

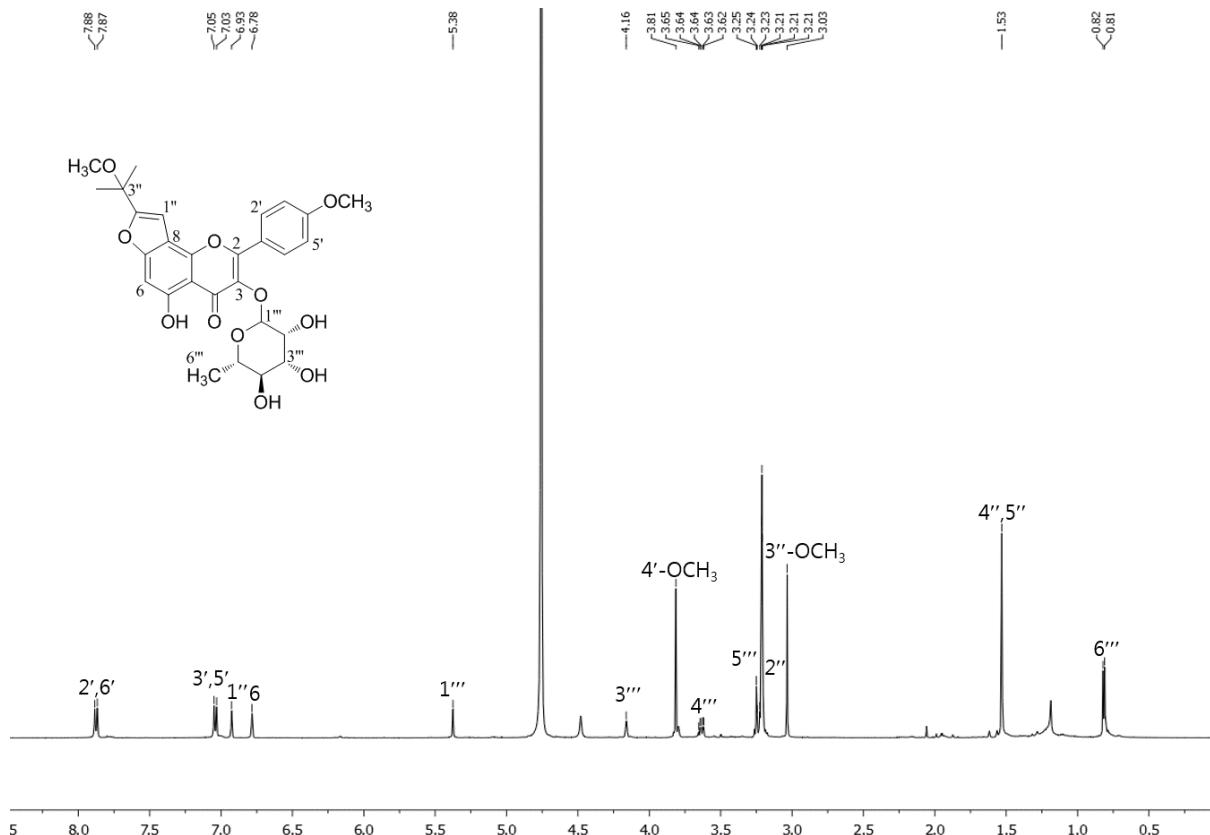
# **Supplementary materials**

## **Effectiveness of prenyl group on flavonoids from *Epimedium koreanum* to bacterial neuraminidase inhibition**

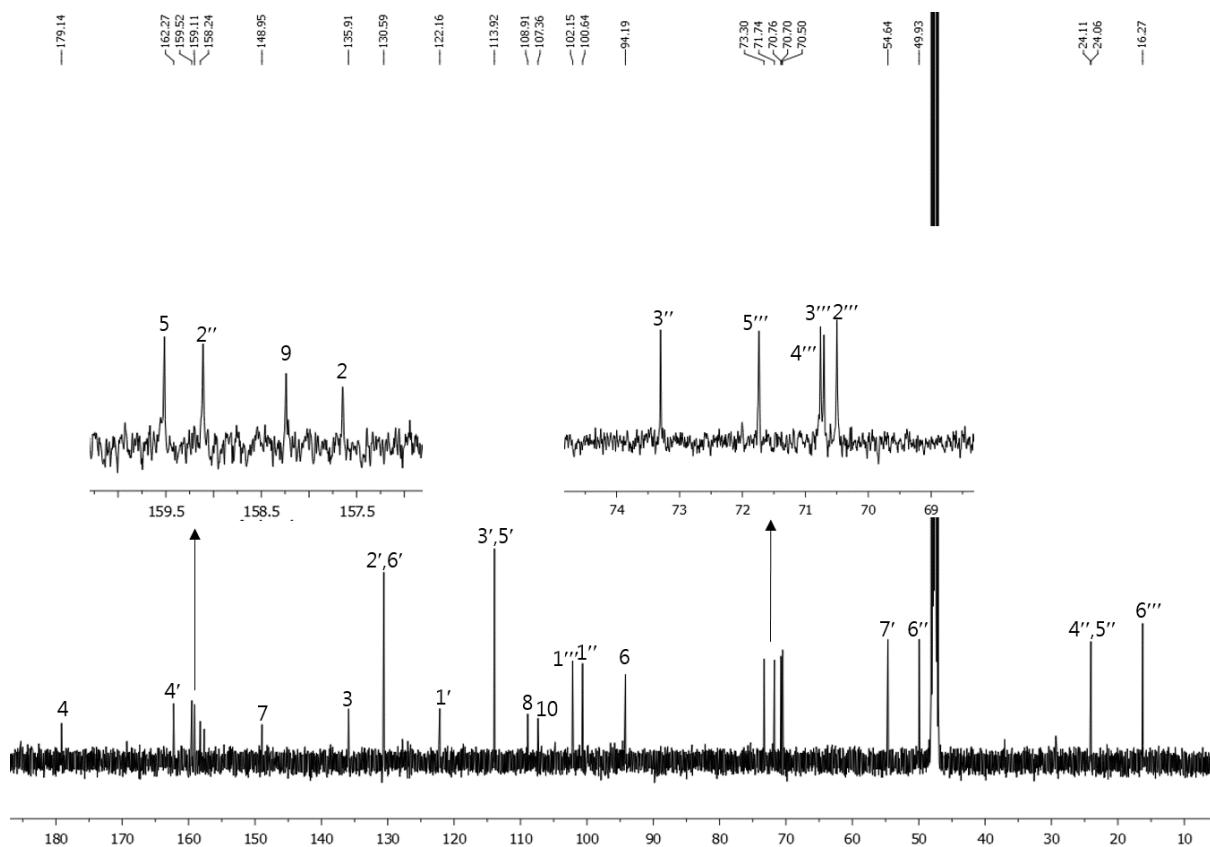
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Division of Applied Life Science (BK21 plus), IALS, Gyeongsang National University, Jinju 52828, Republic of Korea

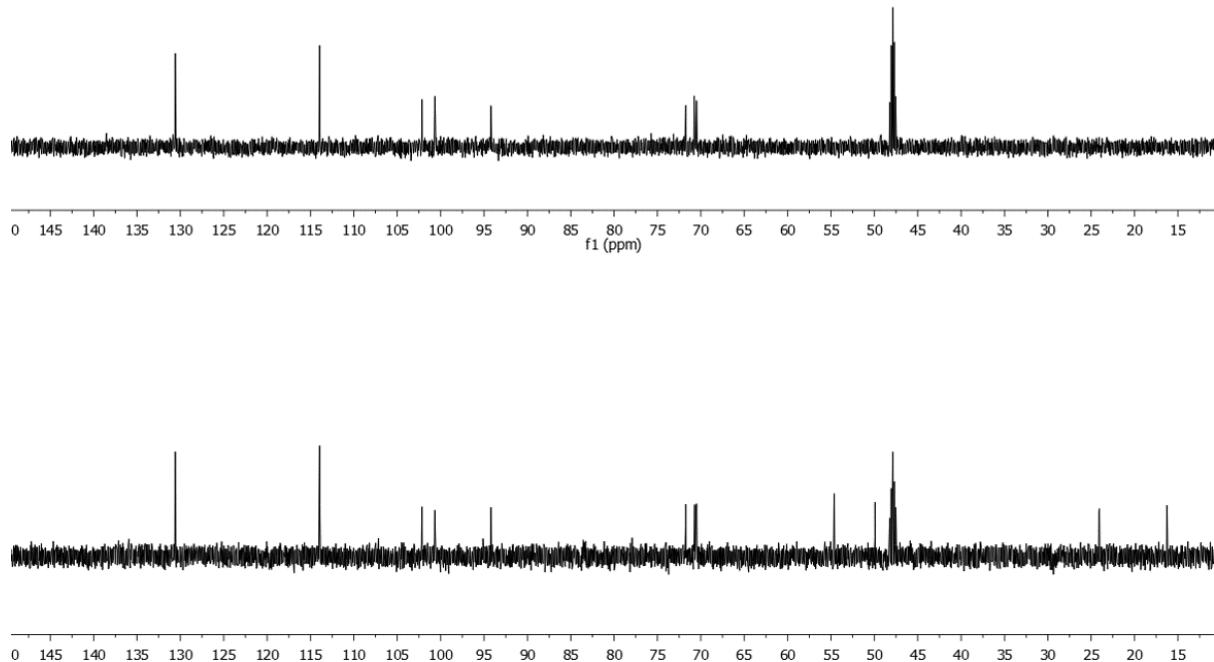
- **Figure S1-32:** 1D, 2D-NMR of isolated compounds **1-8**
- **Figure S33-34:** Enzyme kinetic data of isolated compounds (**2-4** and **6-8**)
- **Figure S35:** Fluorescence quenching effect of compounds (**3-8**, luteolin, and apigenin)



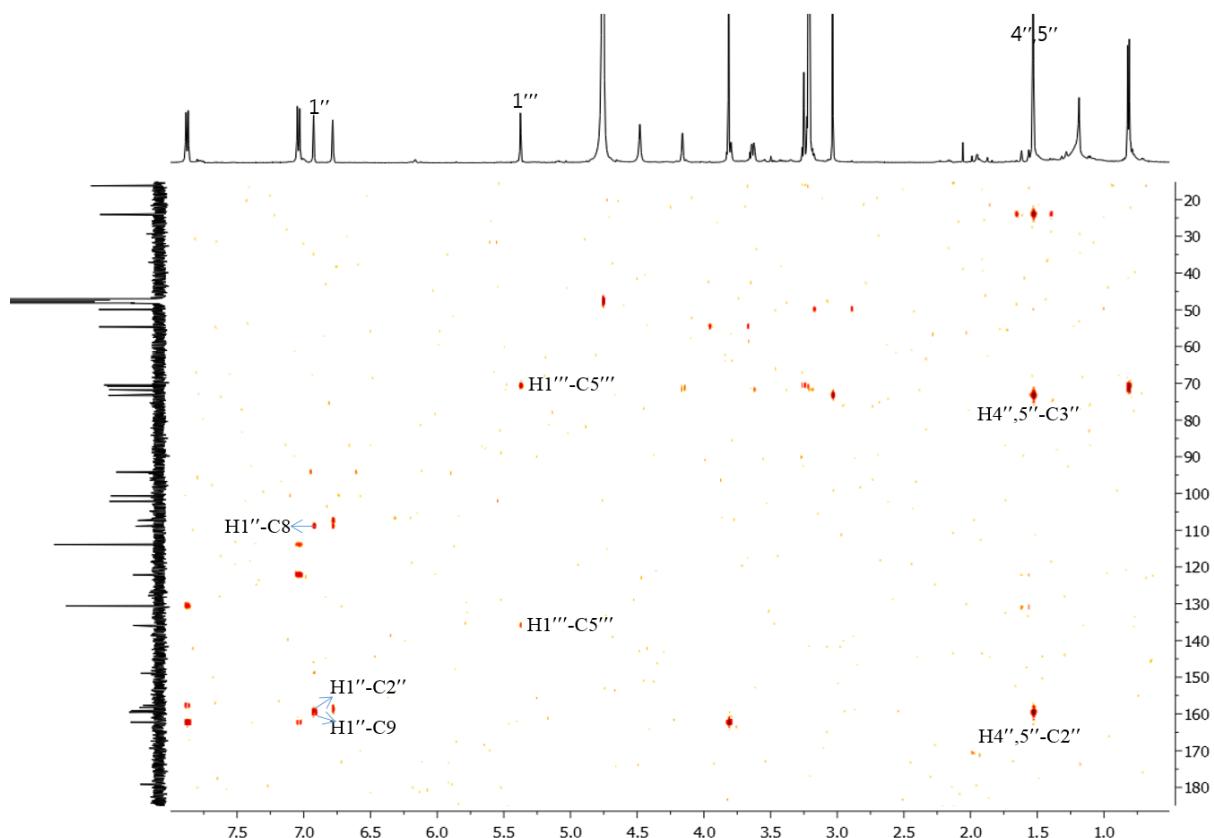
**Figure 1.**  $^1\text{H}$  NMR spectrum of compound 7 (500 MHz, MeOD).



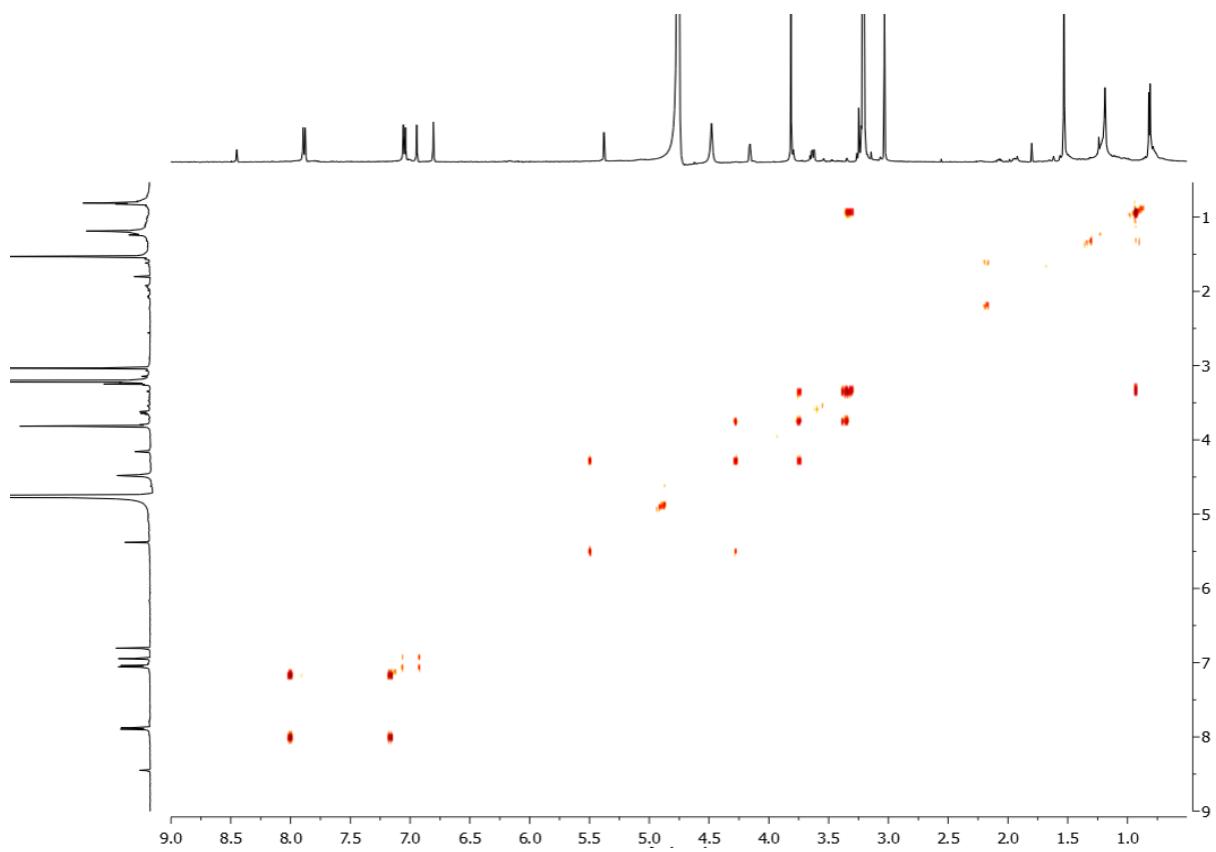
**Figure 2.**  $^{13}\text{C}$  NMR spectrum of compound 7 (500 MHz, MeOD).



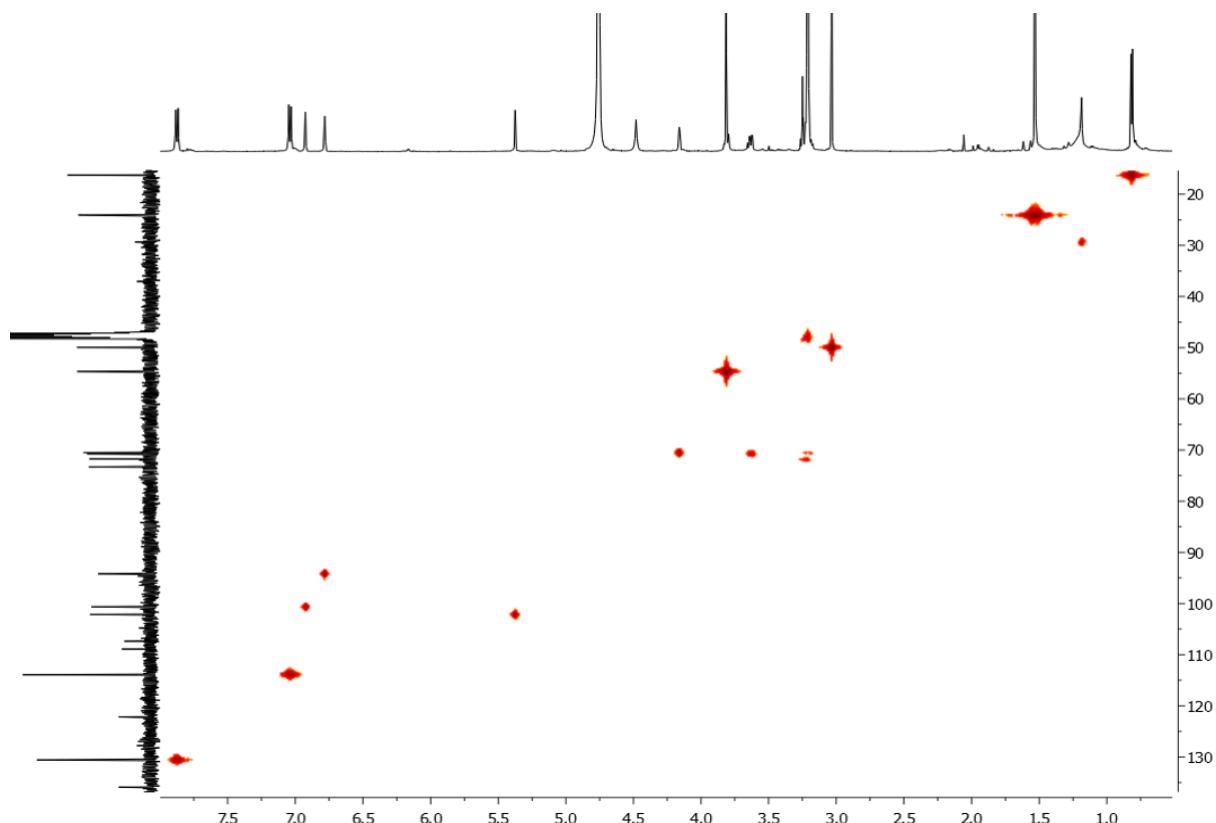
**Figure 3.** DEPT-90 and -135 spectrum of compound 7 (500 MHz, MeOD).



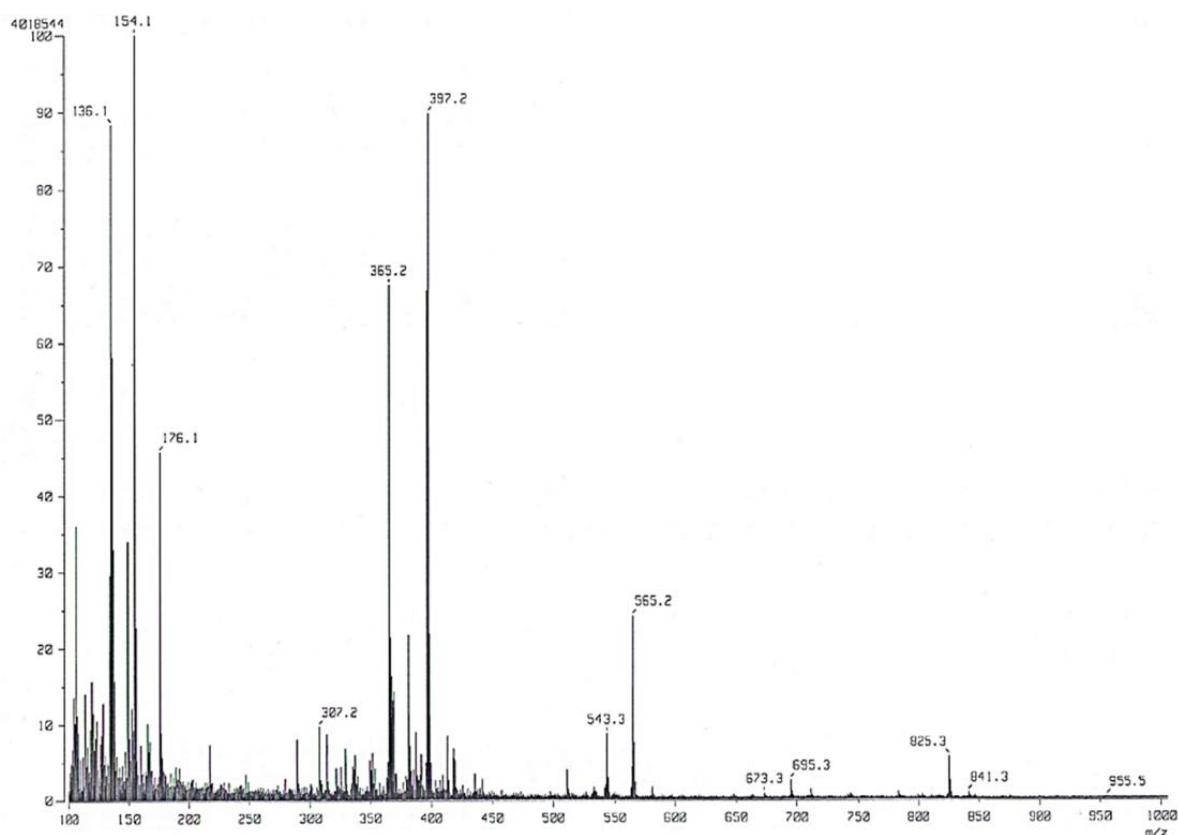
**Figure 4.** HMBC spectrum of compound 7 (500 MHz, MeOD).



**Figure 5.** COSY spectrum of compound 7 (500 MHz, MeOD).



**Figure 6.** HMQC spectrum of compound 7 (500 MHz, MeOD).



[ Elemental Composition ]

Data : HM-7-HR1

Date : 05-Apr-2018 16:38

Sample: -

Note : -

Inlet : Direct

Ion Mode : FAB+

RT : 1.00 min

Scan# : 13

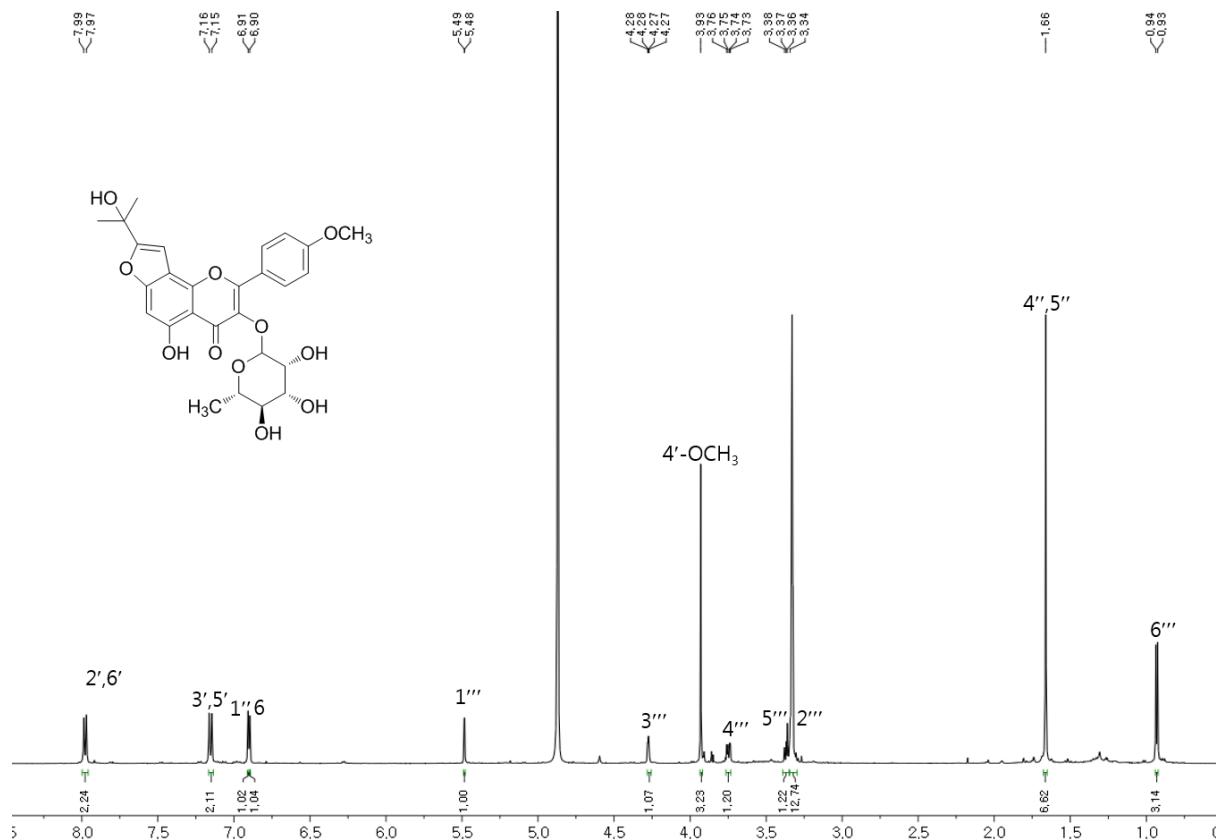
Elements : C 100/1, H 100/1, O 20/1

Mass Tolerance : 100ppm, 10mmu if m/z > 100

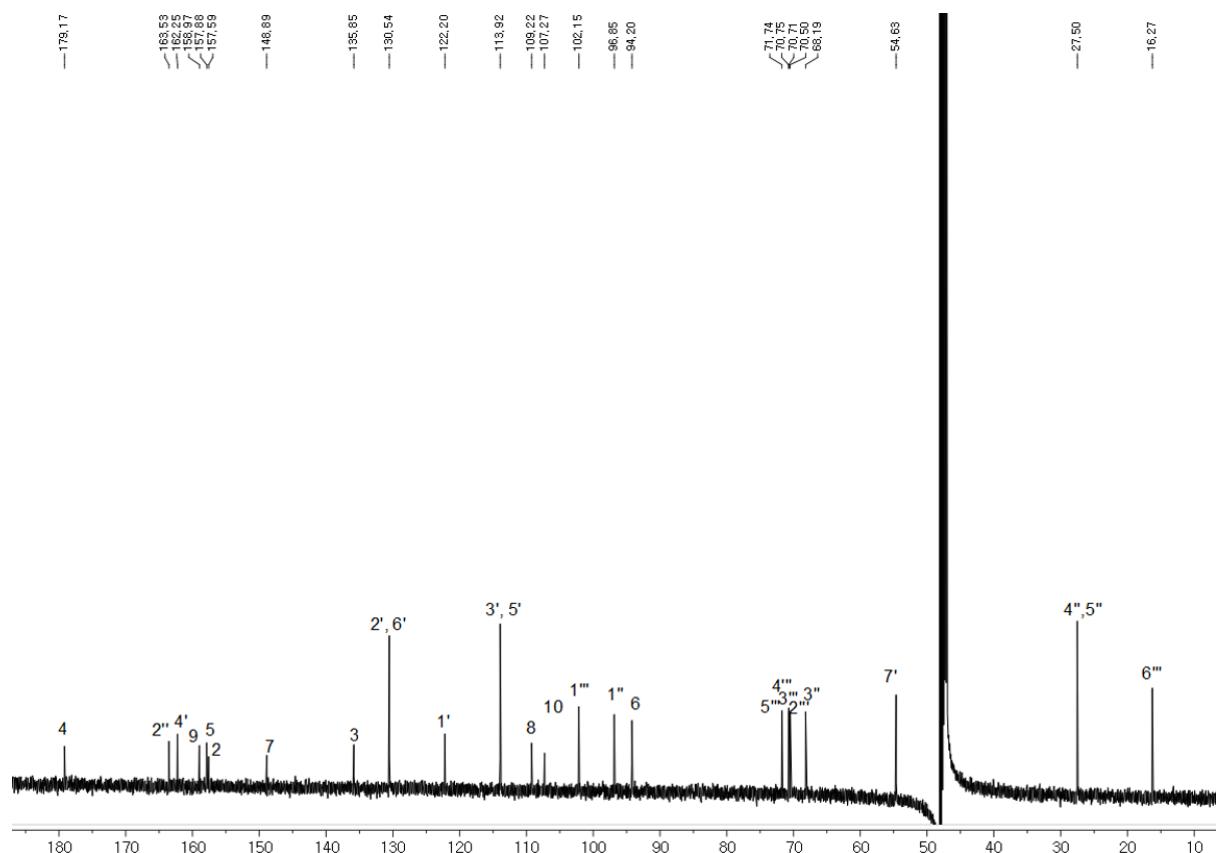
Unsaturation (U.S.) : 0.0 - 20.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
543.1906	11.9	+7.2 / +3.9	13.5	C 28 H 31 O 11
		-3.6 / -2.0	4.5	C 21 H 35 O 16

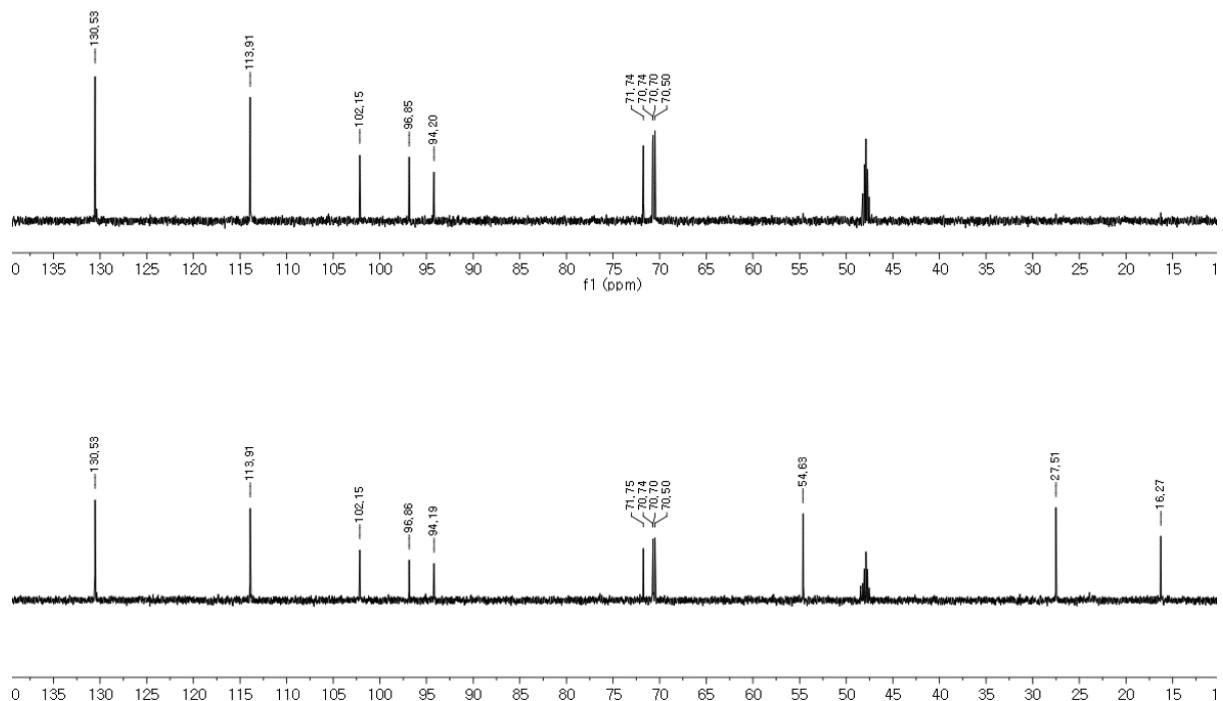
Figure 7. FABMS spectra and HRFABMS data of compound 7.



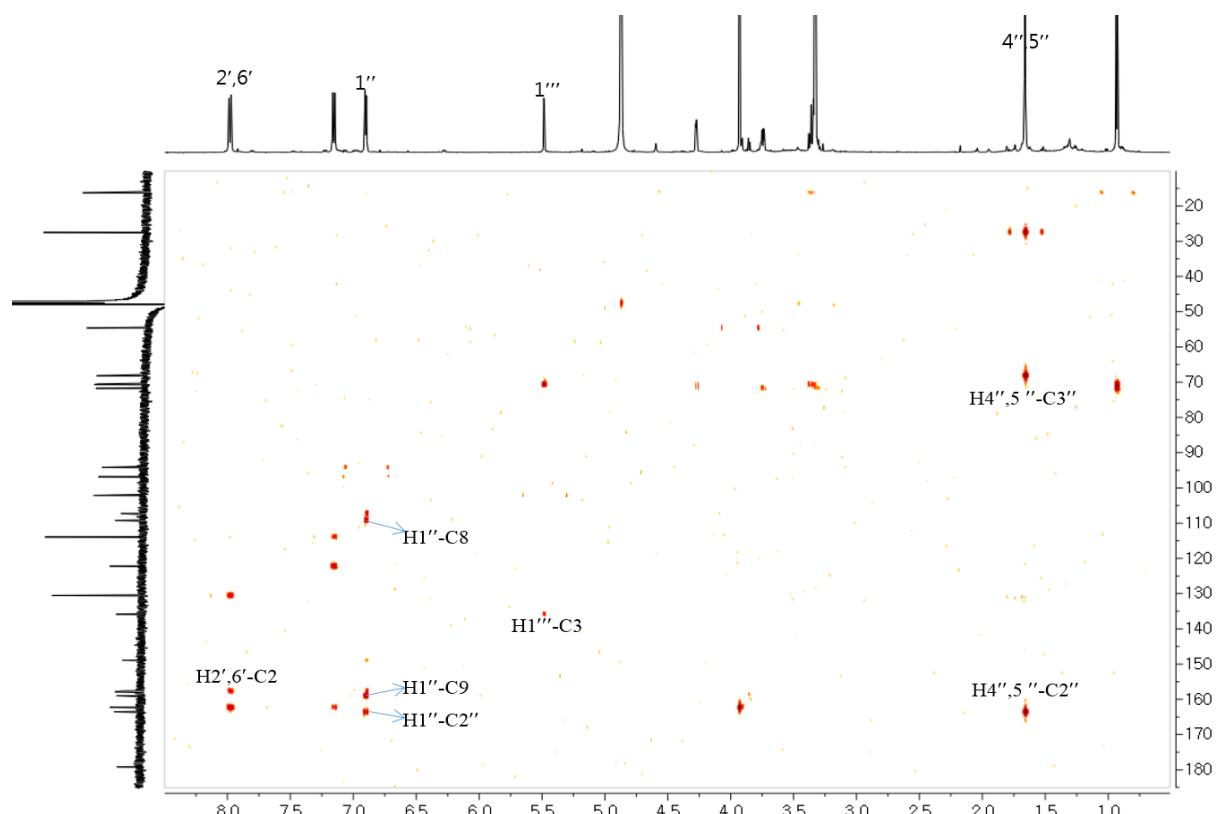
**Figure 8.** <sup>1</sup>H NMR spectrum of compound 8 (500 MHz, MeOD).



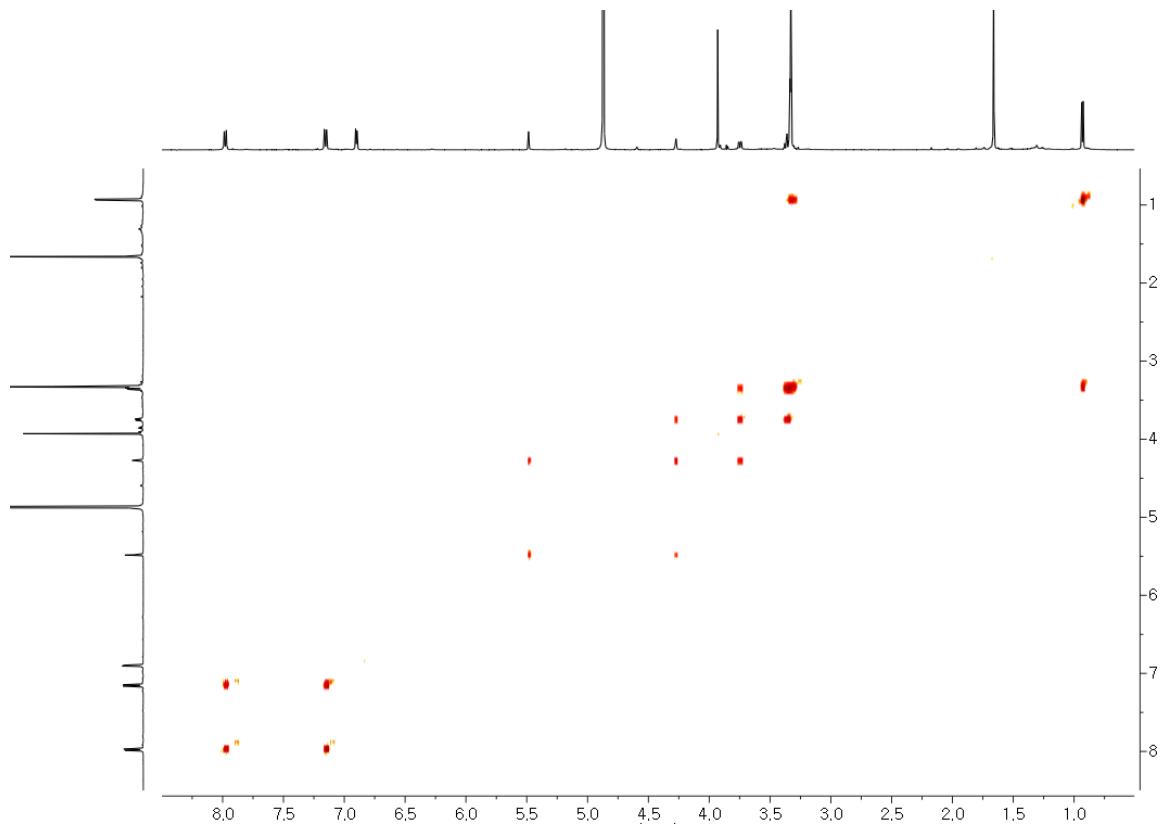
**Figure 9.** <sup>13</sup>C NMR spectrum of compound 8 (125 MHz, MeOD).



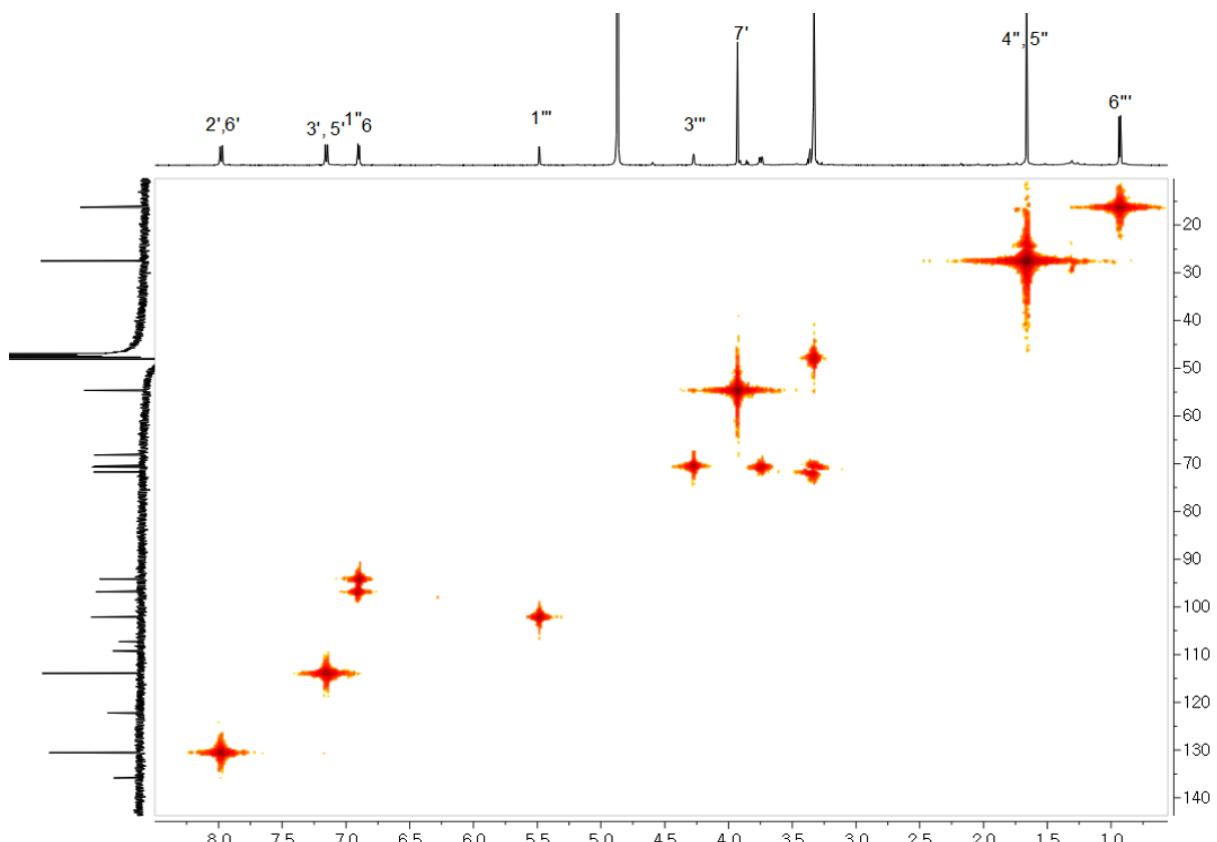
**Figure 10.** DEPT-90 and -135 spectrum of compound **8** (500 MHz, MeOD).



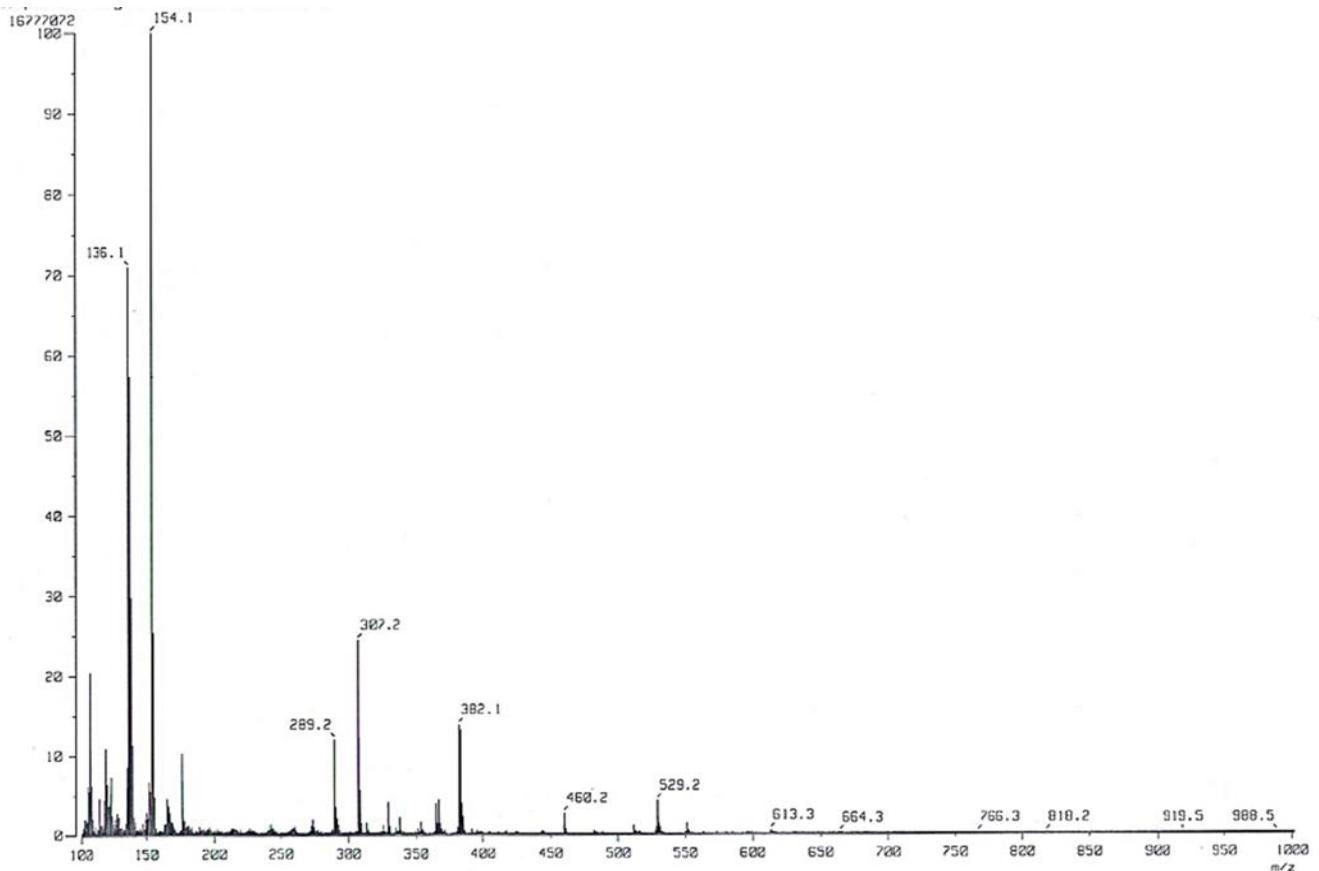
**Figure 11.** HMBC spectrum of compound **8** (500 MHz, MeOD).



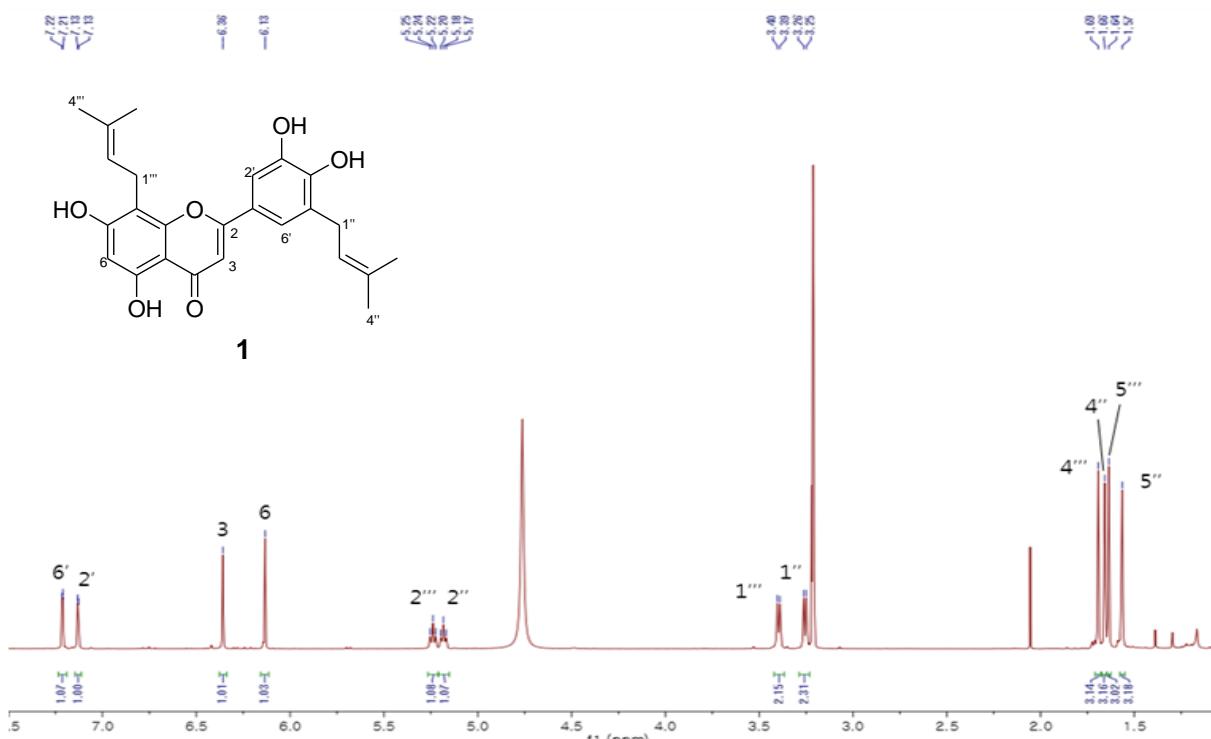
**Figure 12.** COSY spectrum of compound **8** (500 MHz, MeOD).



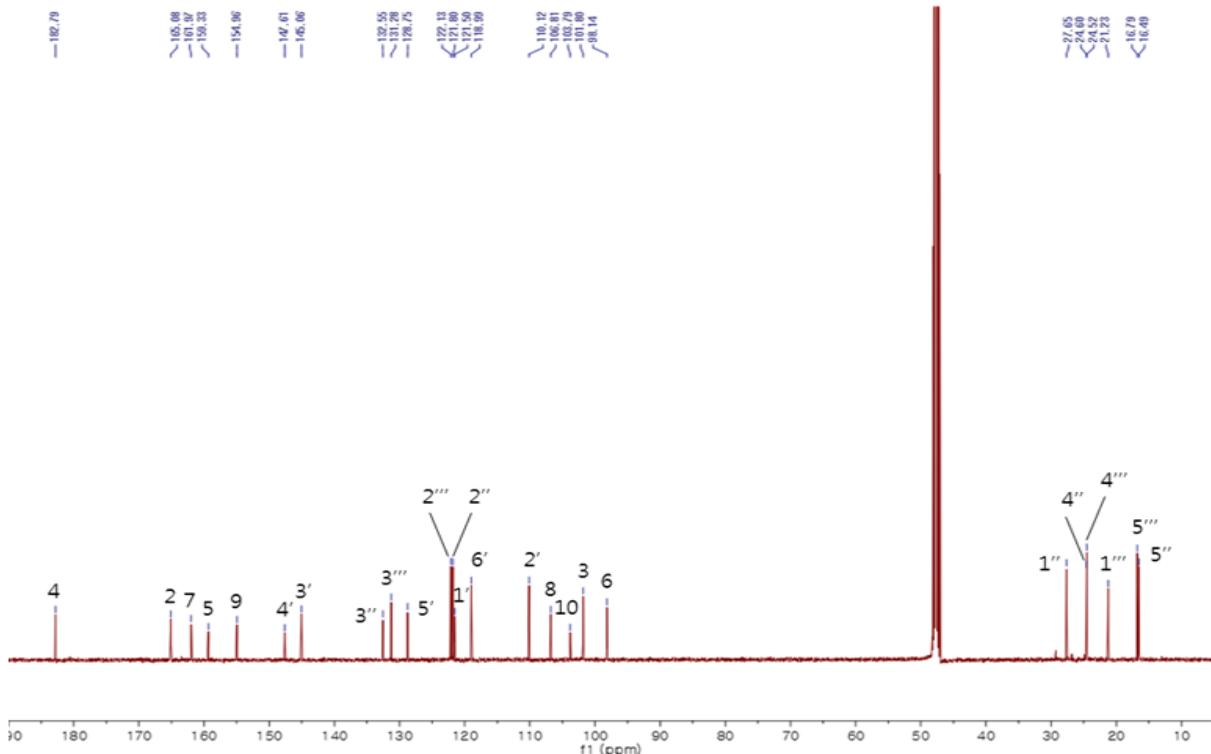
**Figure 13.** HMQC spectrum of compound **8** (500 MHz, MeOD).



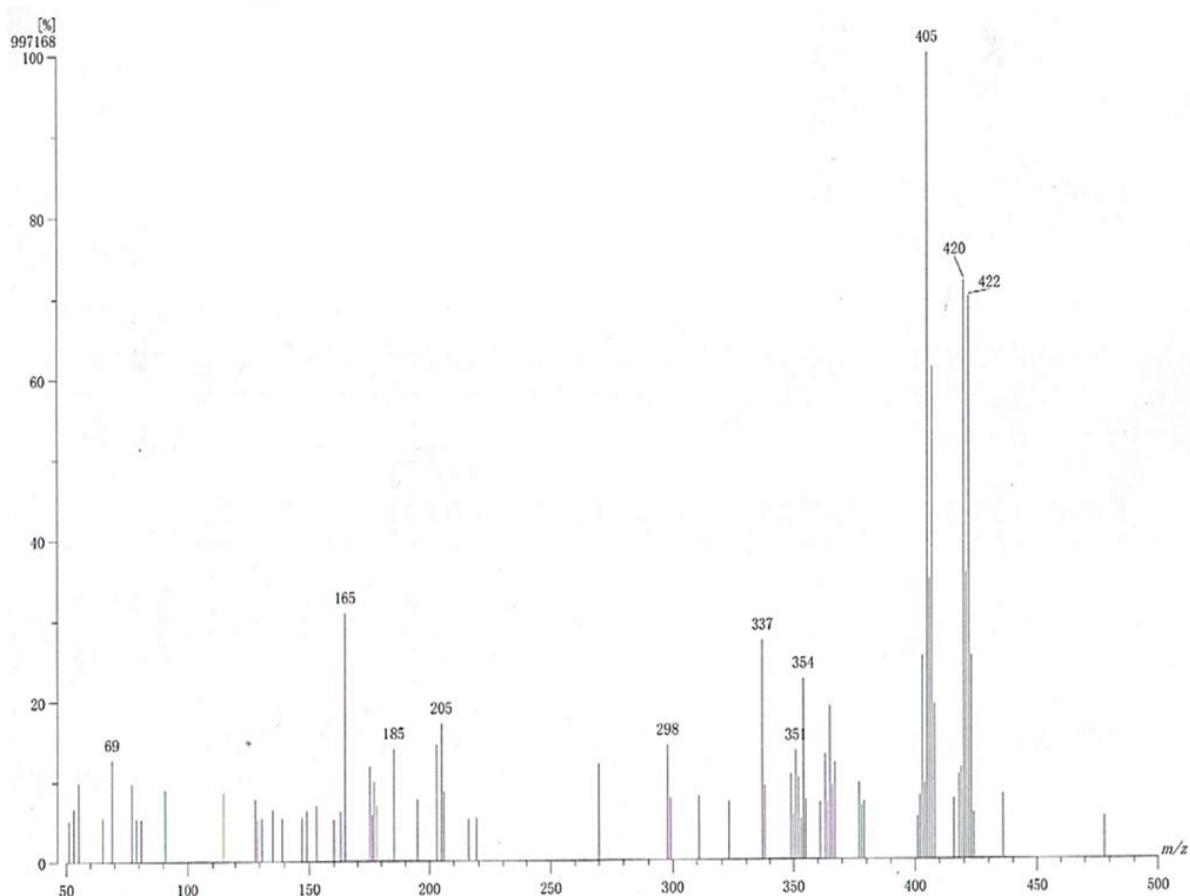
**Figure 14.** FABMS spectra and HRFABMS data of compound **8**.



**Figure 15.** <sup>1</sup>H-NMR spectrum of compound **1** (500 MHz, MeOD)



**Figure 16.** <sup>13</sup>C-NMR spectrum of compound **1** (500 MHz, MeOD)



Data : HM-1-HR      Date : 20-Mar-2018 15:43

Instrument : MStation

Sample :-

Note :-

Inlet : Direct      Ion Mode : EI+

RT : 1.34 min      Scan# : 21

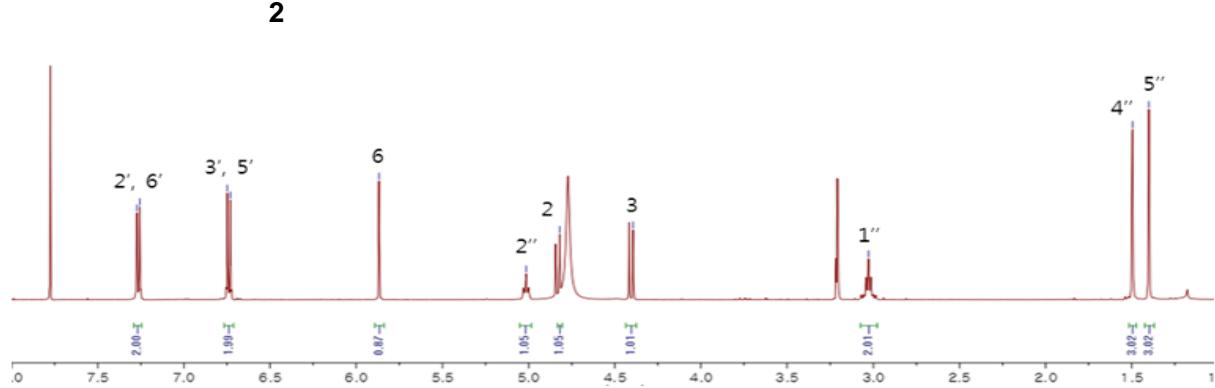
Elements : C 100/1, H 100/1, O 10/1

Mass Tolerance : 1000ppm, 3mmu if m/z > 3

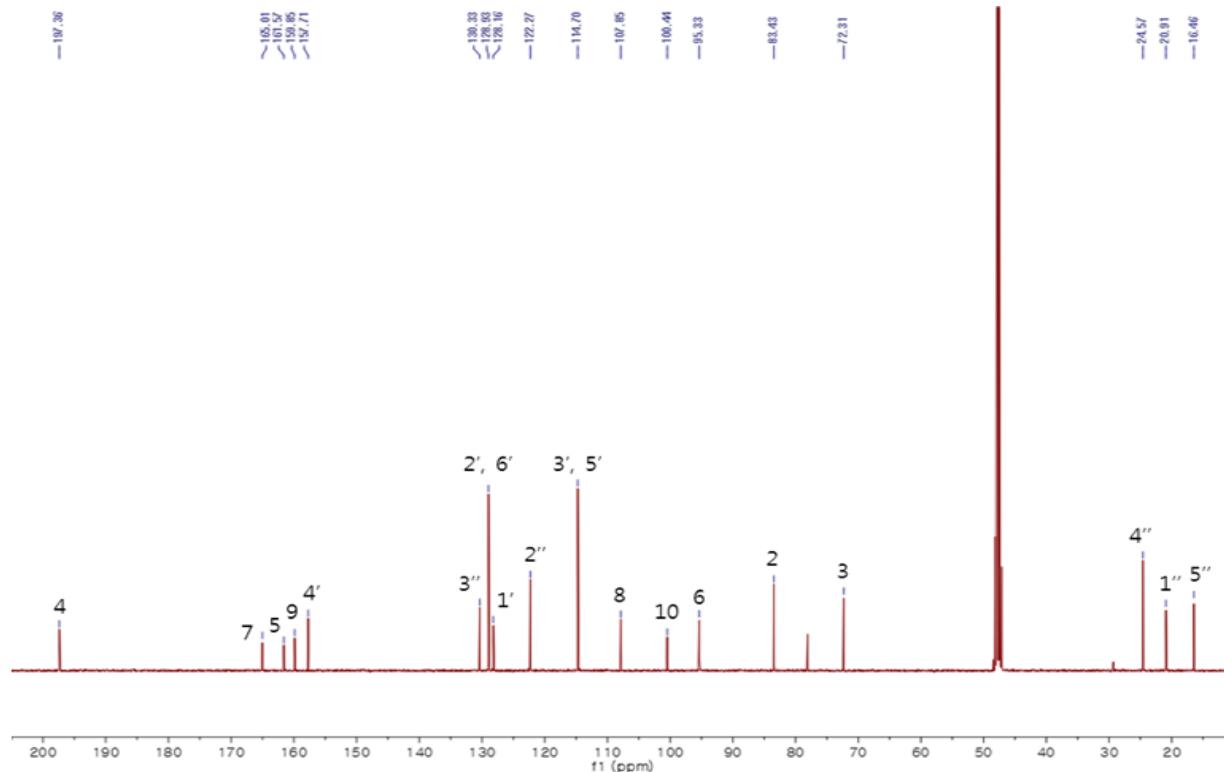
Unsaturation (U.S.) : -0.5 - 20.0

	Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
1	422.1721	27.76	-2.0 / -0.8	13.0	C25 H26 O6

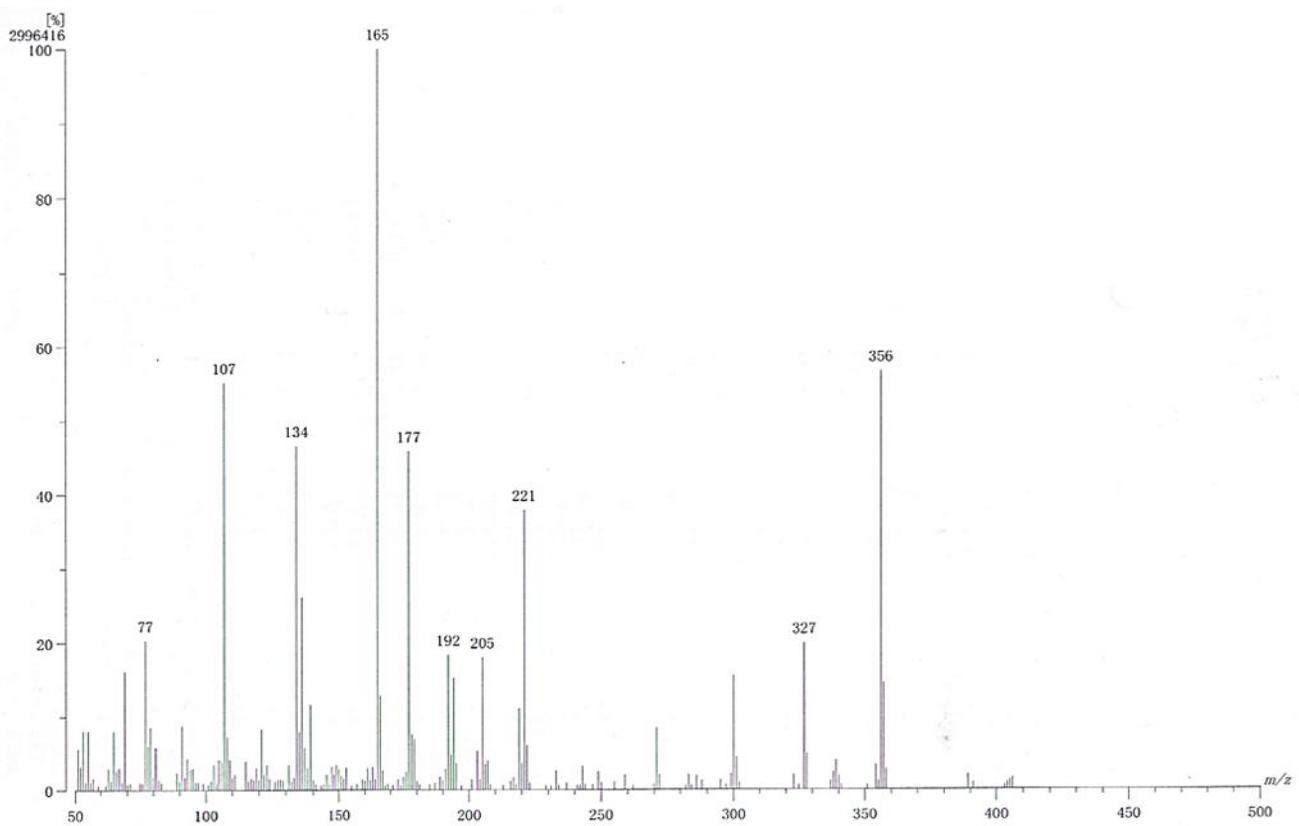
**Figure 17.** EIMS spectrum and HREIMS data of compound **1**



**Figure 18.**  $^1\text{H}$ -NMR spectrum of compound **2** (500 MHz, MeOD)



**Figure 19.**  $^{13}\text{C}$ -NMR spectrum of compound 2 (500 MHz, MeOD)



Data : HM-2-HR      Date : 20-Mar-2018 15:31

Instrument : MStation

Sample :-

Note :-

Inlet : Direct      Ion Mode : EI+

RT : 2.14 min      Scan# : 33

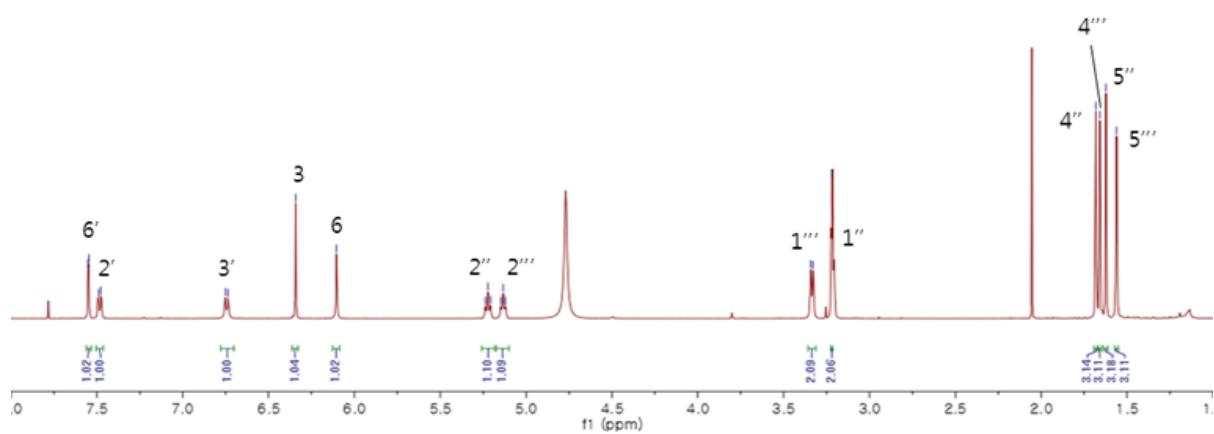
Elements : C 100/1, H 100/1, O 10/1

Mass Tolerance : 1000ppm, 5mmu if  $m/z > 5$

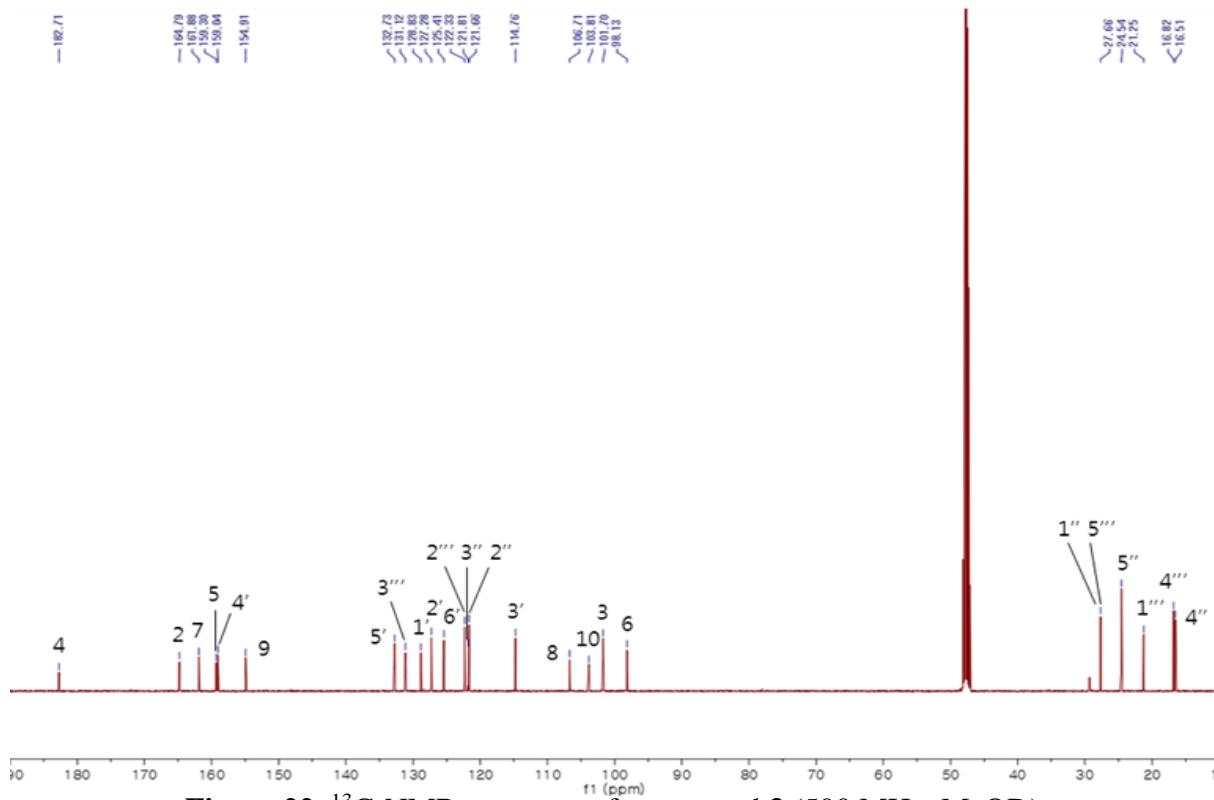
Unsaturation (U.S.) : -0.5 – 30.0

Observed $m/z$	Int %	Err [ppm / mmu]	U.S.	Composition
1      356.1262	35.81	+0.6 / +0.2	11.0	C20 H20 O6

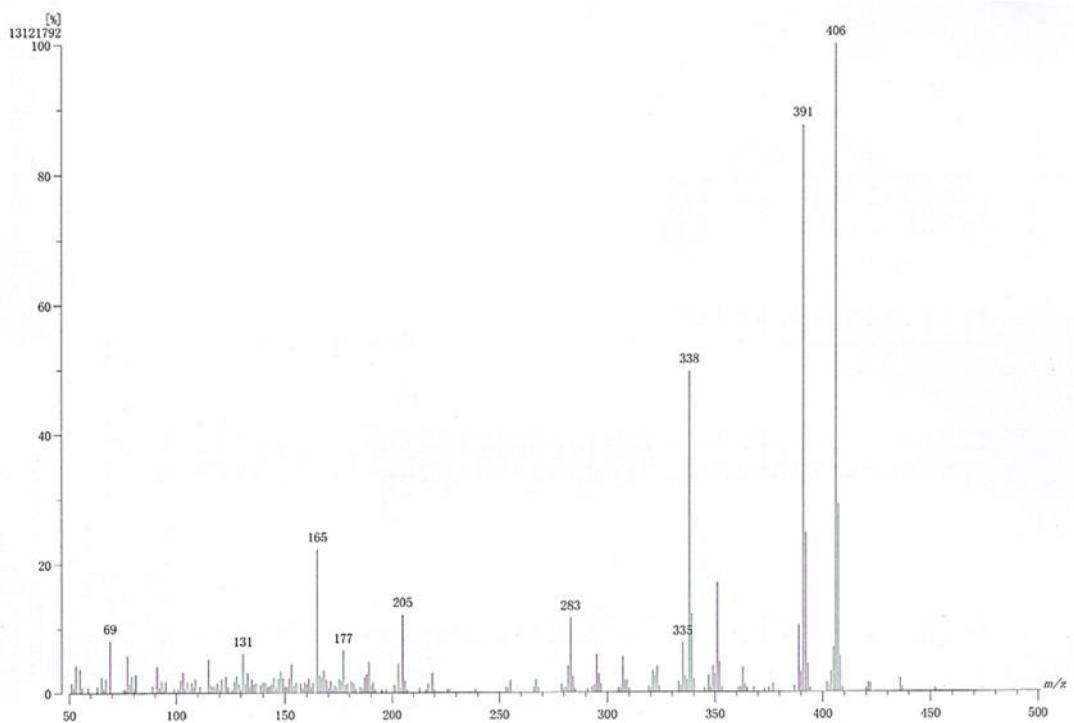
**Figure 20.** EIMS spectrum and HREIMS data of compound 2



**Figure 21.**  $^1\text{H}$ -NMR spectrum of compound **3** (500 MHz, MeOD)



**Figure 22.**  $^{13}\text{C}$ -NMR spectrum of compound **3** (500 MHz, MeOD)



Data : HM-3-HR Date : 20-Mar-2018 15:59

Instrument : MStation

Sample :-

Note :-

Inlet : Direct Ion Mode : EI+

RT : 1.34 min Scan# : 21

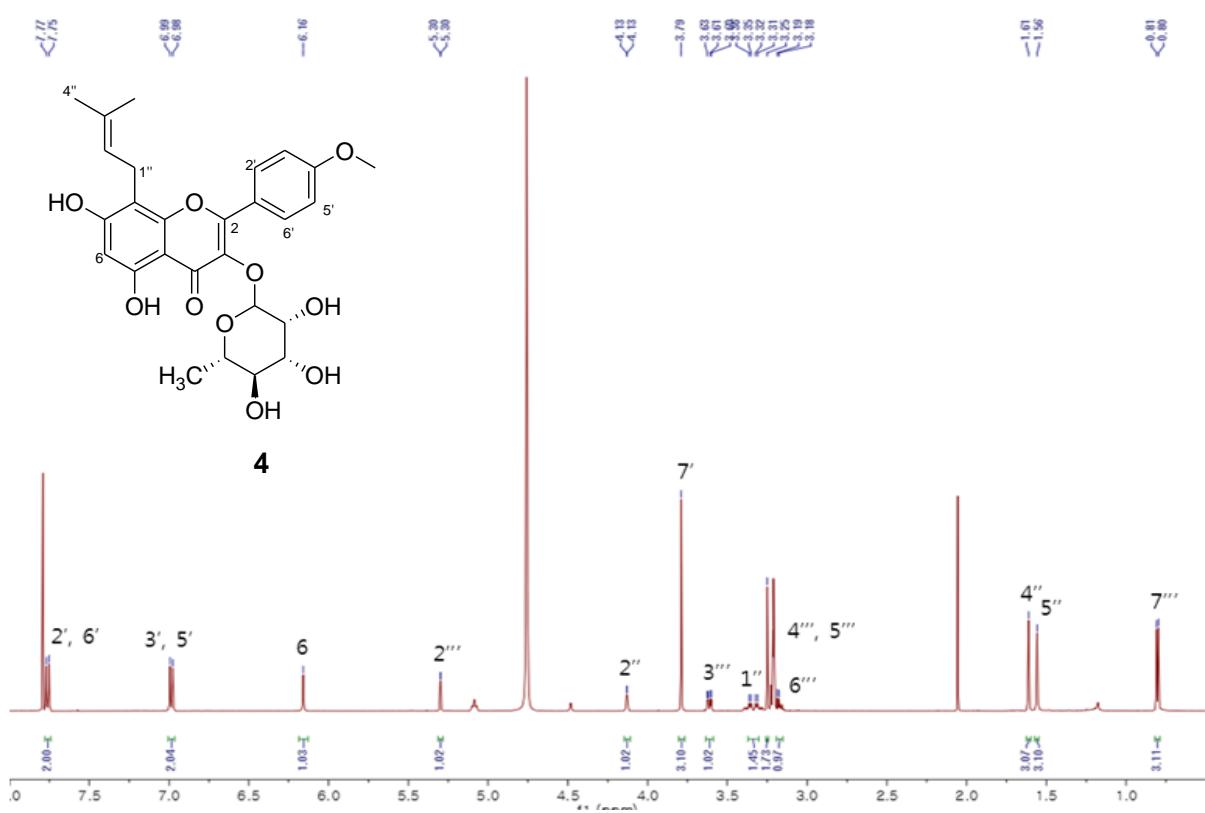
Elements : C 100/1, H 100/1, O 10/1

Mass Tolerance : 1000ppm, 3mmu if  $m/z > 3$

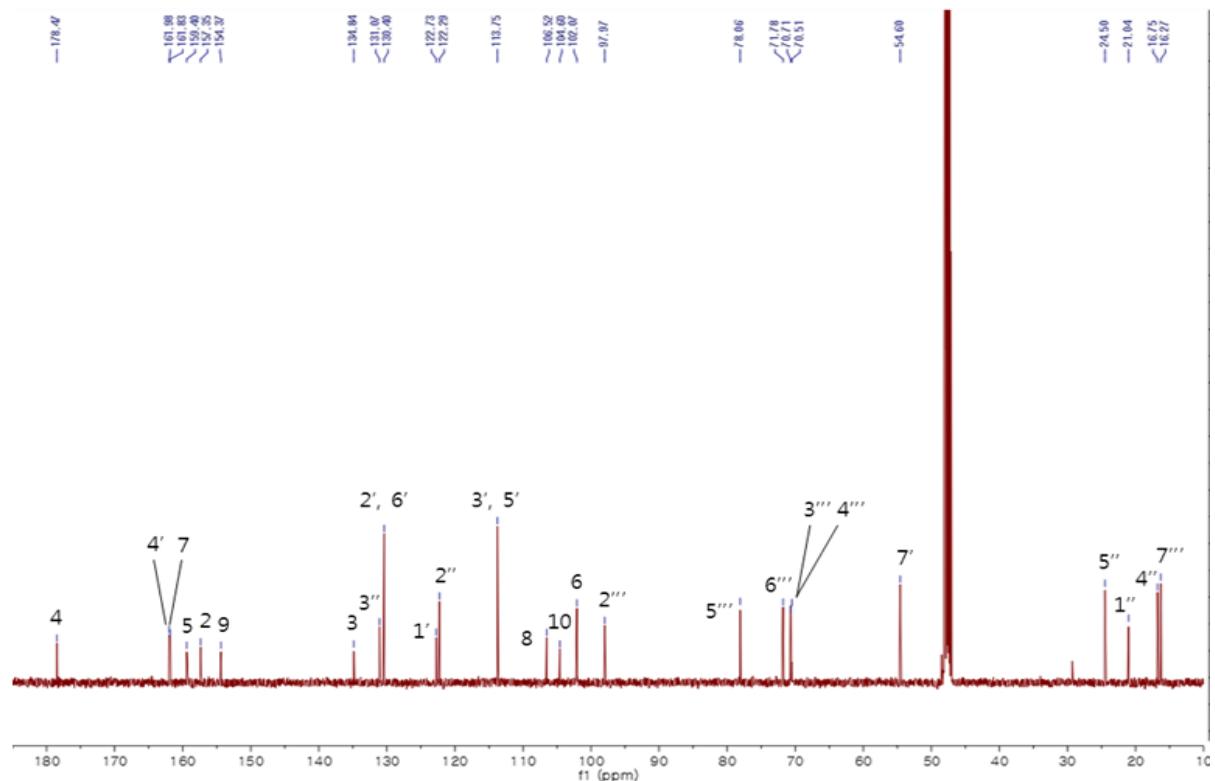
Unsaturation (U.S.) : -0.5 - 20.0

Observed $m/z$	Int%	Err [ppm / mmu]	U.S.	Composition
1 406.1784	100.00	+0.9 / +0.4	13.0	C <sub>25</sub> H <sub>26</sub> O <sub>5</sub>

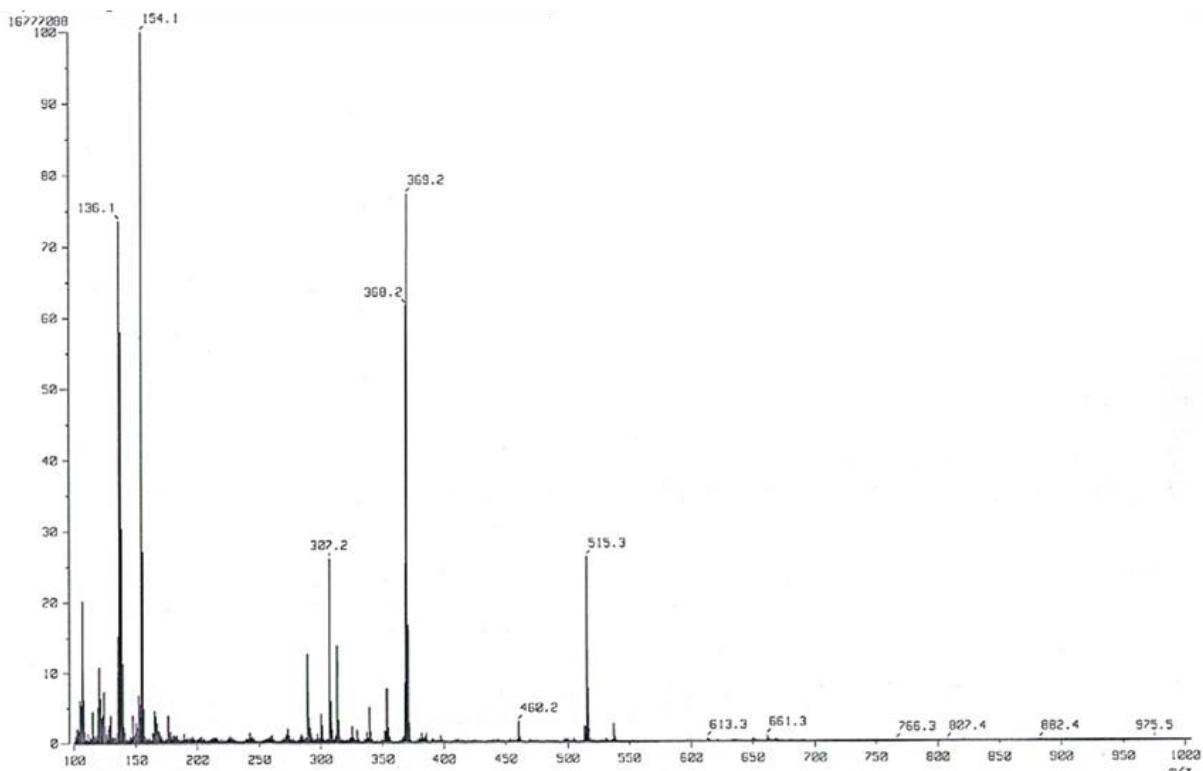
**Figure 23.** EIMS spectrum and HREIMS data of compound 3



**Figure 24.** <sup>1</sup>H-NMR spectrum of compound 4 (500 MHz, MeOD)



**Figure 25.** <sup>13</sup>C-NMR spectrum of compound 4 (500 MHz, MeOD)



[ Elemental Composition ]

Data : HM4-HR1

Date : 05-Apr-2018 15:22

Sample: -

Note : -

Inlet : Direct

Ion Mode : FAB+

RT : 0.84 min

Scan# : 11

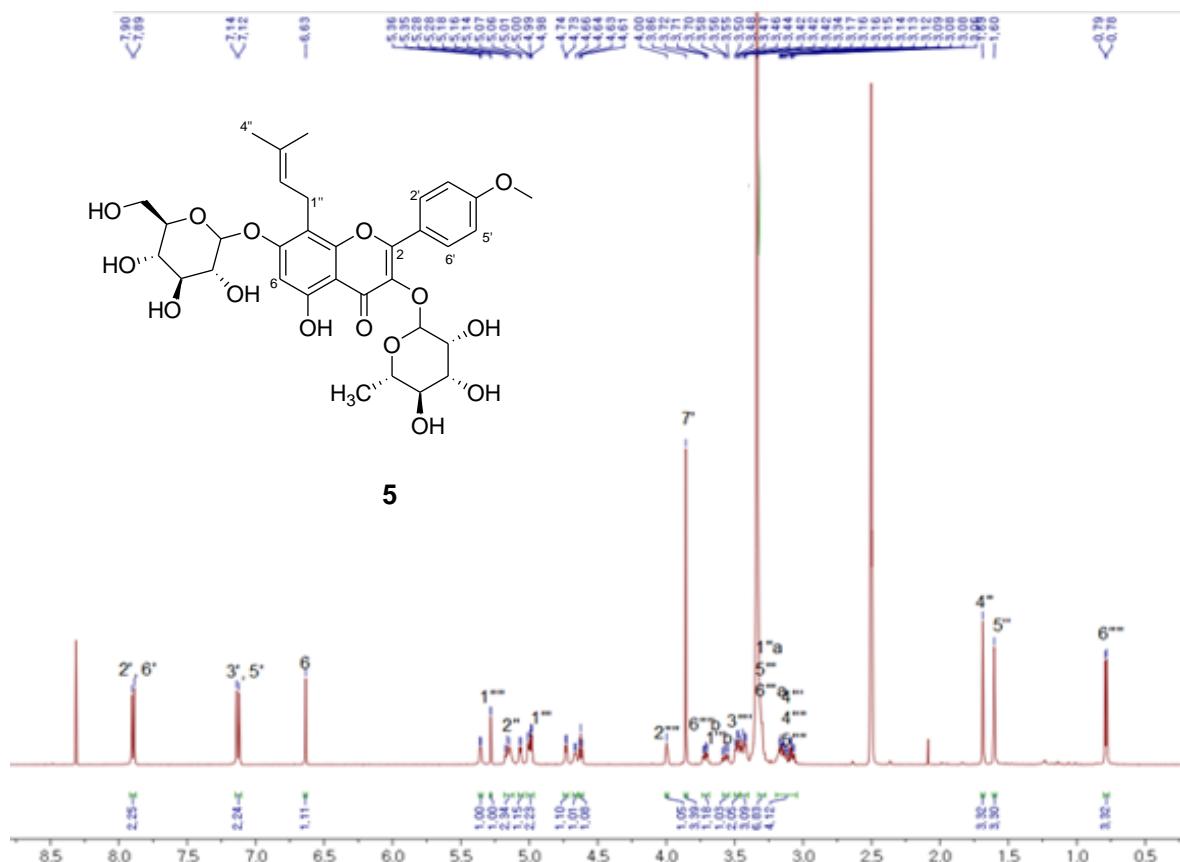
Elements : C 100/1, H 100/1, O 20/1

Mass Tolerance : 100ppm, 10mmu if m/z > 100

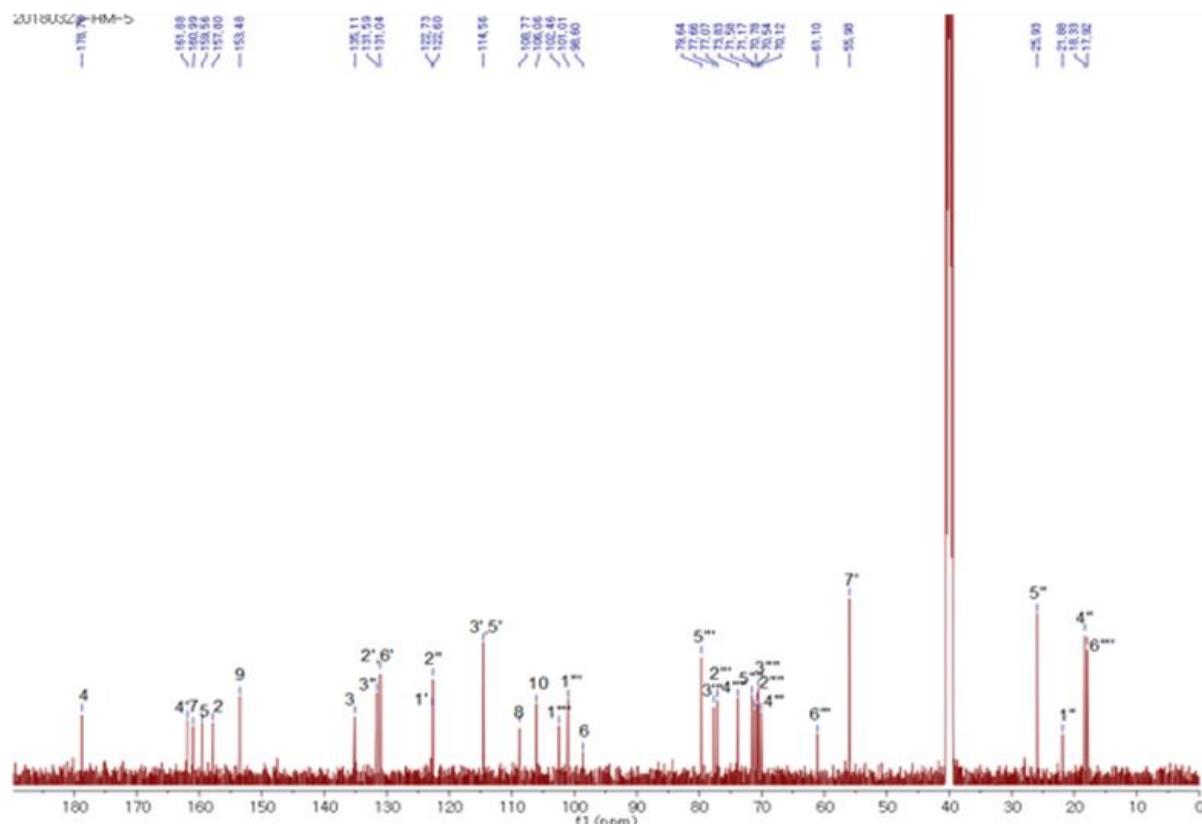
Unsaturation (U.S.) : 0.0 - 20.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
515.1893	10.2	-4.8 / -2.5	12.5	C 27 H 31 O 10
		-16.2 / -8.3	3.5	C 20 H 35 O 15

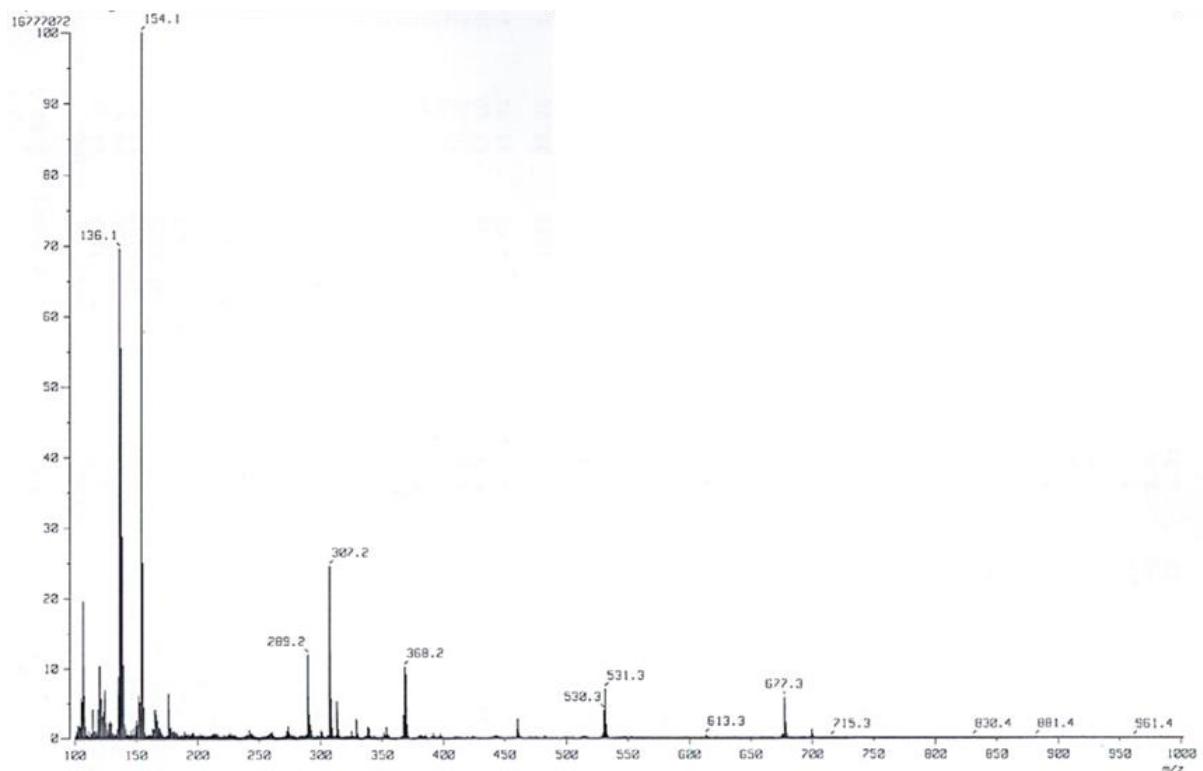
Figure 26. FABMS spectrum and HRFABMS data of compound 4



**Figure 27.**  $^1\text{H}$ -NMR spectrum of compound **5** (500 MHz, DMSO)

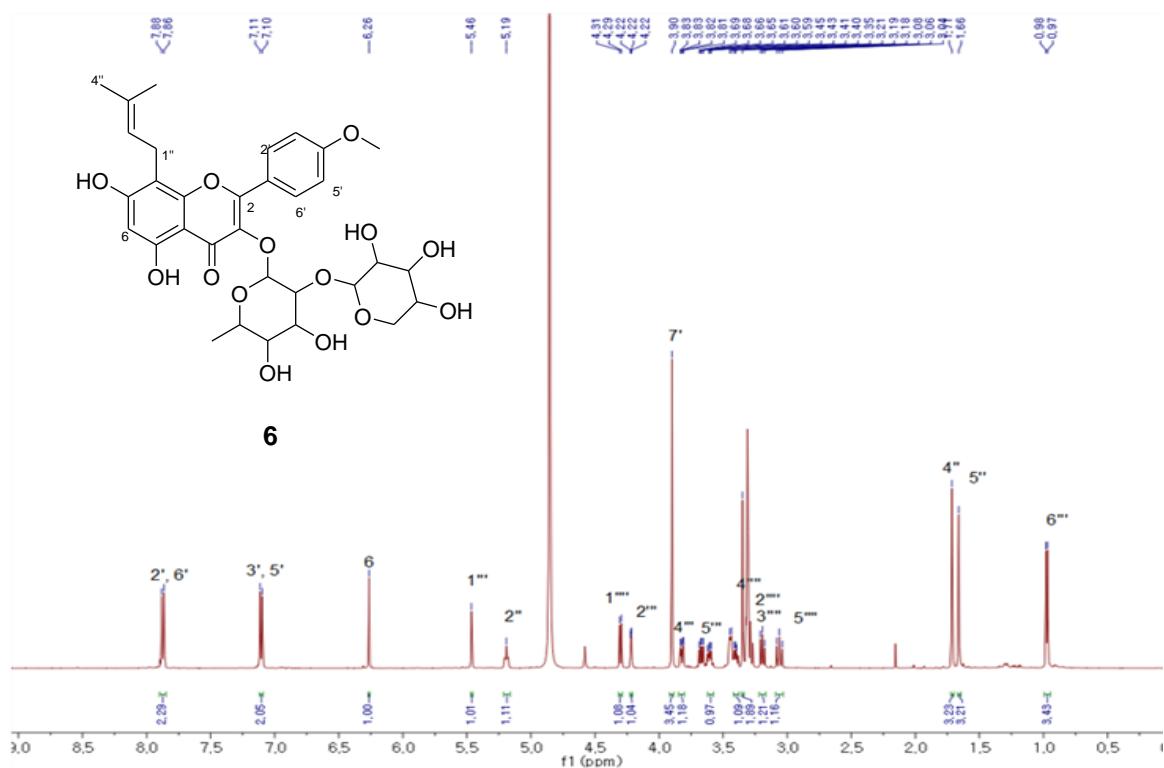


**Figure 28.**  $^{13}\text{C}$ -NMR spectrum of compound 5 (500 MHz, DMSO)

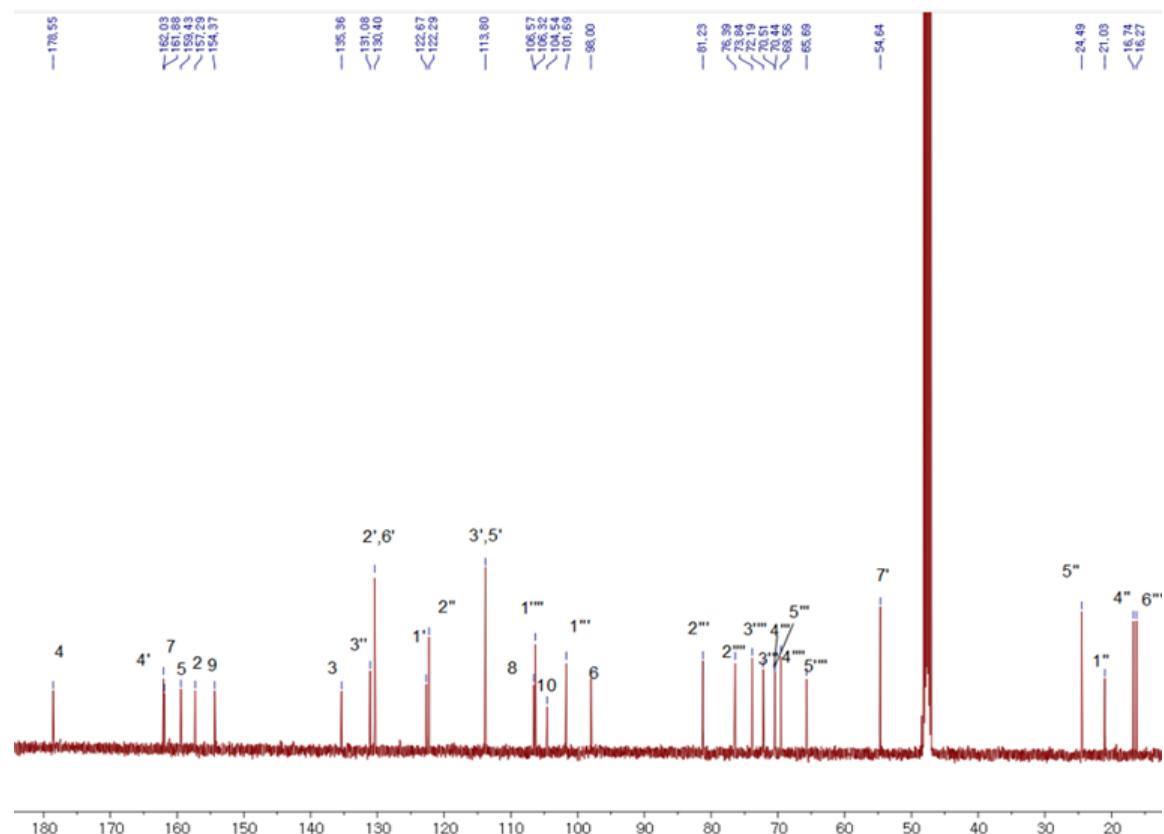


[ Elemental Composition ]  
 Data : HM-5-HR1 Date : 05-Apr-2018 15:58  
 Sample: -  
 Note : -  
 Inlet : Direct Ion Mode : FAB+  
 RT : 1.00 min Scan#: 13  
 Elements : C 100/1, H 100/1, O 20/1  
 Mass Tolerance : 100ppm, 10mmu if m/z > 100  
 Unsaturation (U.S.) : 0.0 - 20.0  
 Observed m/z Int% Err [ppm / mmu] U.S. Composition  
 677.2460 20.1 +2.2 / +1.5 13.5 C 33 H 41 O 15  
 -6.5 / -4.4 4.5 C 26 H 45 O 20

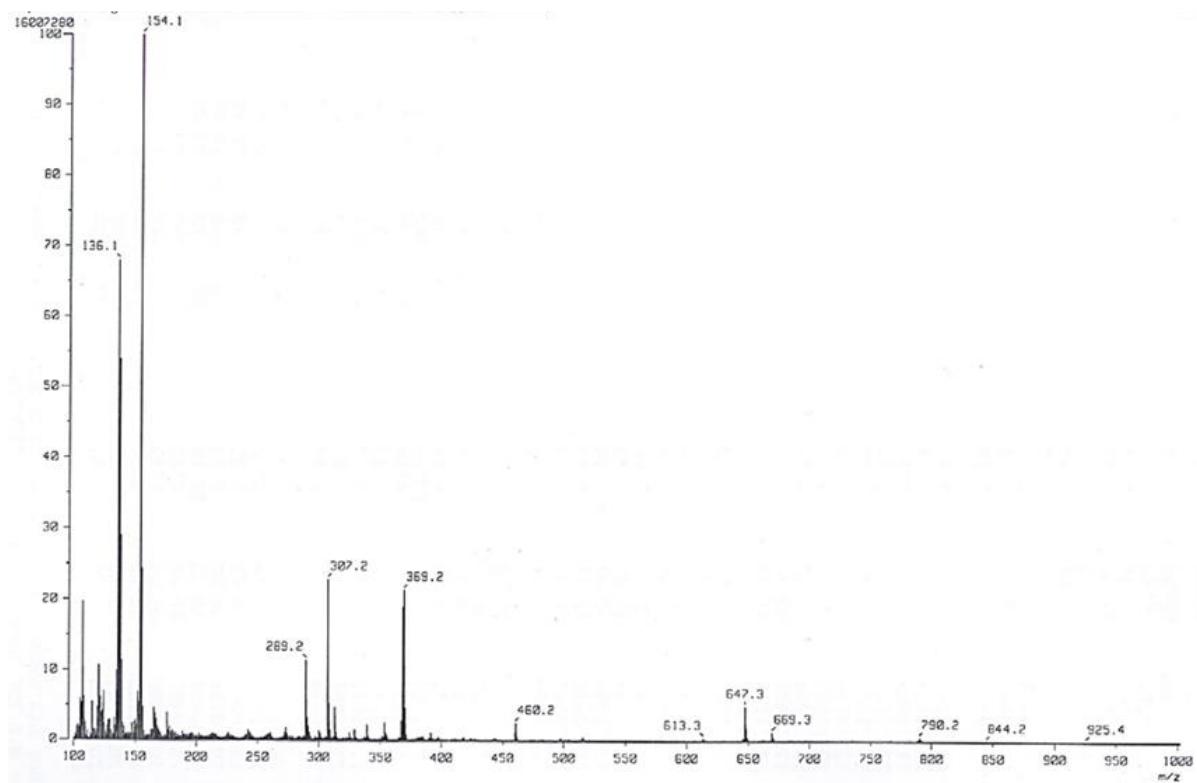
**Figure 29.** FABMS spectrum and HRFABMS data of compound 5



**Figure 30.** <sup>1</sup>H-NMR spectrum of compound **6** (500 MHz, MeOD)



**Figure 31.** <sup>13</sup>C-NMR spectrum of compound **6** (500 MHz, MeOD)



[ Elemental Composition ]

Data : HM-6-HR1

Date : 05-Apr-2018 16:11

Sample: -

Note : -

Inlet : Direct

Ion Mode : FAB+

RT : 0.84 min

Scan# : 11

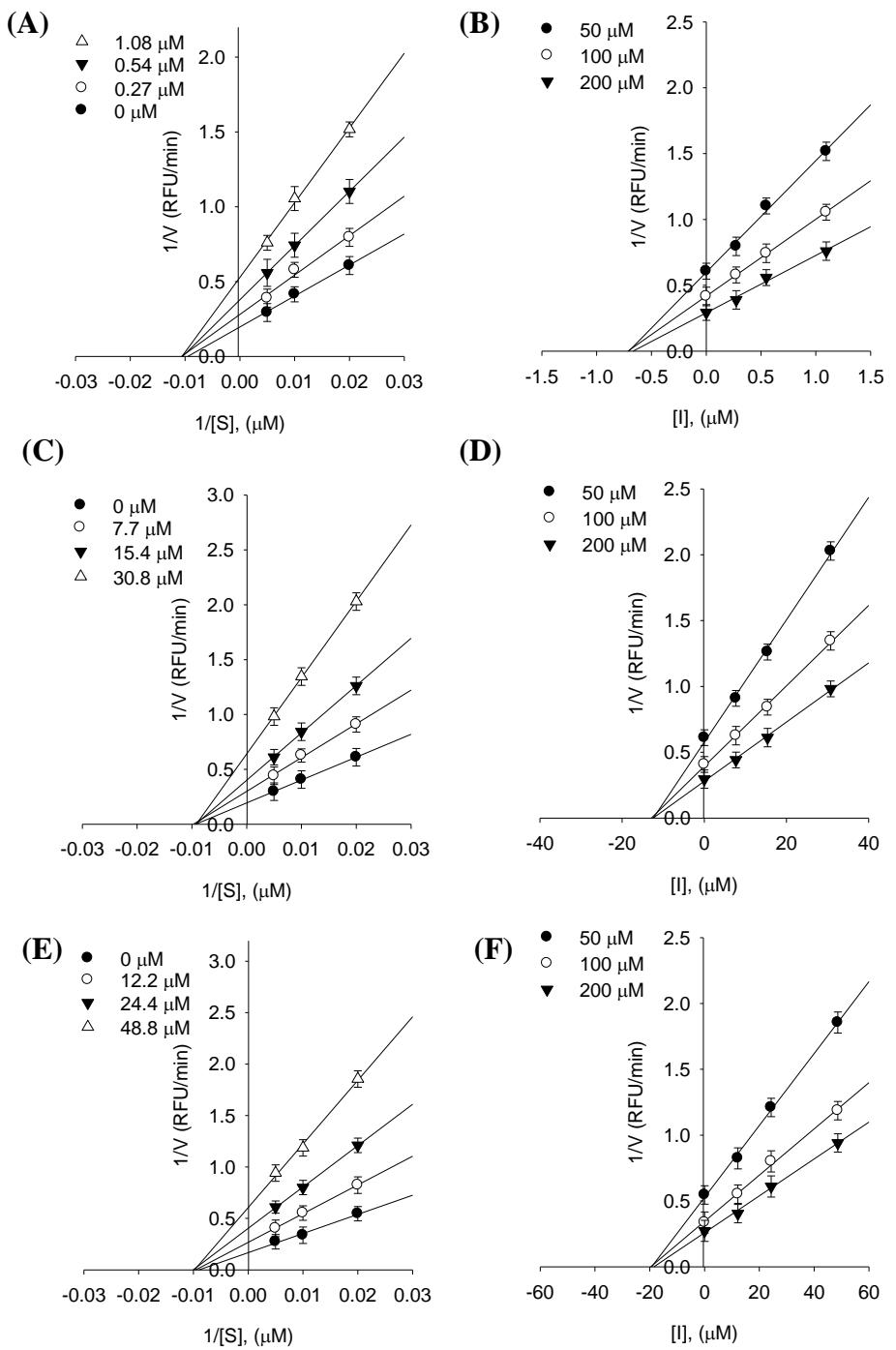
Elements : C 100/1, H 100/1, O 20/1

Mass Tolerance : 100ppm, 10mmu if m/z > 100

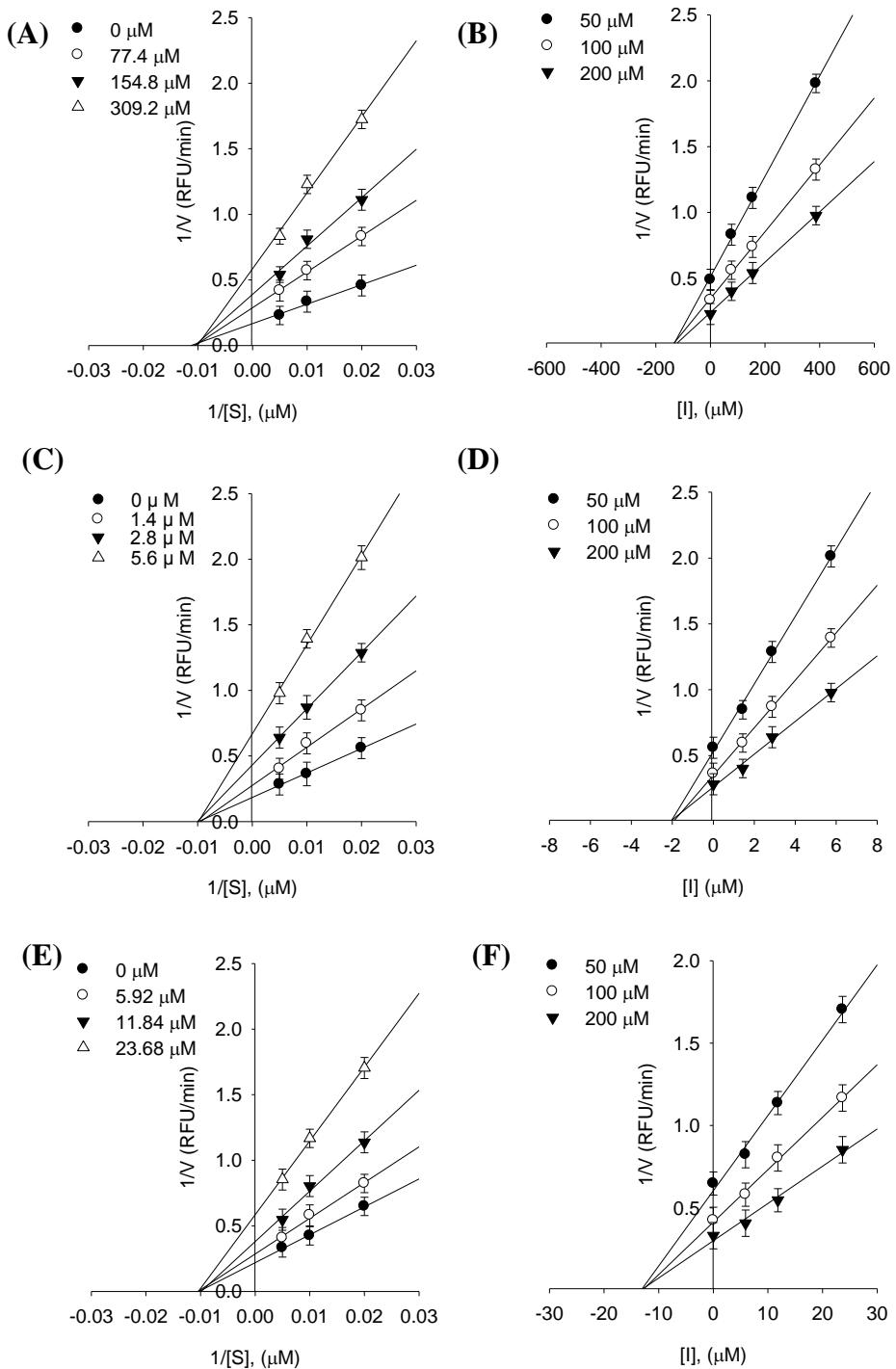
Unsaturation (U.S.) : 0.0 - 20.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
647.2369	27.6	+4.6 / +3.0	13.5	C 32 H 39 O 14
		-4.5 / -2.9	4.5	C 25 H 43 O 19

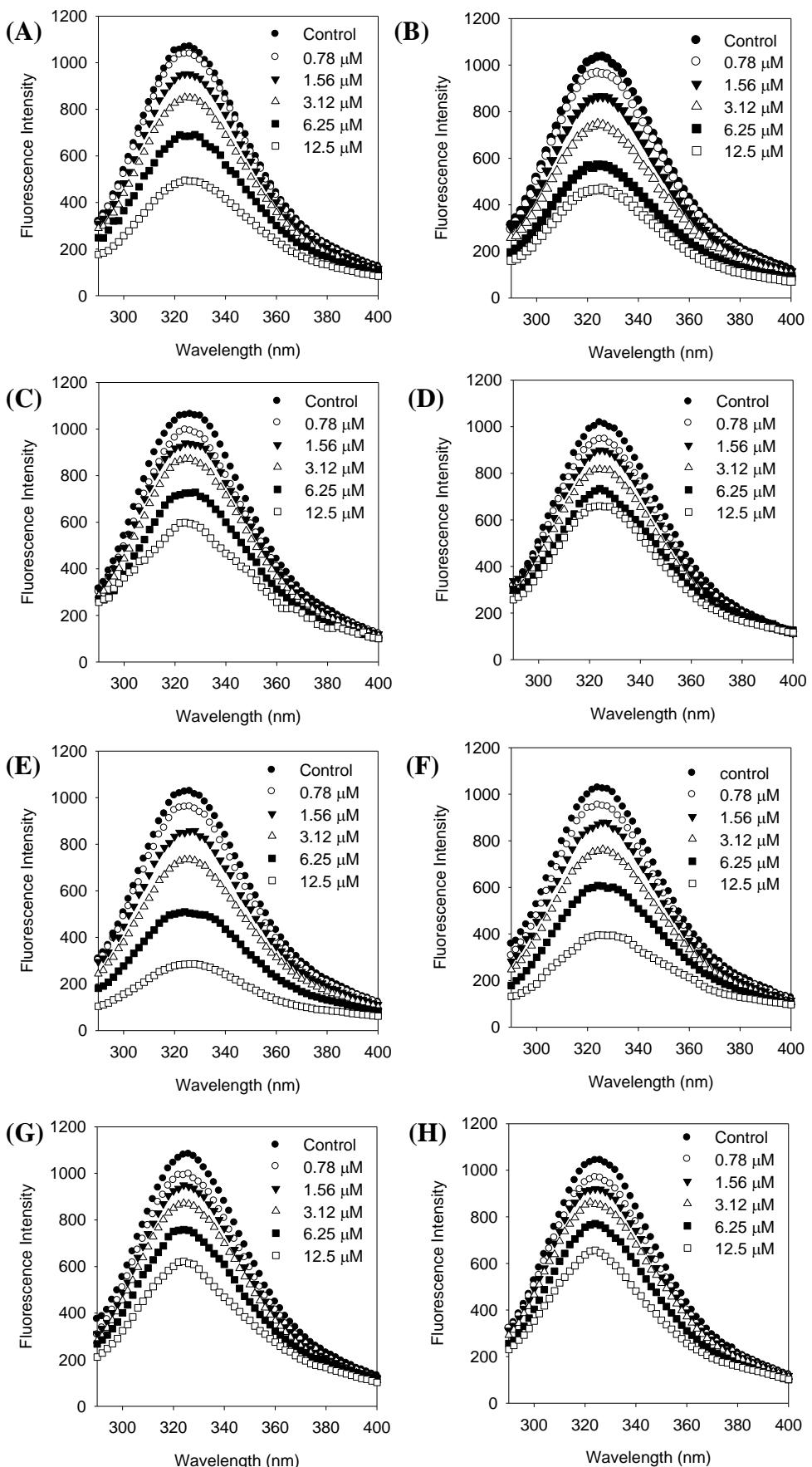
Figure 32. FABMS spectrum and HRFABMS data of compound 6



**Figure 33.** (A, C, E) Lineweaver-Burk plots of compounds **2-4** on bacterial neuraminidase inhibition, (B, D, F) Dixon plots of compounds **2-4** on bacterial neuraminidase inhibition.



**Figure 34.** (A, C, E) Lineweaver-Burk plots of compounds **6-8** on bacterial neuraminidase inhibition, (B, D, F) Dixon plots of compounds **6-8** on bacterial neuraminidase inhibition.



**Figure 35.** Fluorescence quenching effect of (A-H) 3-8, luteolin, and apigenin, respectively.