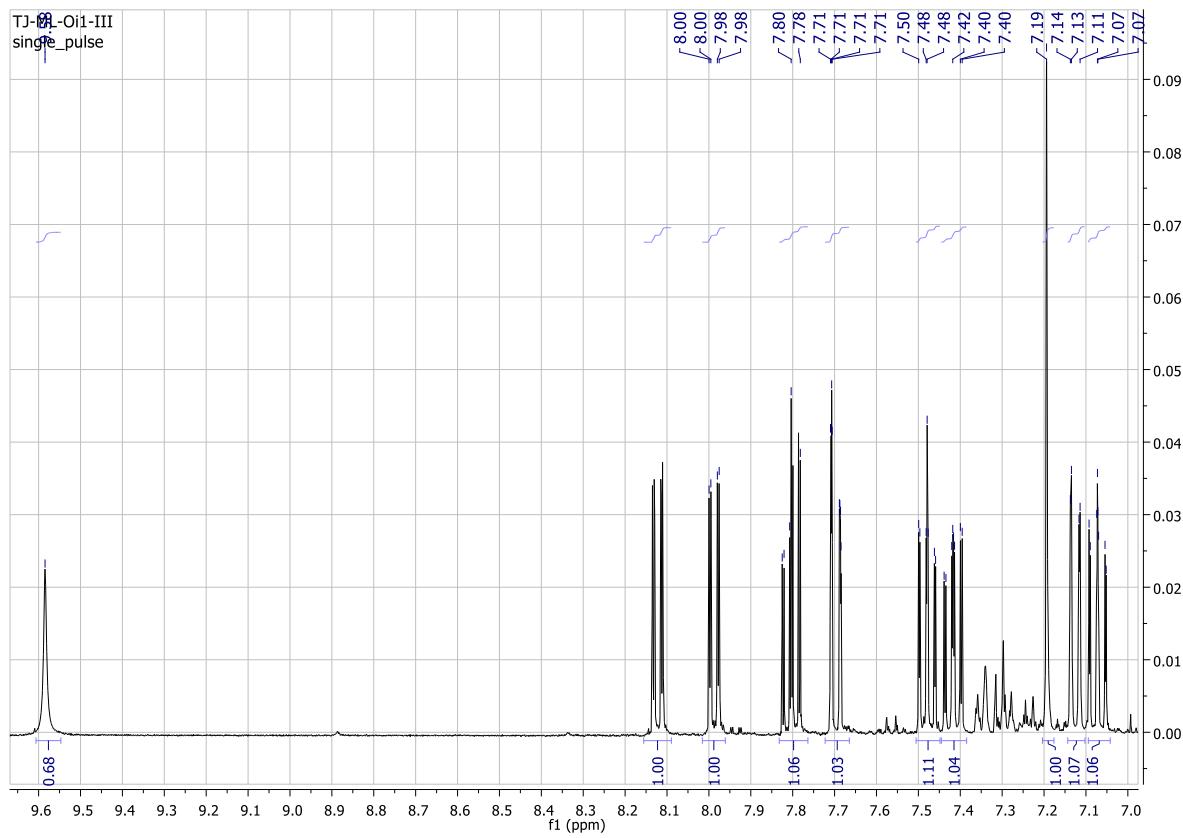


Fig.S30.  $^{13}\text{C}$  NMR spectral of 2'-hydroxyflavone (**10**) (Acetone- $d_6$ , 151 MHz)

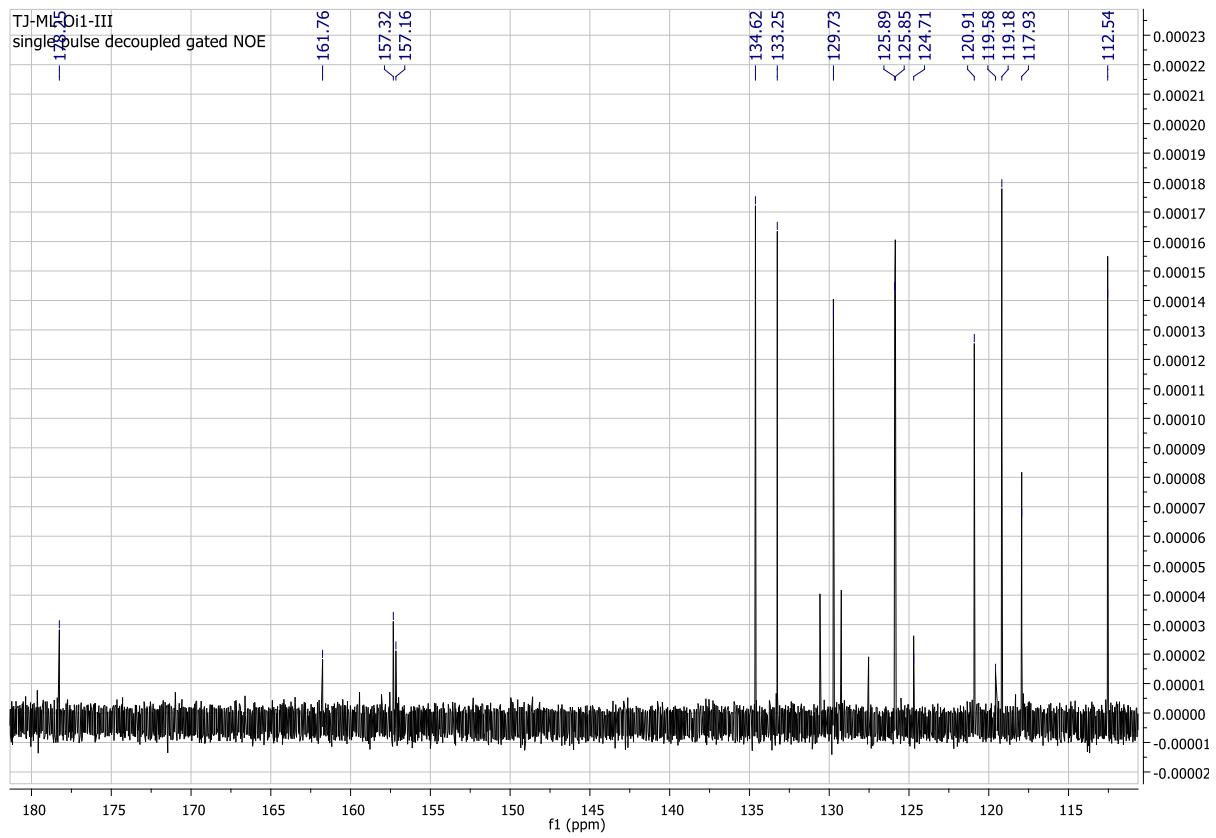


Fig.S31. COSY spectral of 2'-hydroxyflavone (**10**) (Acetone-*d*<sub>6</sub>, 151 MHz)

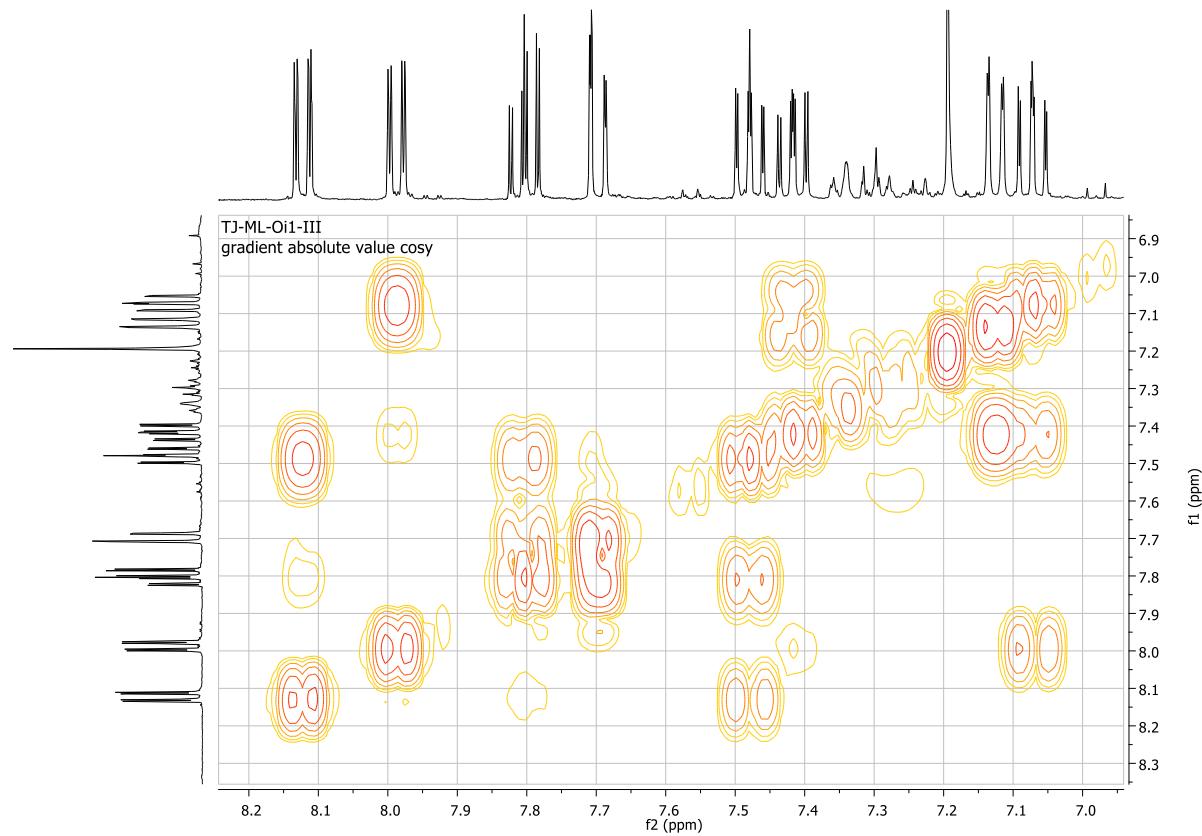


Fig.S32. HMQC spectral of 2'-hydroxyflavone (**10**) (Acetone-*d*<sub>6</sub>, 151 MHz)

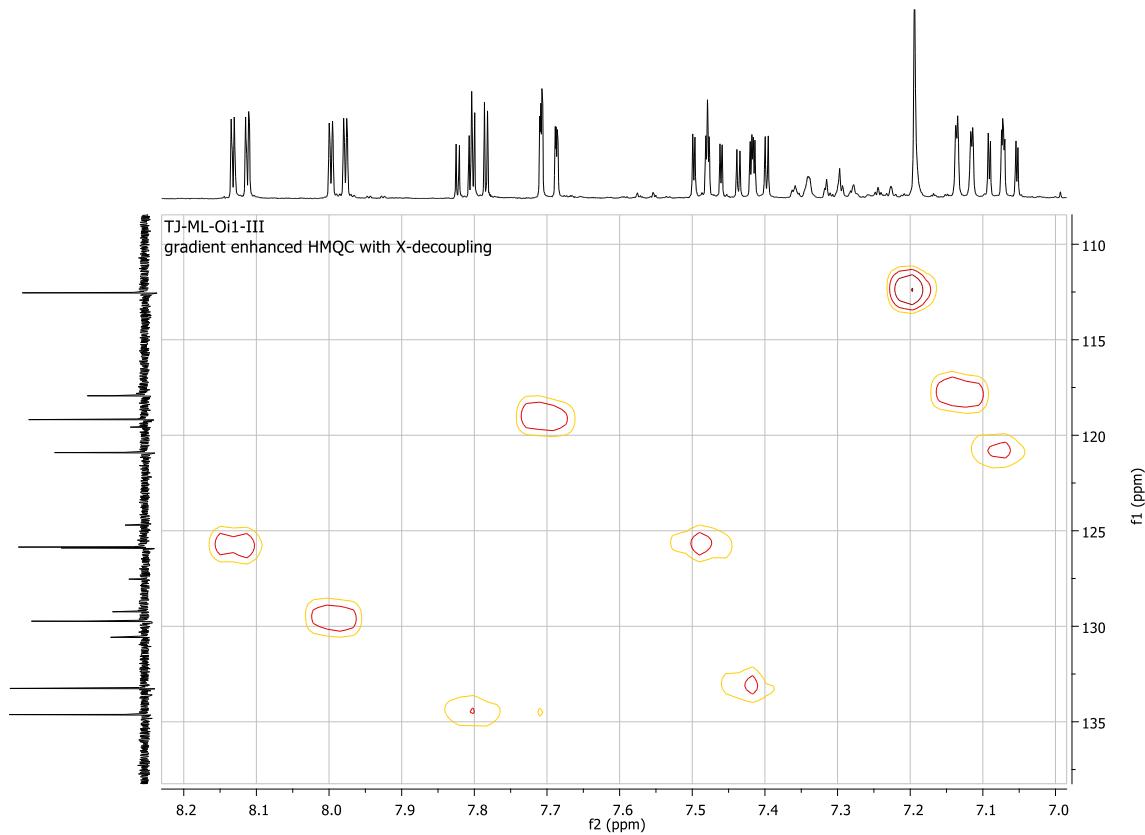


Fig.S33. HMBC spectral of 2'-hydroxyflavone (**10**) (Acetone-*d*<sub>6</sub>, 151 MHz)

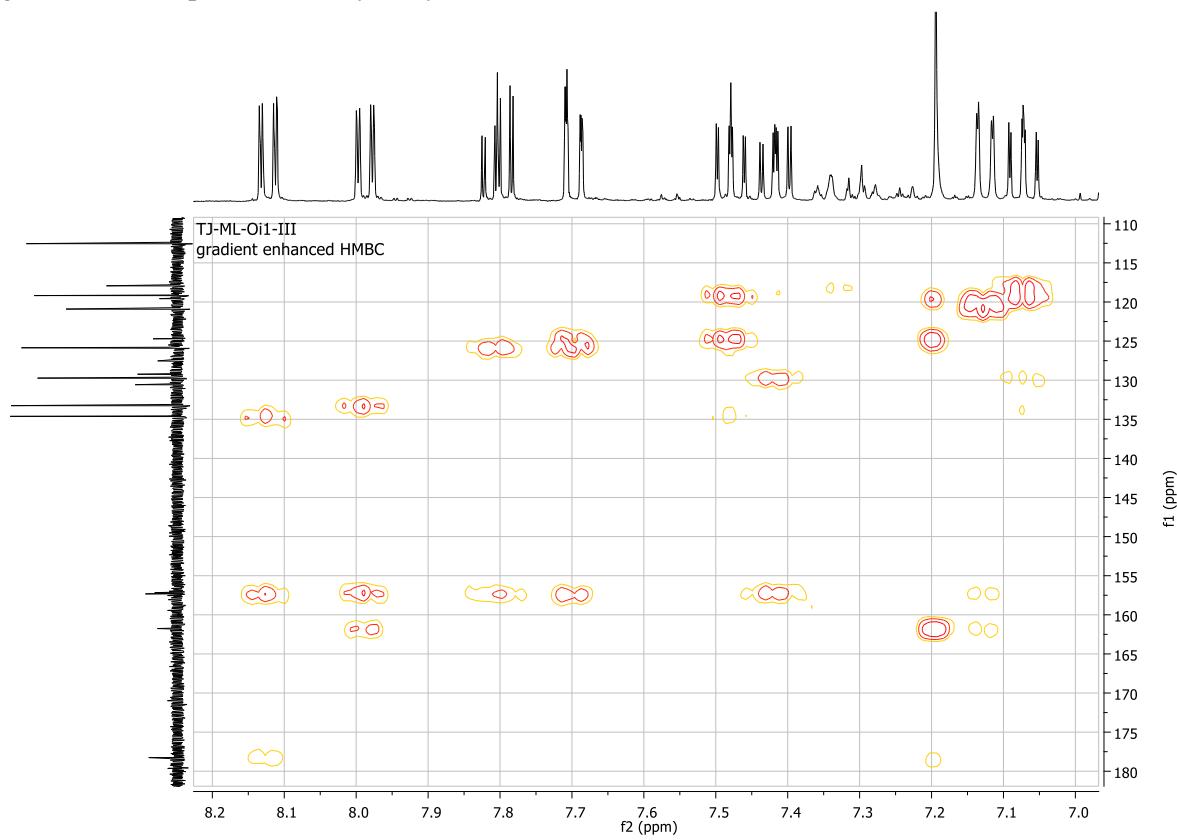
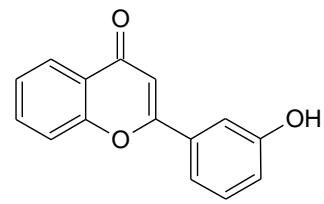


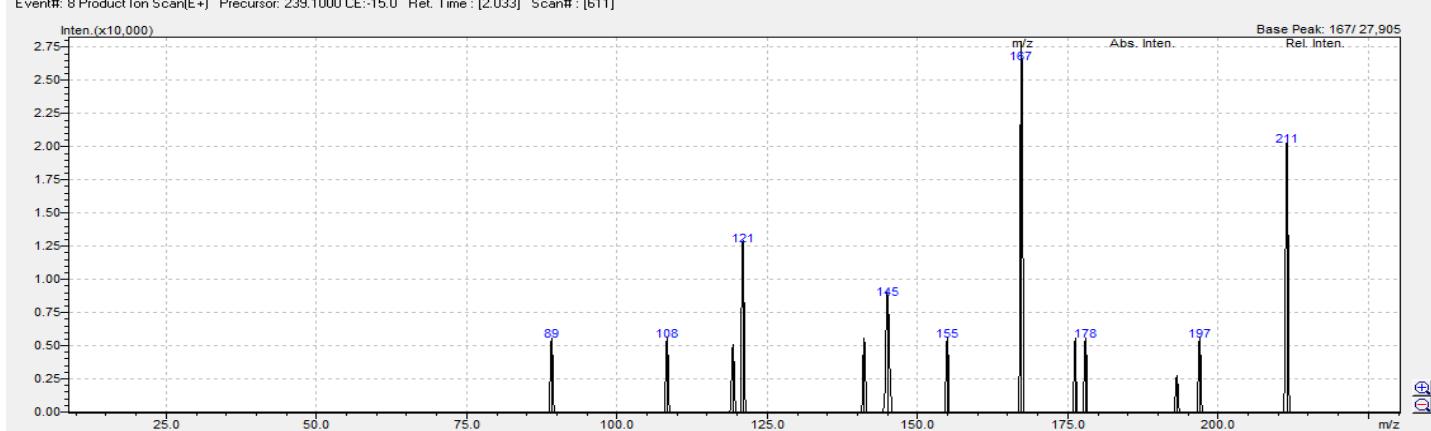
Fig.S34. MS analysis 3'-hydroxyflavone (**11**)



Molecular Formula: C<sub>15</sub>H<sub>10</sub>O<sub>3</sub>  
 Formula Weight: 238.2381  
 Precursor: 239.2000

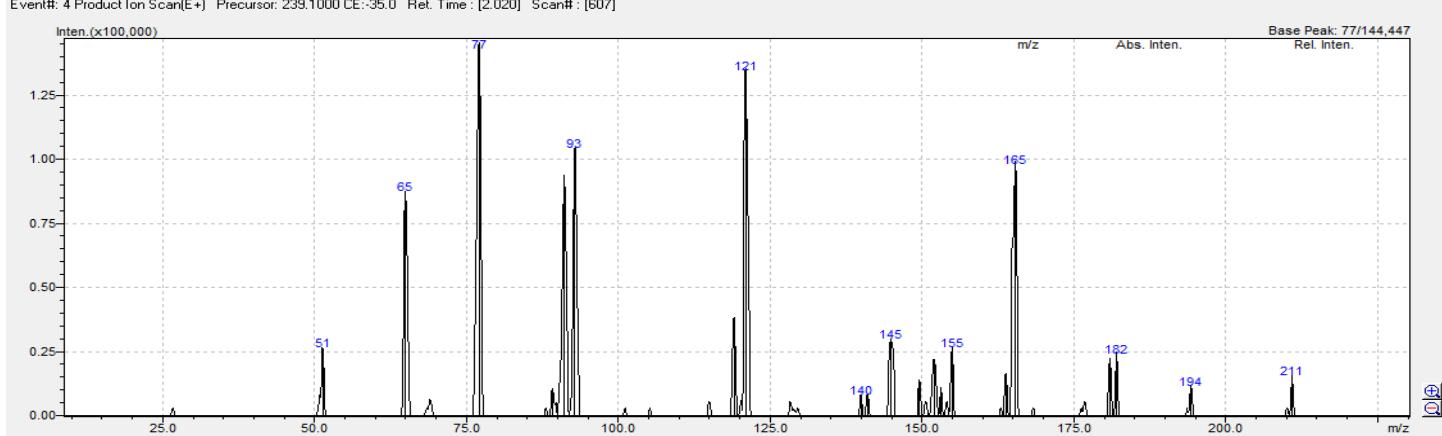
CE: -15.0

Event#: 8 Product Ion Scan(E+) Precursor: 239.1000 CE:-15.0 Ret. Time : [2.033] Scan#: [611]



CE:-35.0

Event#: 4 Product Ion Scan(E+) Precursor: 239.1000 CE:-35.0 Ret. Time : [2.020] Scan#: [607]



CE:-45.0

Event#: 2 Product Ion Scan(E+) Precursor: 239.1000 CE:-45.0 Ret. Time : [2.013] Scan#: [605]

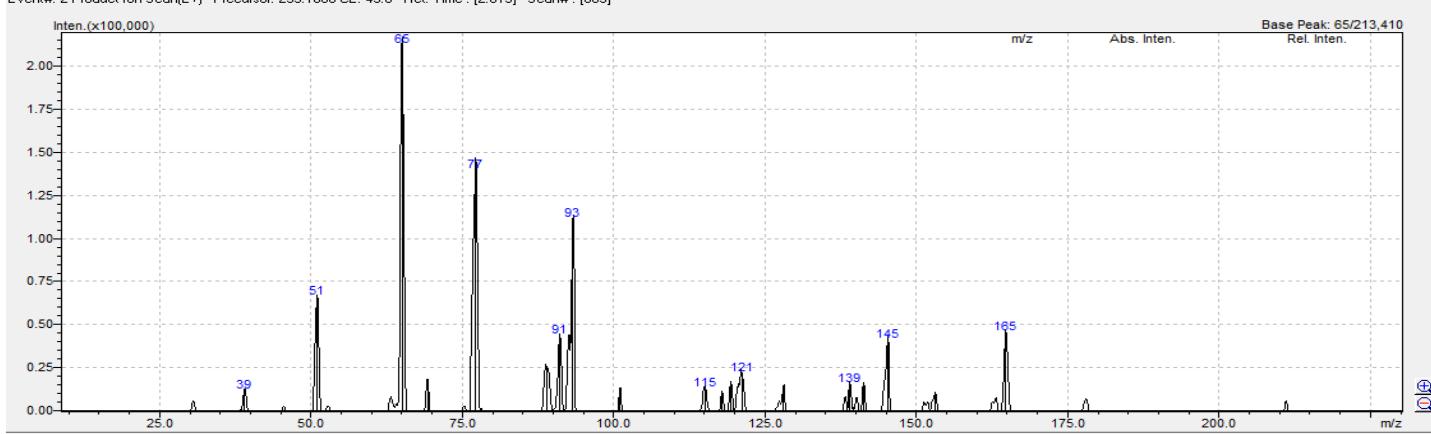


Fig.S35.  $^1\text{H}$  NMR spectral of 3'-hydroxyflavone (**11**) (DMSO- $d_6$ , 600 MHz)

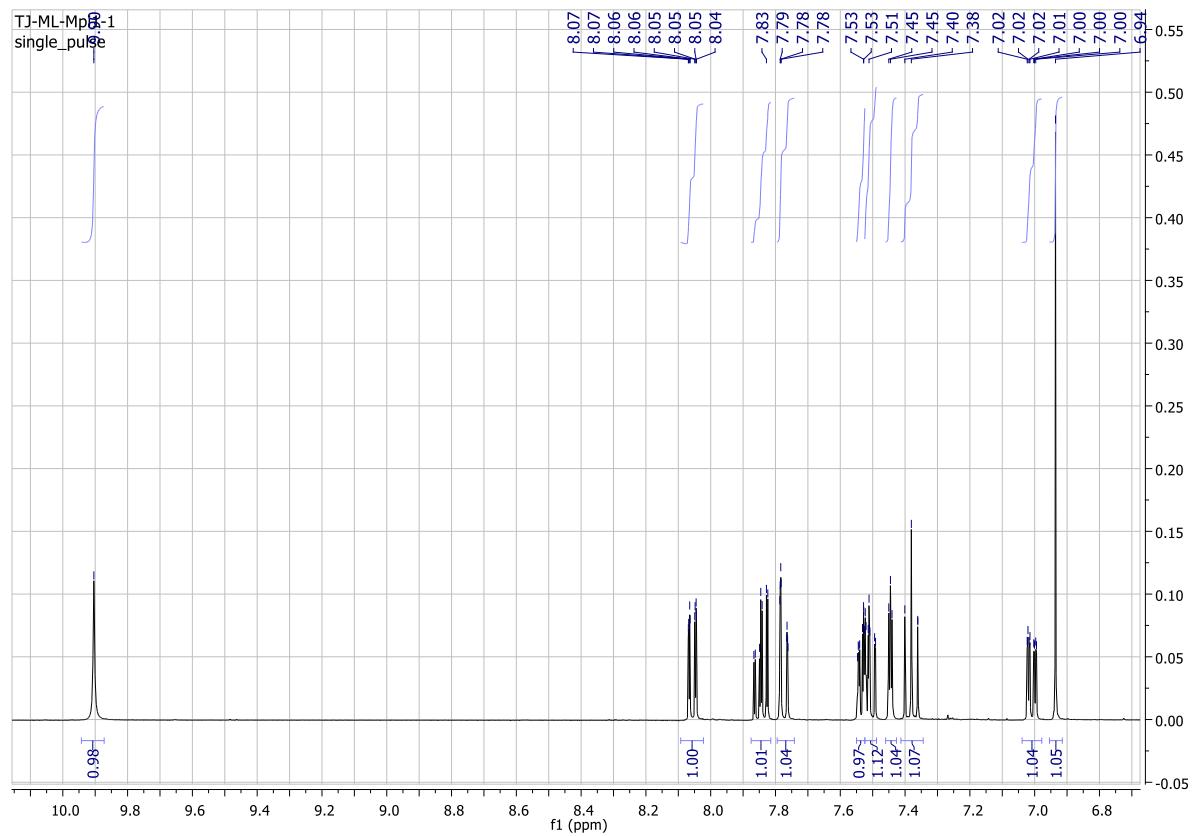


Fig.S36.  $^{13}\text{C}$  NMR spectral of 3'-hydroxyflavone (**11**) (DMSO- $d_6$ , 151 MHz)

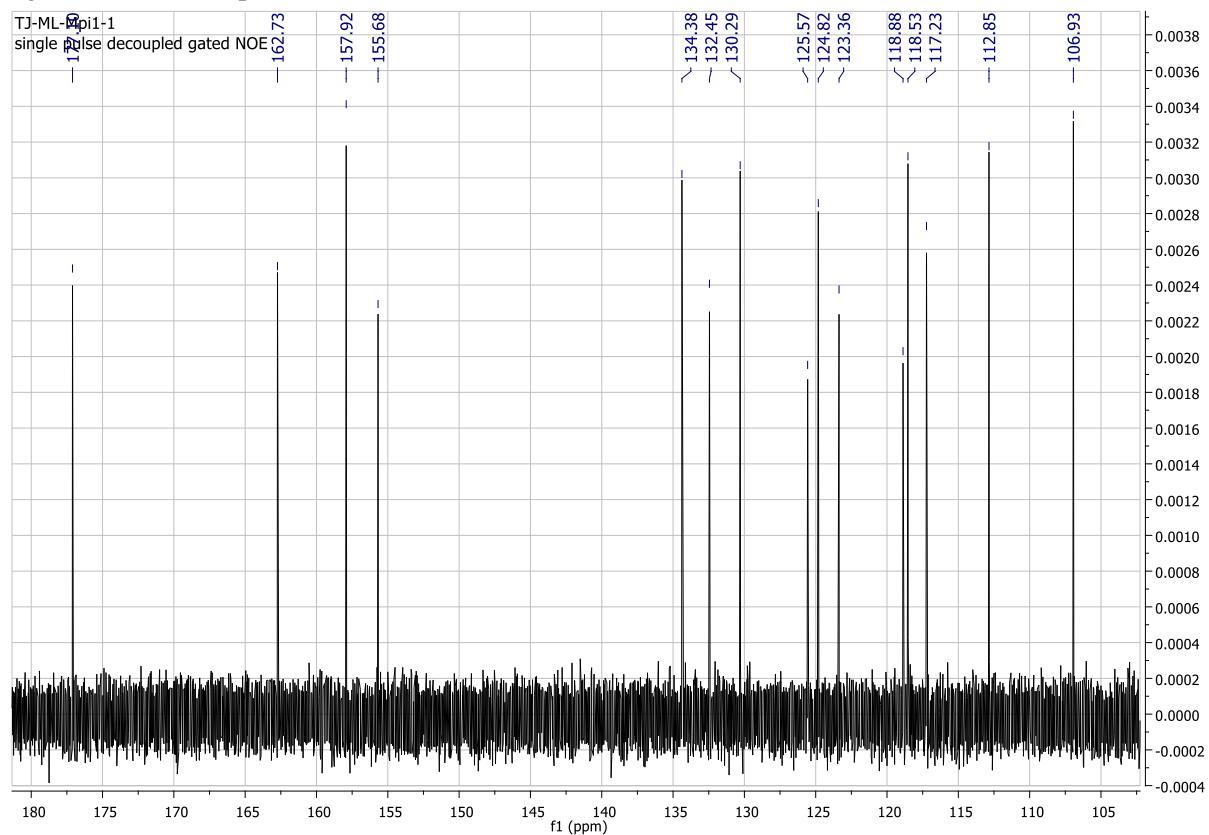


Fig.S37. COSY spectral of 3'-hydroxyflavone (**11**) (DMSO-*d*<sub>6</sub>, 151 MHz)

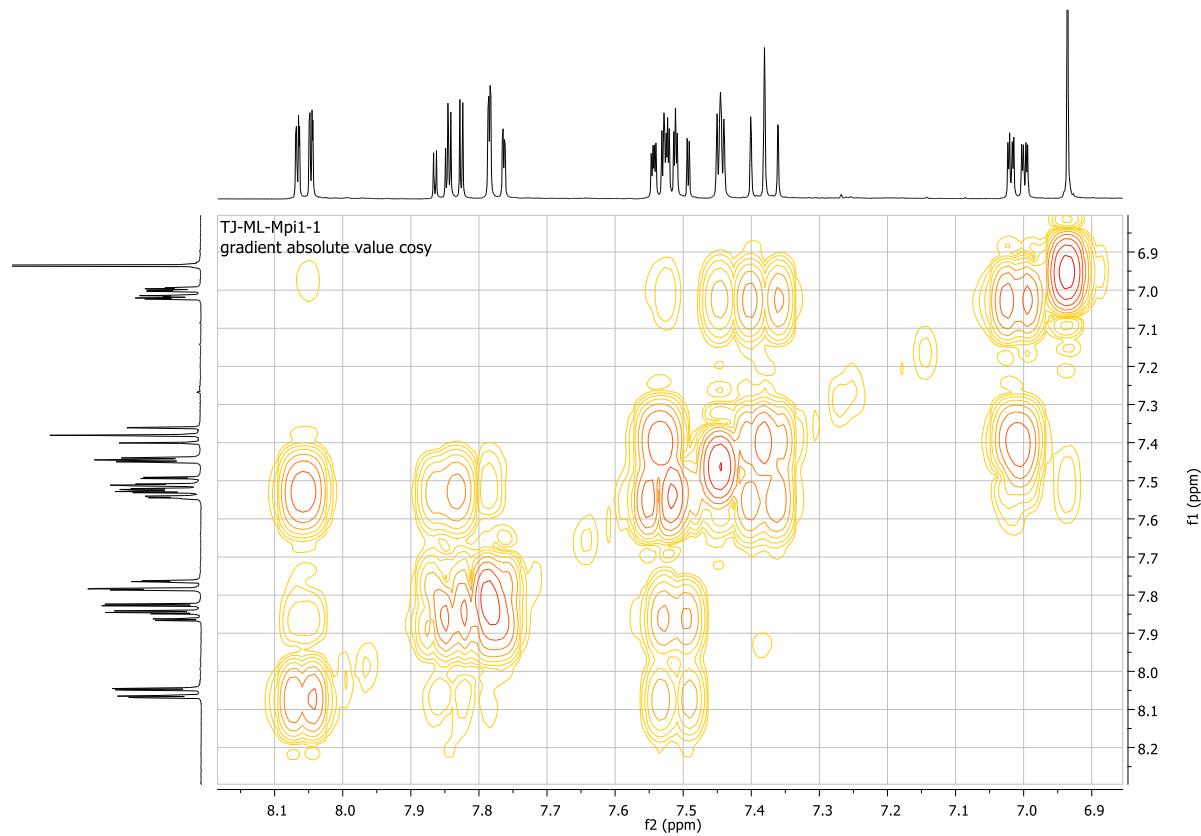


Fig.S38. HMQC spectral of 3'-hydroxyflavone (**11**) (DMSO-*d*<sub>6</sub>, 151 MHz)

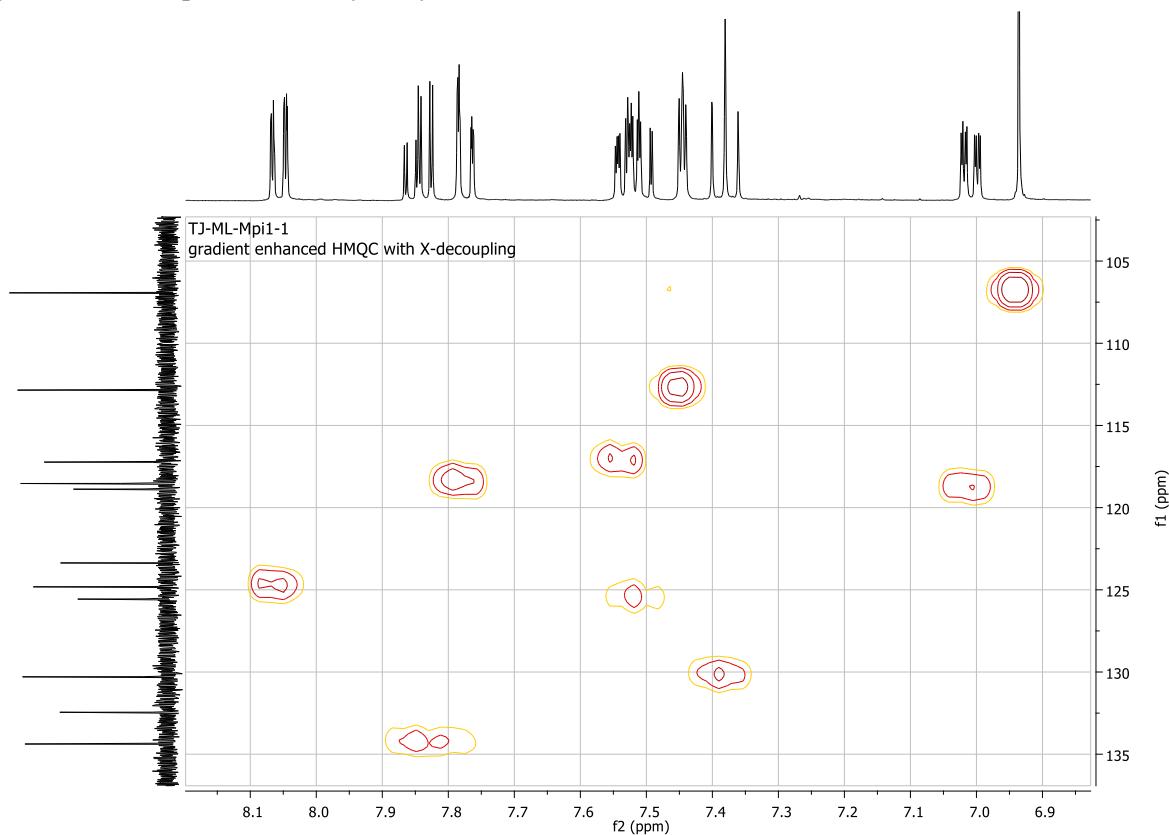


Fig.S39. HMBC spectral of 3'-hydroxyflavone (**11**) (DMSO-*d*<sub>6</sub>, 151 MHz)

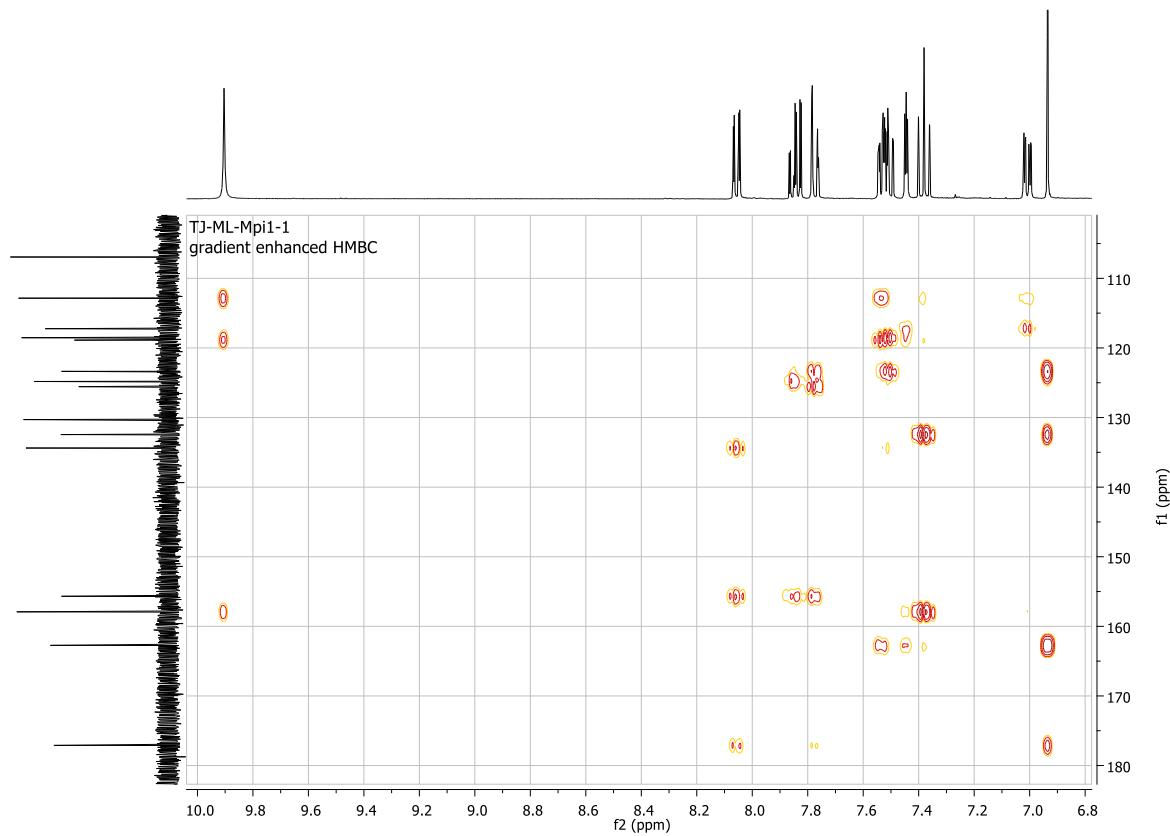
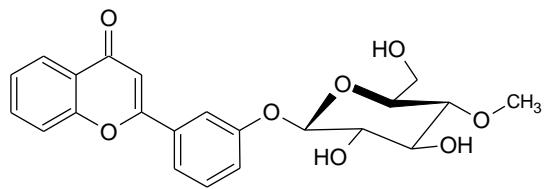


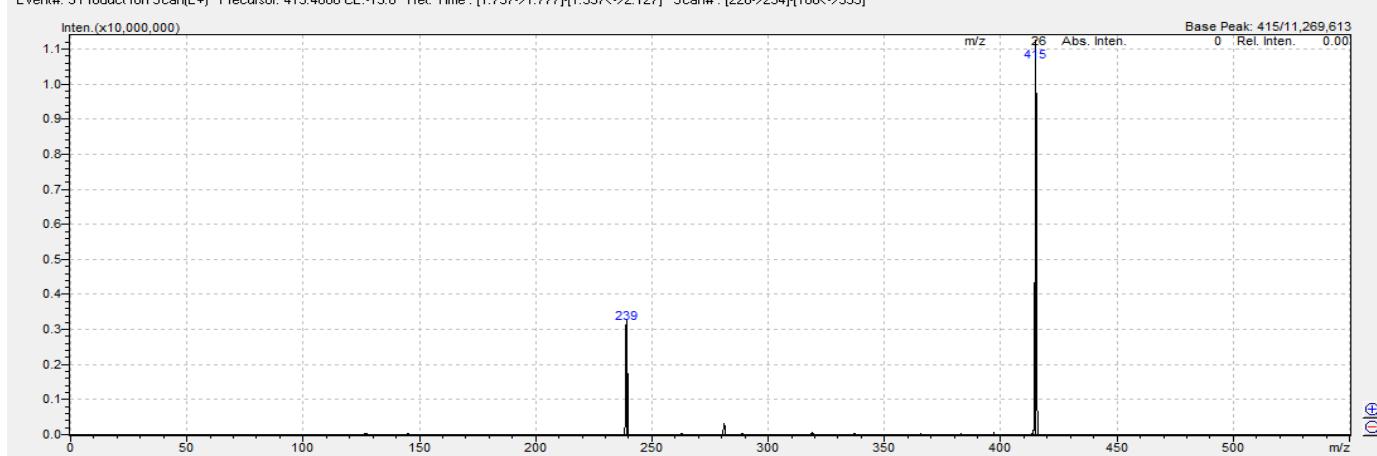
Fig.S40. MS analysis flavone 3'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**12**)

Molecular Formula = C<sub>22</sub>H<sub>22</sub>O<sub>8</sub>  
 Formula Weight = 414.40528  
 Precursor = 415.4000



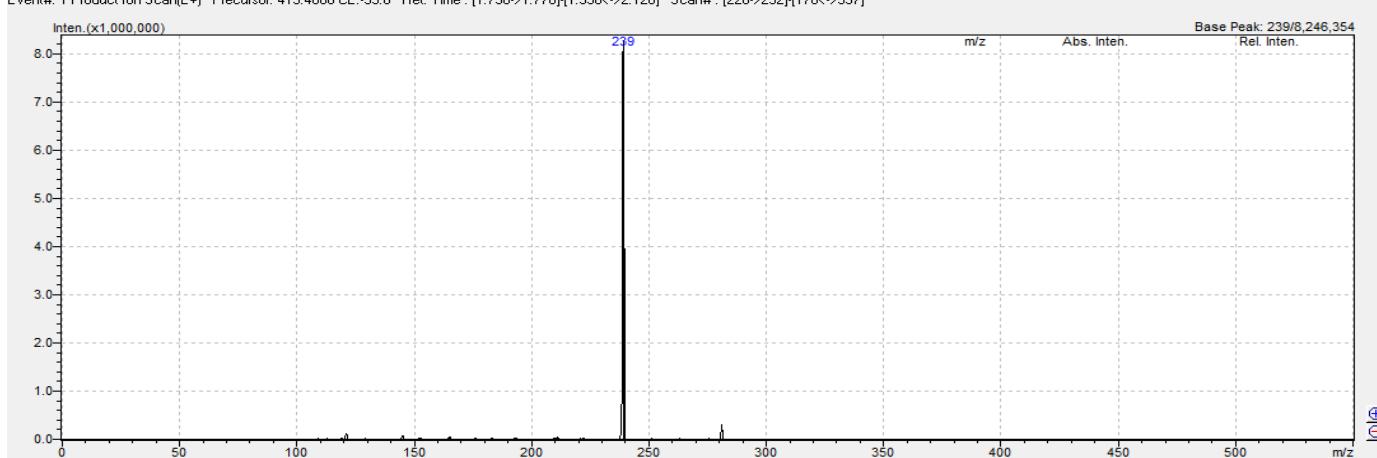
CE: -15.0

Event#: 3 Product Ion Scan(E+) Precursor: 415.4000 CE:-15.0 Ret. Time : [1.757>1.777][1.597<>2.127] Scan# : [228>234][180<>339]



CE:-35.0

Event#: 1 Product Ion Scan(E+) Precursor: 415.4000 CE:-35.0 Ret. Time : [1.750>1.770][1.590<>2.120] Scan# : [226>232][178<>337]



CE:-45.0

Event#: 2 Product Ion Scan(E+) Precursor: 415.4000 CE:-45.0 Ret. Time : [1.753>1.773][1.593<>2.123] Scan# : [227>233][179<>338]



Fig.S41.  $^1\text{H}$  NMR spectral of flavone 3'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**12**) (DMSO- $d_6$ , 600 MHz)

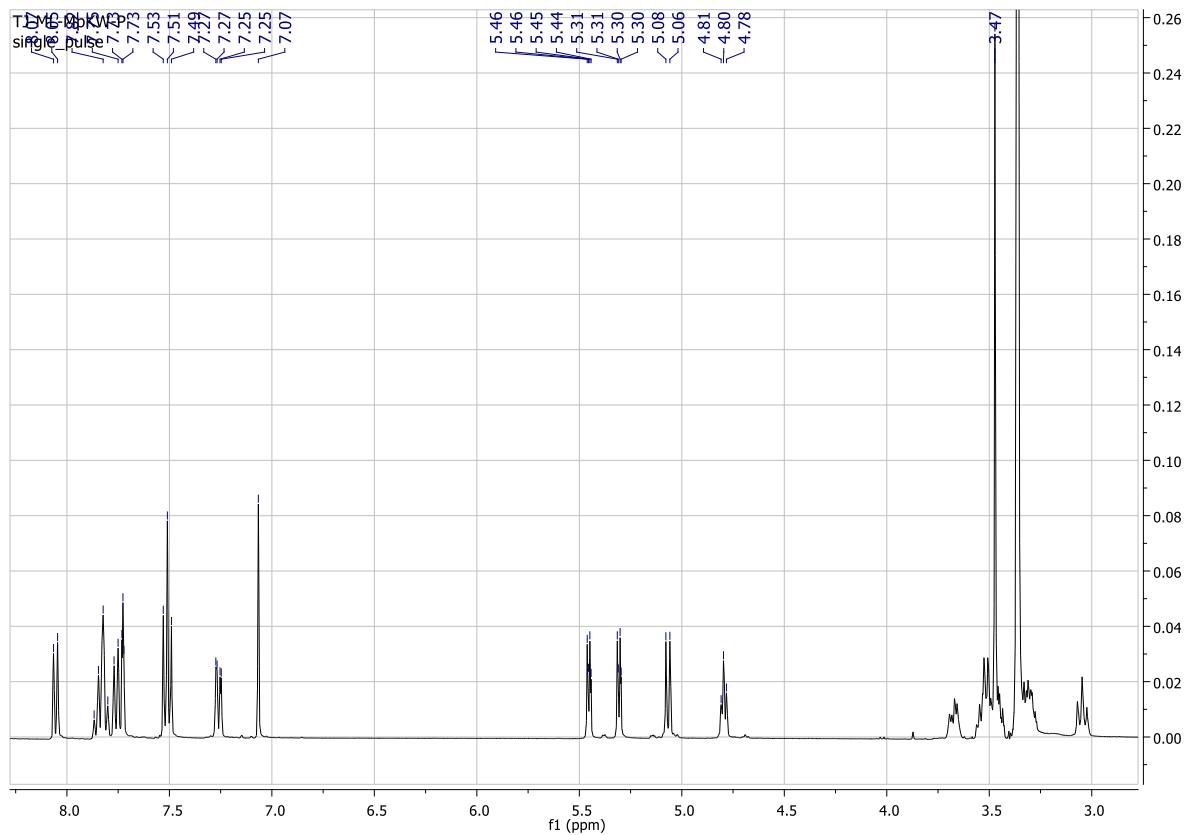


Fig.S42. Flavone part of the  $^1\text{H}$  NMR spectral flavone 3'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**12**) (DMSO- $d_6$ , 600 MHz)

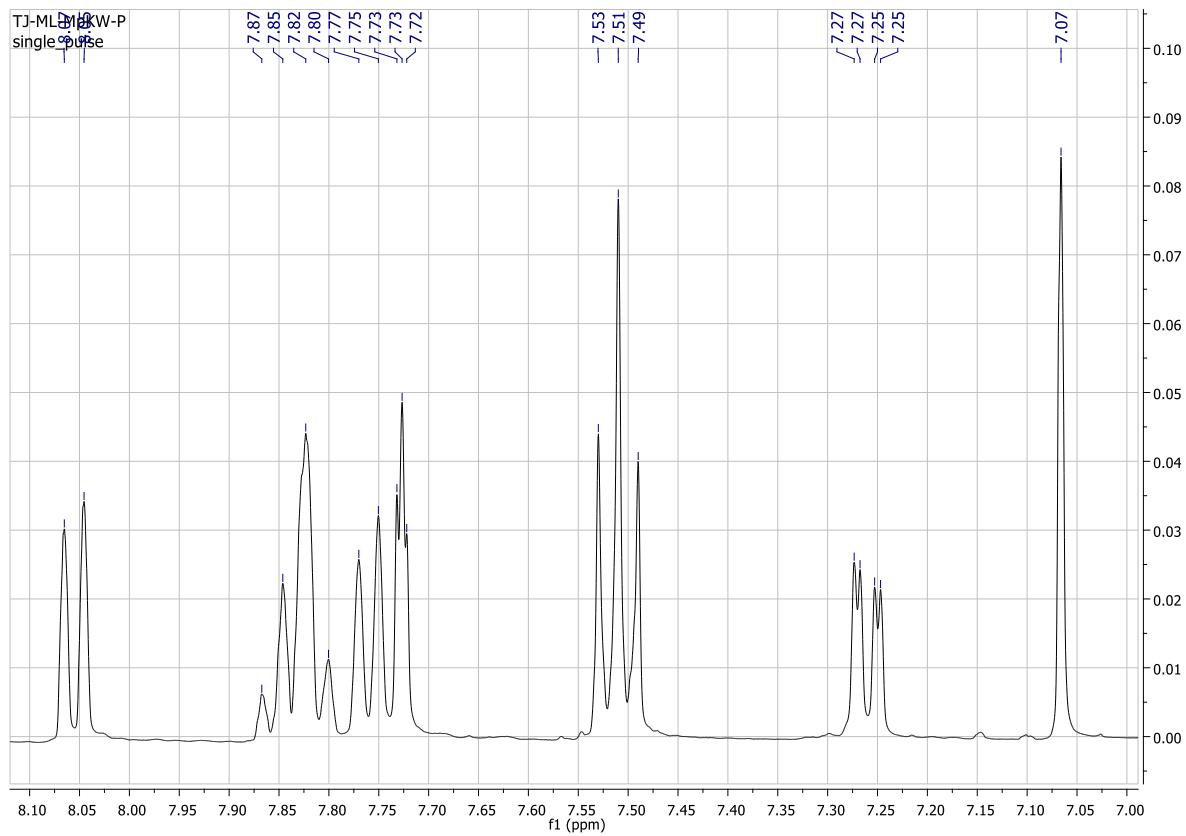


Fig.S43. Glucopyranoside part of the  $^1\text{H}$  NMR spectral flavone 3'-*O*- $\beta$ -D-(4''-*O*-methyl)-glucopyranoside (**12**) ( $\text{DMSO}-d_6$ , 600 MHz)

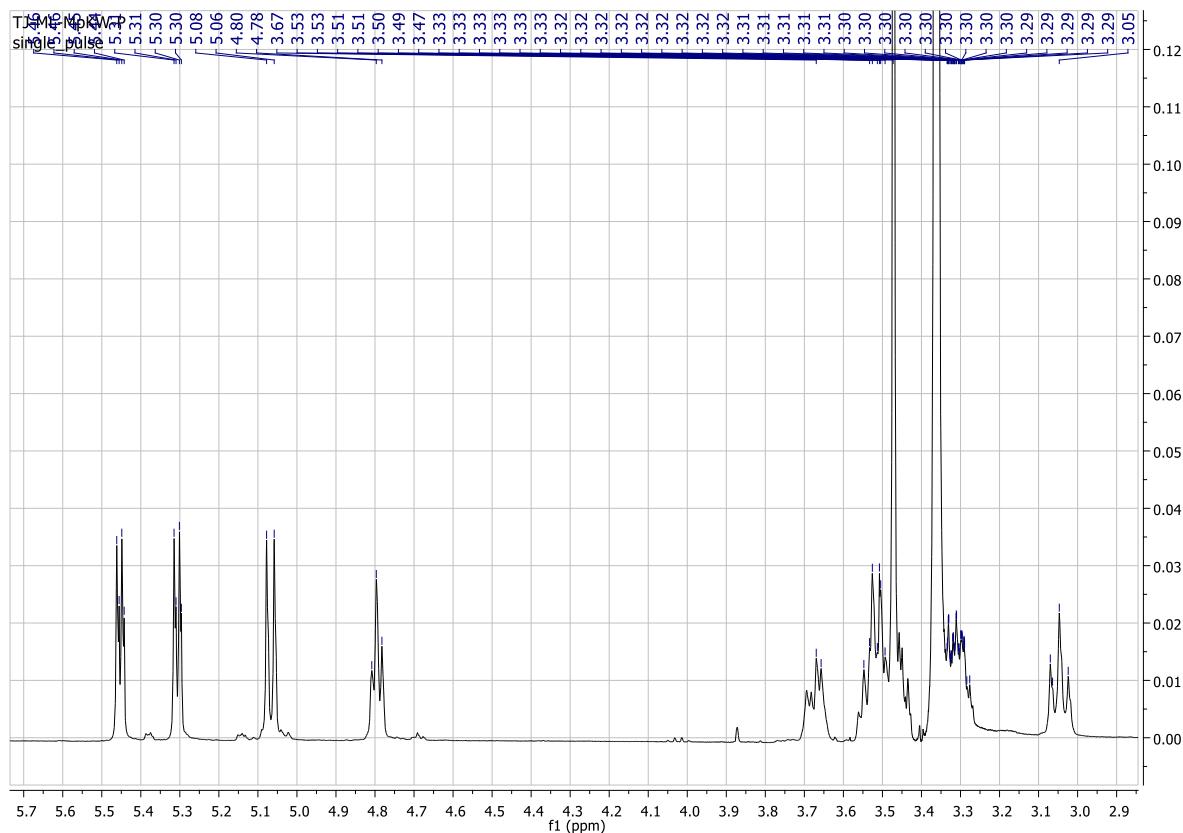


Fig.S44.  $^{13}\text{C}$  NMR spectral of flavone 3'-*O*- $\beta$ -D-(4''-*O*-methyl)-glucopyranoside (**12**) (DMSO- $d_6$ , 151 MHz)

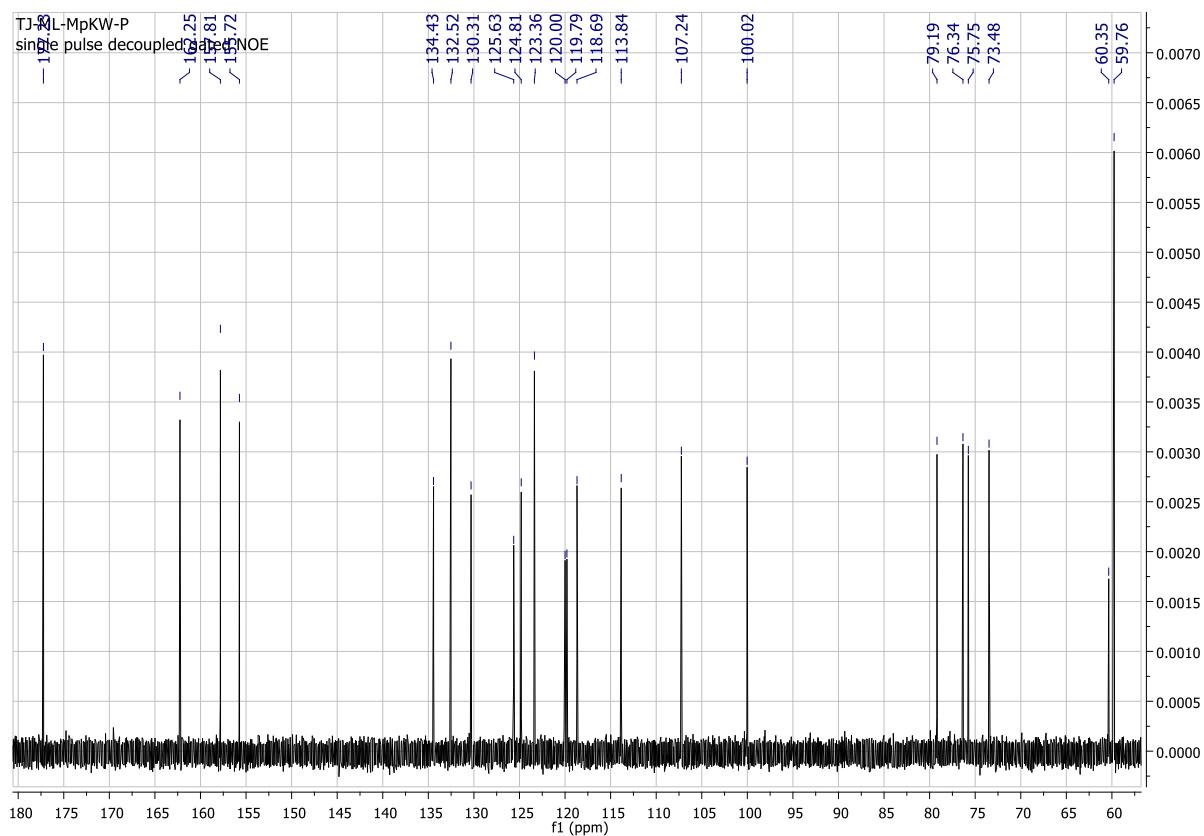


Fig.S45. HMQC spectral of flavone 3'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**12**) (DMSO- $d_6$ , 151 MHz)

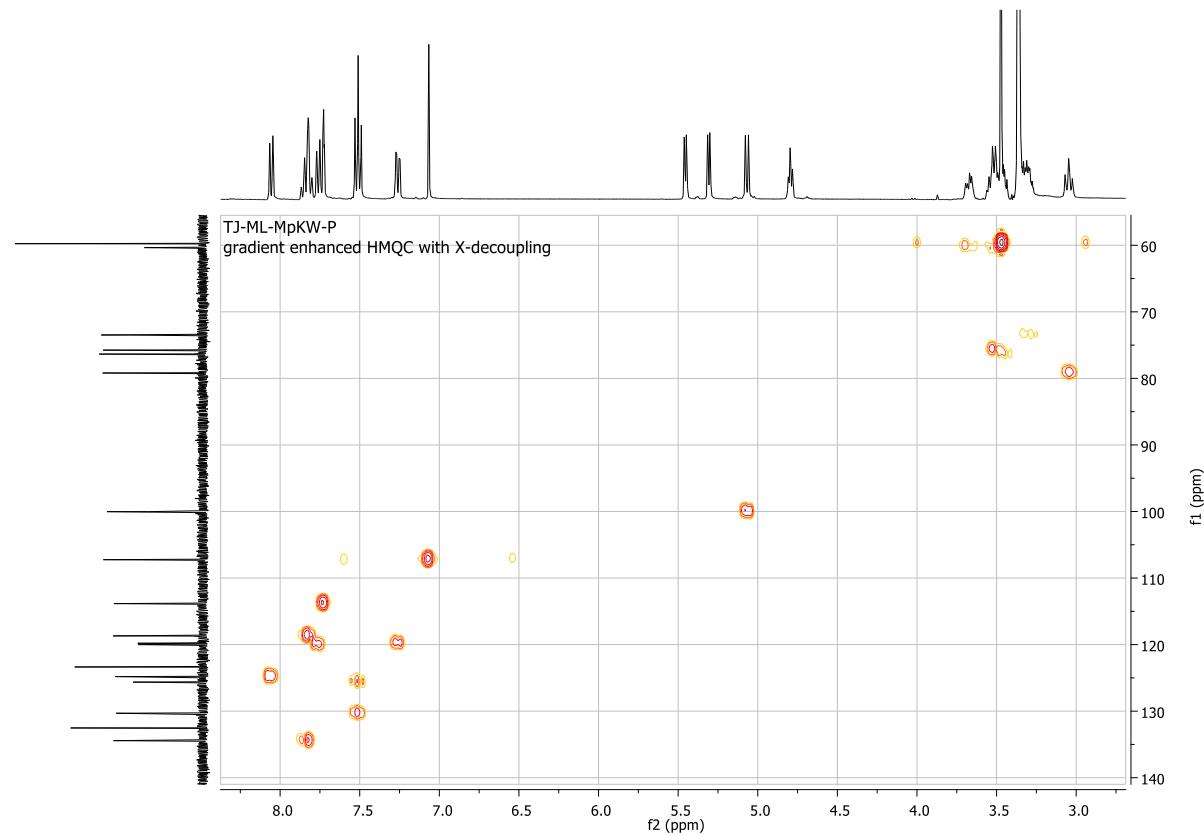


Fig.S46. HMBC spectral of flavone 3'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**12**) (DMSO- $d_6$ , 151 MHz)

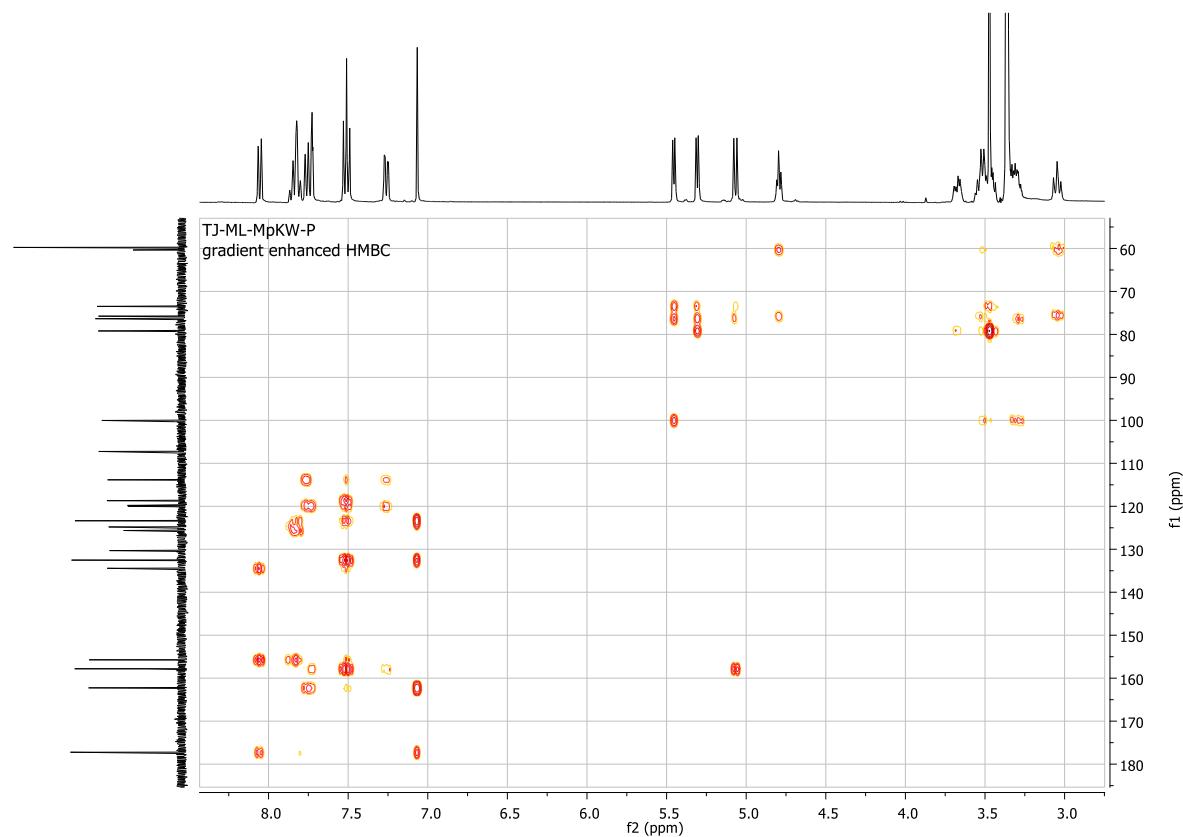
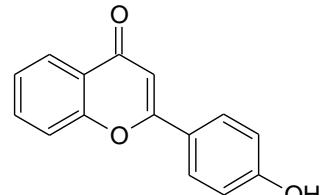


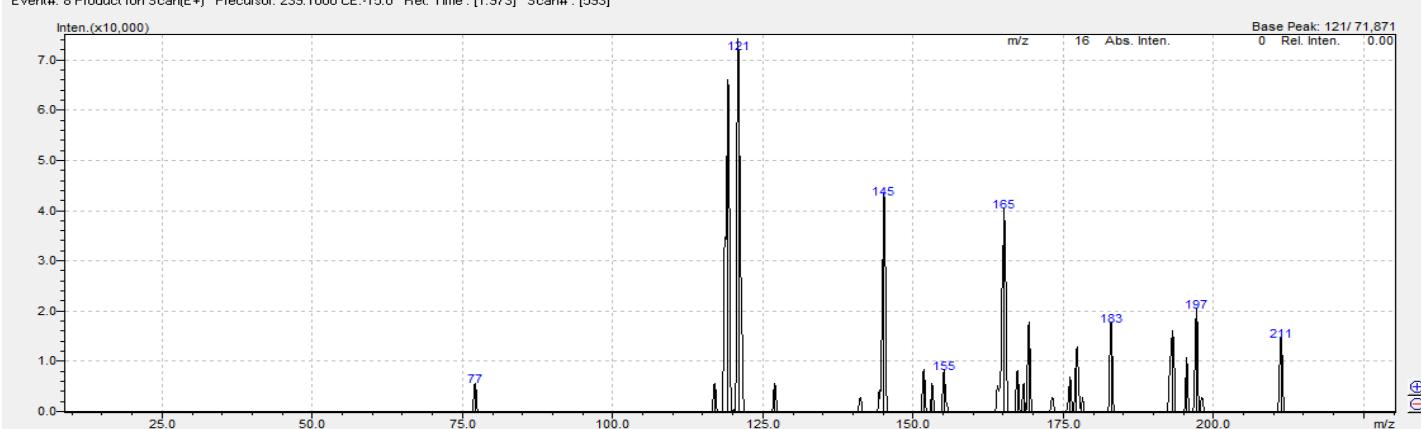
Fig.S47. MS analysis 4'-hydroxyflavone (**13**)



Molecular Formula: C<sub>15</sub>H<sub>10</sub>O<sub>3</sub>  
 Formula Weight: 238.2381  
 Precursor: 239.2000

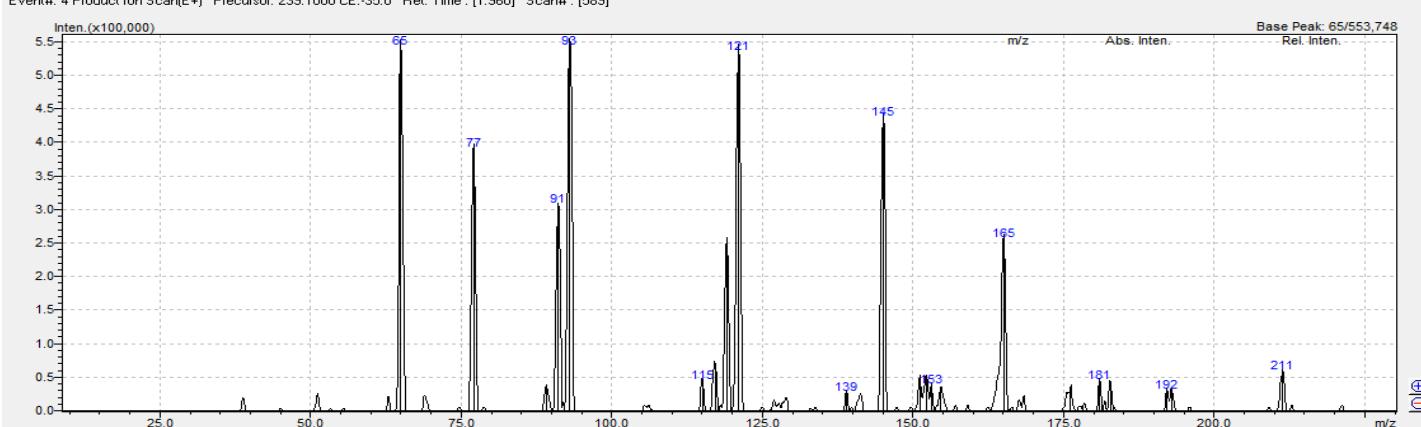
CE: -15.0

Event#: 8 Product Ion Scan(E+) Precursor: 239.1000 CE:-15.0 Ret. Time : [1.973] Scan# : [593]



CE:-35.0

Event#: 4 Product Ion Scan(E+) Precursor: 239.1000 CE:-35.0 Ret. Time : [1.960] Scan# : [589]



CE:-45.0

Event#: 2 Product Ion Scan(E+) Precursor: 239.1000 CE:-45.0 Ret. Time : [1.953] Scan# : [587]

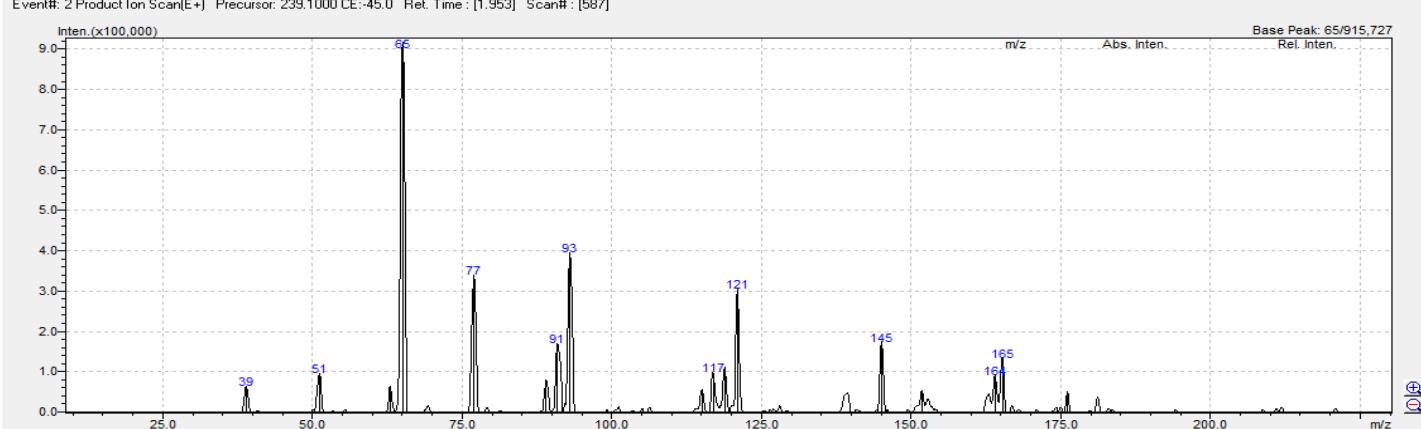


Fig.S48.  $^1\text{H}$  NMR spectral of 4'-hydroxyflavone (**13**) (DMSO- $d_6$ , 600 MHz)

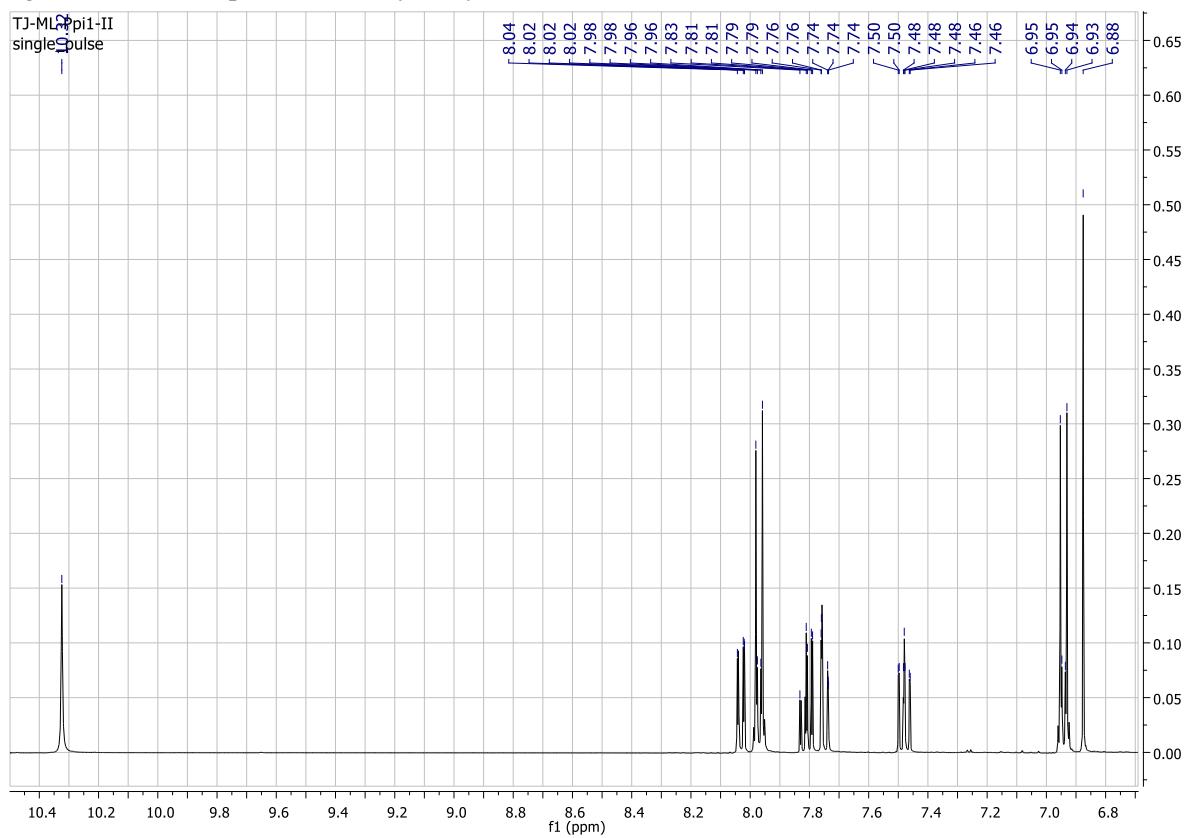


Fig.S49.  $^{13}\text{C}$  NMR spectral of 4'-hydroxyflavone (**13**) (DMSO- $d_6$ , 151 MHz)

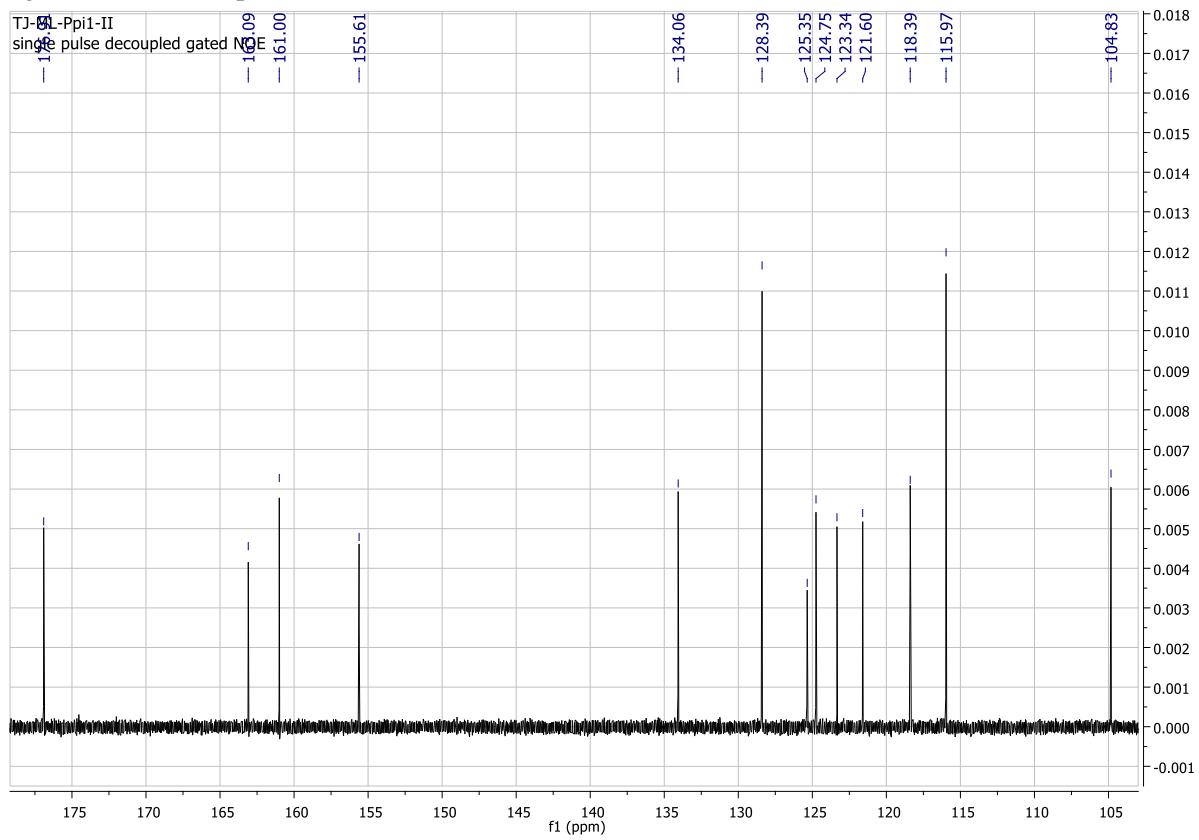


Fig.S50. COSY spectral of 4'-hydroxyflavone (**13**) (DMSO-*d*<sub>6</sub>, 151 MHz)

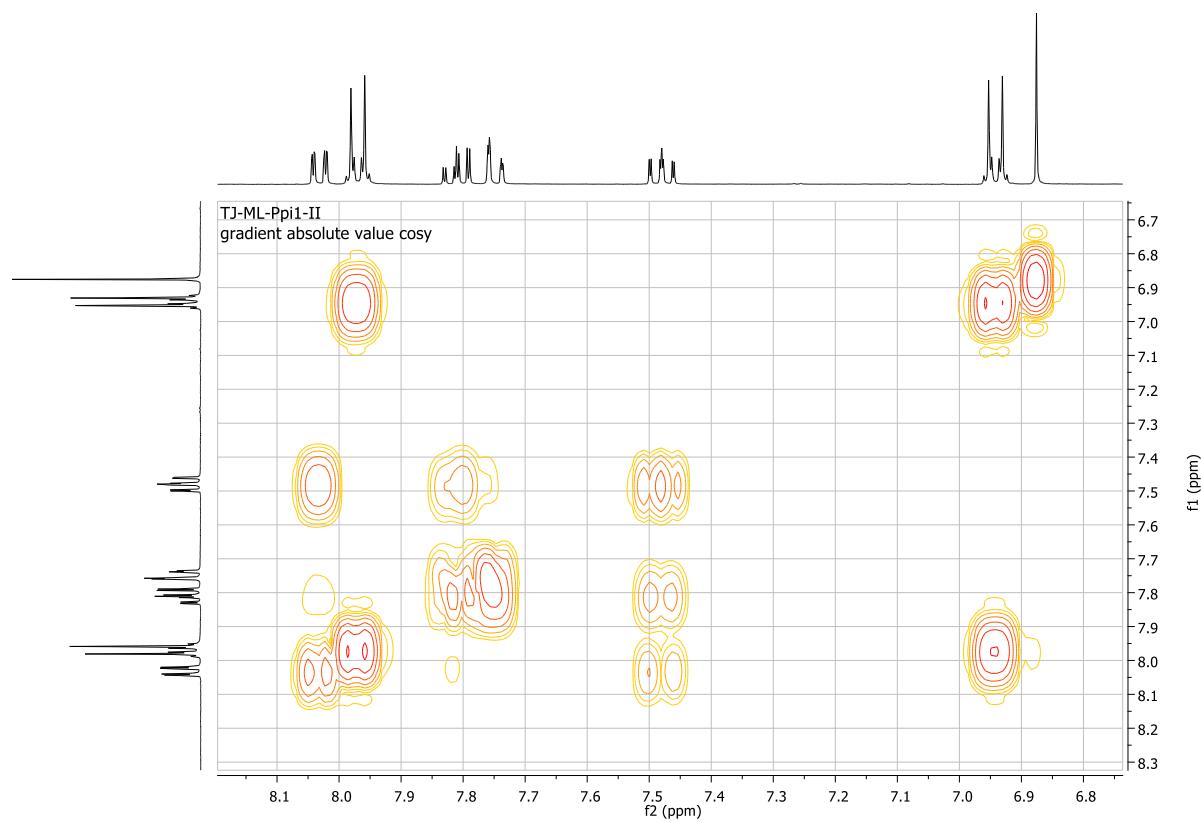


Fig.S51. HMQC spectral of 4'-hydroxyflavone (**13**) (DMSO-*d*<sub>6</sub>, 151 MHz)

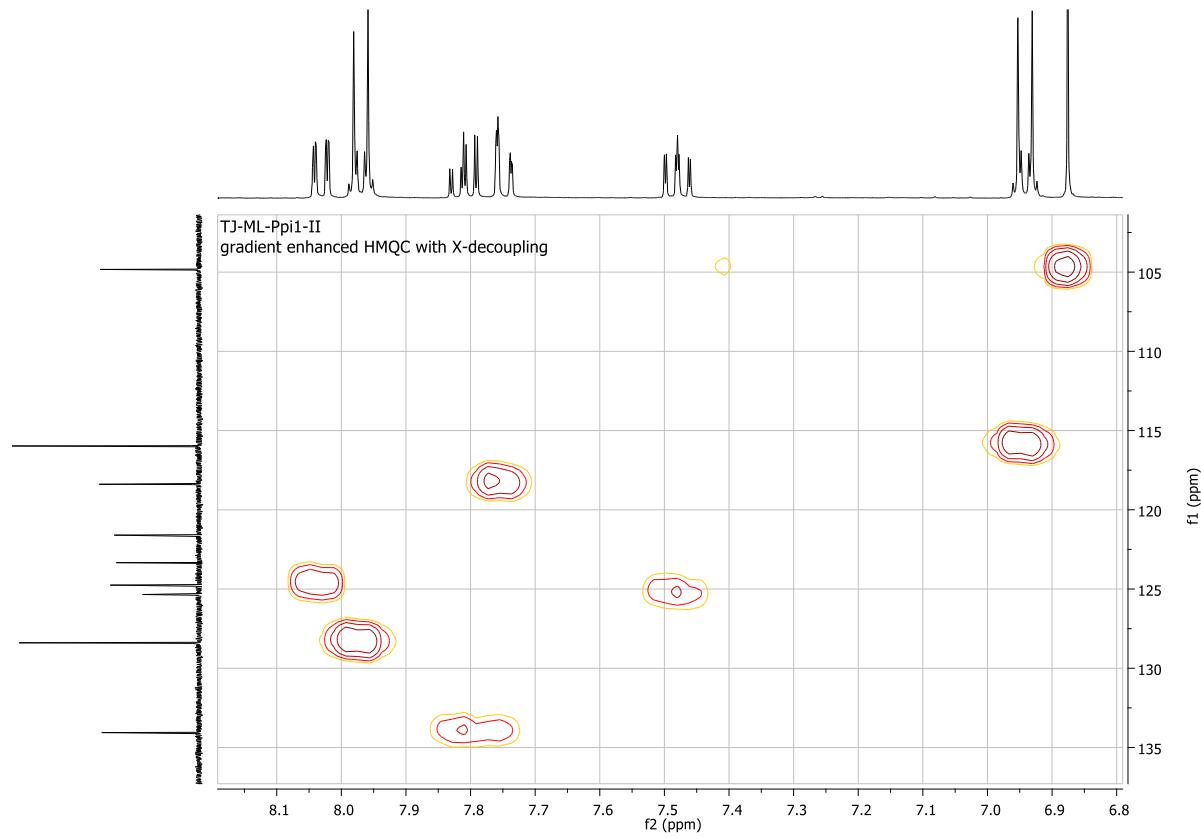


Fig.S52. HMBC spectral of 4'-hydroxyflavone (**13**) (DMSO-*d*<sub>6</sub>, 151 MHz)

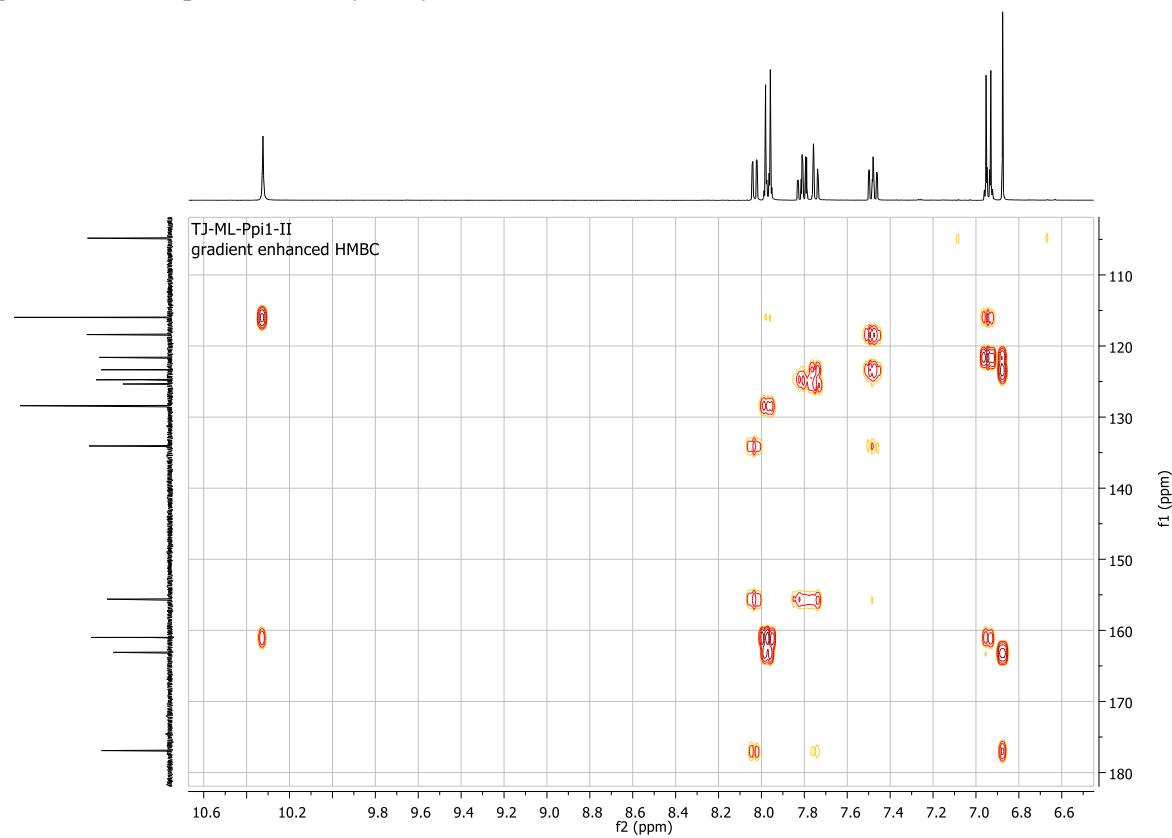
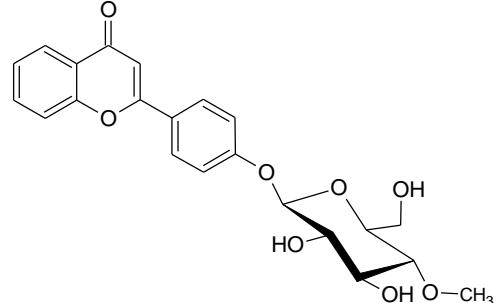


Fig.S53. MS analysis flavone 4'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**14**)

Molecular Formula = C<sub>22</sub>H<sub>22</sub>O<sub>8</sub>  
 Formula Weight = 414.40528  
 Precursor = 415.4000



CE: -15.0

Event#: 8 Product Ion Scan(E+) Precursor: 415.2000 CE:-15.0 Ret. Time : [2.213] Scan# : [665]



CE:-35.0

Event#: 4 Product Ion Scan(E+) Precursor: 415.2000 CE:-35.0 Ret. Time : [2.290] Scan# : [688]



CE:-45.0

Event#: 2 Product Ion Scan(E+) Precursor: 415.2000 CE:-45.0 Ret. Time : [2.283] Scan# : [686]



Fig.S54.  $^1\text{H}$  NMR spectral of flavone 4'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**14**) (DMSO- $d_6$ , 600 MHz)

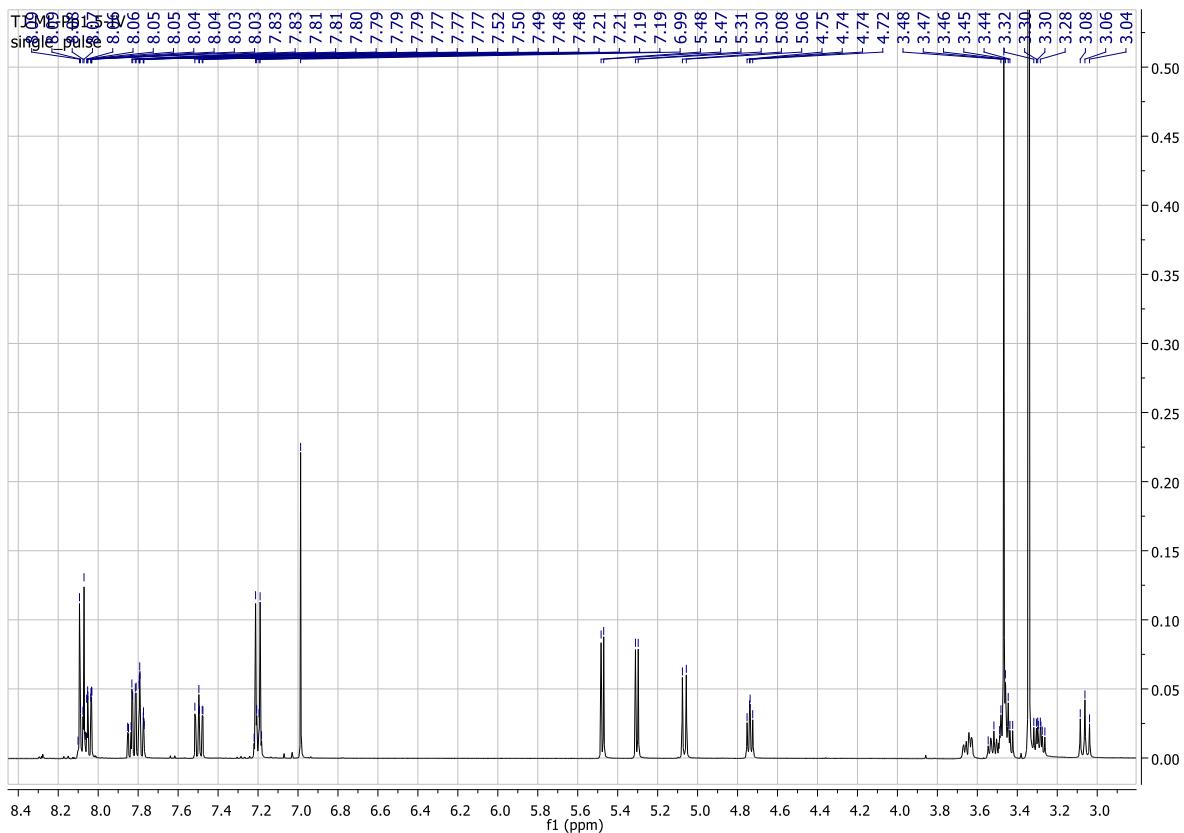


Fig.S55. Flavone part of the  $^1\text{H}$  NMR spectral flavone 4'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**14**) (DMSO- $d_6$ , 600 MHz)

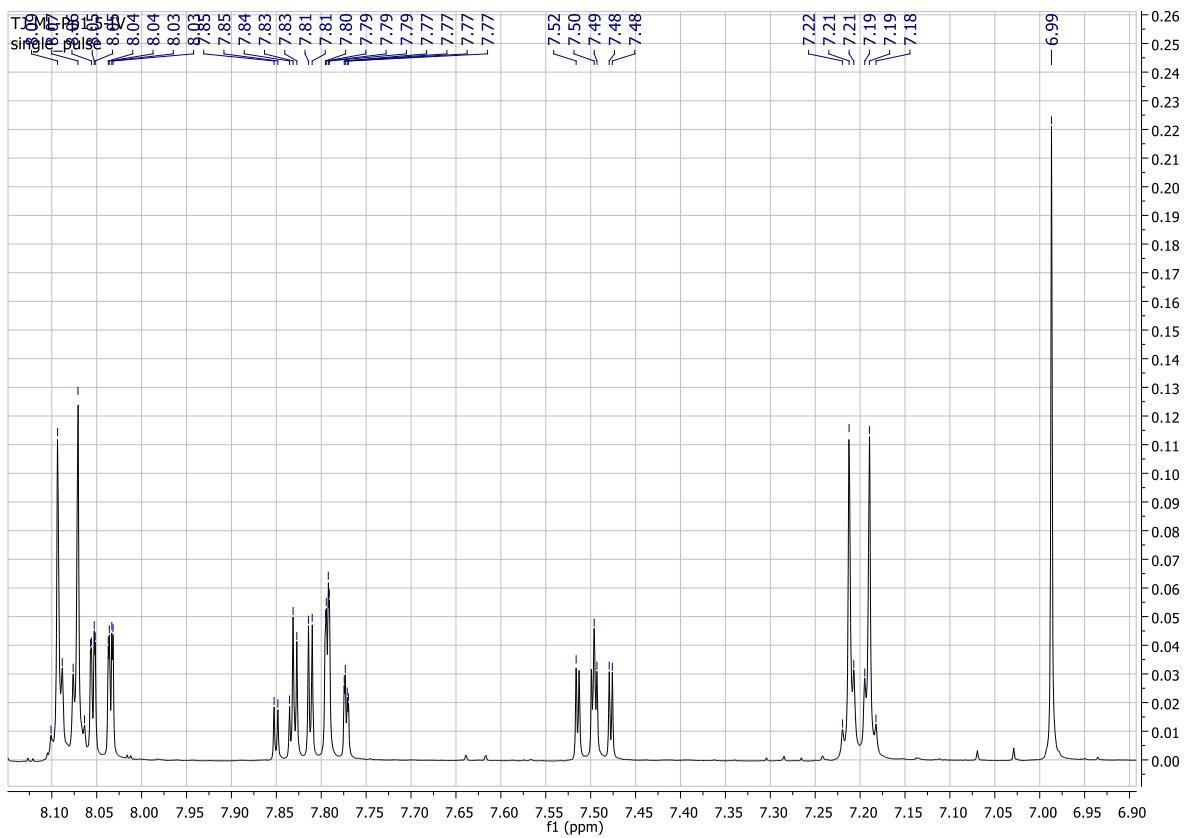


Fig.S56. Glucopyranoside part of the  $^1\text{H}$  NMR spectral flavone 4'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**14**) (DMSO- $d_6$ , 600 MHz)

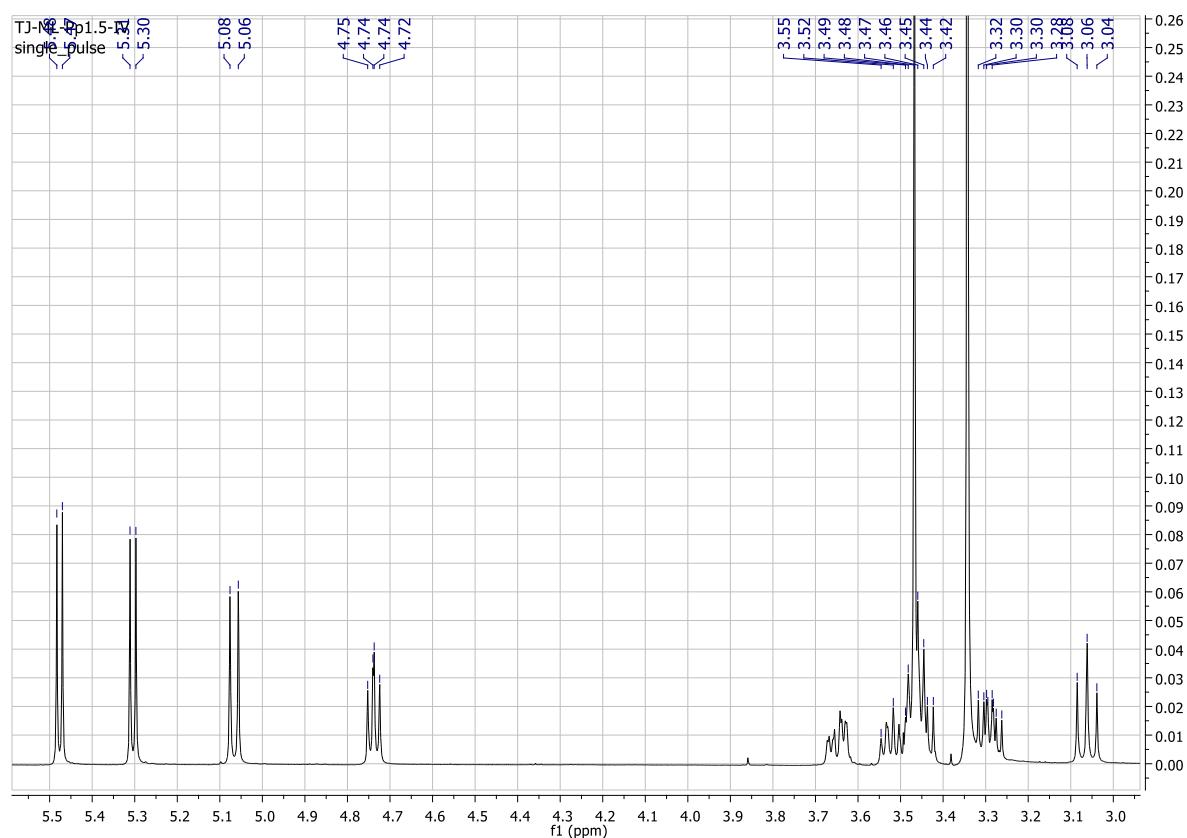


Fig.S57.  $^{13}\text{C}$  NMR spectral of flavone 4'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**14**) (DMSO- $d_6$ , 151 MHz)

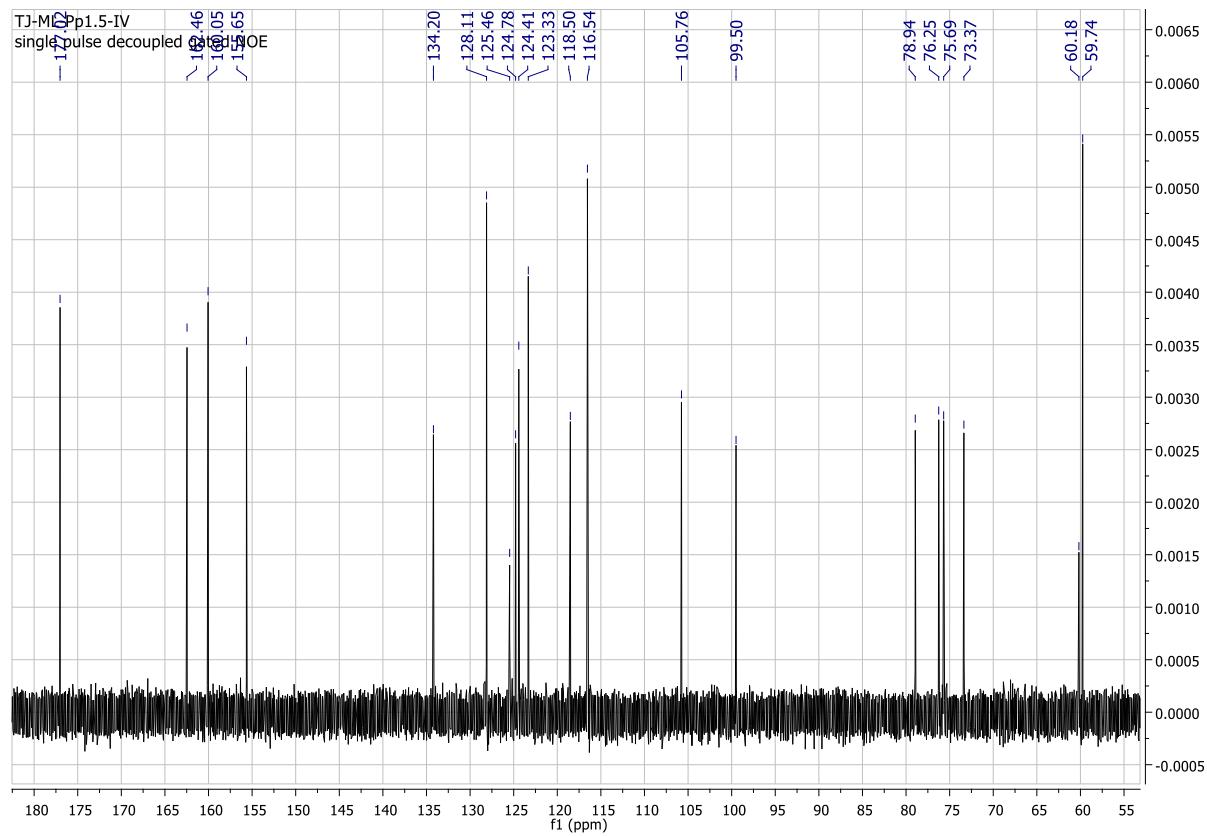


Fig.S58. COSY spectral of flavone 4'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**14**) (DMSO- $d_6$ , 151 MHz)

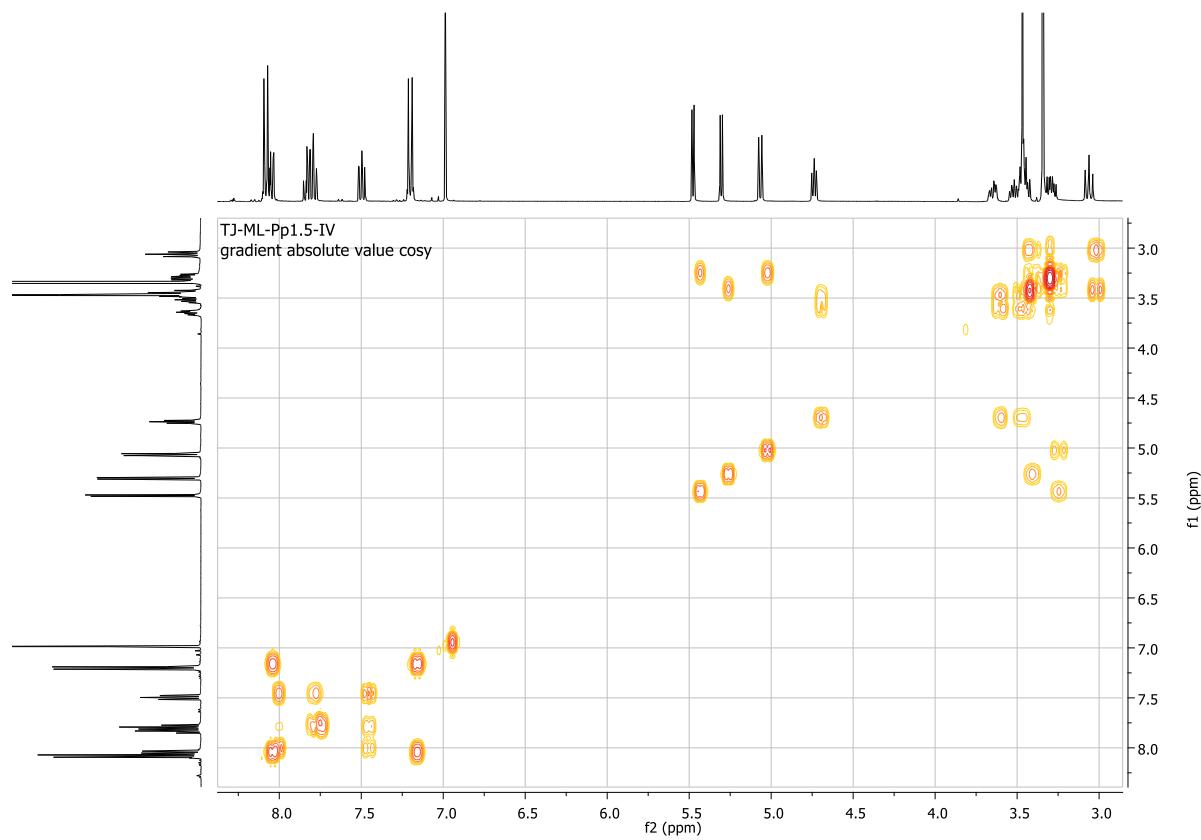


Fig.S59. HMQC spectral of flavone 4'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**14**) (DMSO- $d_6$ , 151 MHz)

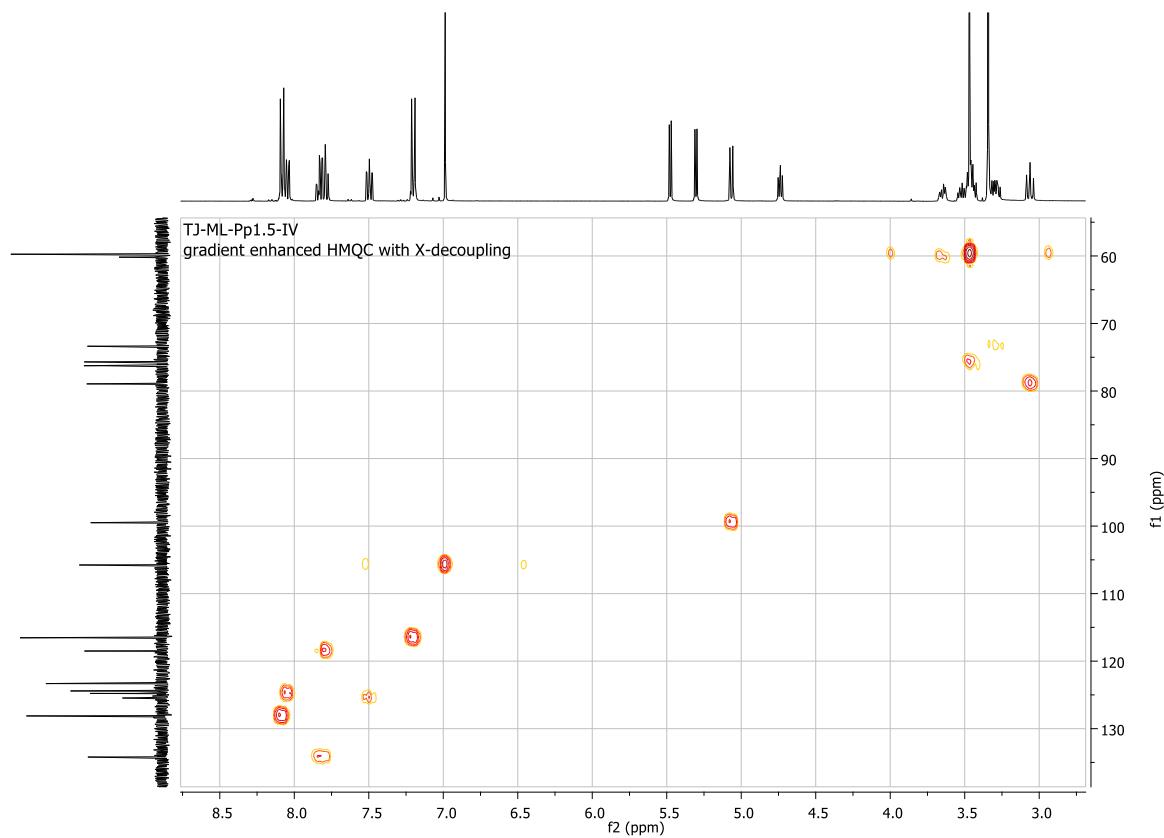


Fig.S60. HMBC spectral of flavone 4'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**14**) (DMSO- $d_6$ , 151 MHz)

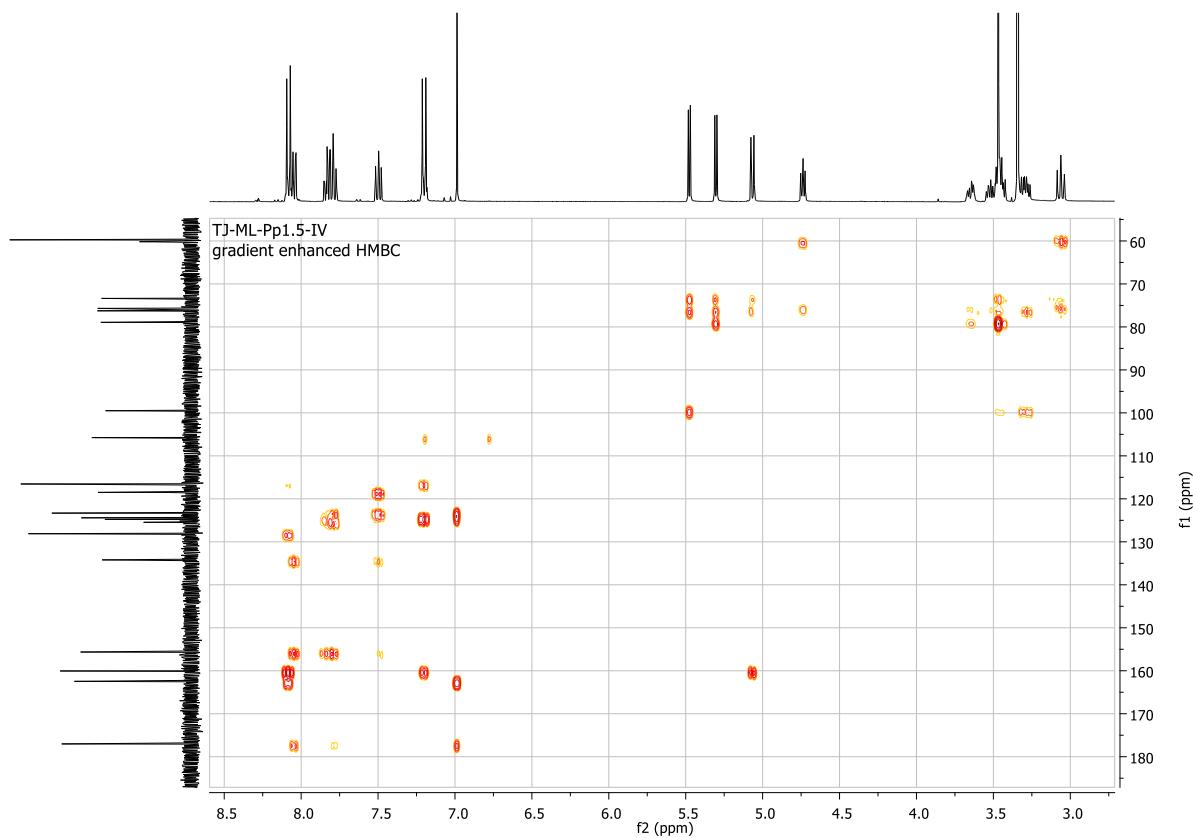
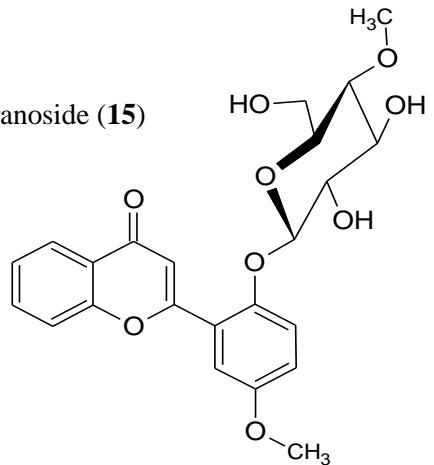


Fig.S61. MS analysis 5'-methoxyflavone 2'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**15**)

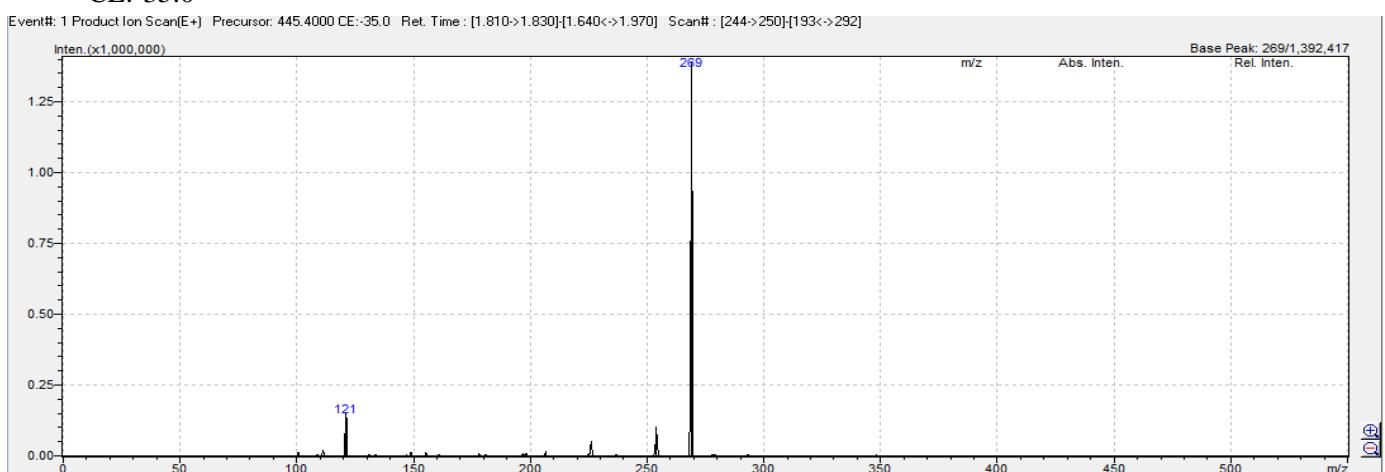
Molecular Formula = C<sub>23</sub>H<sub>24</sub>O<sub>9</sub>  
 Formula Weight = 444.43126  
 Precursor = 445.4000



CE: -15.0



CE:-35.0



CE:-45.0

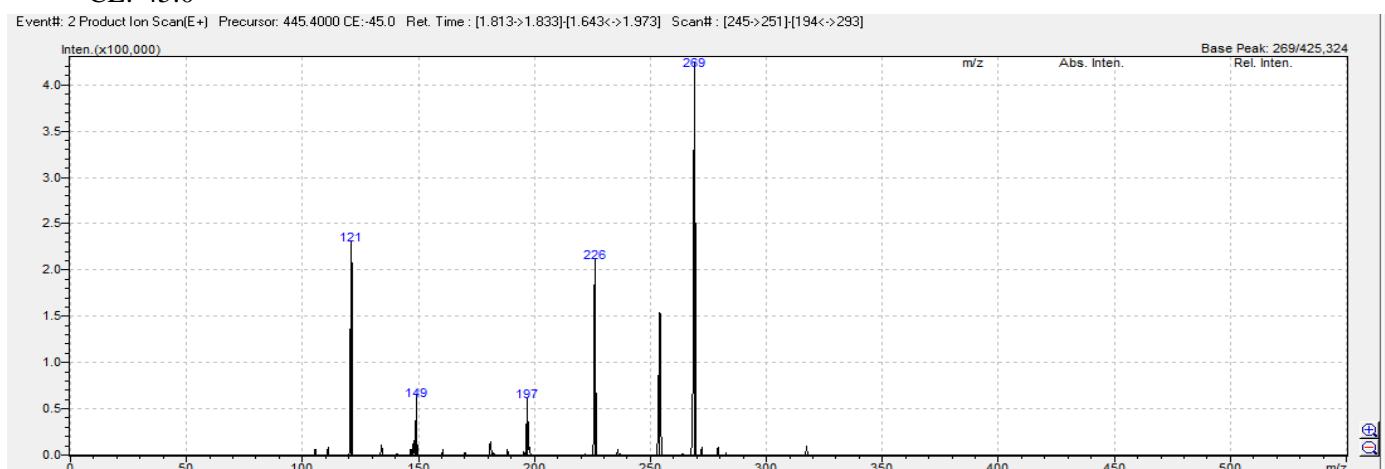


Fig.S62.  $^1\text{H}$  NMR spectral of 5'-methoxyflavone 2'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**15**) (DMSO- $d_6$ , 600 MHz)

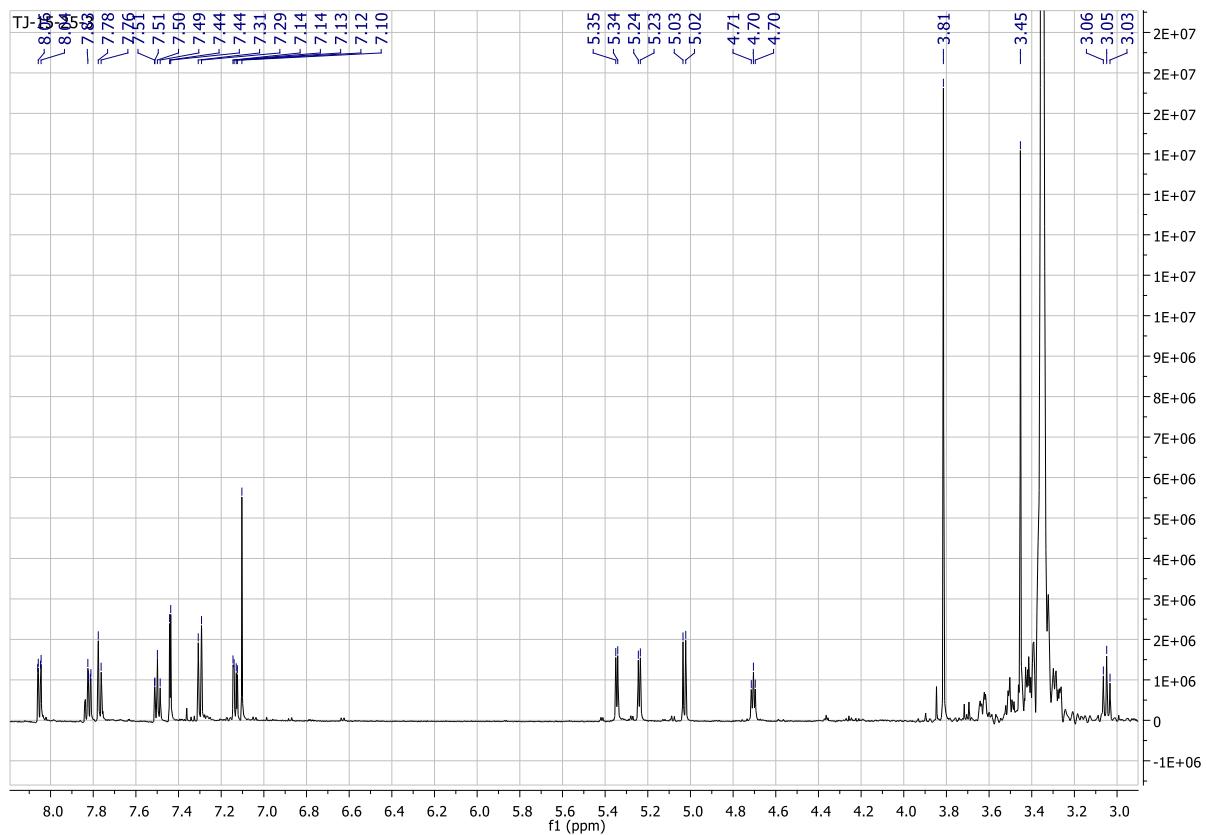


Fig.S63. Flavone part of the  $^1\text{H}$  NMR spectral 5'-methoxyflavone 2'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**15**) (DMSO- $d_6$ , 600 MHz)

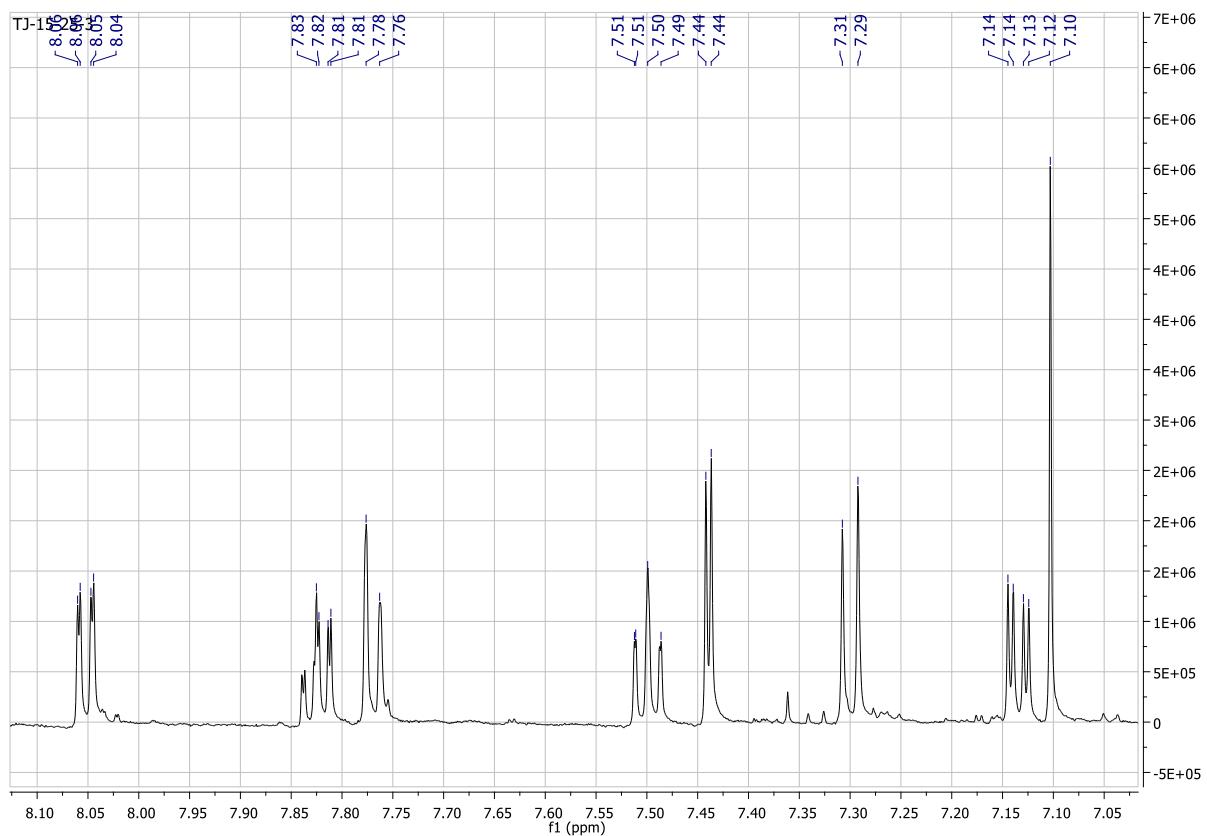


Fig.S64. Glucopyranoside part of the  $^1\text{H}$  NMR spectral  $5'$ -methoxyflavone  $2'$ - $O$ - $\beta$ -D-( $4''$ - $O$ -methyl)-glucopyranoside (**15**) (DMSO- $d_6$ , 600 MHz)

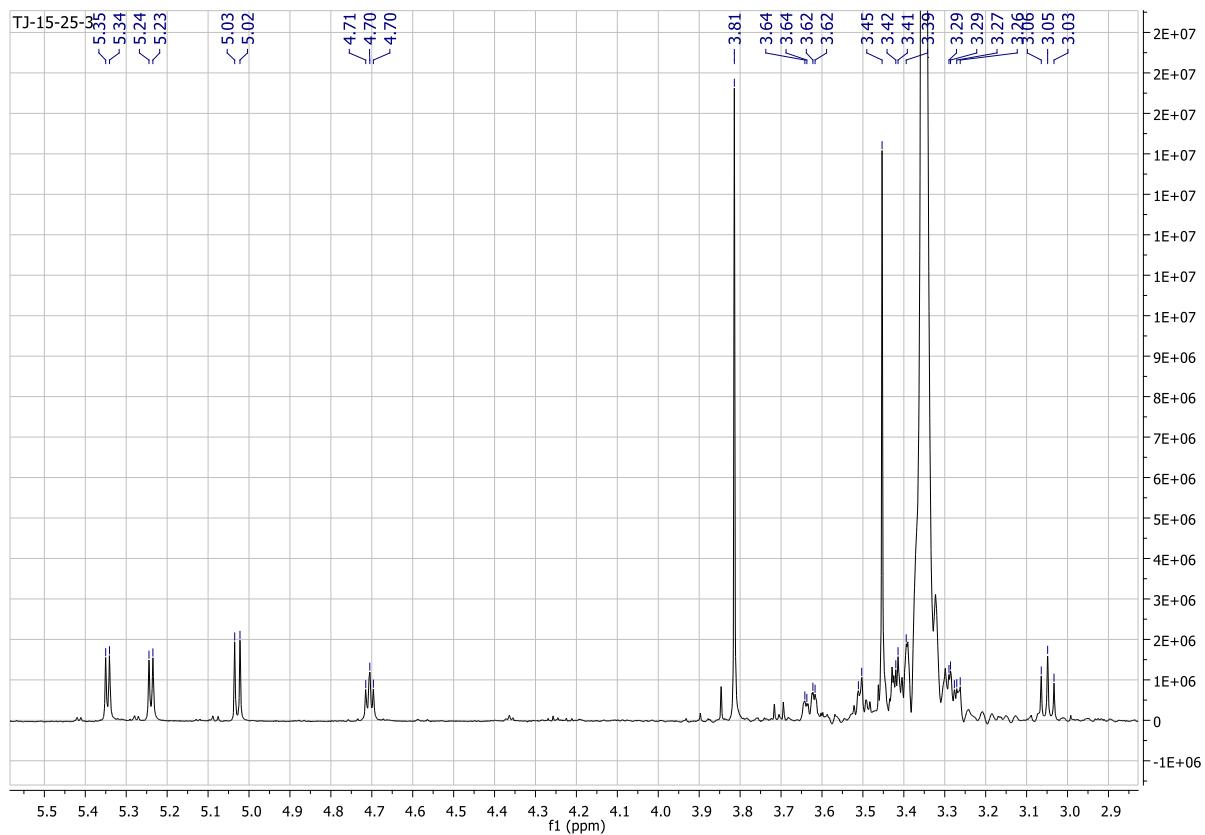


Fig.S65.  $^{13}\text{C}$  NMR spectral of  $5'$ -methoxyflavone  $2'$ - $O$ - $\beta$ -D-( $4''$ - $O$ -methyl)-glucopyranoside (**15**) (DMSO- $d_6$ , 151 MHz)

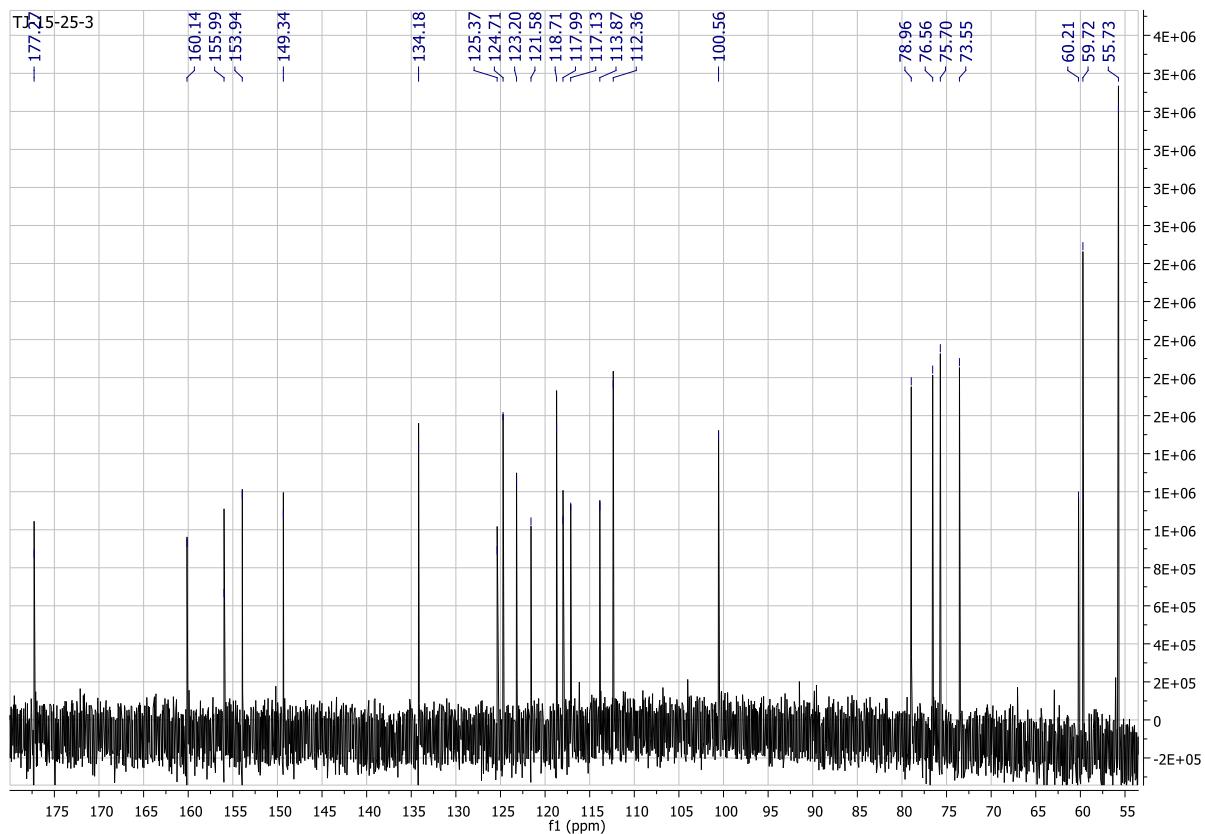


Fig.S66. COSY spectral of 5'-methoxyflavone 2'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**15**) (DMSO- $d_6$ , 151 MHz)

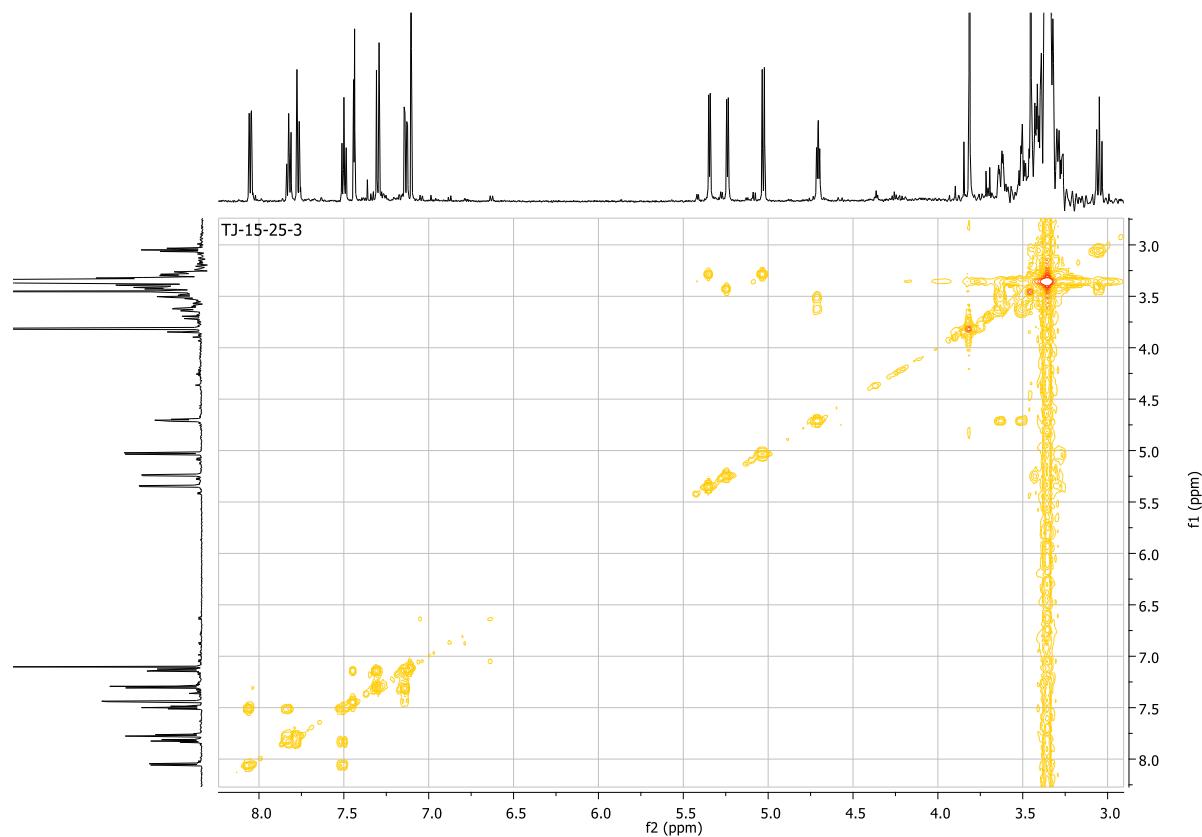


Fig.S67. HMQC spectral of 5'-methoxyflavone 2'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**15**) (DMSO- $d_6$ , 151 MHz)

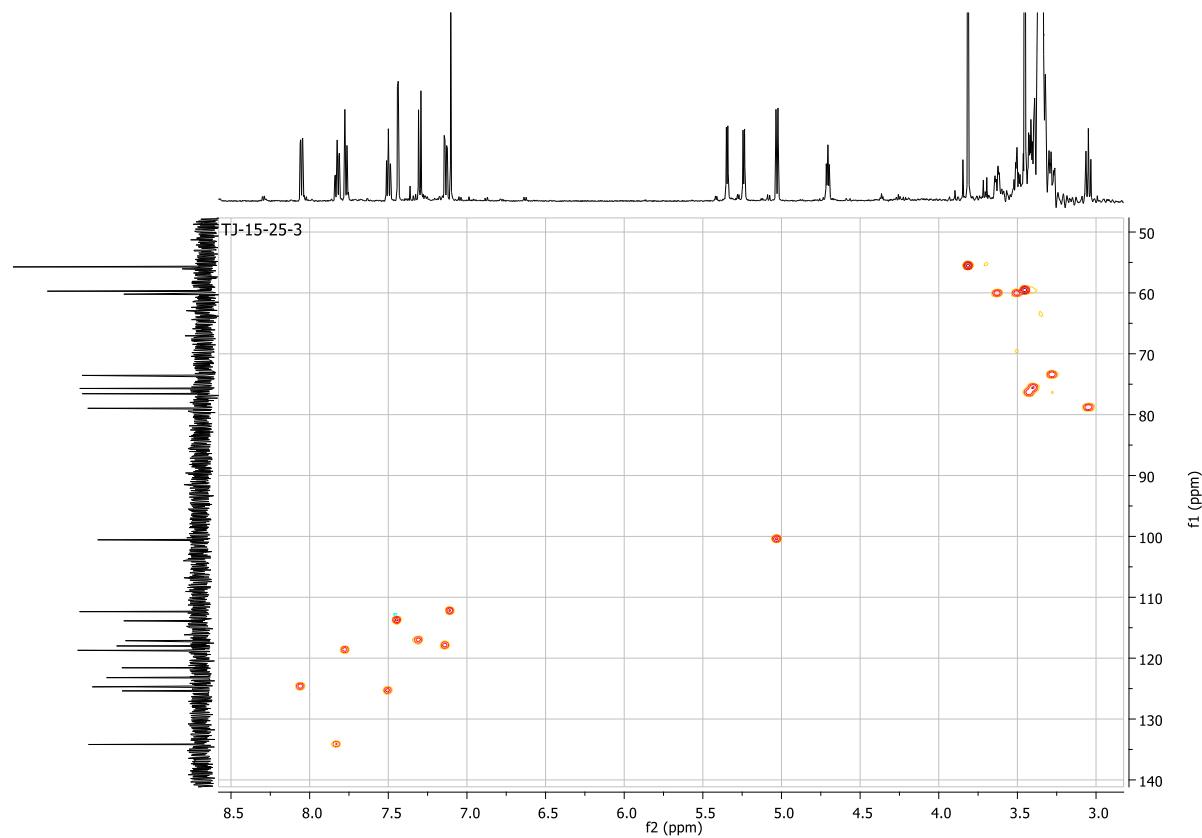


Fig.S68. HMBC spectral of 5'-methoxyflavone 2'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**15**) (DMSO-*d*<sub>6</sub>, 151 MHz)

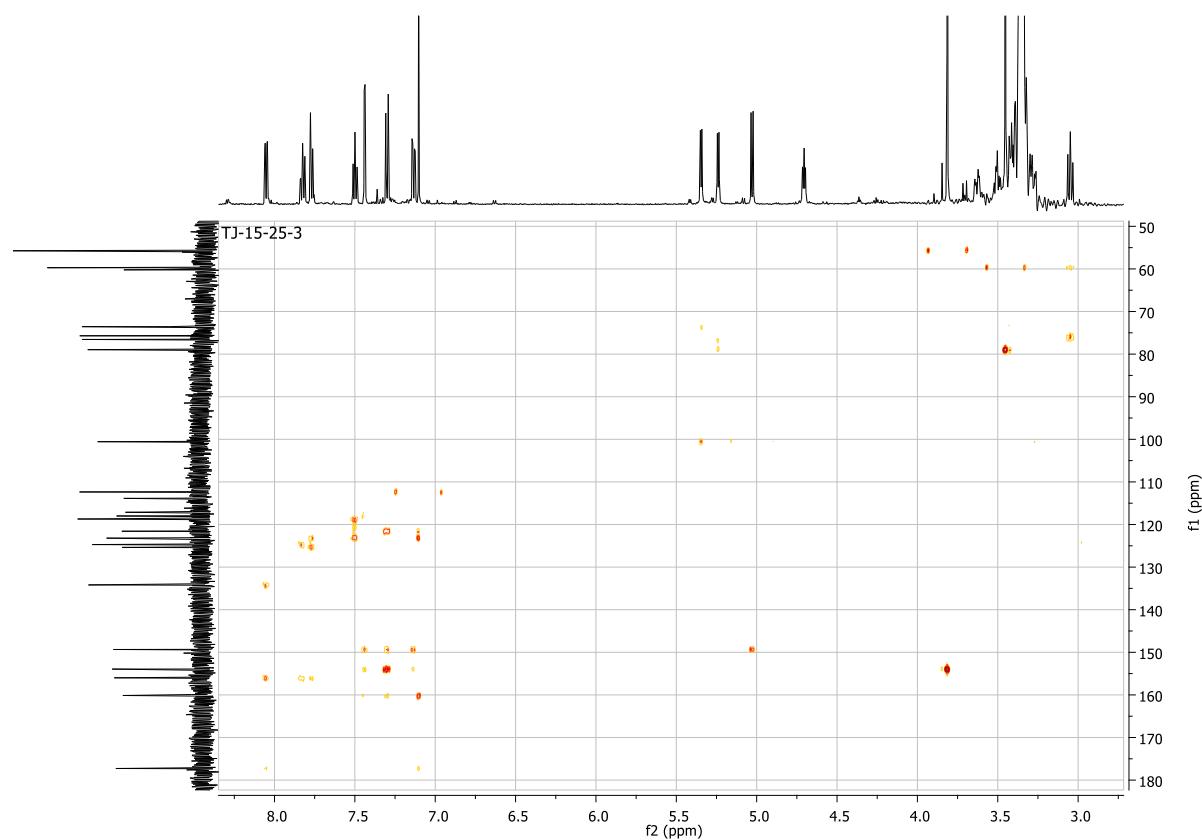
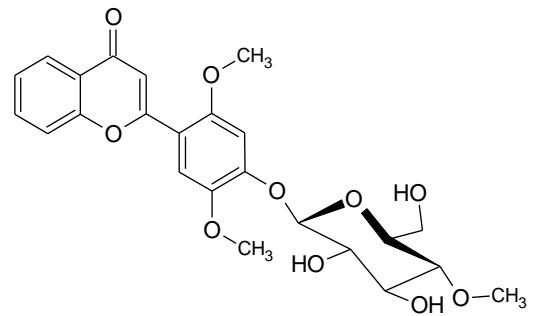


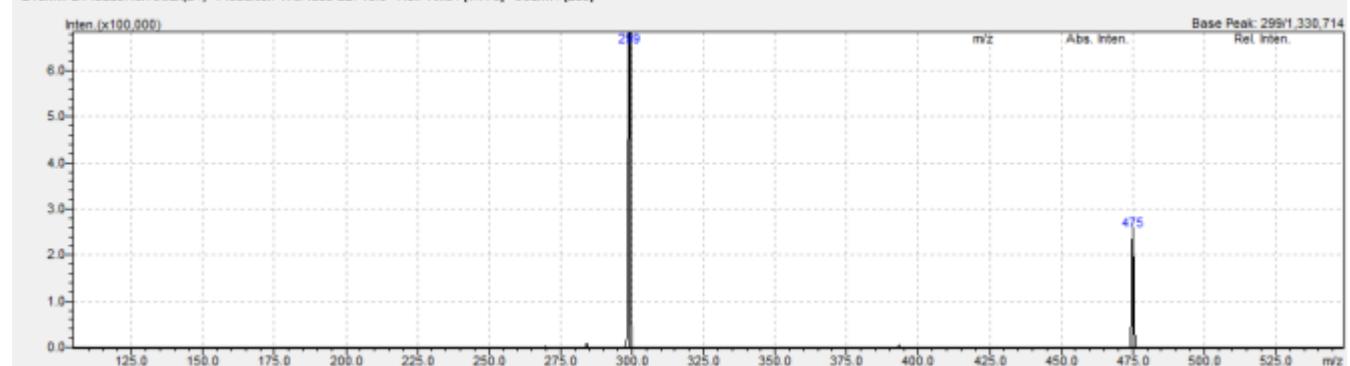
Fig.S69. MS analysis 2',5'-dimethoxyflavone 4'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**16**)

Molecular Formula = C<sub>24</sub>H<sub>26</sub>O<sub>10</sub>  
 Formula Weight = 474.45724  
 Precursor: =475.4000



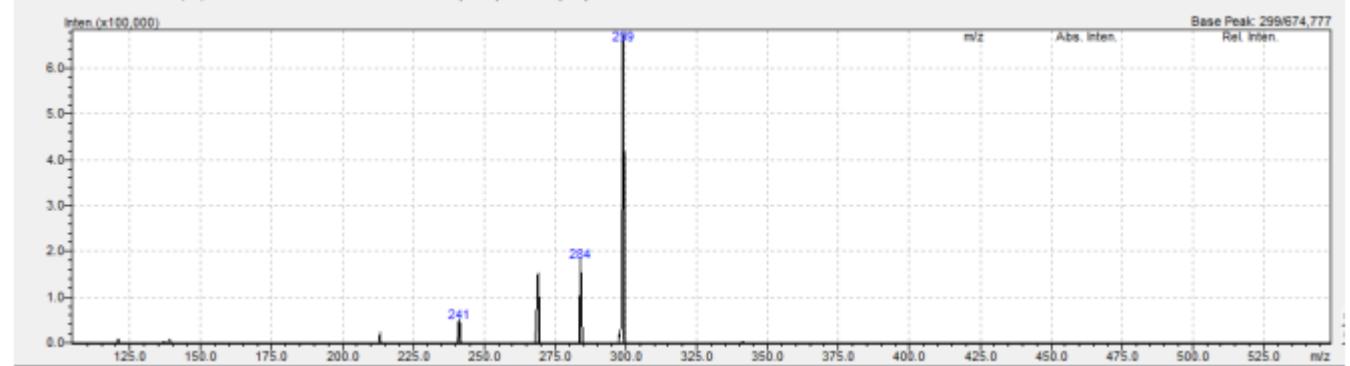
CE: -15

Event#: 2 Product Ion Scan(E+) Precursor: 475.4000 CE:-15.0 Ret. Time : [1.773] Scan#: [233]



CE:-35

Event#: 3 Product Ion Scan(E+) Precursor: 475.4000 CE:-35.0 Ret. Time : [1.777] Scan#: [234]



CE:-45

Event#: 1 Product Ion Scan(E+) Precursor: 475.4000 CE:-45.0 Ret. Time : [1.760] Scan#: [229]

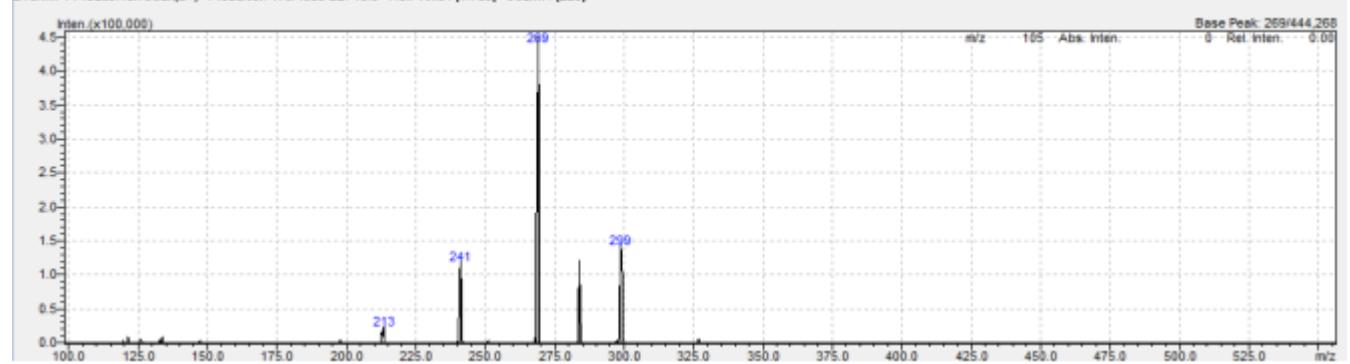


Fig.S70.  $^1\text{H}$  NMR spectral of 2',5'-dimethoxyflavone 4'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**16**) (DMSO- $d_6$ , 600 MHz)

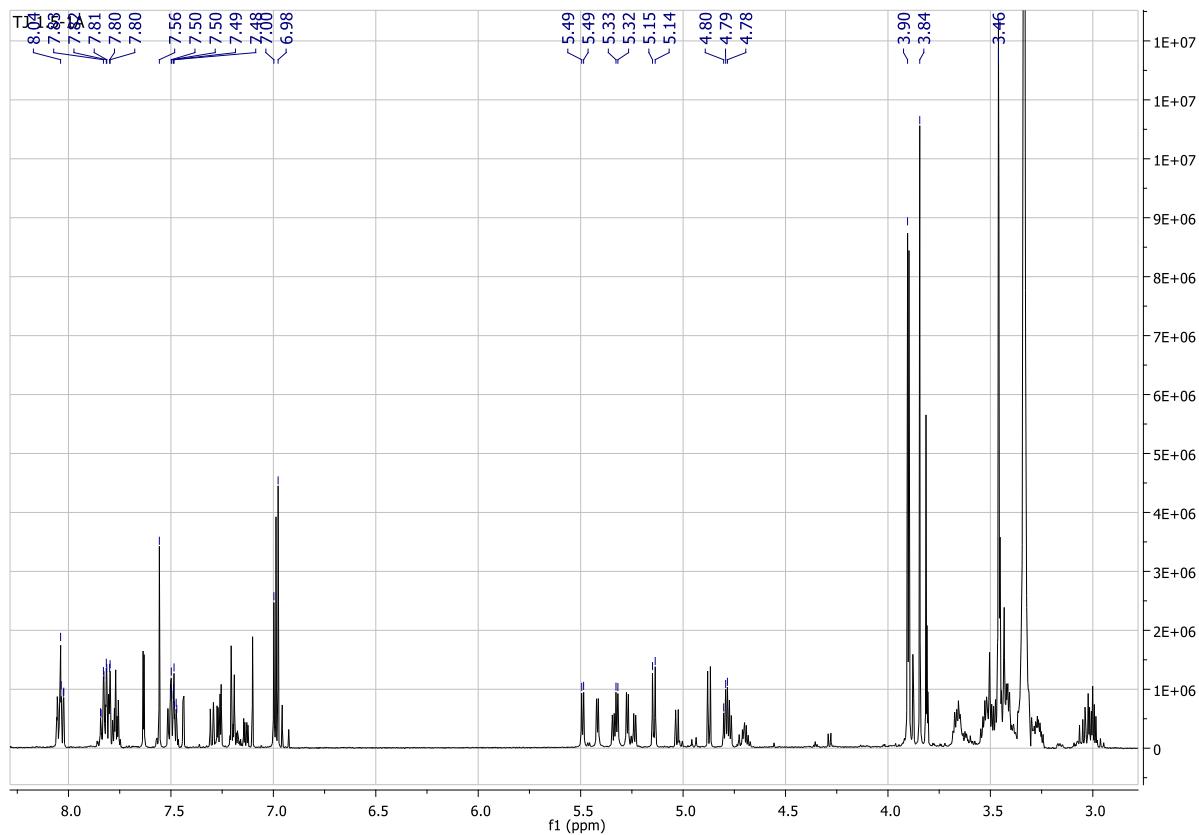


Fig.S71. Flavone part of the  $^1\text{H}$  NMR spectral 2',5'-dimethoxyflavone 4'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**16**) (DMSO- $d_6$ , 600 MHz)

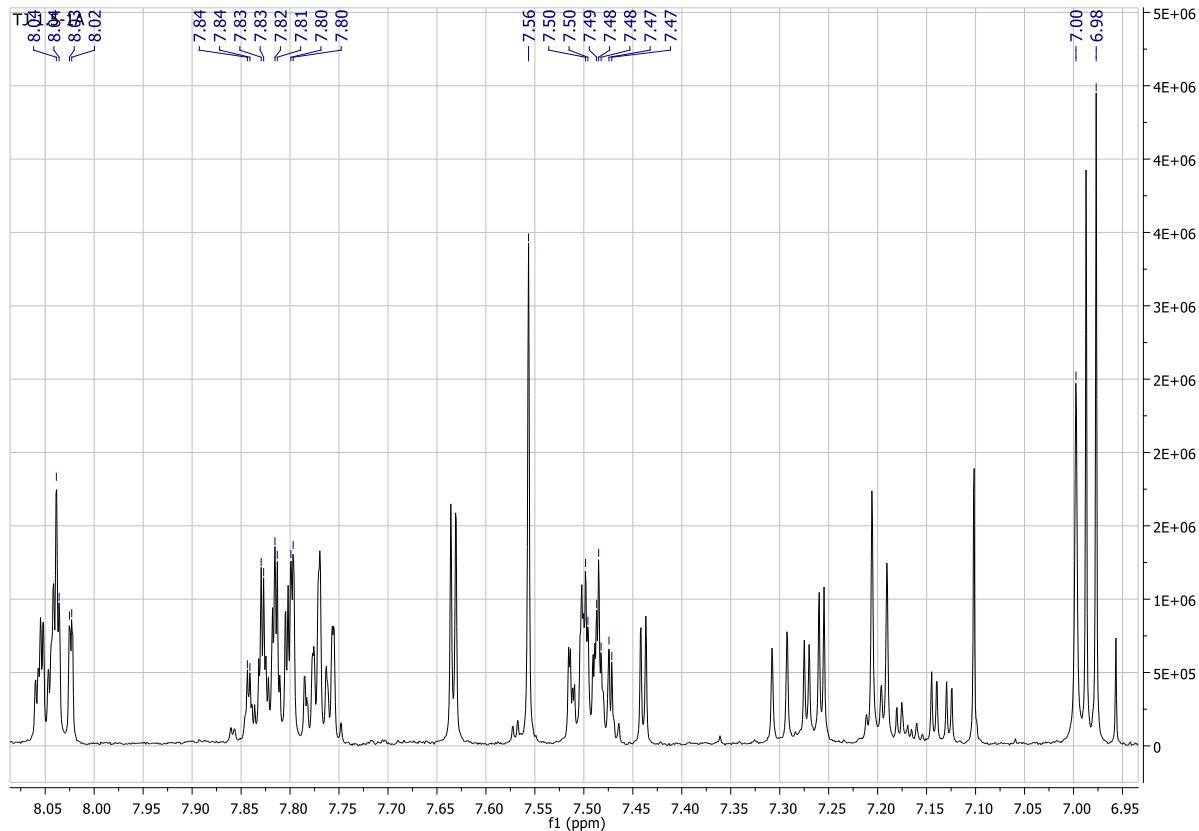


Fig.S72. Glucopyranoside part of the  $^1\text{H}$  NMR spectral  $2',5'$ -dimethoxyflavone  $4'-O$ - $\beta$ -D-( $4''$ -O-methyl)-glucopyranoside (**16**) (DMSO- $d_6$ , 600 MHz)

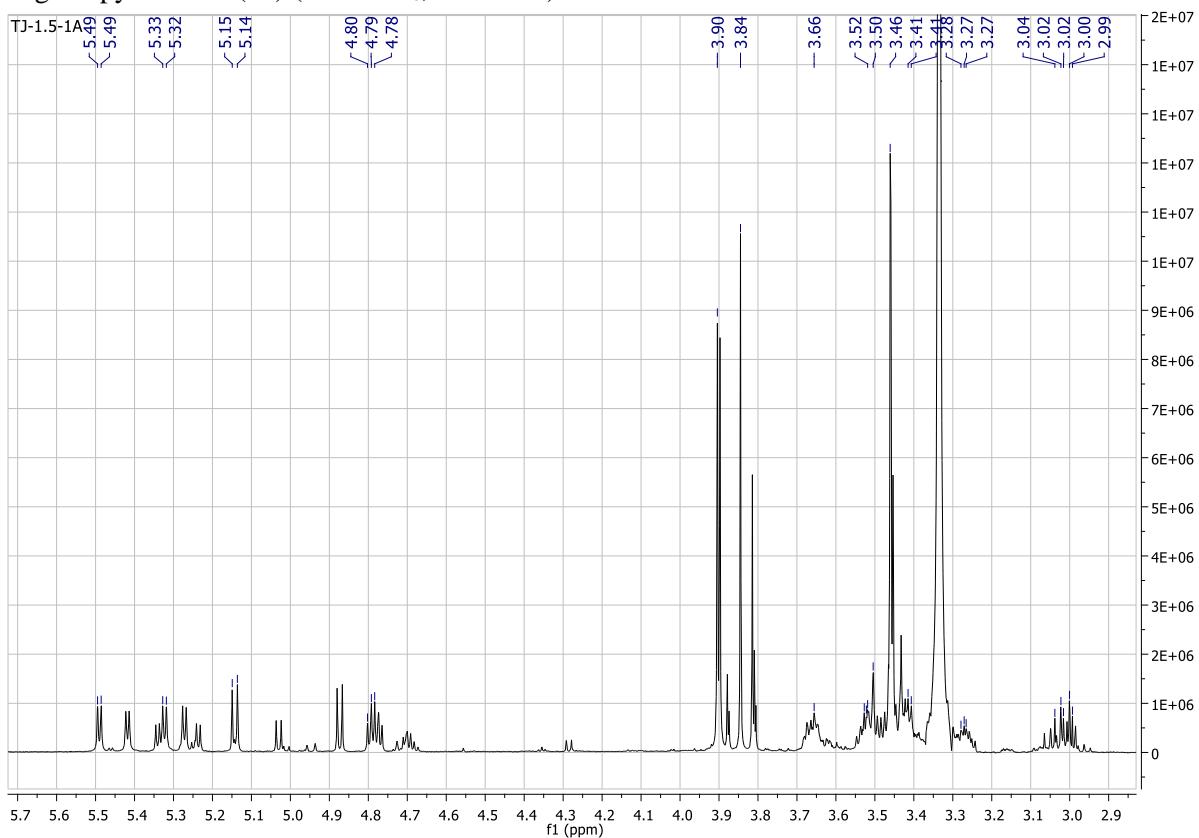


Fig.S73.  $^{13}\text{C}$  NMR spectral of  $2',5'$ -dimethoxyflavone  $4'-O$ - $\beta$ -D-( $4''$ -O-methyl)-glucopyranoside (**16**) (DMSO- $d_6$ , 151 MHz)

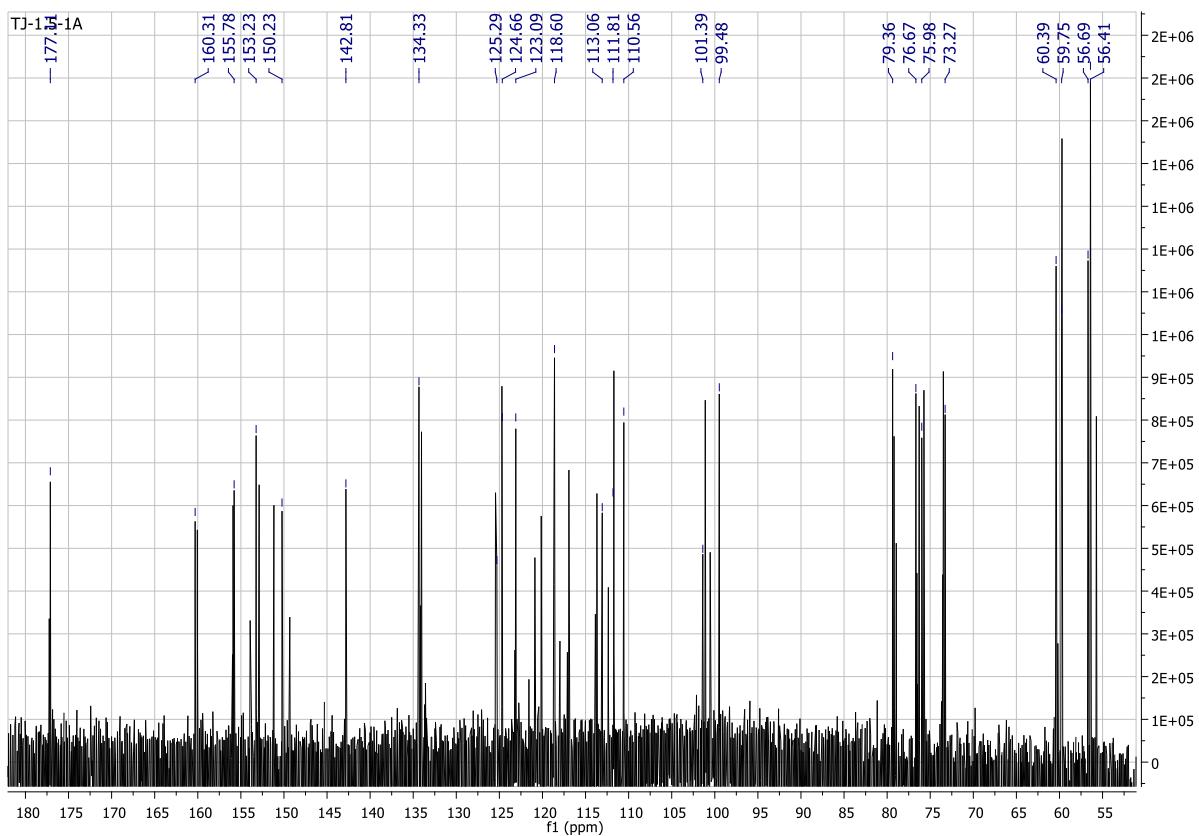


Fig.S74. COSY spectral of 2',5'-dimethoxyflavone 4'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**16**) (DMSO- $d_6$ , 151 MHz)

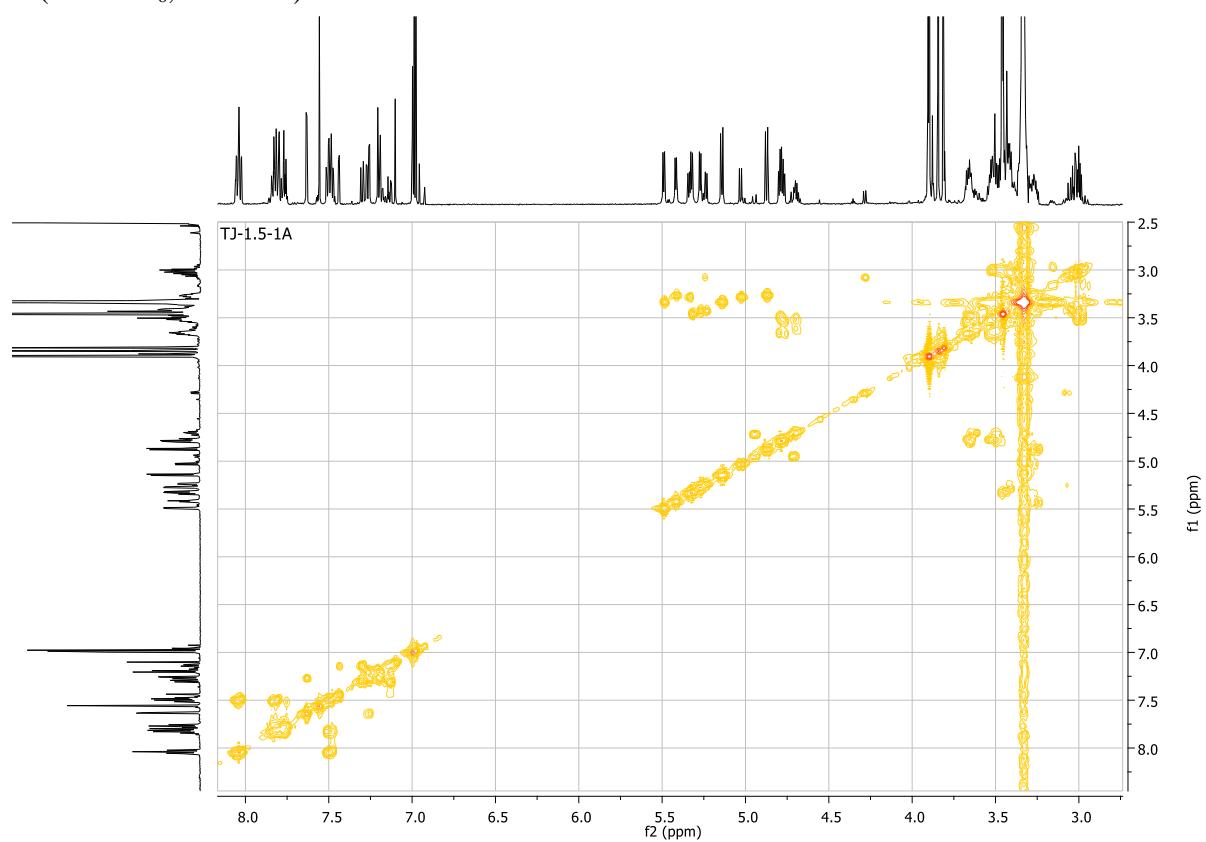


Fig.S75. HMQC spectral of 2',5'-dimethoxyflavone 4'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**16**) (DMSO- $d_6$ , 151 MHz)

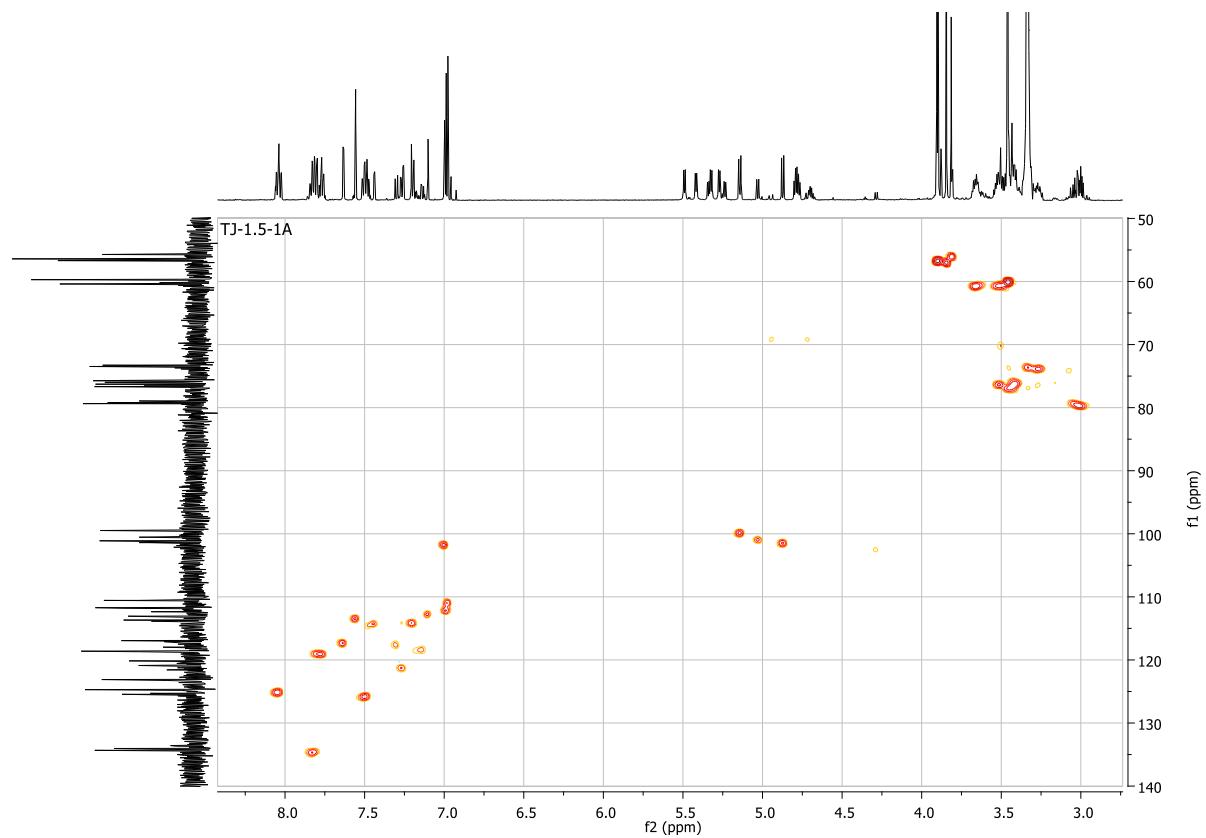


Fig.S76. HMBC spectral of 2',5'-dimethoxyflavone 4'-*O*-β-D-(4"-*O*-methyl)-glucopyranoside (**16**) (DMSO-*d*<sub>6</sub>, 151 MHz)

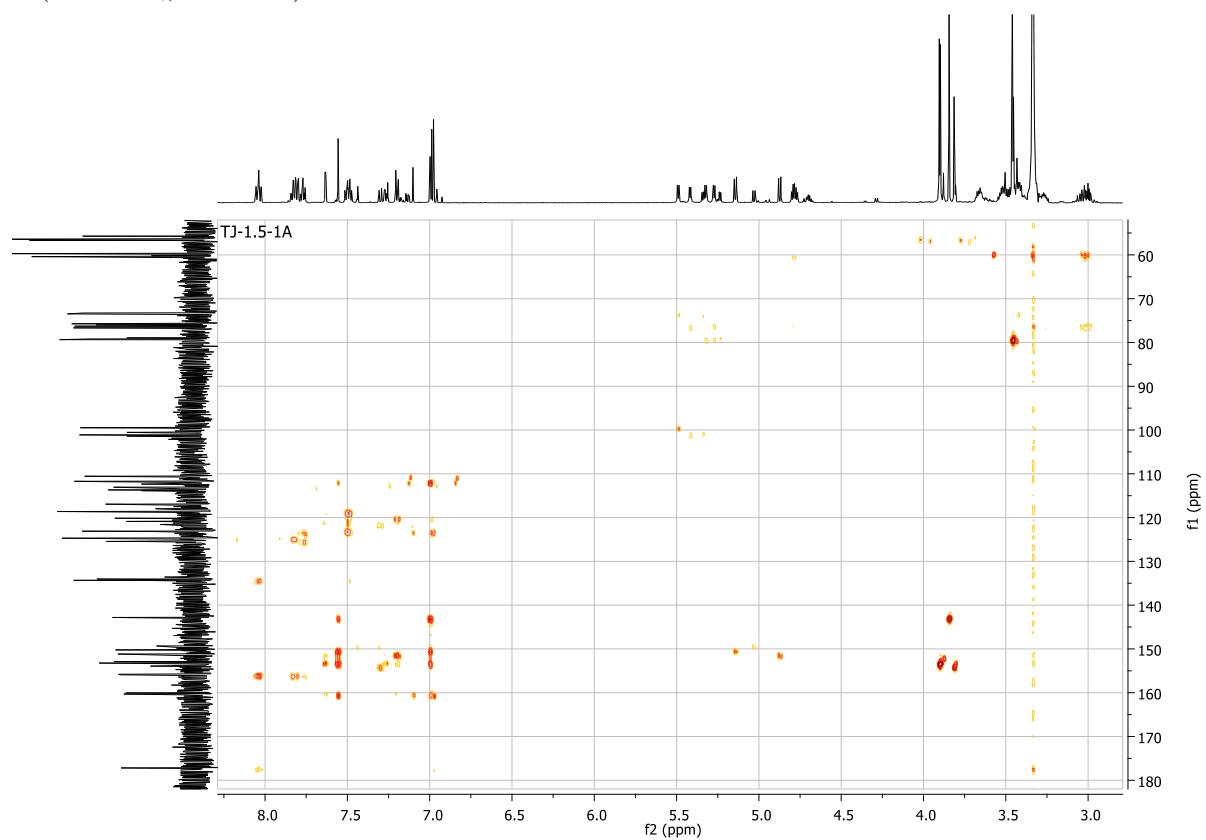
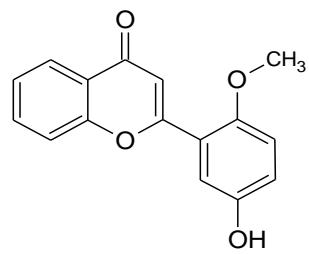


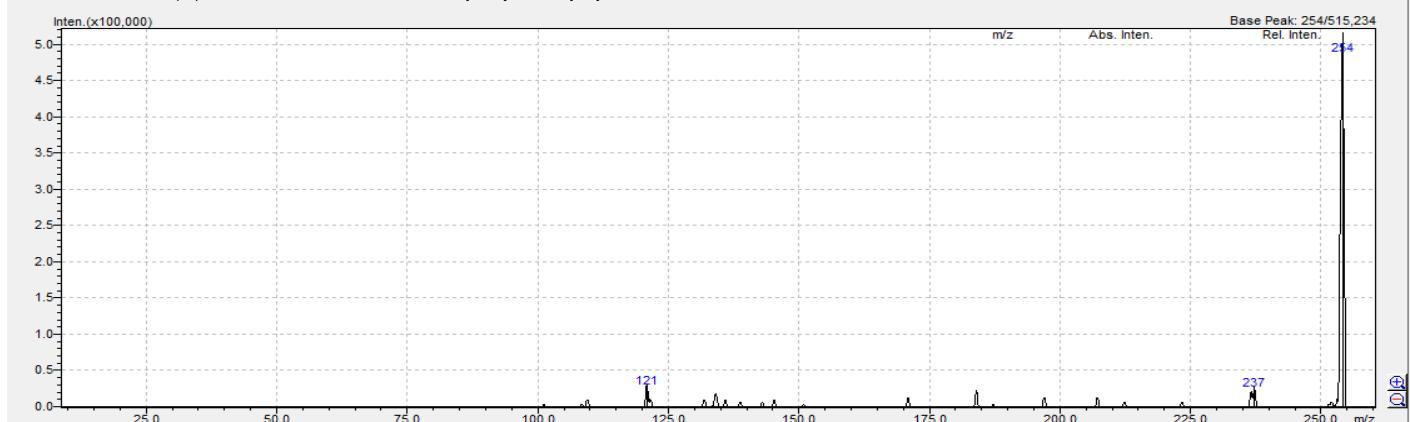
Fig.S77. MS analysis 5'-hydroxy-2'-methoxyflavone (**17**)



Molecular Formula: C<sub>16</sub>H<sub>12</sub>O<sub>4</sub>  
 Formula Weight: 268.26408  
 Precursor: 269.2000

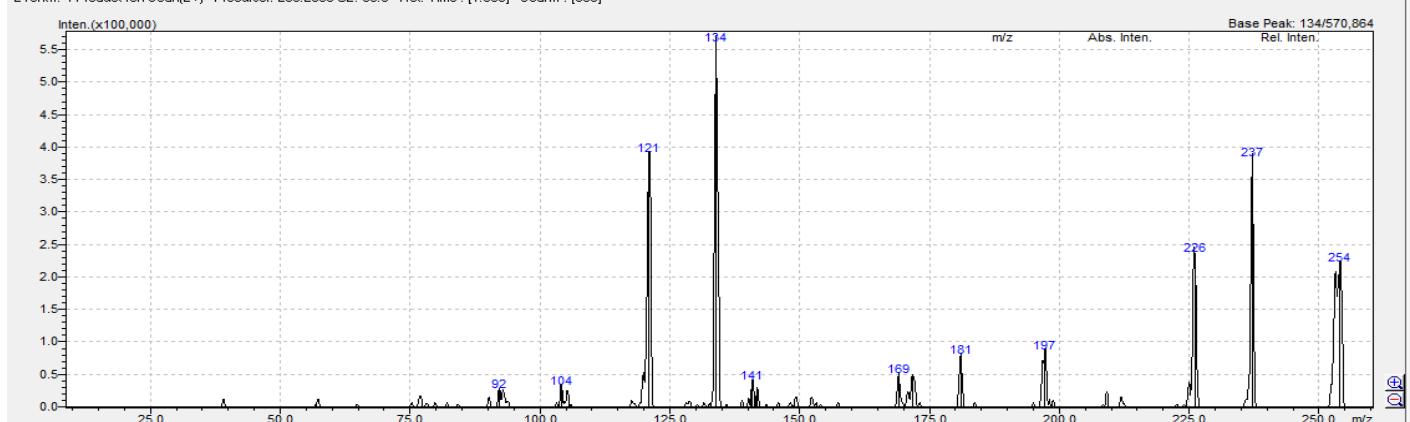
CE: -15.0

Event#: 8 Product Ion Scan(E+) Precursor: 269.2000 CE:-15.0 Ret. Time : [2.003] Scan#: [602]



CE:-35.0

Event#: 4 Product Ion Scan(E+) Precursor: 269.2000 CE:-35.0 Ret. Time : [1.990] Scan#: [598]



CE:-45.0

Event#: 2 Product Ion Scan(E+) Precursor: 269.2000 CE:-45.0 Ret. Time : [1.983] Scan#: [596]

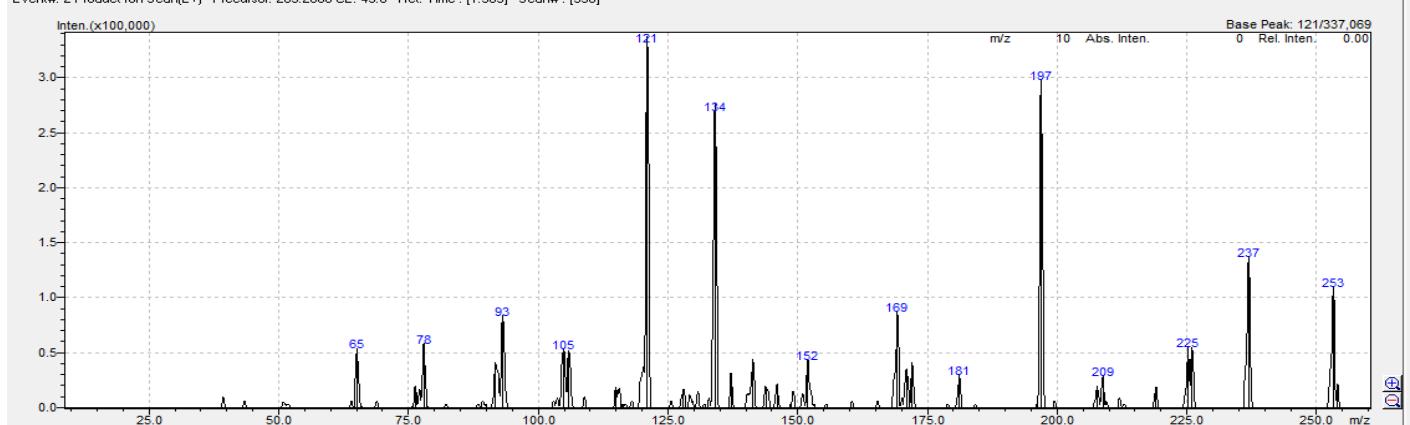


Fig.S78.  $^1\text{H}$  NMR spectral of 5'-hydroxy-2'-methoxyflavone (**17**) (DMSO- $d_6$ , 600 MHz)

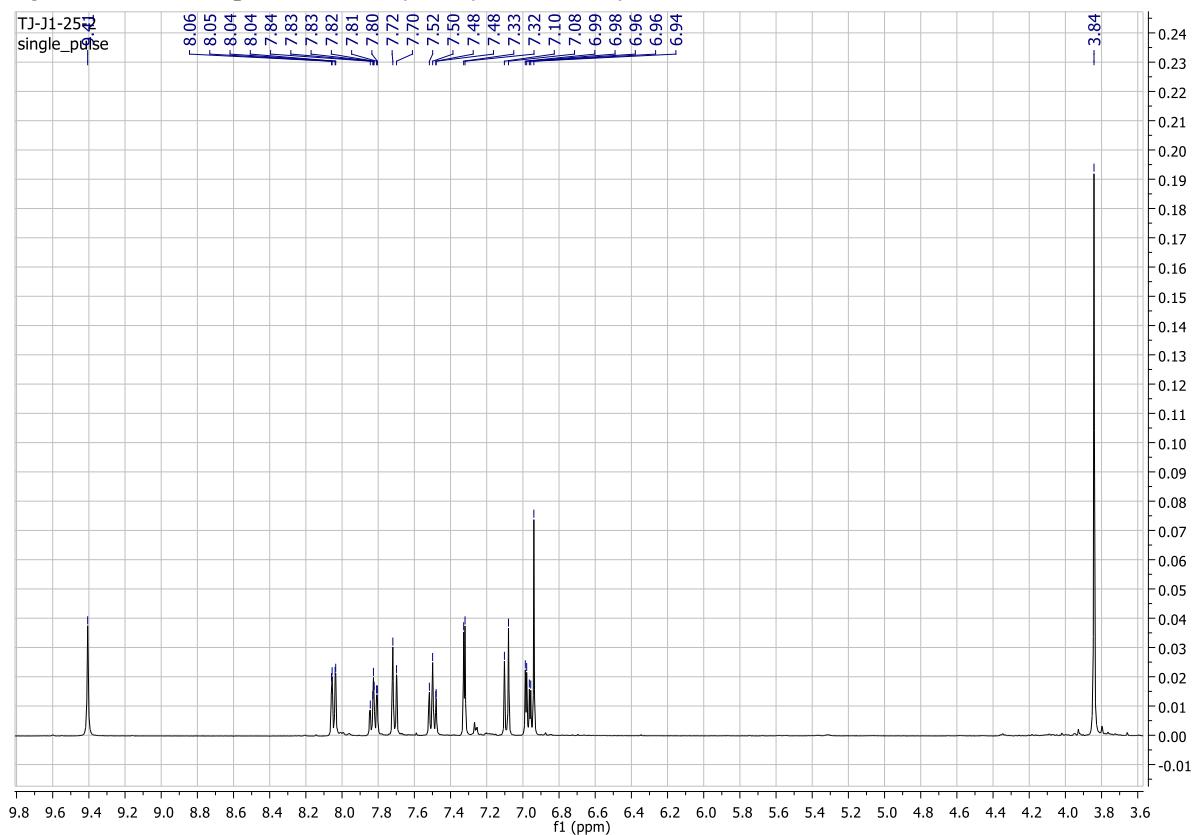


Fig.S79.  $^{13}\text{C}$  NMR spectral of 5'-hydroxy-2'-methoxyflavone (**17**) (DMSO- $d_6$ , 151 MHz)

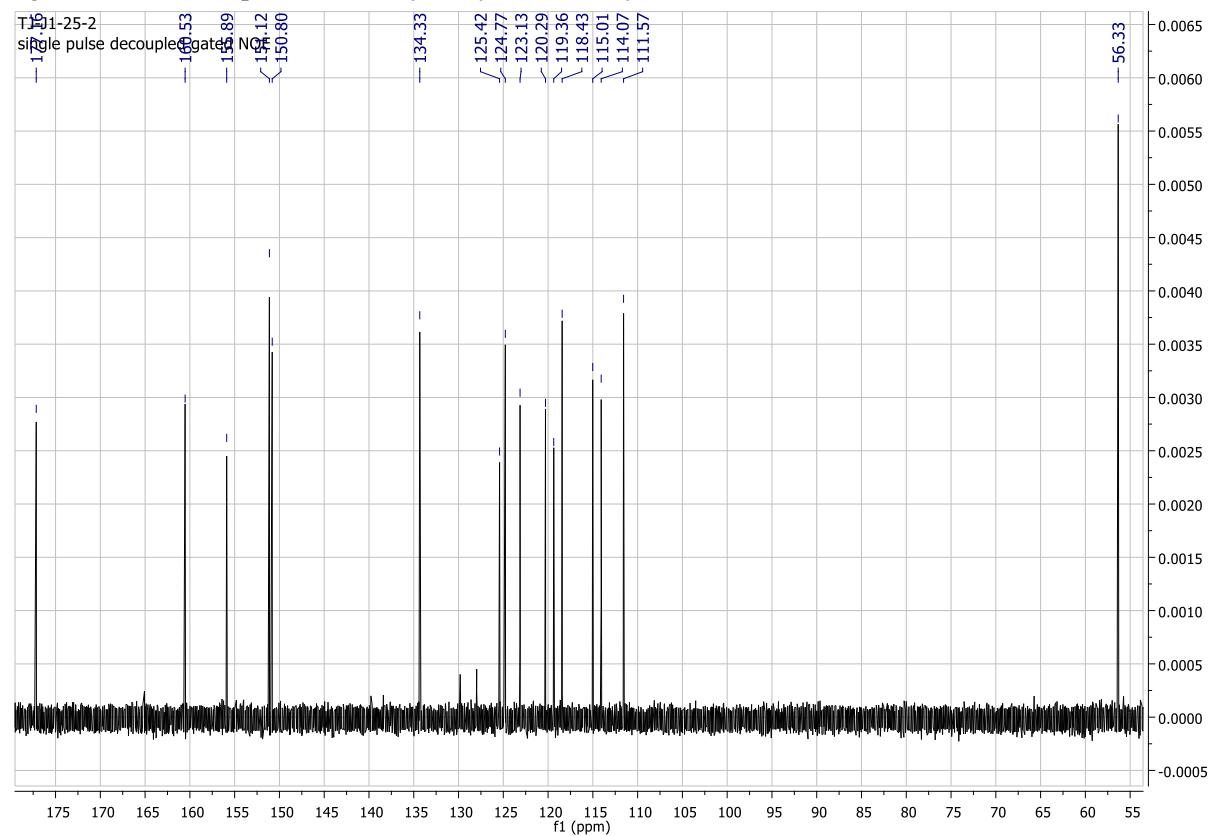


Fig.S80. COSY spectral of 5'-hydroxy-2'-methoxyflavone (**17**) (DMSO-*d*<sub>6</sub>, 151 MHz)

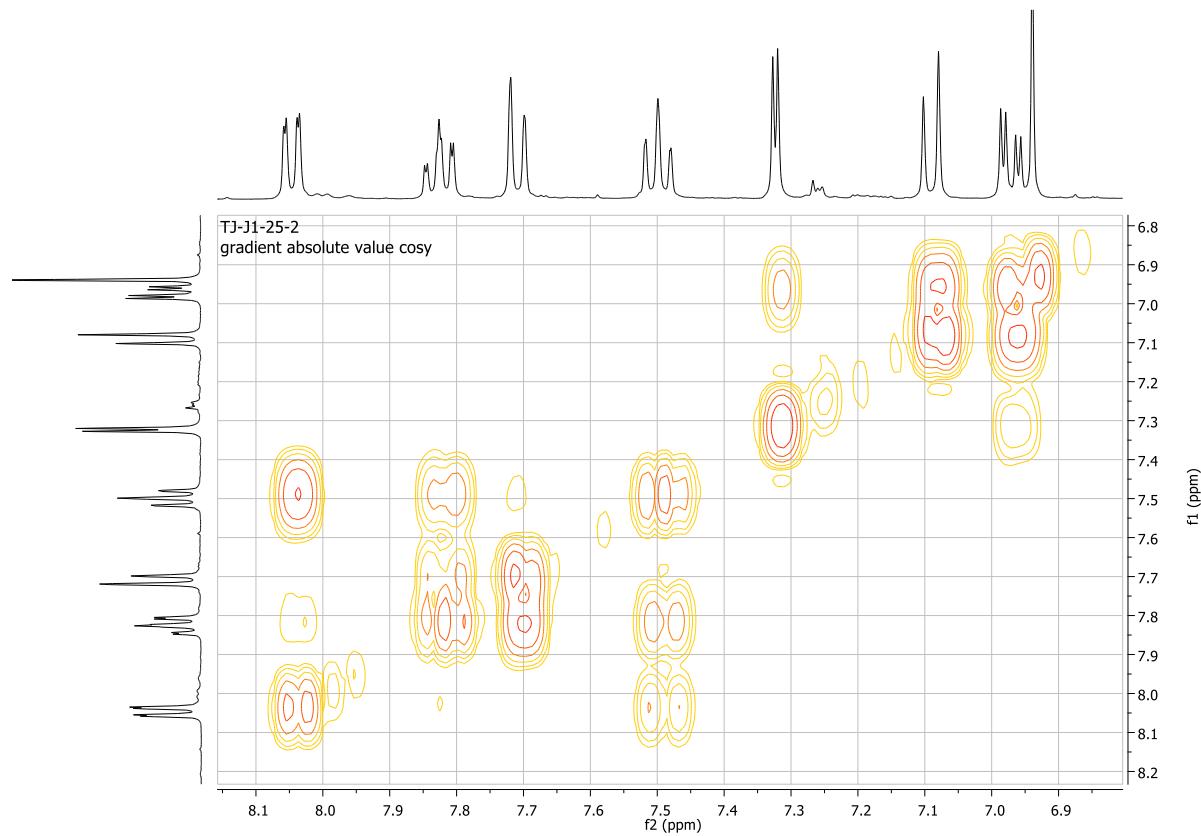


Fig.S81. HMQC spectral of 5'-hydroxy-2'-methoxyflavone (**17**) (DMSO-*d*<sub>6</sub>, 151 MHz)

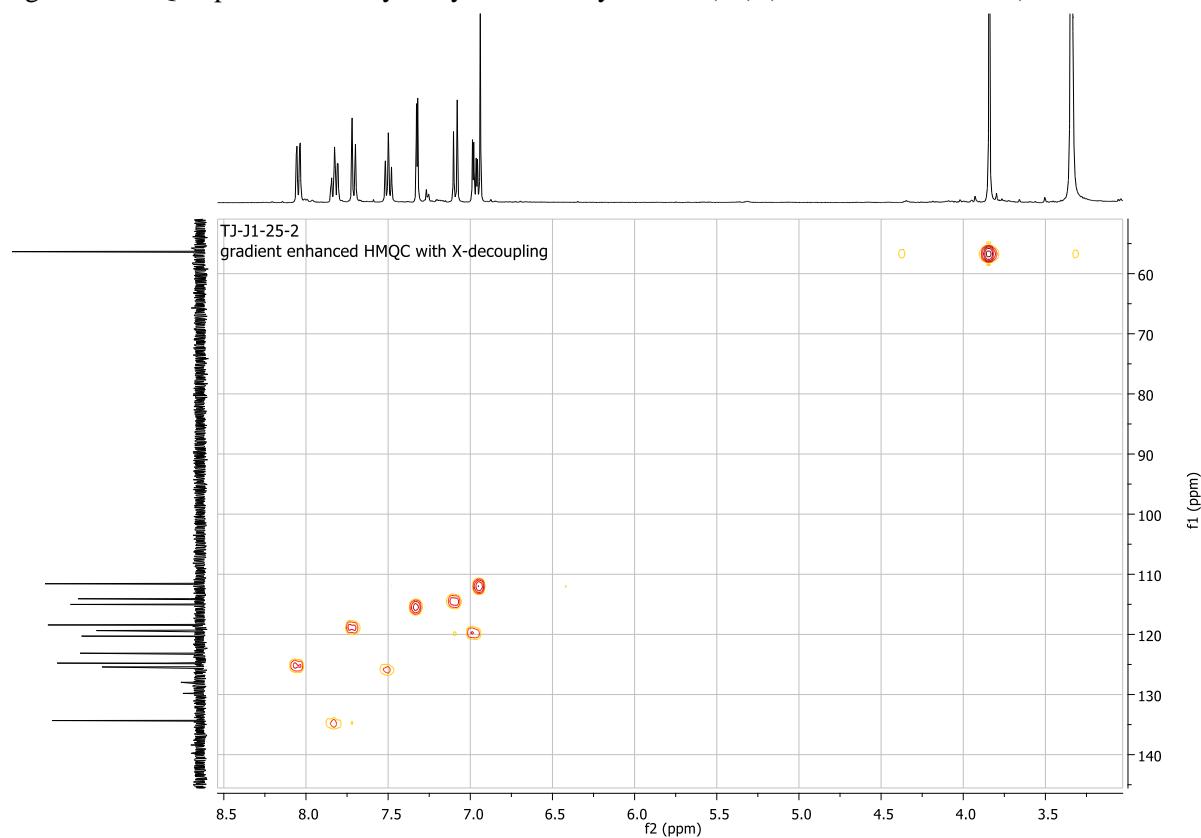


Fig.S82. HMBC spectral of 5'-hydroxy-2'-methoxyflavone (**17**) (DMSO-*d*<sub>6</sub>, 151 MHz)

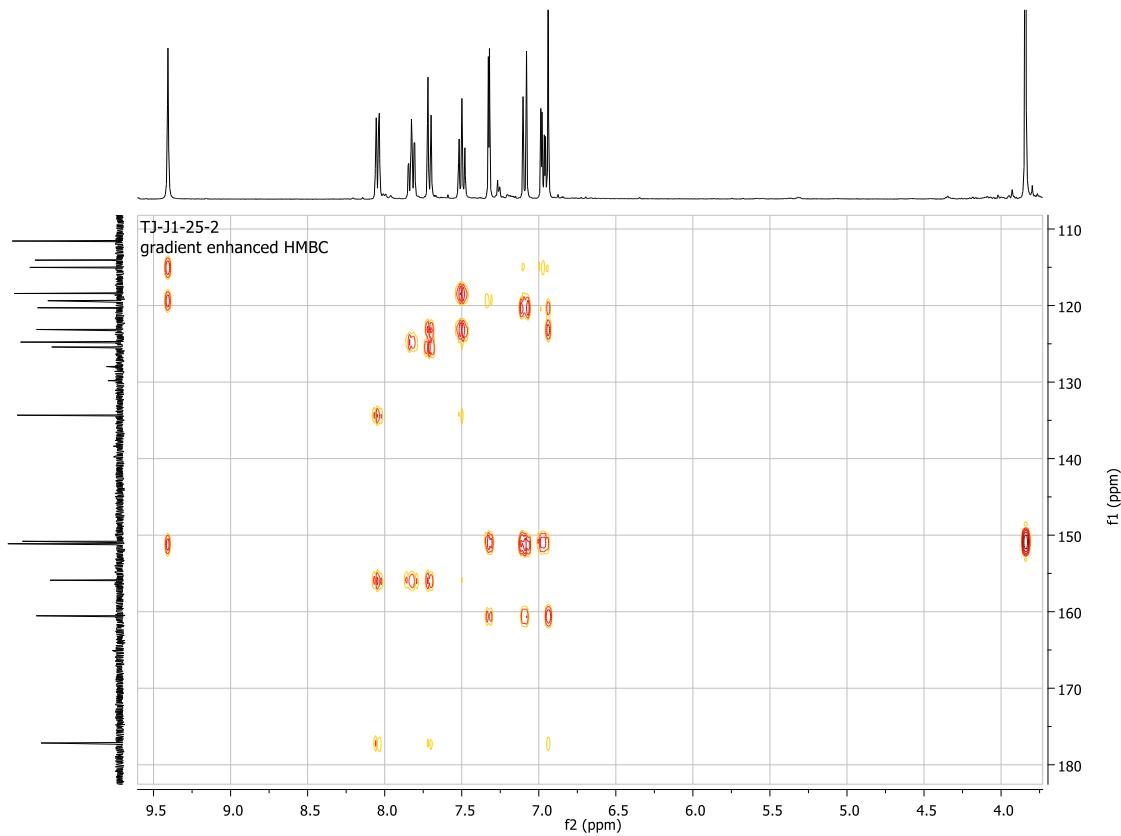
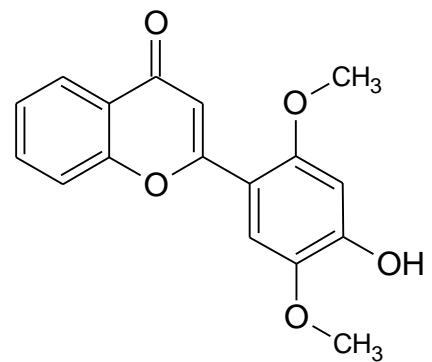


Fig.S83. MS analysis 4'-hydroxy-2',5'-dimethoxyflavone (**18**)

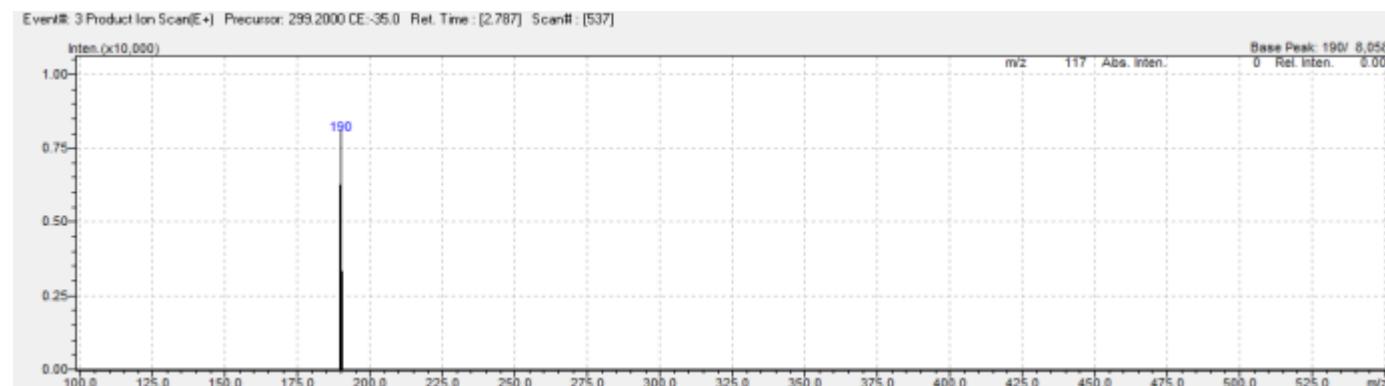


Molecular Formula = C<sub>17</sub>H<sub>14</sub>O<sub>5</sub>  
 Formula Weight = 298.29006  
 Precursor: = 299.2000

CE: -15



CE:-35



CE:-45



Fig.S84.  $^1\text{H}$  NMR spectral of 5'-hydroxy-2'-methoxyflavone (**17**) and 4'-hydroxy-2',5'-dimethoxyflavone (**18**) ( $\text{DMSO}-d_6$ , 600 MHz)

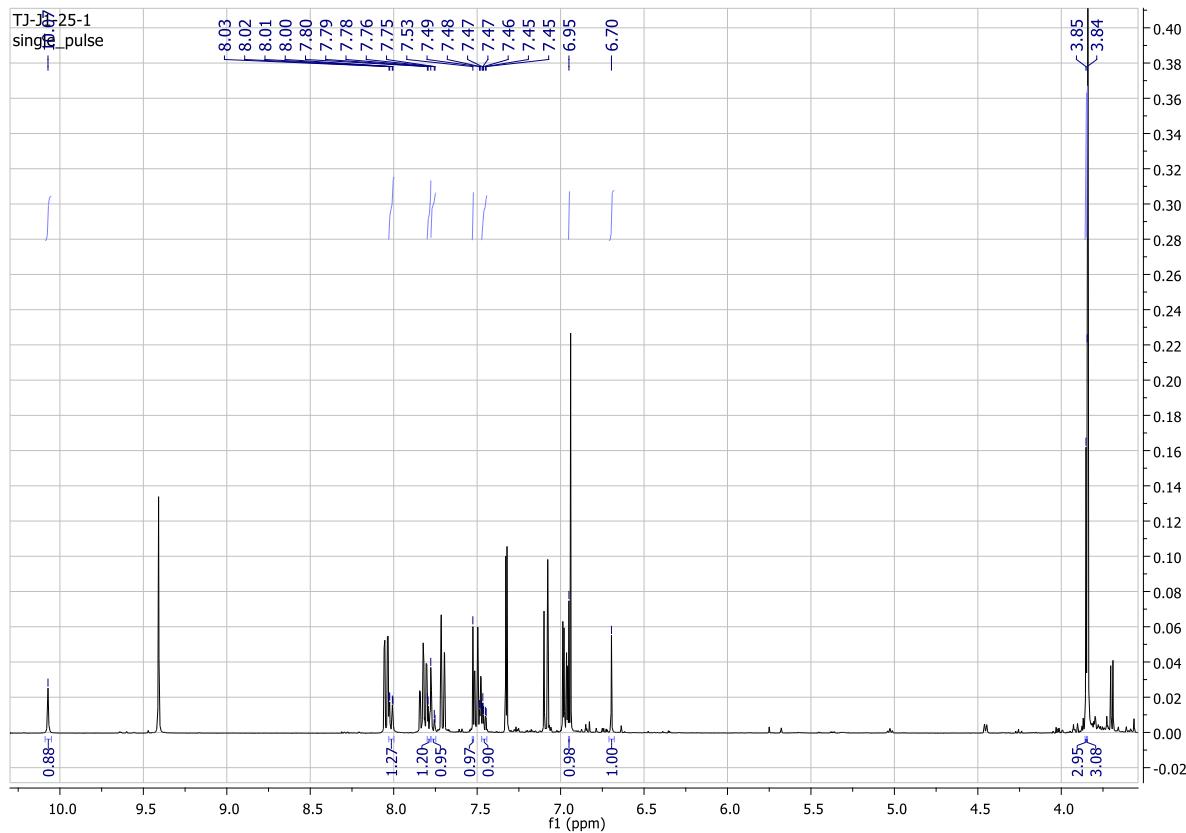


Fig.S85. Part of the  $^1\text{H}$  NMR spectral 5'-hydroxy-2'-methoxyflavone (**17**) and 4'-hydroxy-2',5'-dimethoxyflavone (**18**) (DMSO- $d_6$ , 600 MHz)

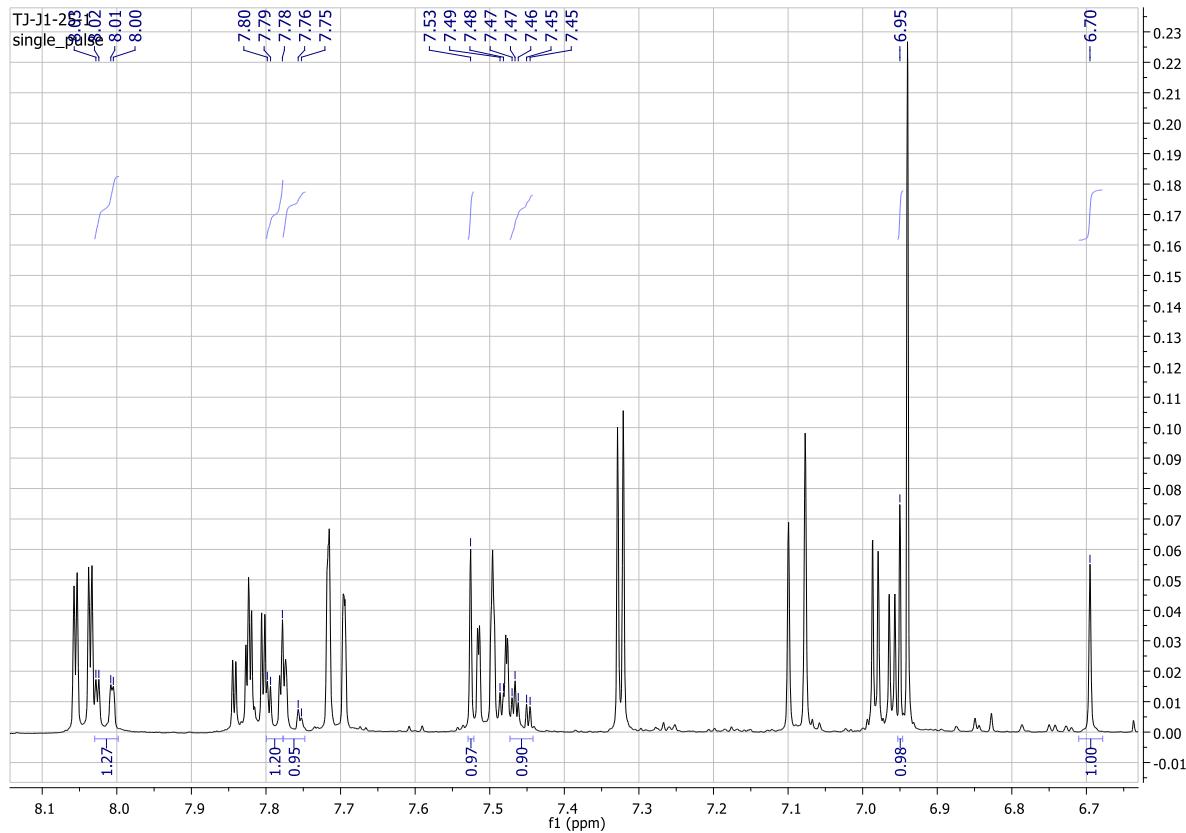


Fig.S86.  $^{13}\text{C}$  NMR spectral of 5'-hydroxy-2'-methoxyflavone (**18**) and 4'-hydroxy-2',5'-dimethoxyflavone (**18**) (DMSO- $d_6$ , 151 MHz)

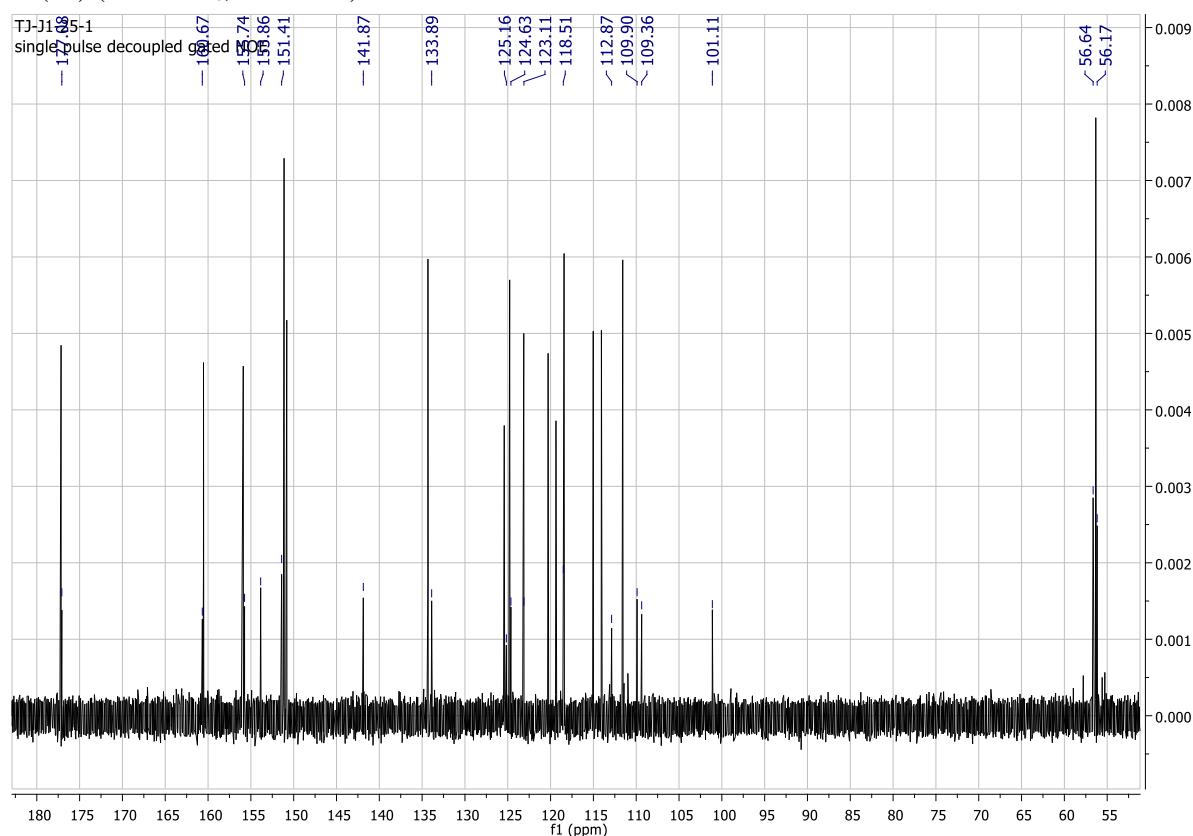


Fig.S87. HMQC spectral of 5'-hydroxy-2'-methoxyflavone (**17**) and 4'-hydroxy-2',5'-dimethoxyflavone (**18**) (DMSO- $d_6$ , 151 MHz)

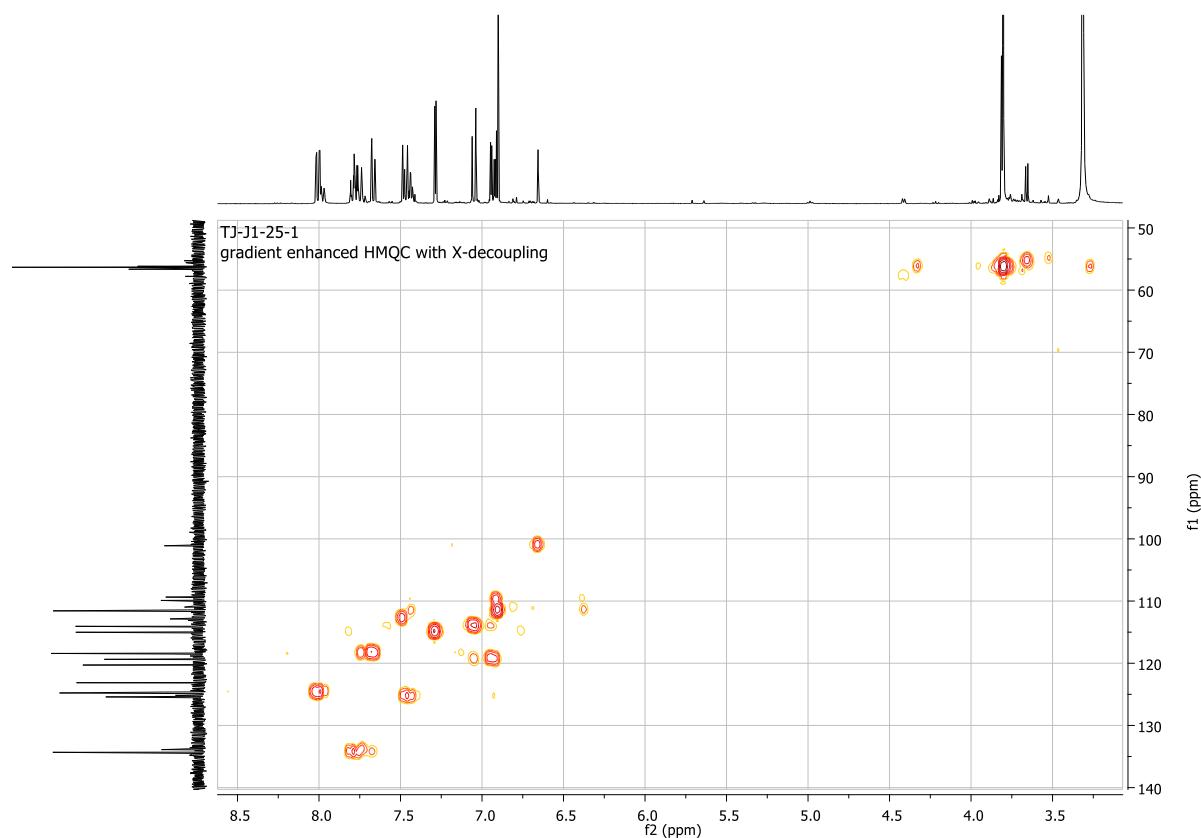


Fig.S88. HMBC spectral of 5'-hydroxy-2'-methoxyflavone (**17**) and 4'-hydroxy-2',5'-dimethoxyflavone (**18**) (DMSO-*d*<sub>6</sub>, 151 MHz)

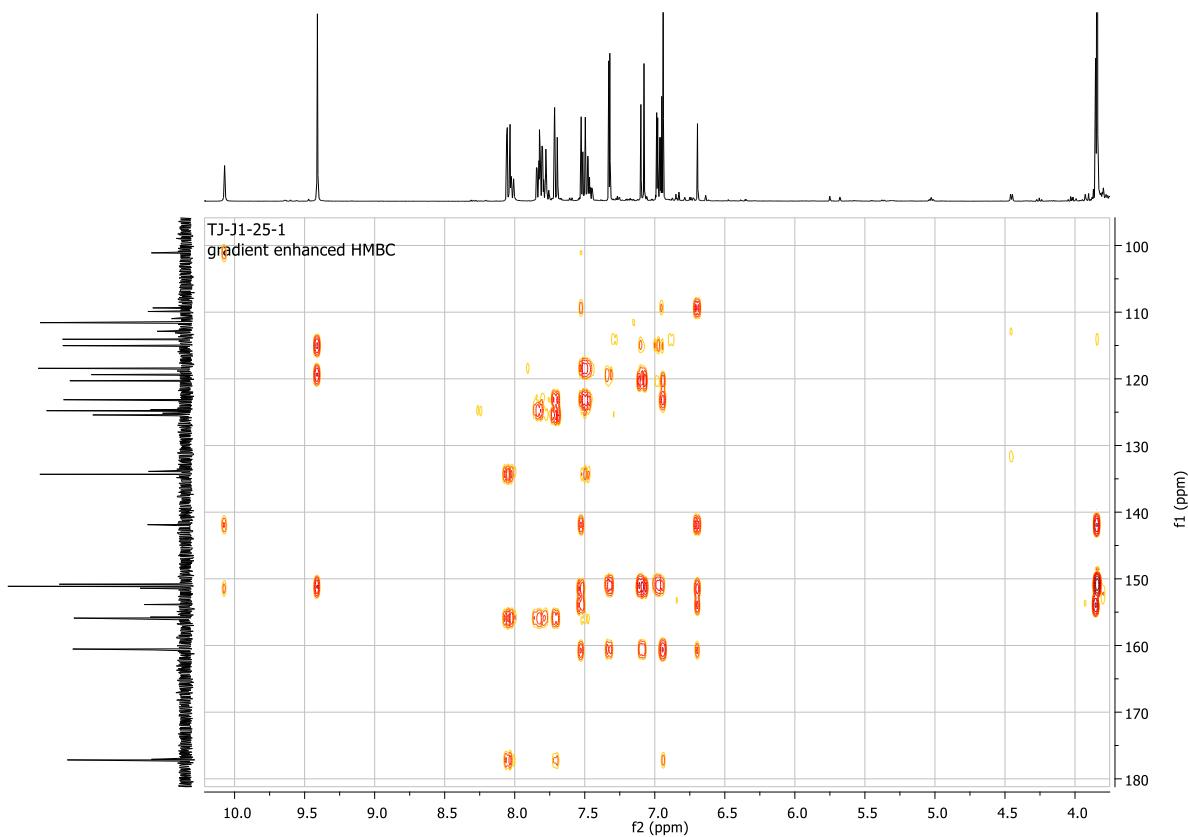
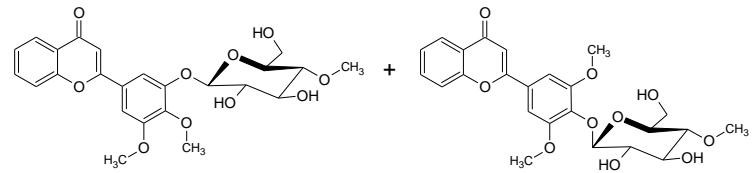


Fig.S89. MS analysis 4',5'-dimethoxyflavone 5'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**19**) and 3',5'-dimethoxyflavone 4'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**20**)

Molecular Formula = C<sub>24</sub>H<sub>26</sub>O<sub>10</sub>  
 Formula Weight = 474.45724  
 Precursor = 475.4000



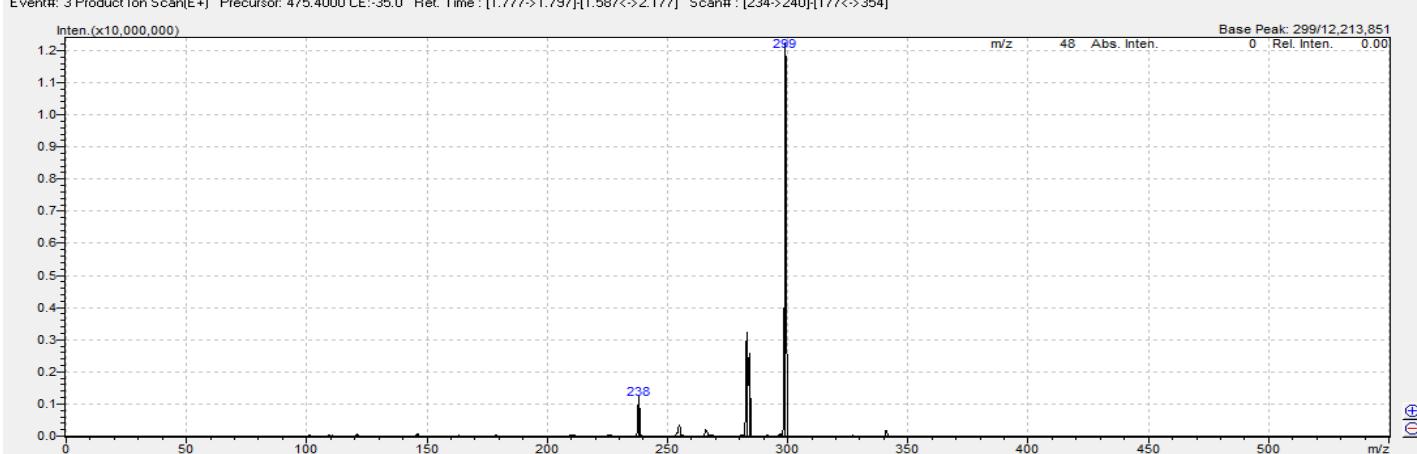
CE: -15.0

Event#: 2 Product Ion Scan(E+) Precursor: 475.4000 CE:-15.0 Ret. Time : [1.773->1.793][1.583->2.173] Scan# : [233->239][176<->353]



CE:-35.0

Event#: 3 Product Ion Scan(E+) Precursor: 475.4000 CE:-35.0 Ret. Time : [1.777->1.797][1.587->2.177] Scan# : [234->240][177<->354]



CE:-45.0

Event#: 1 Product Ion Scan(E+) Precursor: 475.4000 CE:-45.0 Ret. Time : [1.770->1.790][1.580->2.170] Scan# : [232->238][175<->352]

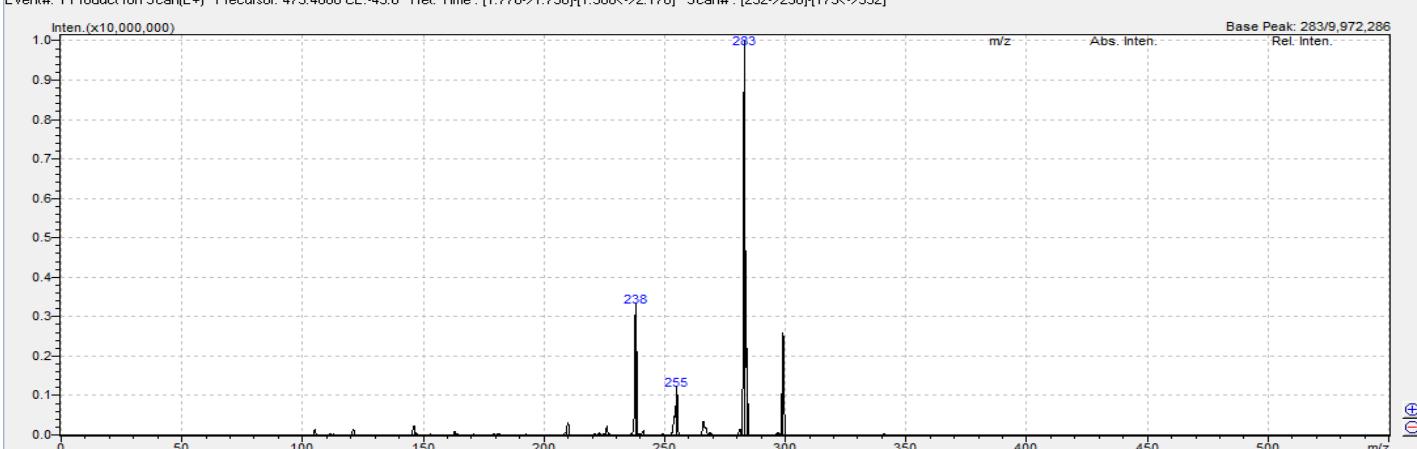


Fig.S90.  $^1\text{H}$  NMR spectral of 4',5'-dimethoxyflavone 5'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**19**) and 3',5'-dimethoxyflavone 4'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**20**) (DMSO- $d_6$ , 600 MHz)

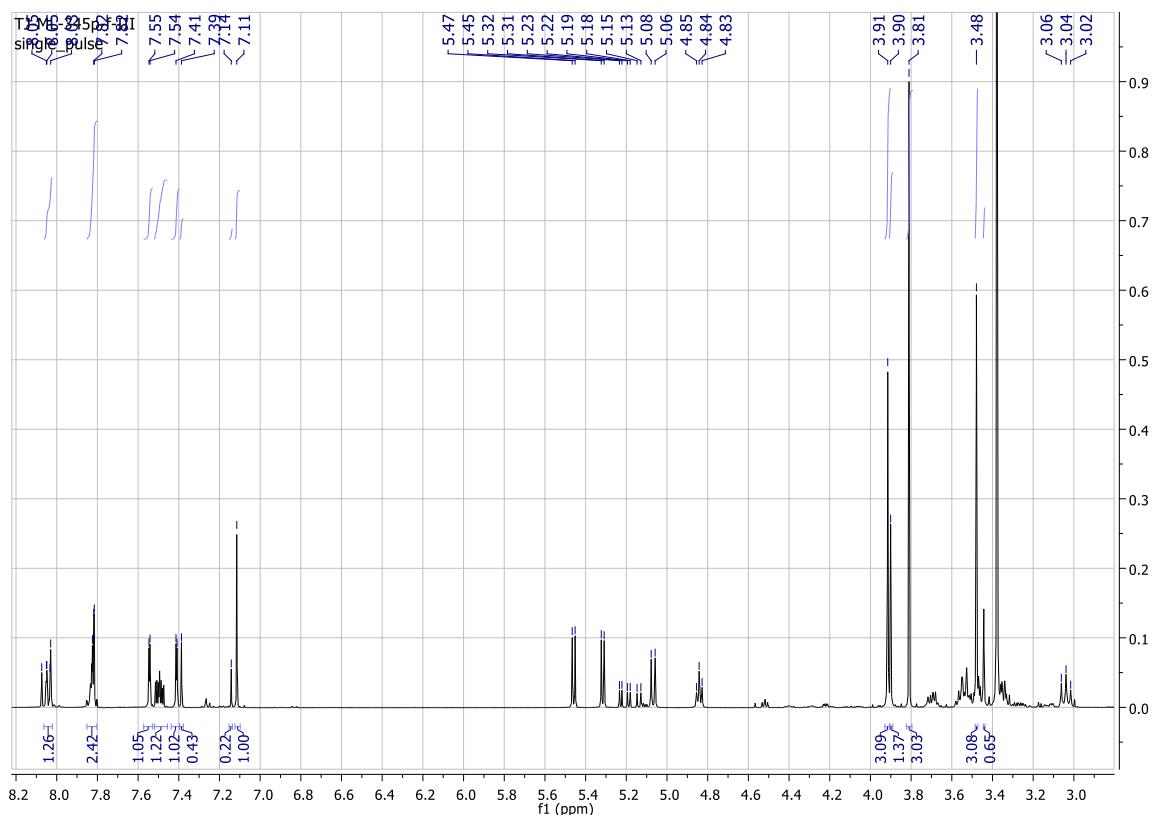


Fig.S91. Flavone part of the  $^1\text{H}$  NMR spectral 4',5'-dimethoxyflavone 5'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**19**) and 3',5'-dimethoxyflavone 4'- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**20**) (DMSO- $d_6$ , 600 MHz)

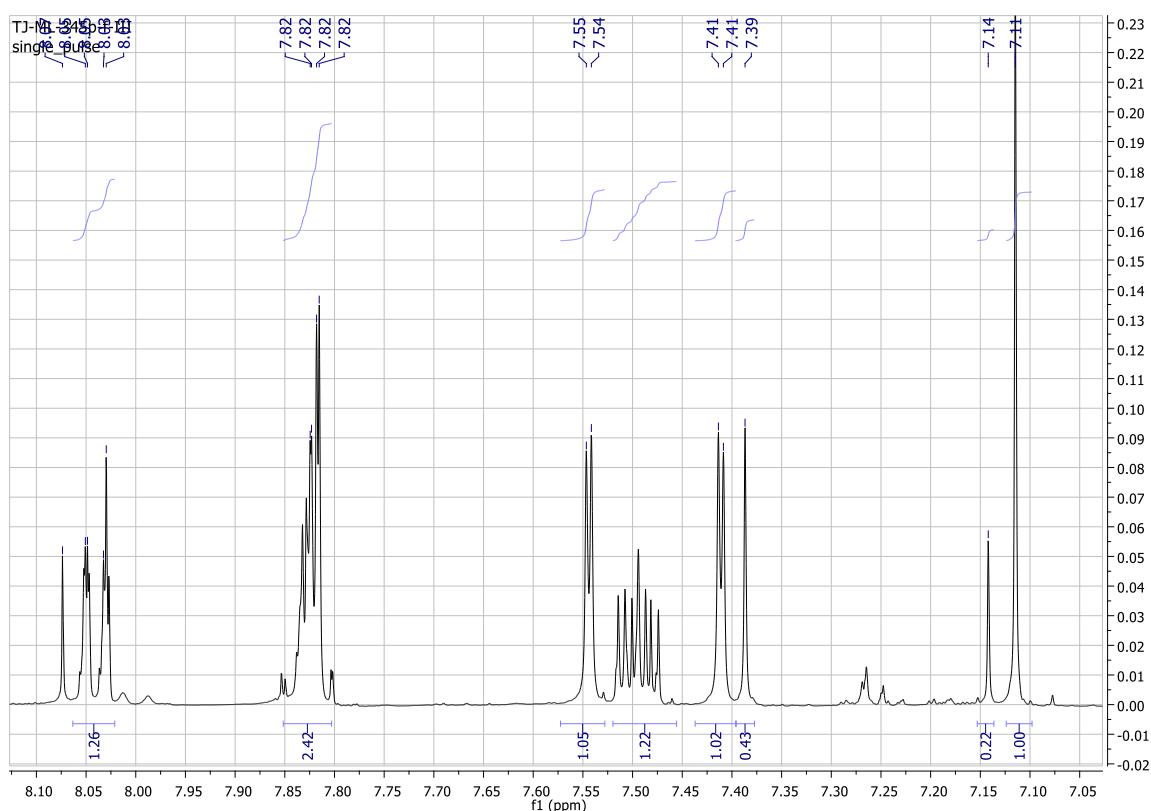


Fig.S92. Glycoside part of the  $^1\text{H}$  NMR spectral  $4',5'$ -dimethoxyflavone  $5'-O-\beta\text{-D-(4''-O-methyl)-glucopyranoside}$  (**19**) and  $3',5'$ -dimethoxyflavone  $4'-O-\beta\text{-D-(4''-O-methyl)-glucopyranoside}$  (**20**) (DMSO- $d_6$ , 600 MHz)

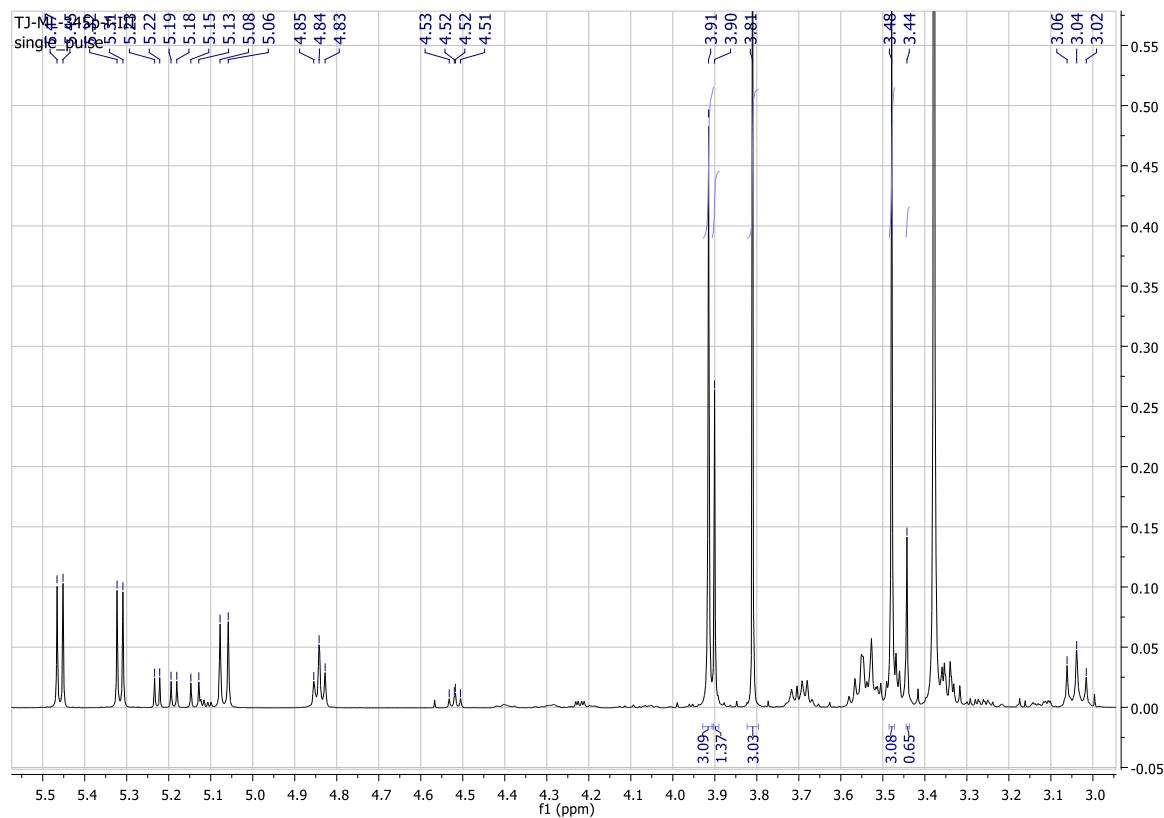


Fig.S93.  $^{13}\text{C}$  NMR spectral of  $4',5'$ -dimethoxyflavone  $5'-O-\beta\text{-D-(4''-O-methyl)-glucopyranoside}$  (**19**) and  $3',5'$ -dimethoxyflavone  $4'-O-\beta\text{-D-(4''-O-methyl)-glucopyranoside}$  (**20**) (DMSO- $d_6$ , 151 MHz)

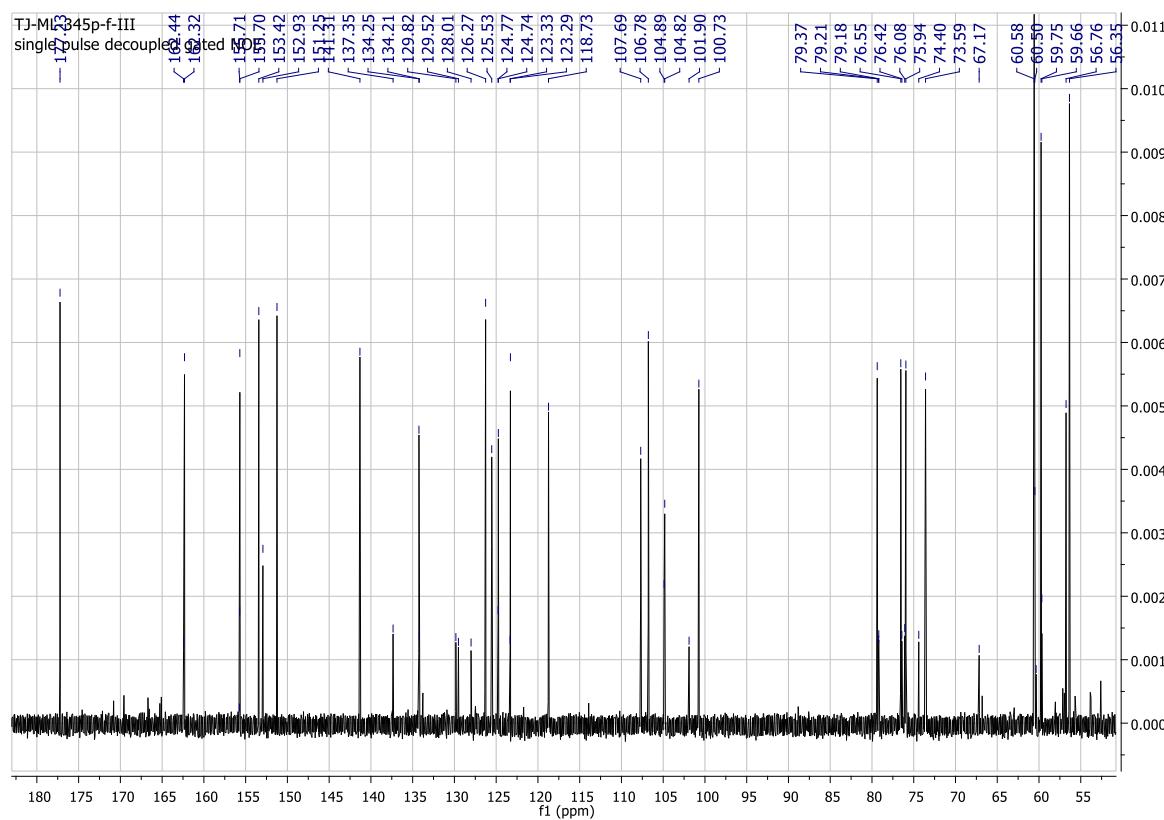


Fig.S94. HMQC spectral of 4',5'-dimethoxyflavone 5'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**19**) and 3',5'-dimethoxyflavone 4'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**20**) (DMSO- $d_6$ , 151 MHz)

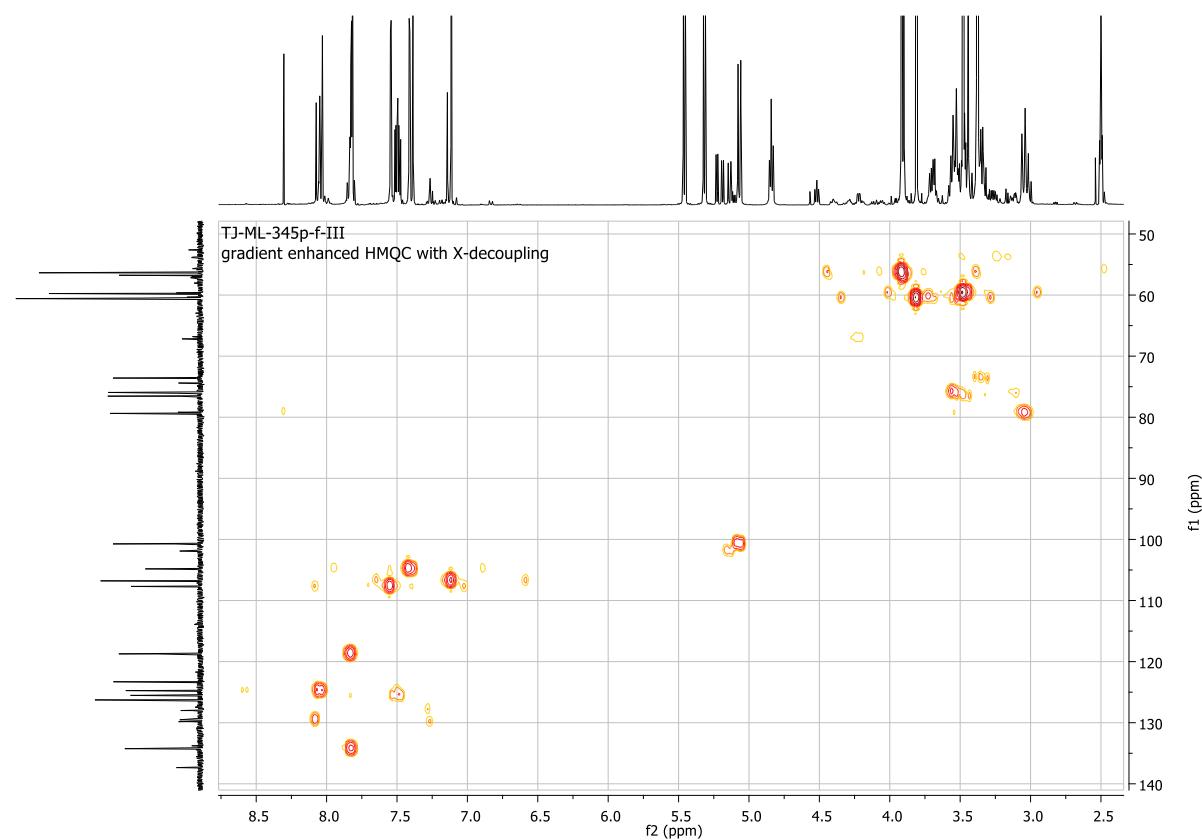


Fig.S95. HMBC spectral of 4',5'-dimethoxyflavone 5'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**19**) and 3',5'-dimethoxyflavone 4'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**20**) (DMSO- $d_6$ , 151 MHz)

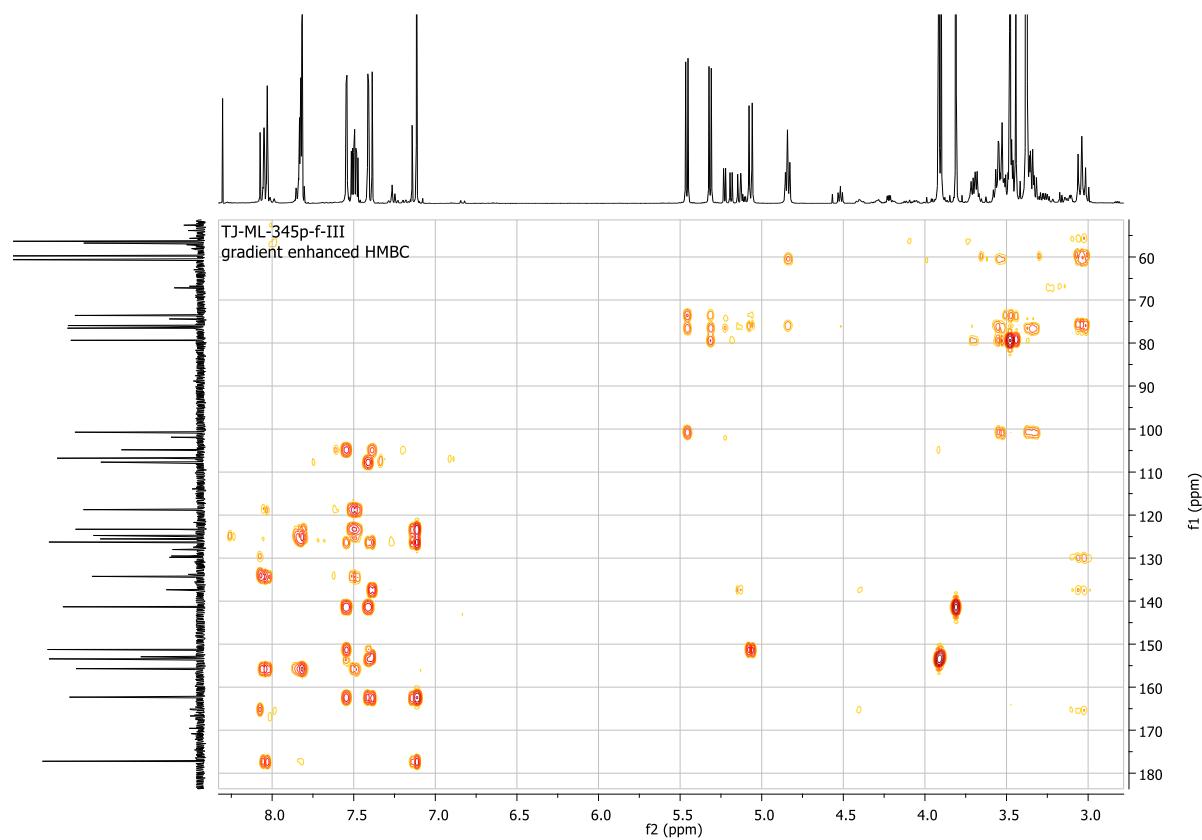
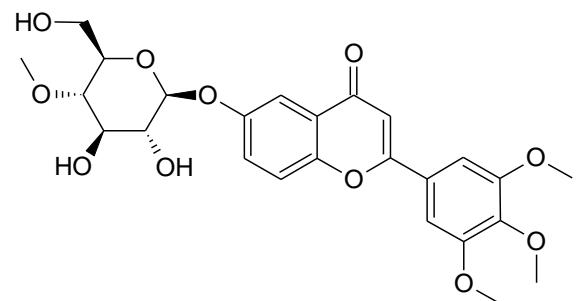


Fig.S96. MS analysis 3',4',5'-trimethoxyflavone 6-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**21**)

Molecular Formula = C<sub>25</sub>H<sub>28</sub>O<sub>11</sub>  
 Formula Weight = 504.48322  
 Precursor: =505.4000



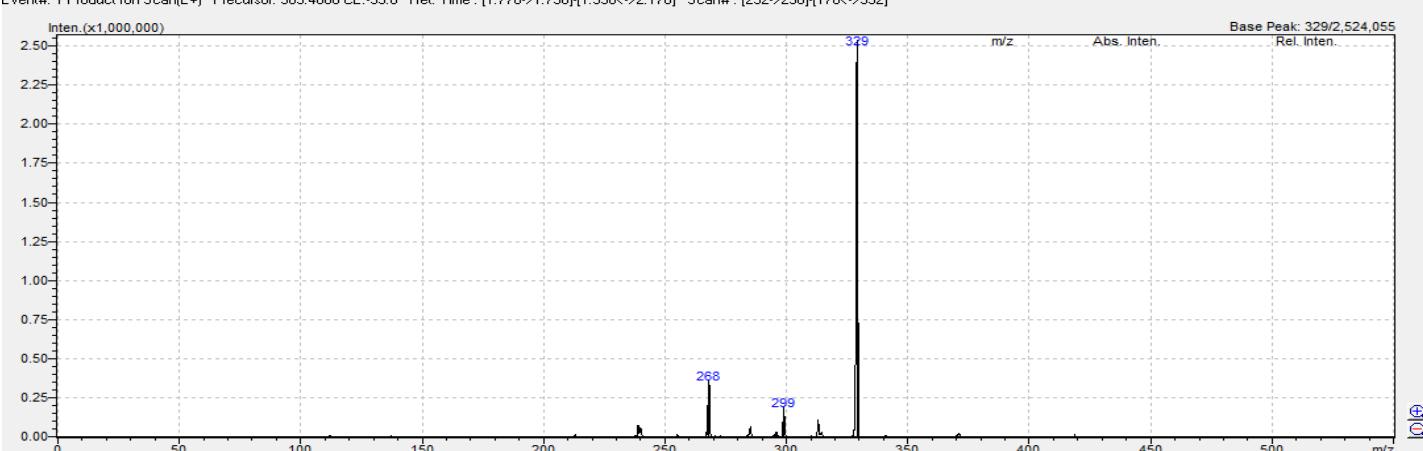
CE: -15.0

Event#: 3 Product Ion Scan(E+) Precursor: 505.4000 CE:-15.0 Ret. Time : [1.777->1.797][1.597<>2.177] Scan#: [234->240][180<>354]



CE:-35.0

Event#: 1 Product Ion Scan(E+) Precursor: 505.4000 CE:-35.0 Ret. Time : [1.770->1.790][1.590<>2.170] Scan#: [232->238][178<>352]



CE:-45.0

Event#: 2 Product Ion Scan(E+) Precursor: 505.4000 CE:-45.0 Ret. Time : [1.773->1.793][1.593<>2.173] Scan#: [233->239][179<>353]

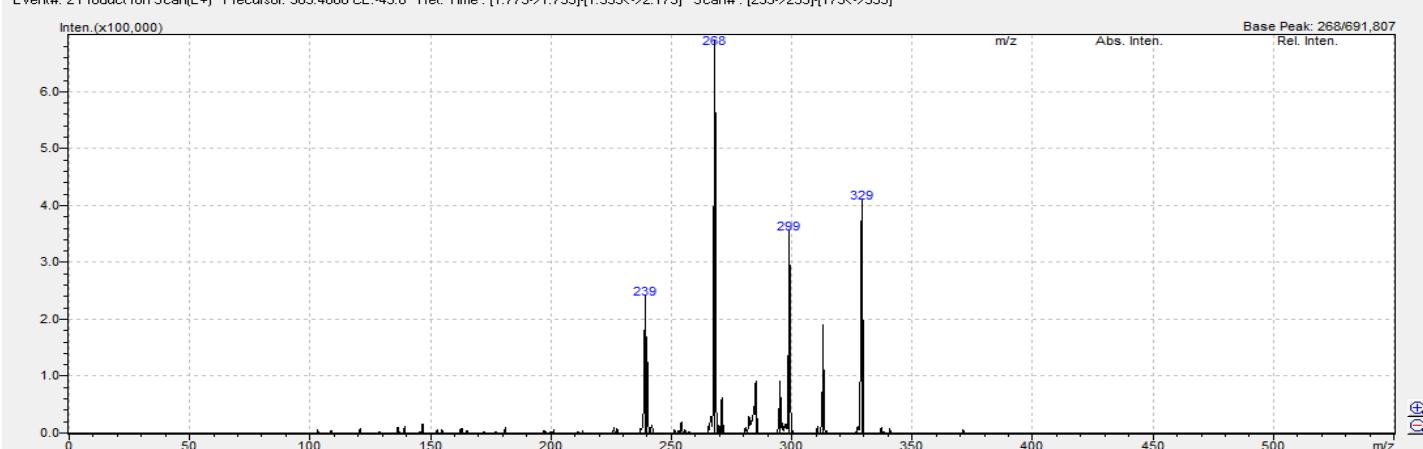


Fig.S97.  $^1\text{H}$  NMR spectral of 3',4',5'-trimethoxyflavone 6-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**21**) (DMSO- $d_6$ , 600 MHz)

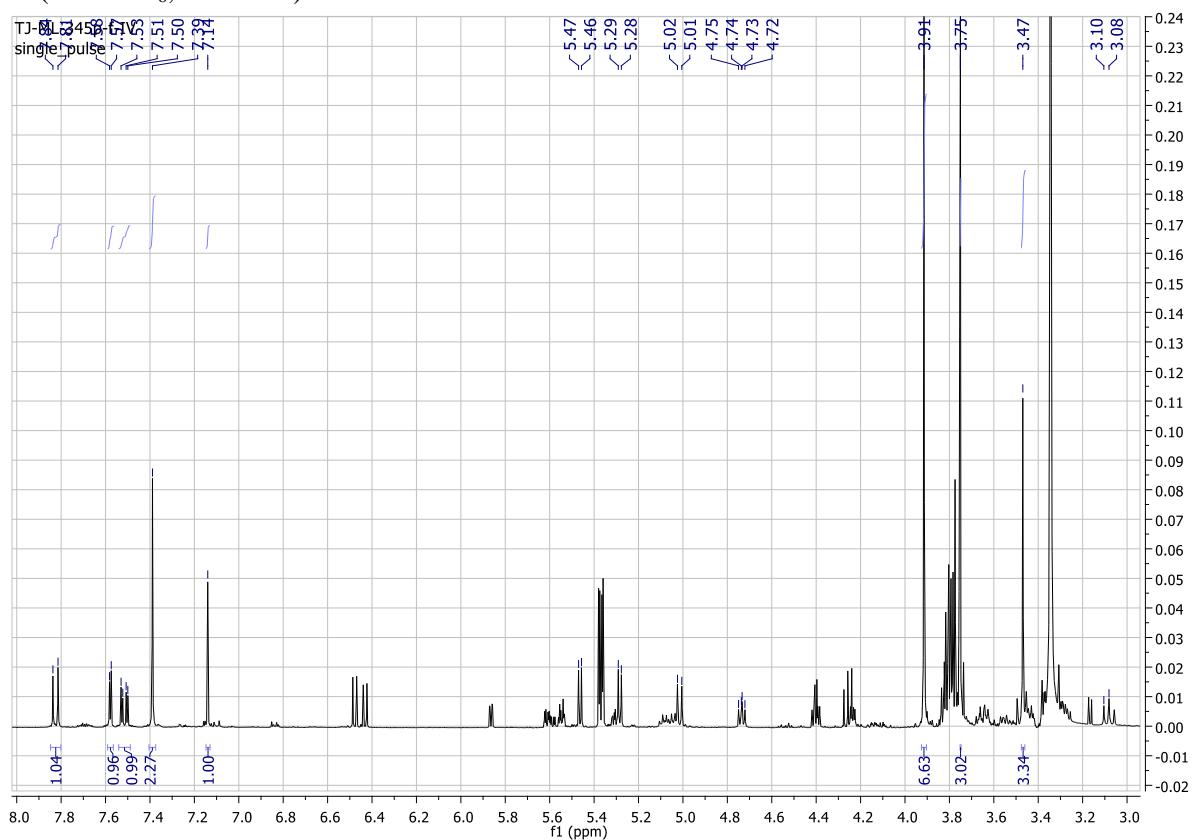


Fig.S98. Flavone part of the  $^1\text{H}$  NMR spectral 3',4',5'-trimethoxyflavone 6-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**21**) (DMSO- $d_6$ , 600 MHz)

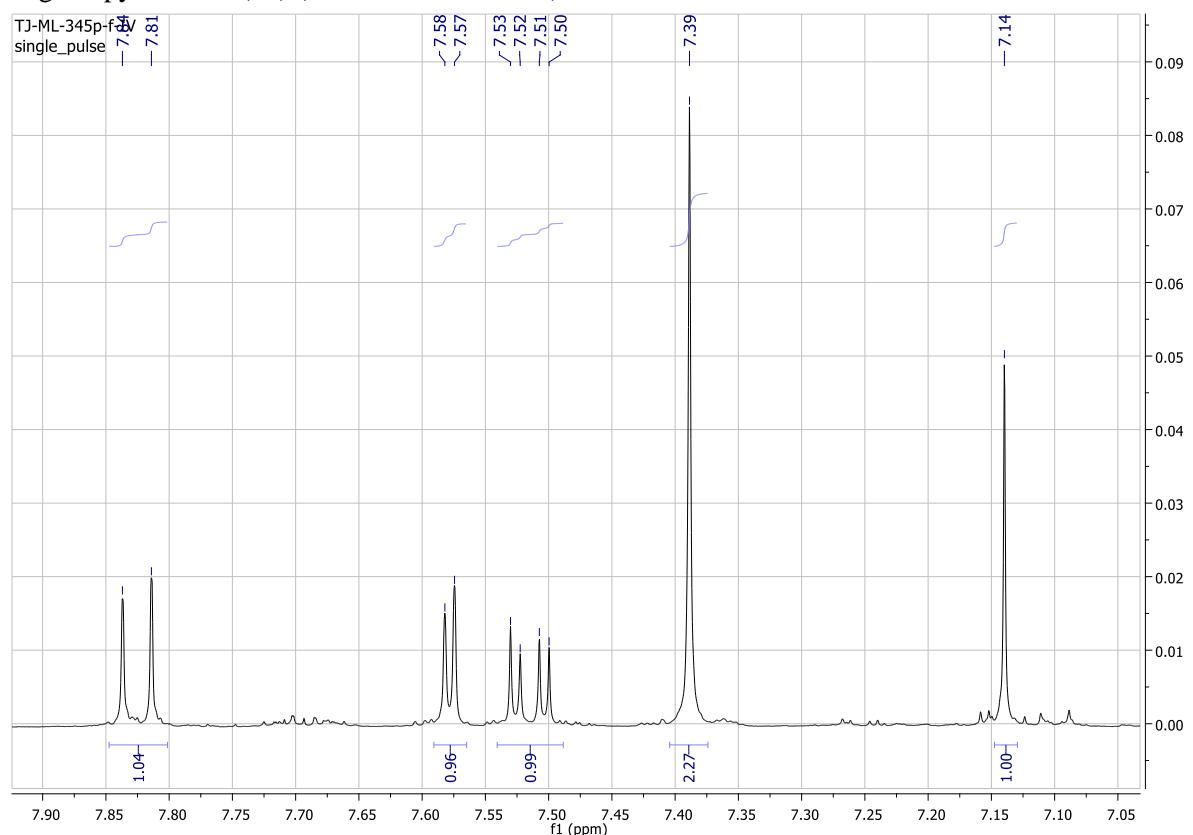


Fig.S99. Glucopyranoside part of the  $^1\text{H}$  NMR spectral 3',4',5'-trimethoxyflavone 6- $O$ - $\beta$ -D-(4"- $O$ -methyl)-glucopyranoside (**21**) (DMSO- $d_6$ , 600 MHz)

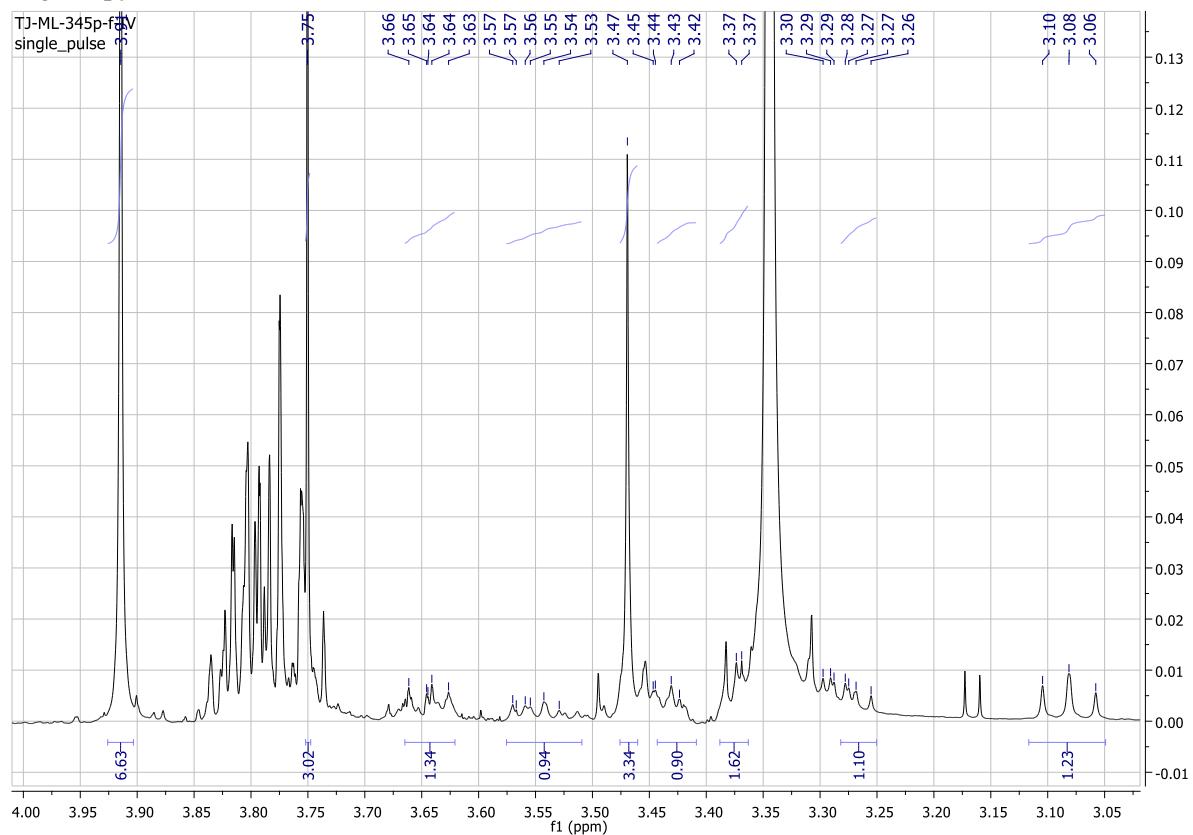


Fig.S100.  $^{13}\text{C}$  NMR spectral of 3',4',5'-trimethoxyflavone 6- $O$ - $\beta$ -D-(4''- $O$ -methyl)-glucopyranoside (**21**) (DMSO- $d_6$ , 151 MHz)

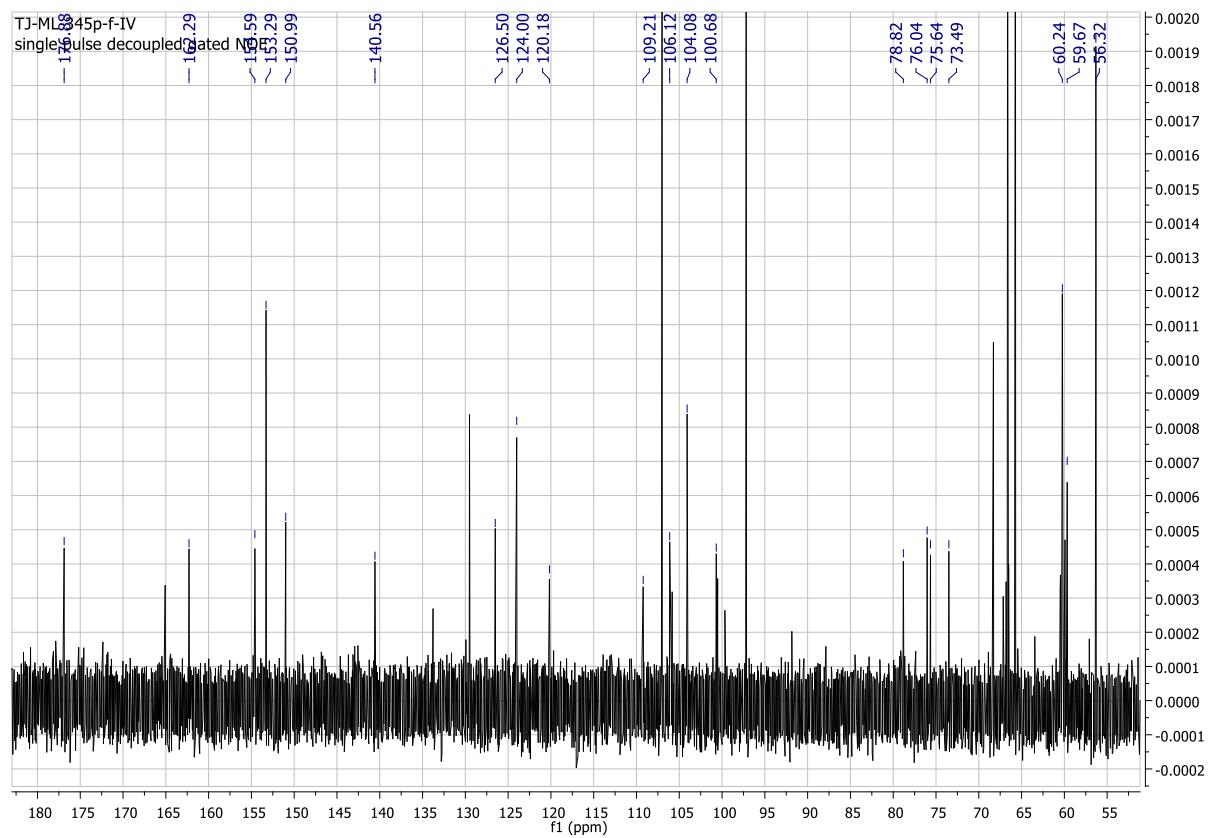


Fig.S101. HMQC spectral of 3',4',5'-trimethoxyflavone 6-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**21**) (DMSO- $d_6$ , 151 MHz)

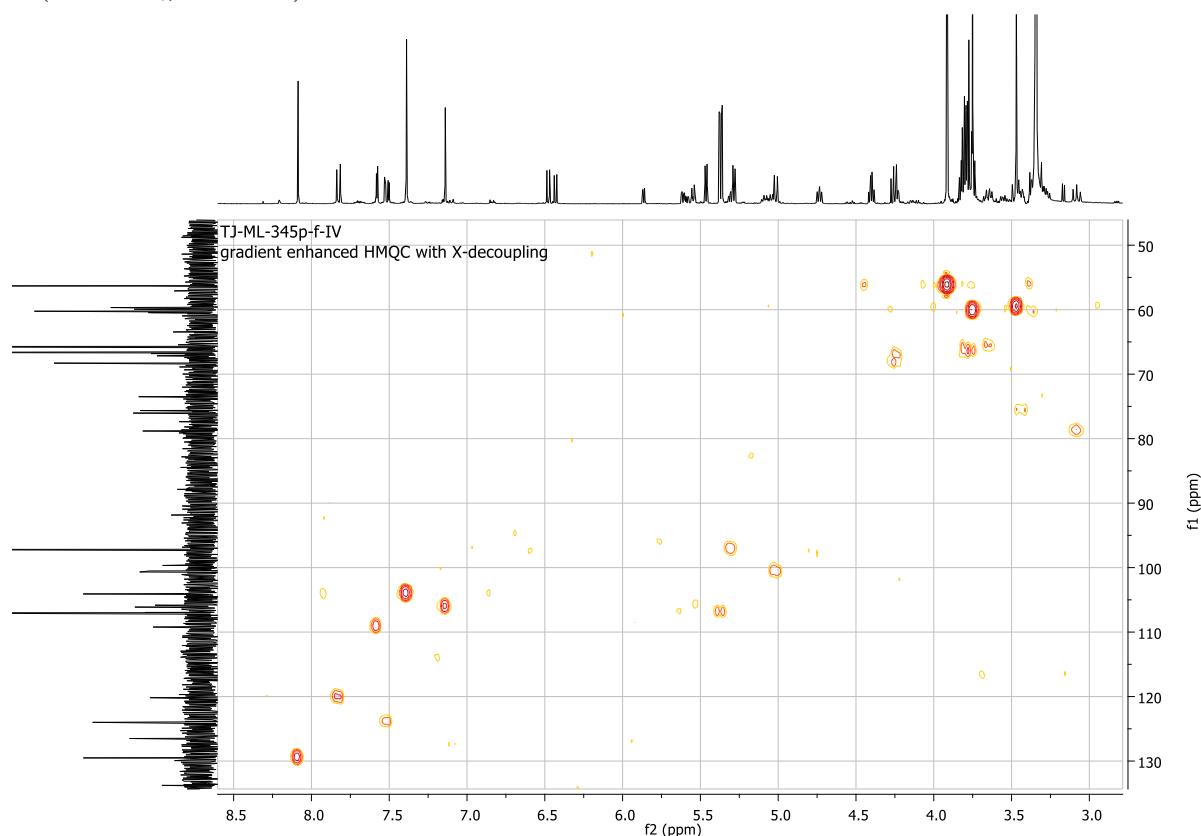


Fig.S102. HMBC spectral of 3',4',5'-trimethoxyflavone 6-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**21**) (DMSO- $d_6$ , 151 MHz)

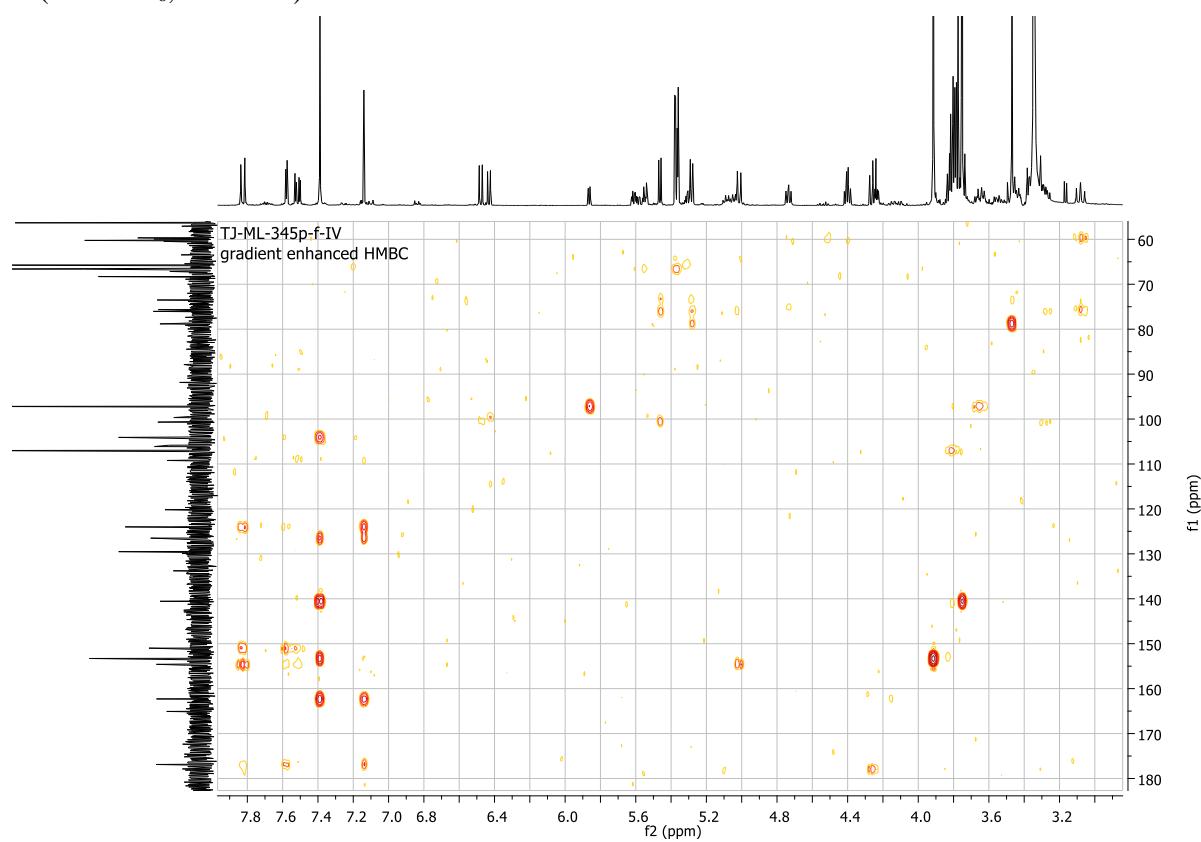
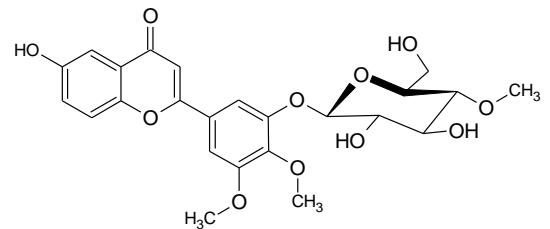


Fig.S103. MS analysis 6-hydroxy-4',5'-dimethoxyflavone 3'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (22)

Molecular Formula = C<sub>24</sub>H<sub>26</sub>O<sub>11</sub>  
 Formula Weight = 490.45664  
 Precursor: = 491.4000



CE:-15

Event#: 2 Product Ion Scan(E+) Precursor: 491.4000 CE:-15.0 Ret. Time : [1.733] Scan#: [221]



CE:-35

Event#: 3 Product Ion Scan(E+) Precursor: 491.4000 CE:-35.0 Ret. Time : [1.737] Scan#: [222]



CE:-45

Event#: 1 Product Ion Scan(E+) Precursor: 491.4000 CE:-45.0 Ret. Time : [1.720] Scan#: [217]

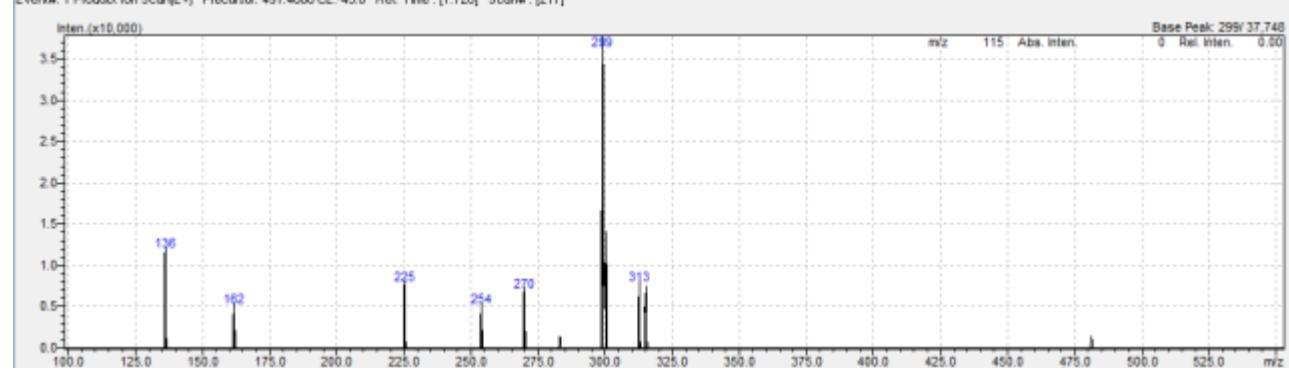


Fig.S104.  $^1\text{H}$  NMR spectral of 6-hydroxy-4',5'-dimethoxyflavone 3'- $O$ - $\beta$ -D-(4"- $O$ -methyl)-glucopyranoside (**22**) (DMSO- $d_6$ , 600 MHz)

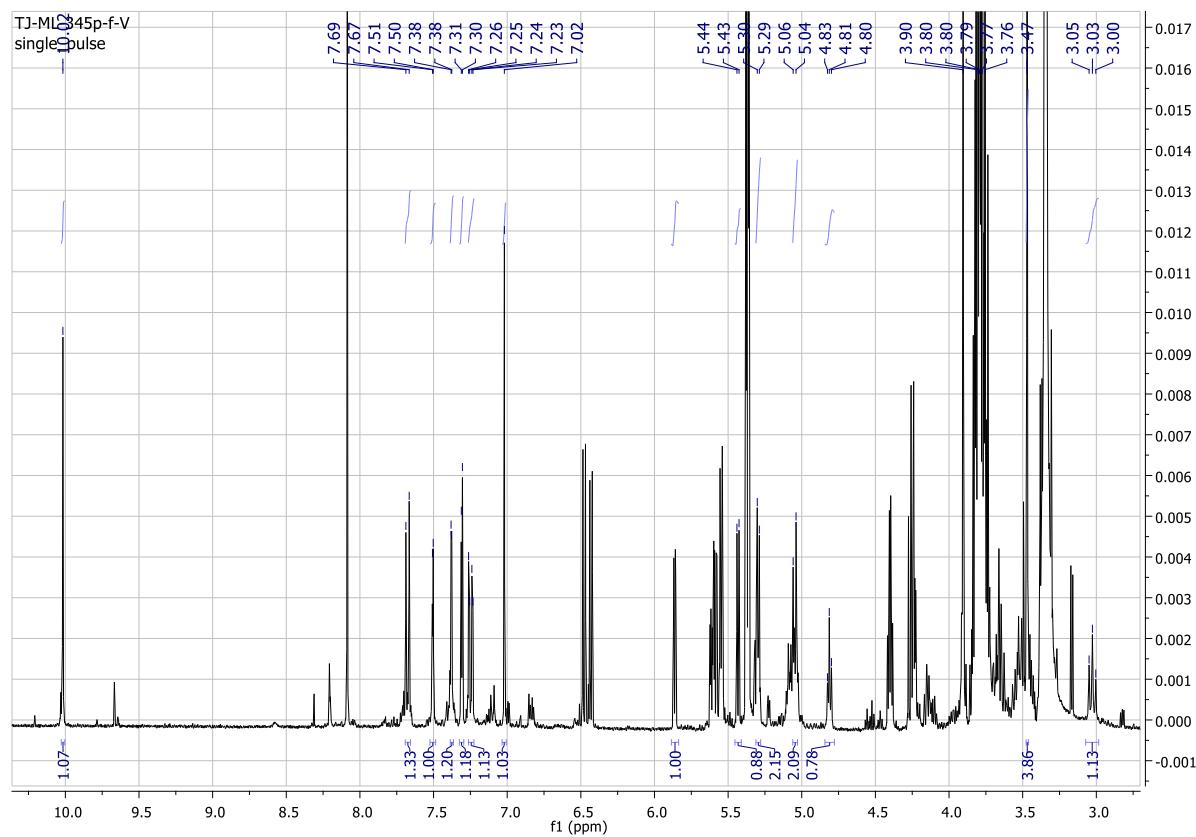


Fig.S105. Flavone part of the  $^1\text{H}$  NMR spectral 6-hydroxy-4',5'-dimethoxyflavone 3'- $O$ - $\beta$ -D-(4"- $O$ -methyl)-glucopyranoside (**22**) (DMSO- $d_6$ , 600 MHz)

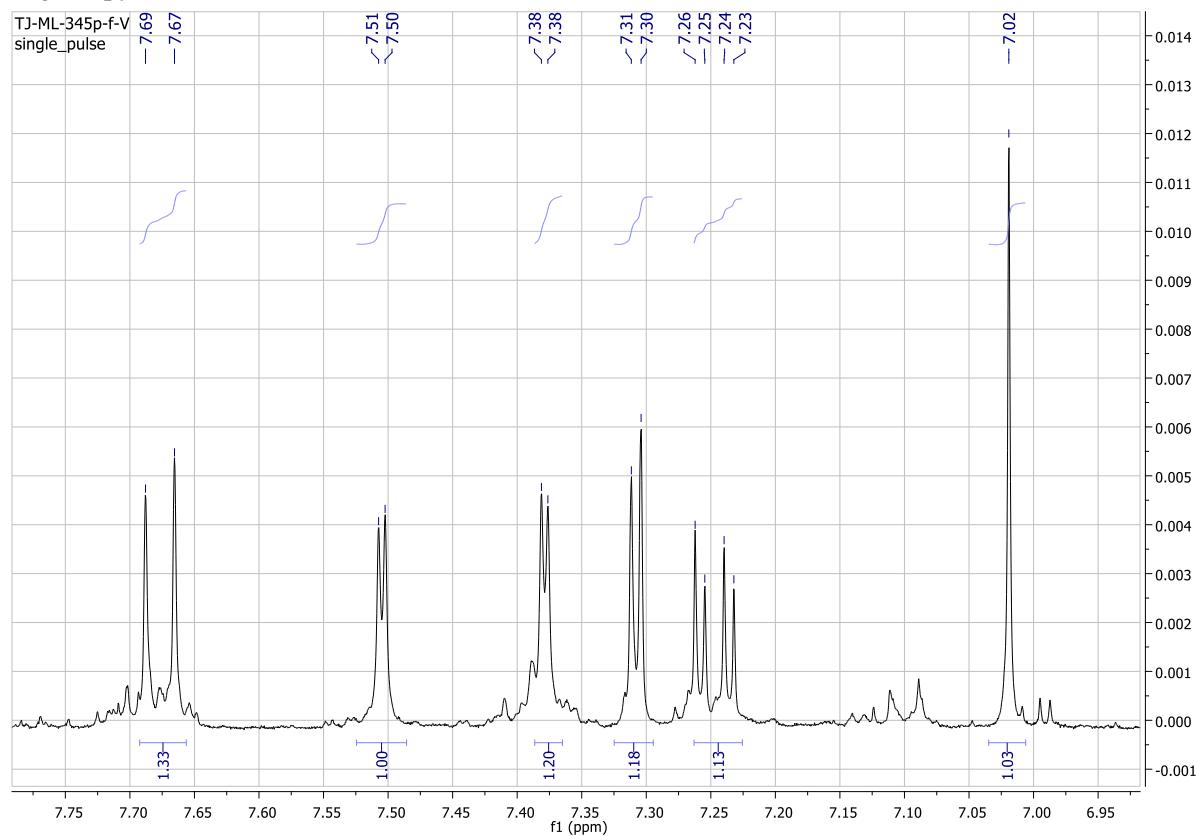


Fig.S106. Glucopyranoside part of the  $^1\text{H}$  NMR spectral 6-hydroxy-4',5'-dimethoxyflavone 3'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**22**) (DMSO- $d_6$ , 600 MHz)

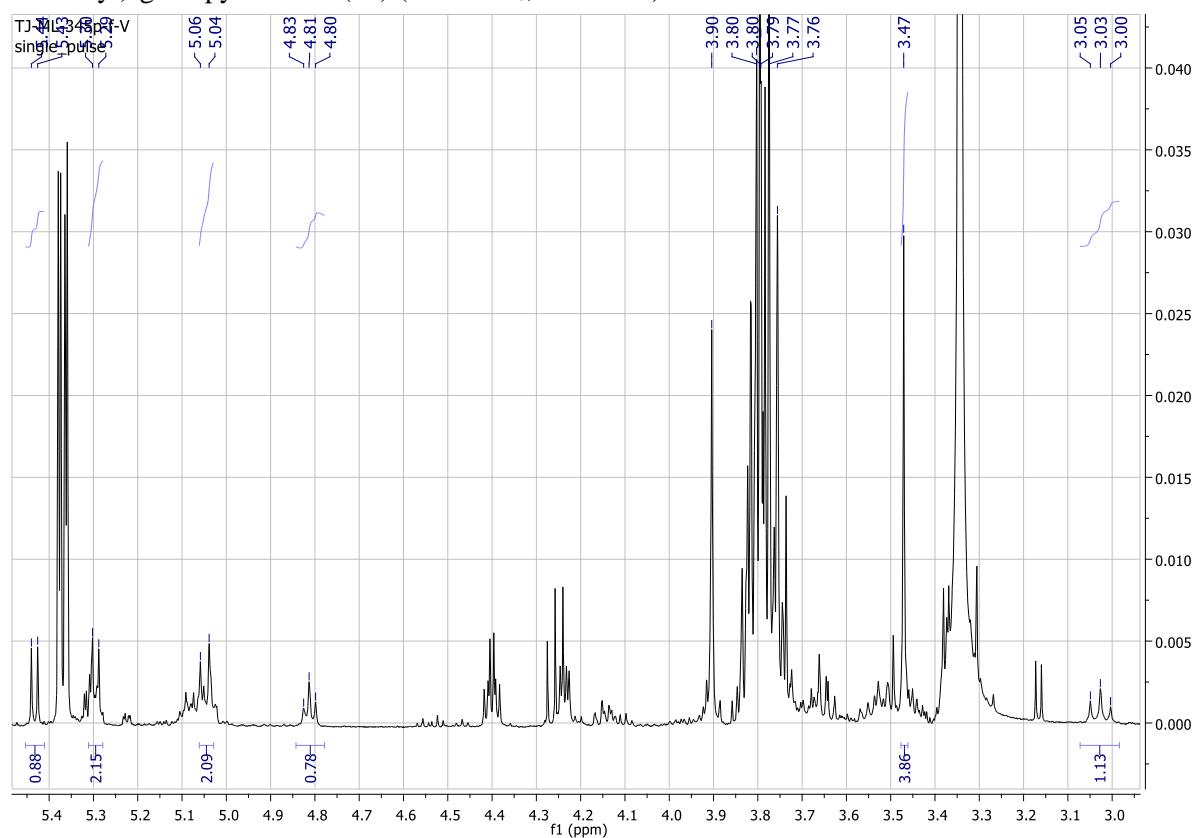


Fig.S107.  $^{13}\text{C}$  NMR spectral of 6-hydroxy-4',5'-dimethoxyflavone 3'-O- $\beta$ -D-(4''-O-methyl)-glucopyranoside (**22**) (DMSO- $d_6$ , 151 MHz)

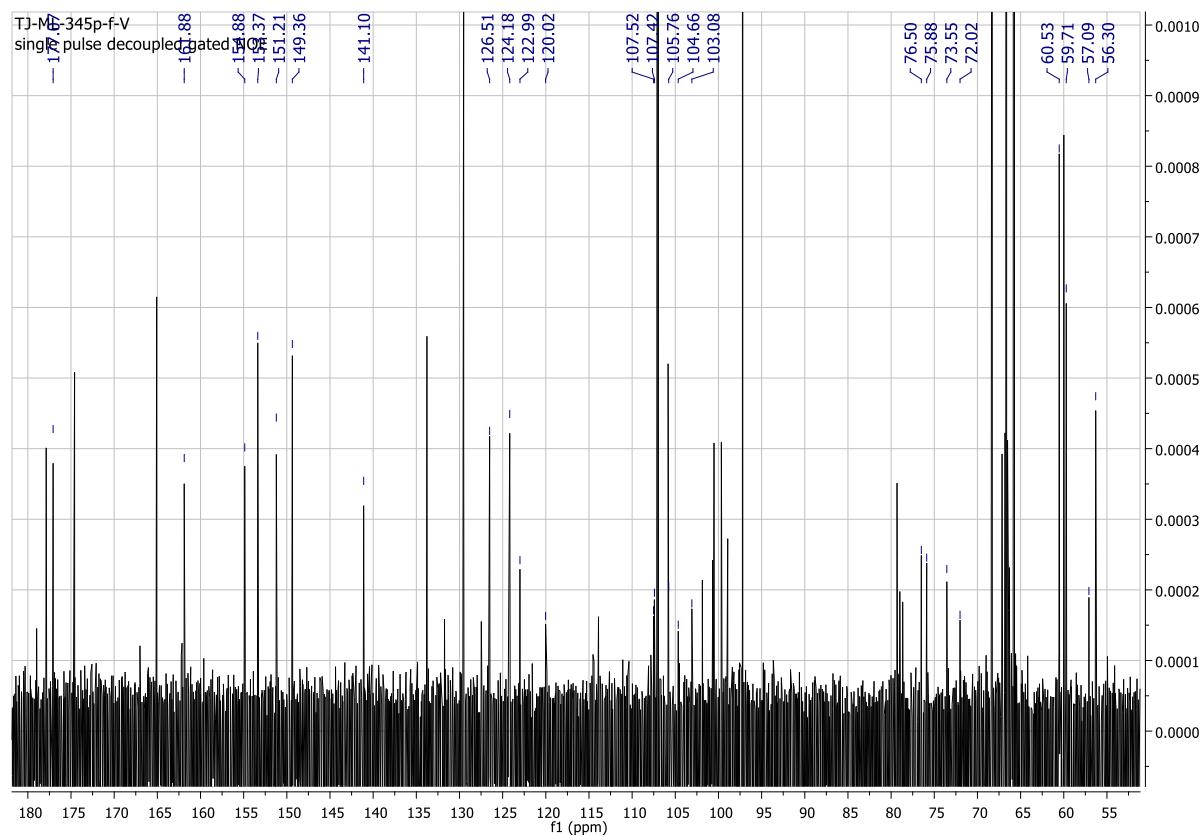


Fig.S108. HMQC spectral of 6-hydroxy-4',5'-dimethoxyflavone 3'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**22**) (DMSO-*d*<sub>6</sub>, 151 MHz)

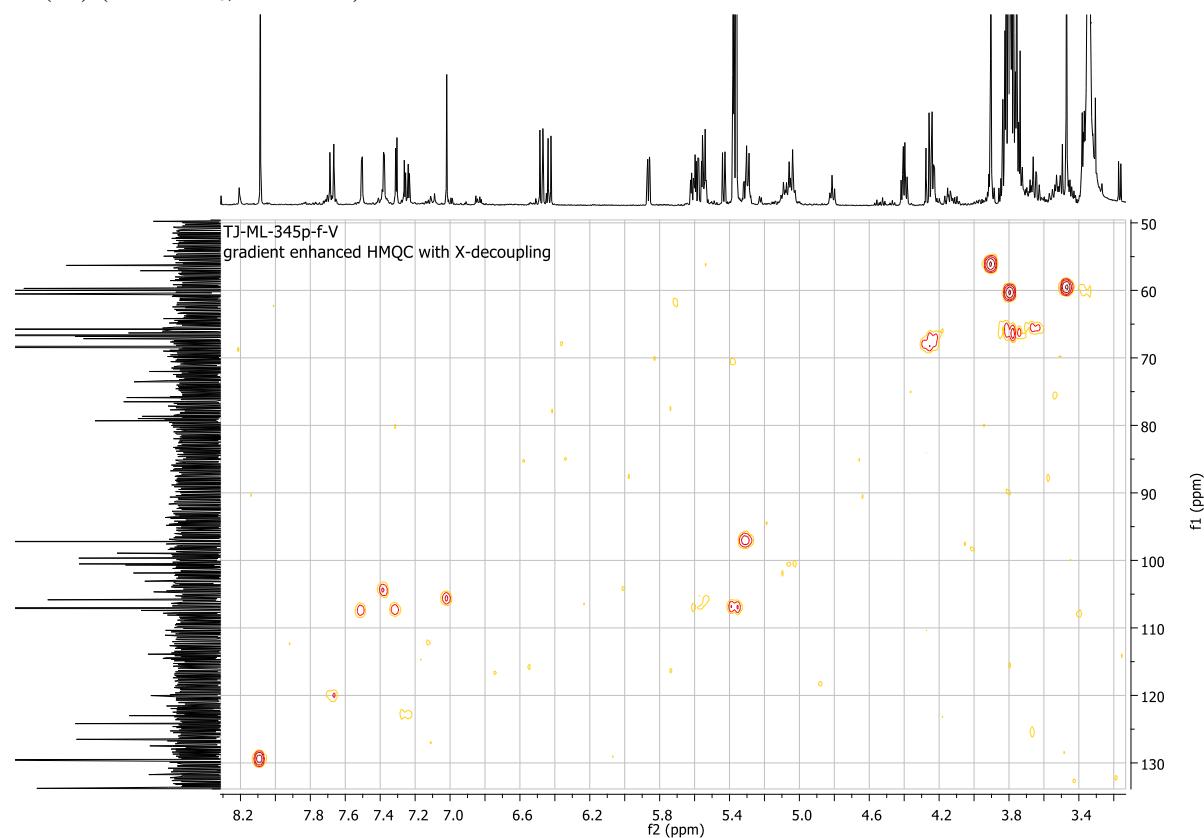


Fig.S109. HMBC spectral of 6-hydroxy-4',5'-dimethoxyflavone 3'-O- $\beta$ -D-(4"-O-methyl)-glucopyranoside (**22**) (DMSO-*d*<sub>6</sub>, 151 MHz)

