Supplementary materials

Xanthine Oxidase Inhibition and Anti-LDL Oxidation by Prenylated Isoflavones from *Flemingia philippinensis* root

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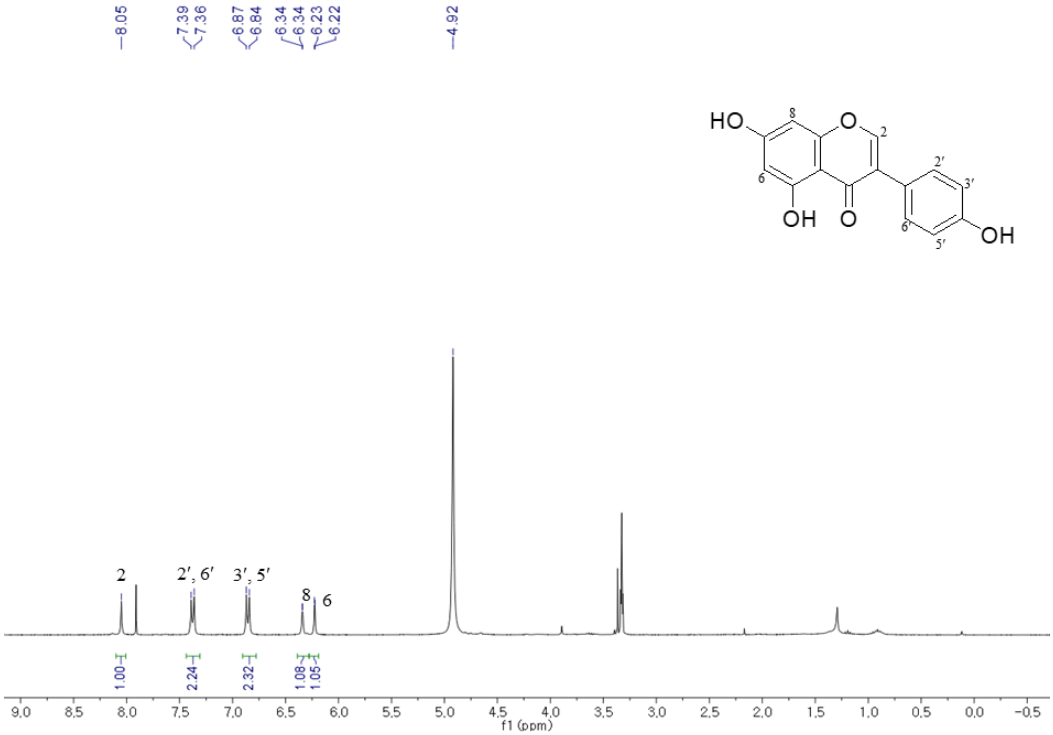

Figure S1. ^{1}H-NMR spectrum of compound **1** (500 MHz, CD_3OD)

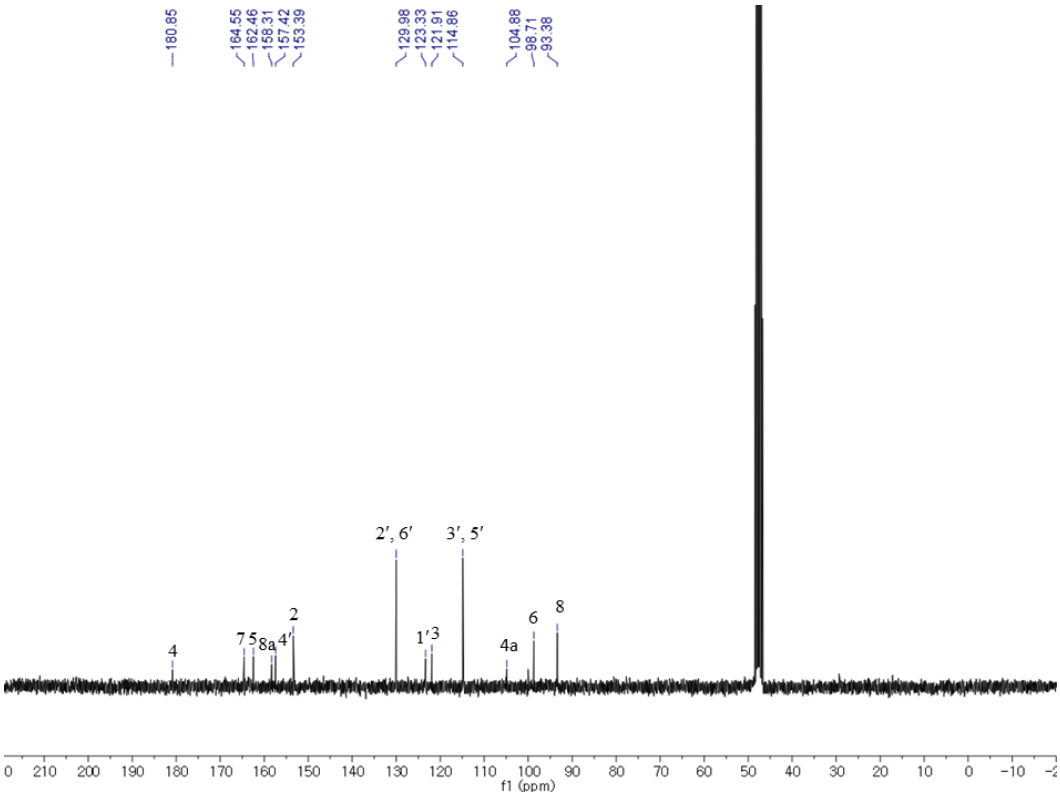

Figure S2. ^{13}C-NMR spectrum of compound **1** (125 MHz, CD_3OD)

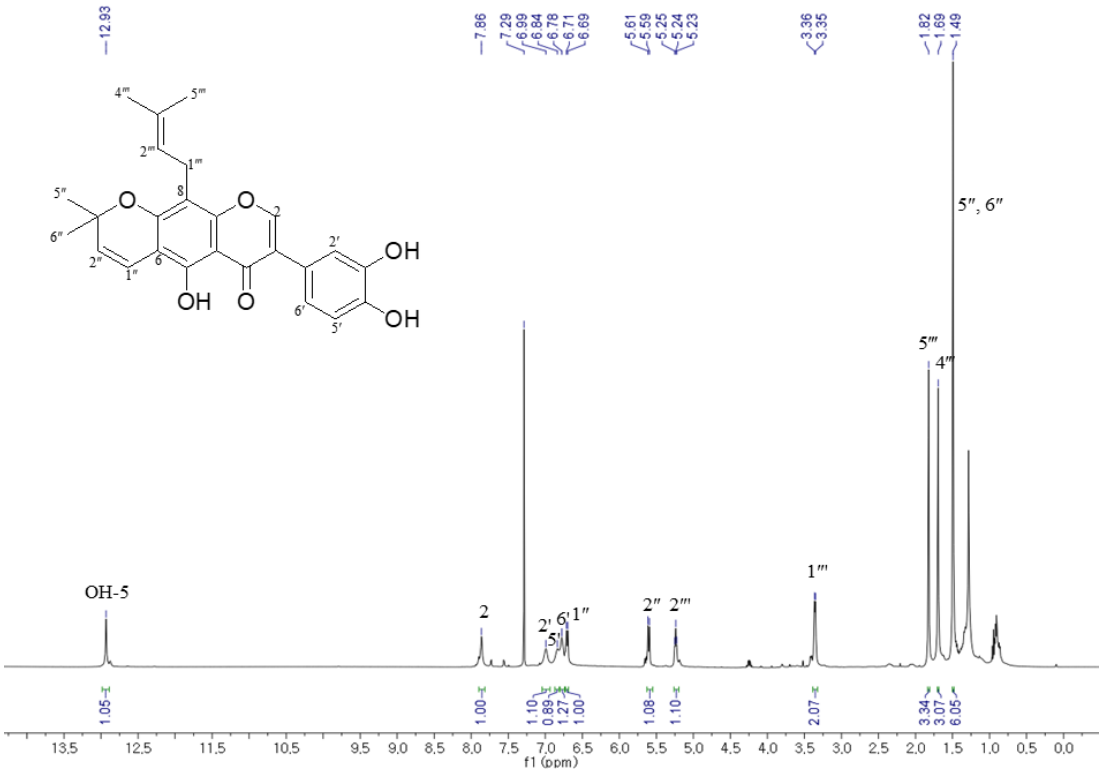

Figure S3. ^{1}H-NMR spectrum of compound **2** (500 MHz, $CDCl_3$)

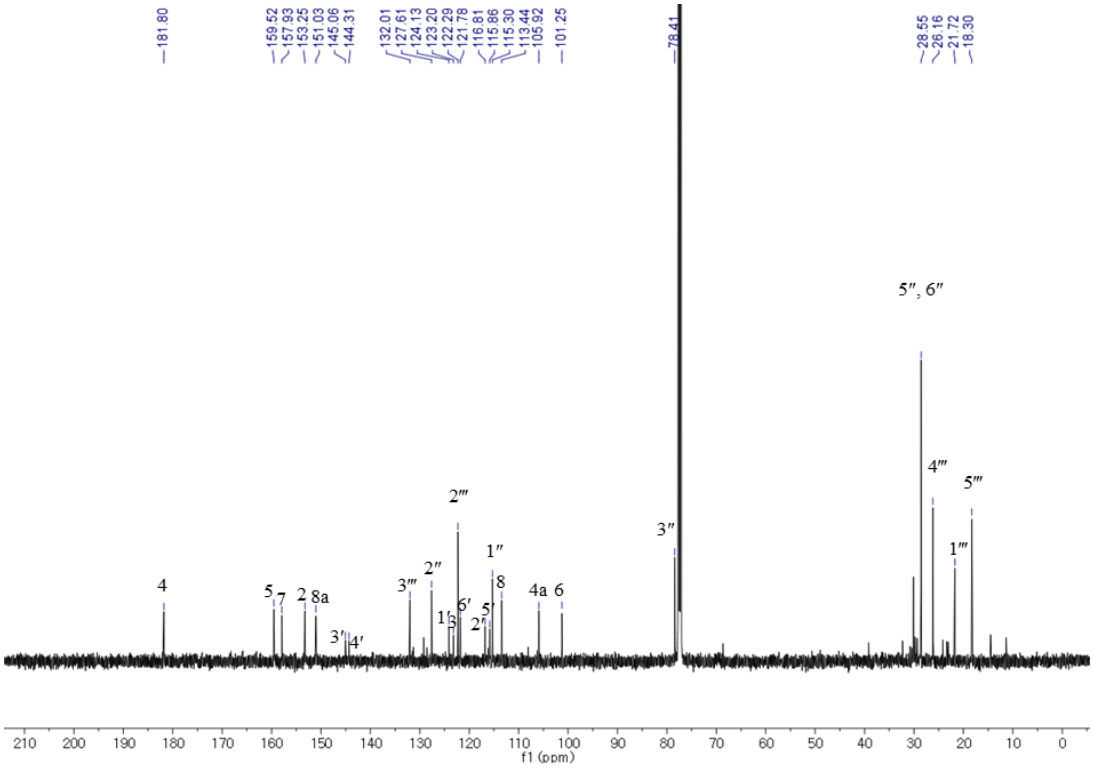

Figure S4. ^{13}C-NMR spectrum of compound **2** (125 MHz, $CDCl_3$)

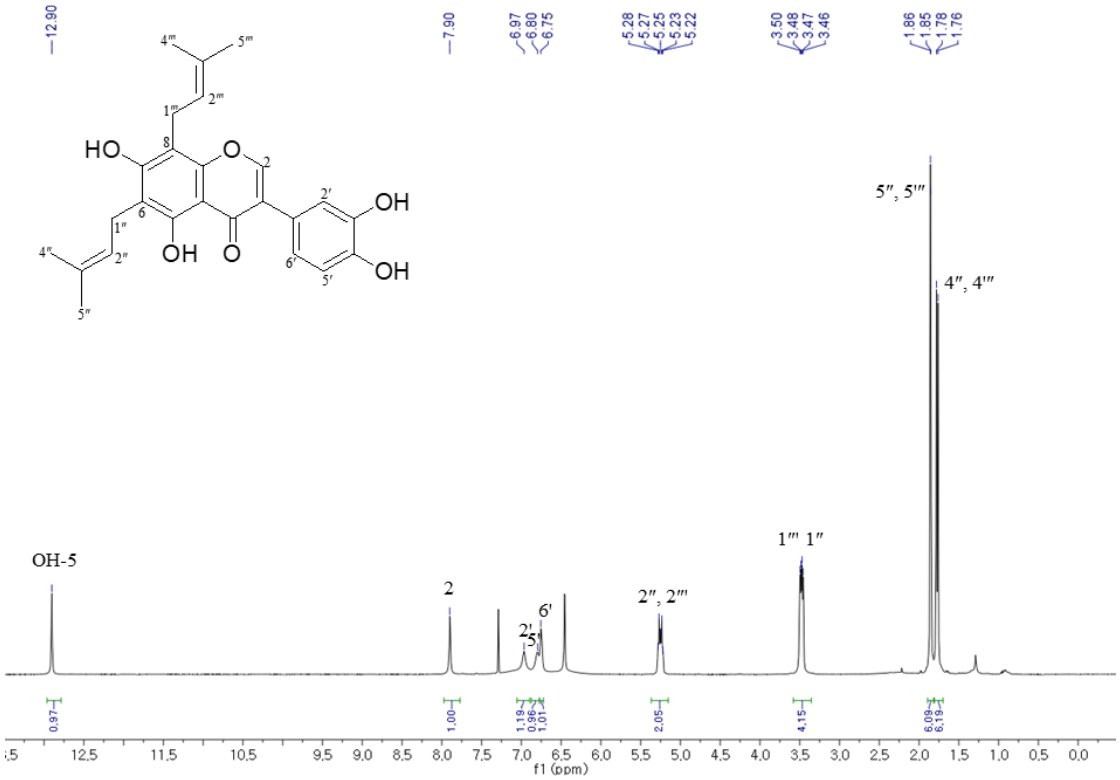

Figure S5. ^{1}H-NMR spectrum of compound **3** (500 MHz, Acetone-d_6)

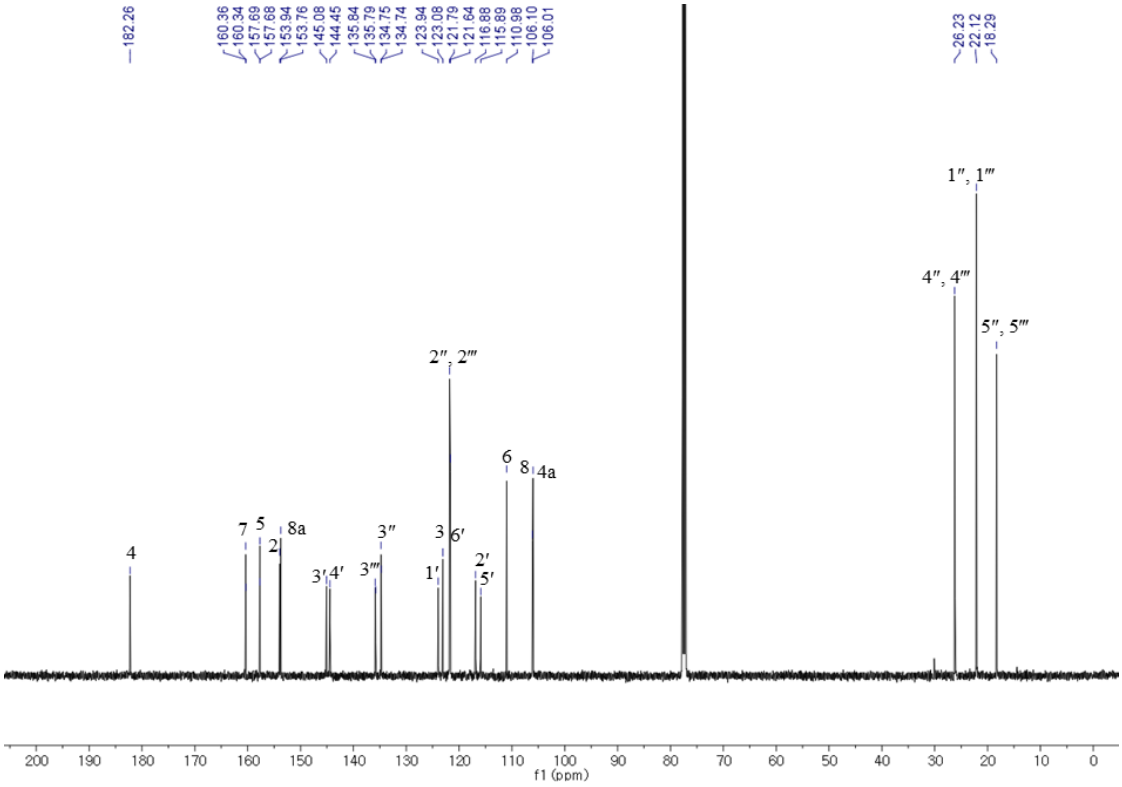

Figure S6. ^{13}C-NMR spectrum of compound **3** (125 MHz, Acetone-d_6)

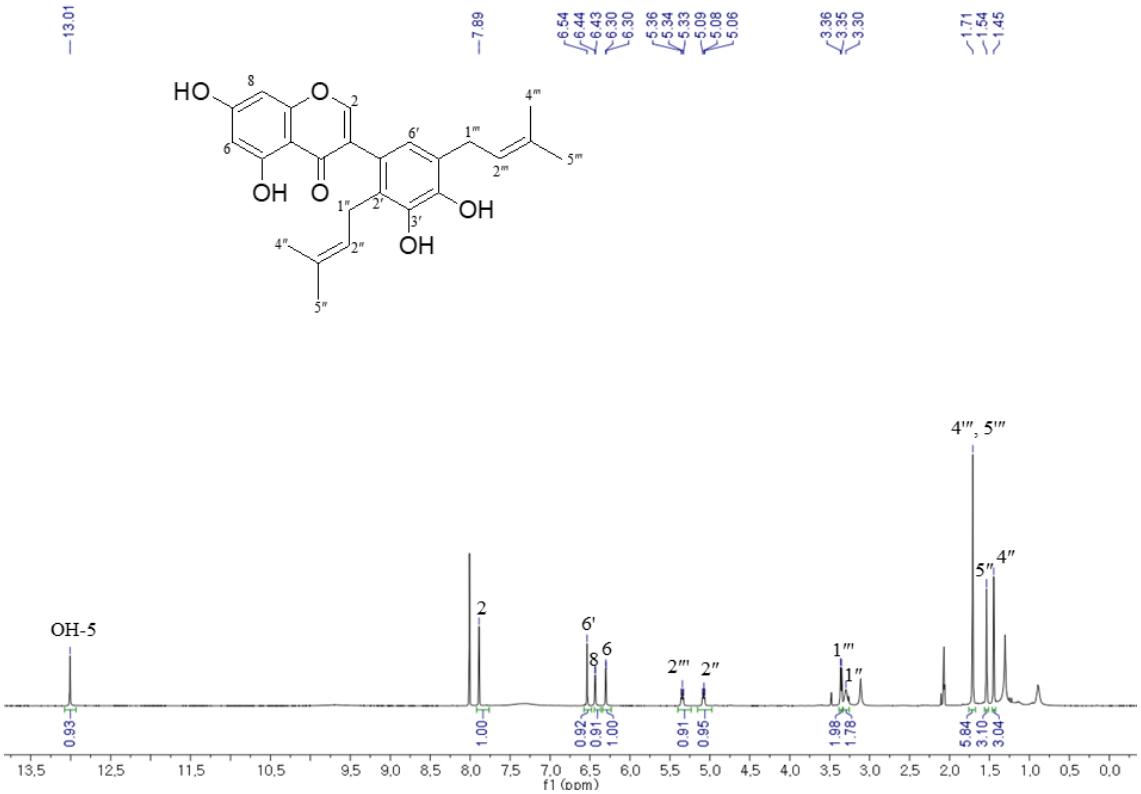

Figure S7. ^{1}H-NMR spectrum of compound **4** (500 MHz, Acetone-d_6)

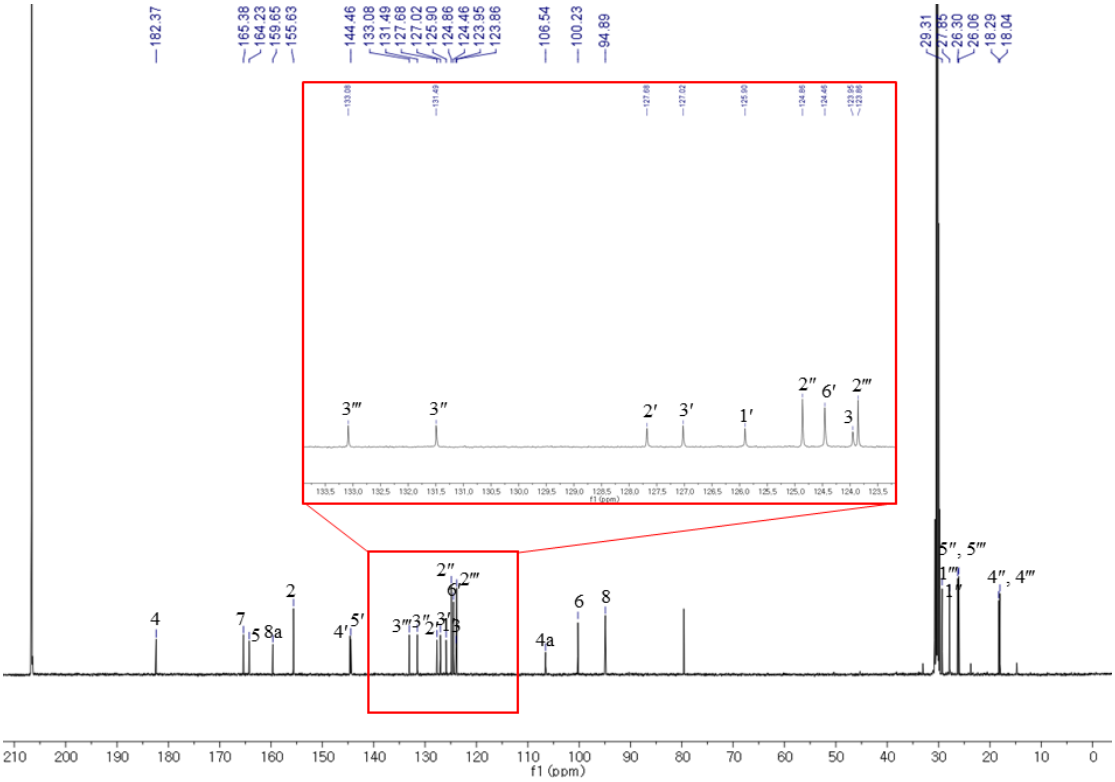

Figure S8. ^{13}C-NMR spectrum of compound **4** (125 MHz, Acetone-d_6)

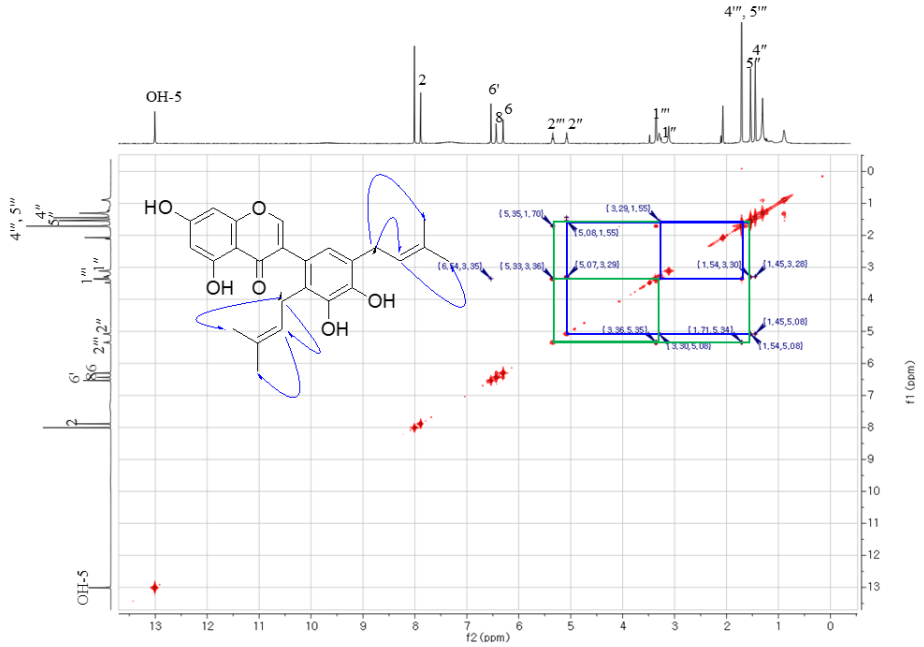

Figure S9. COSY spectrum of compound **4** (500 MHz, Acetone-d_6)

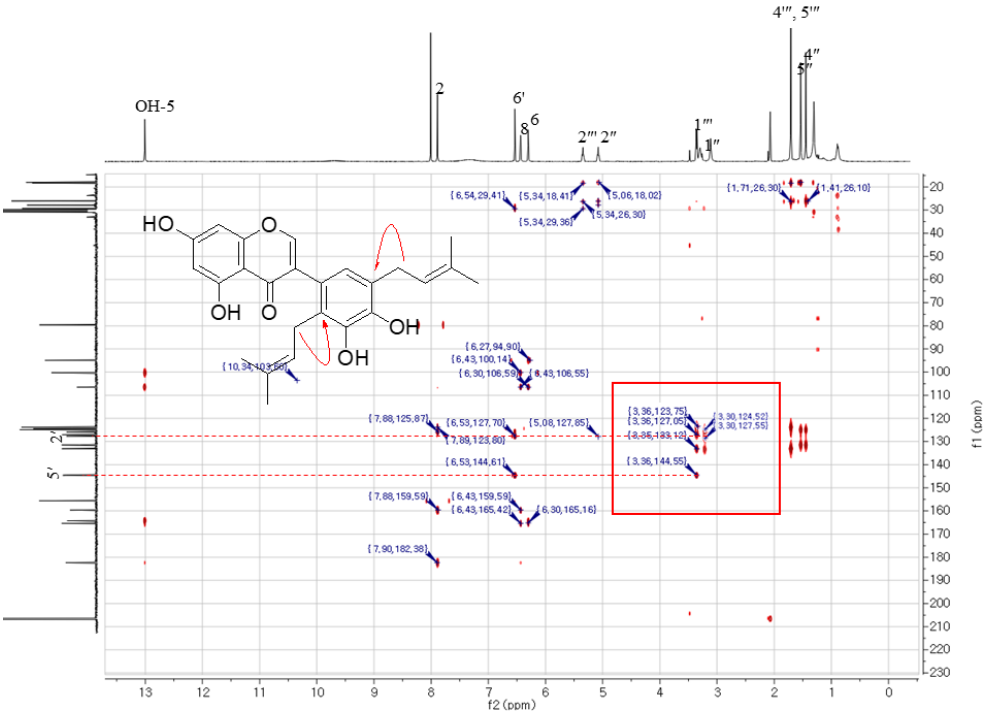

Figure S10. HMBC spectrum of compound **4** (500 MHz, Acetone-d_6)

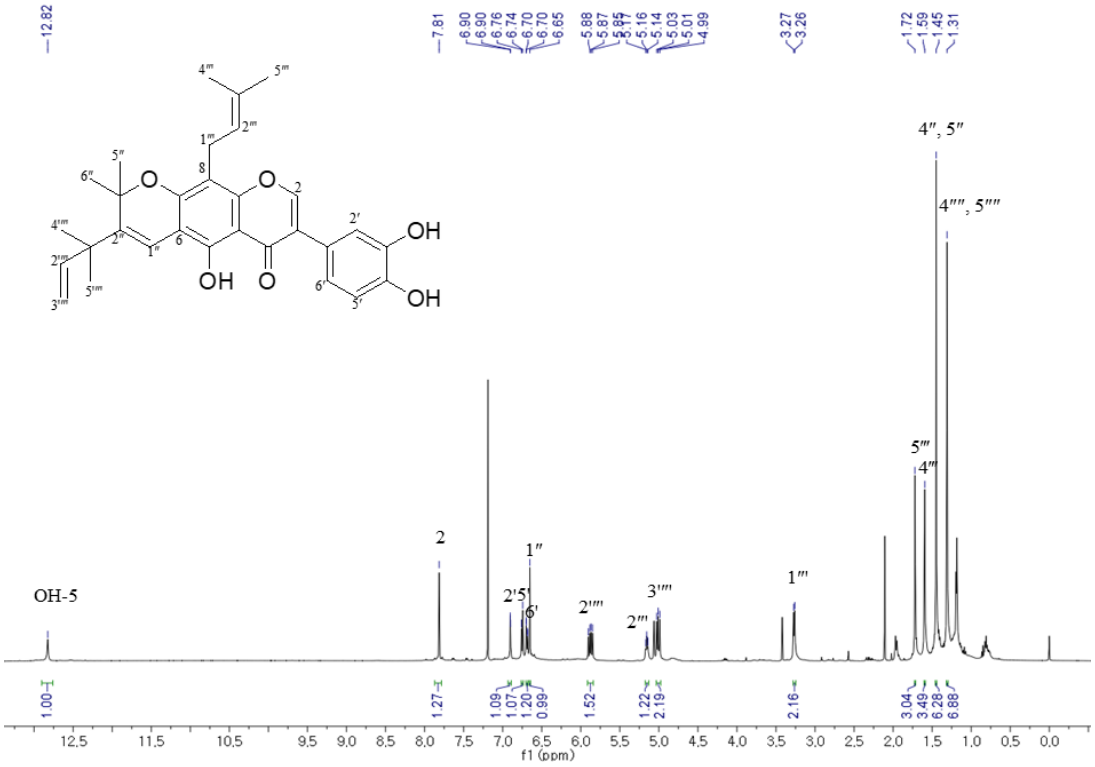

Figure S11. ^{1}H-NMR spectrum of compound **5** (500 MHz, $CDCl_3$)

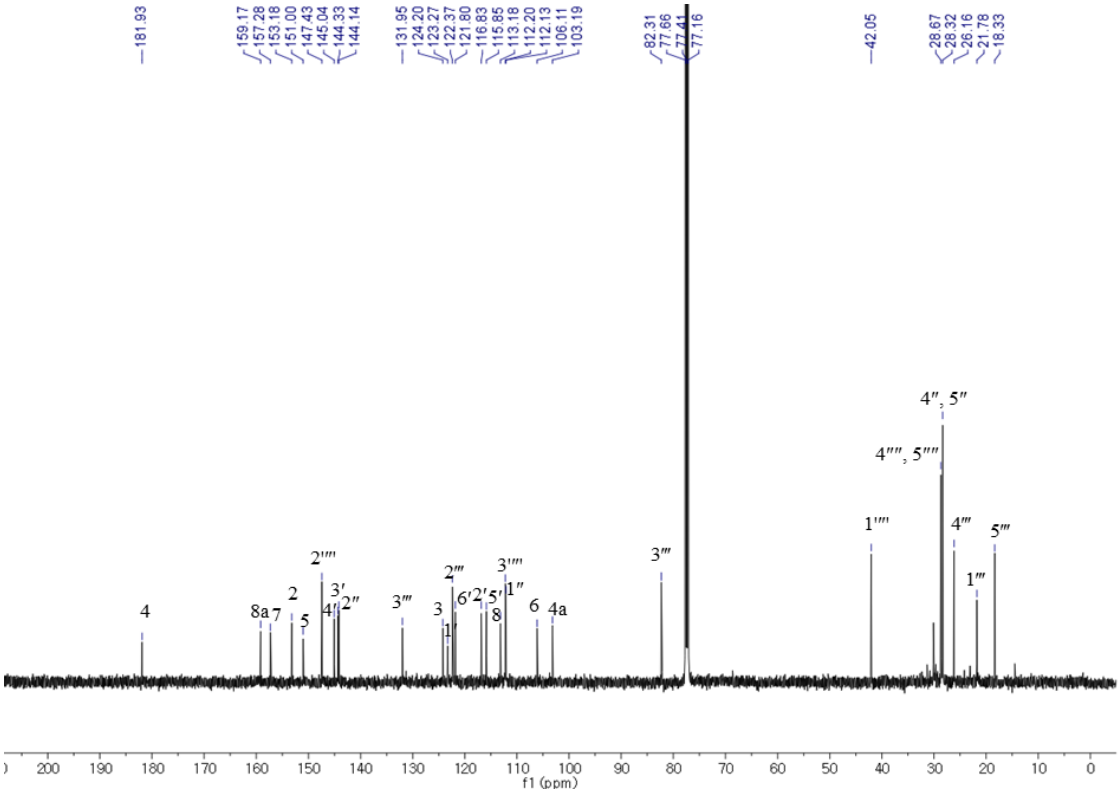

Figure S12. ^{13}C-NMR spectrum of compound **5** (125 MHz, $CDCl_3$)

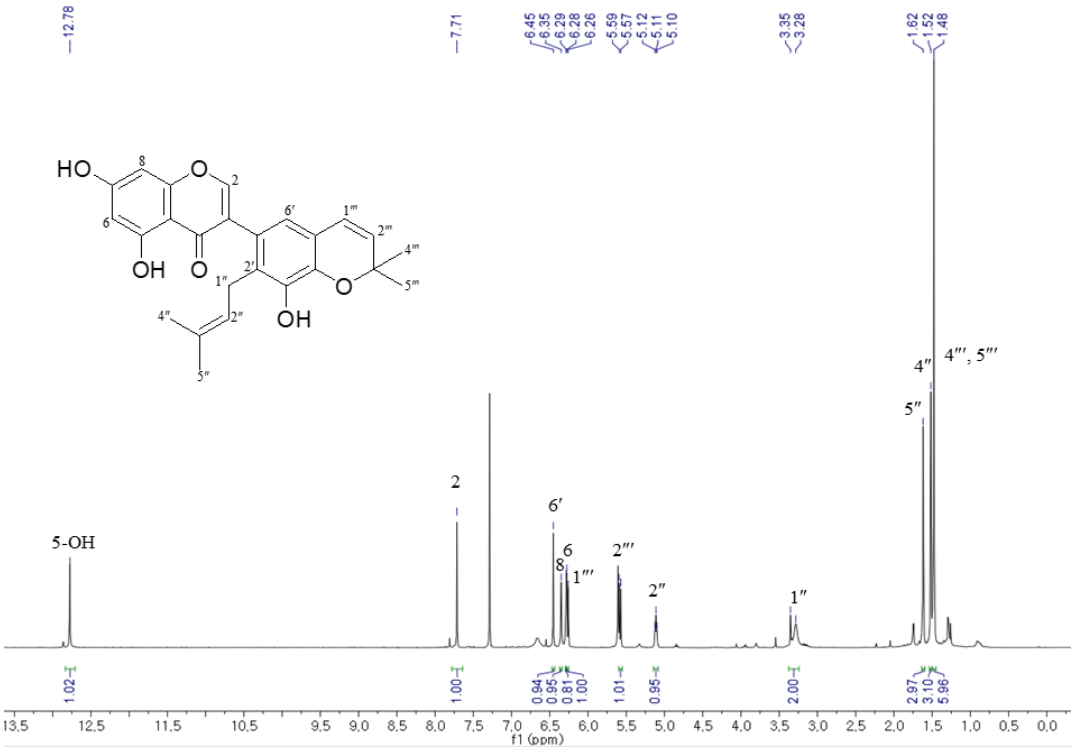

Figure S13. ^{1}H-NMR spectrum of compound **6** (500 MHz, $CDCl_3$)

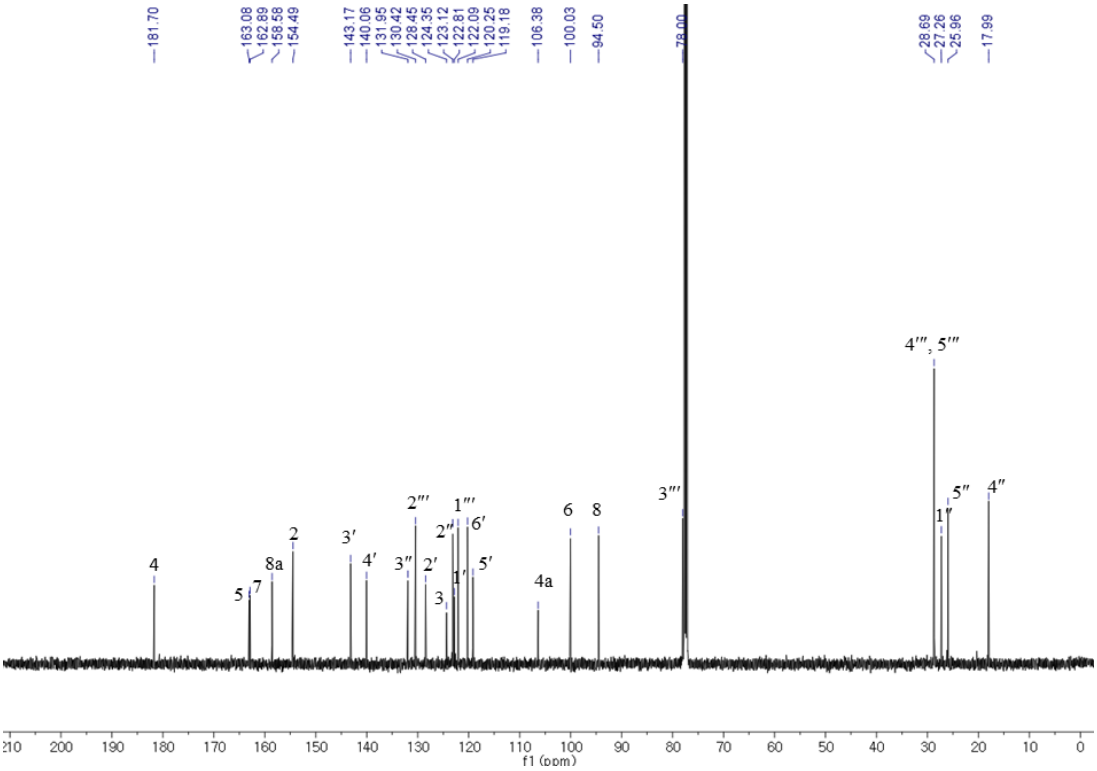

Figure S14. ^{13}C-NMR spectrum of compound **6** (125 MHz, $CDCl_3$)

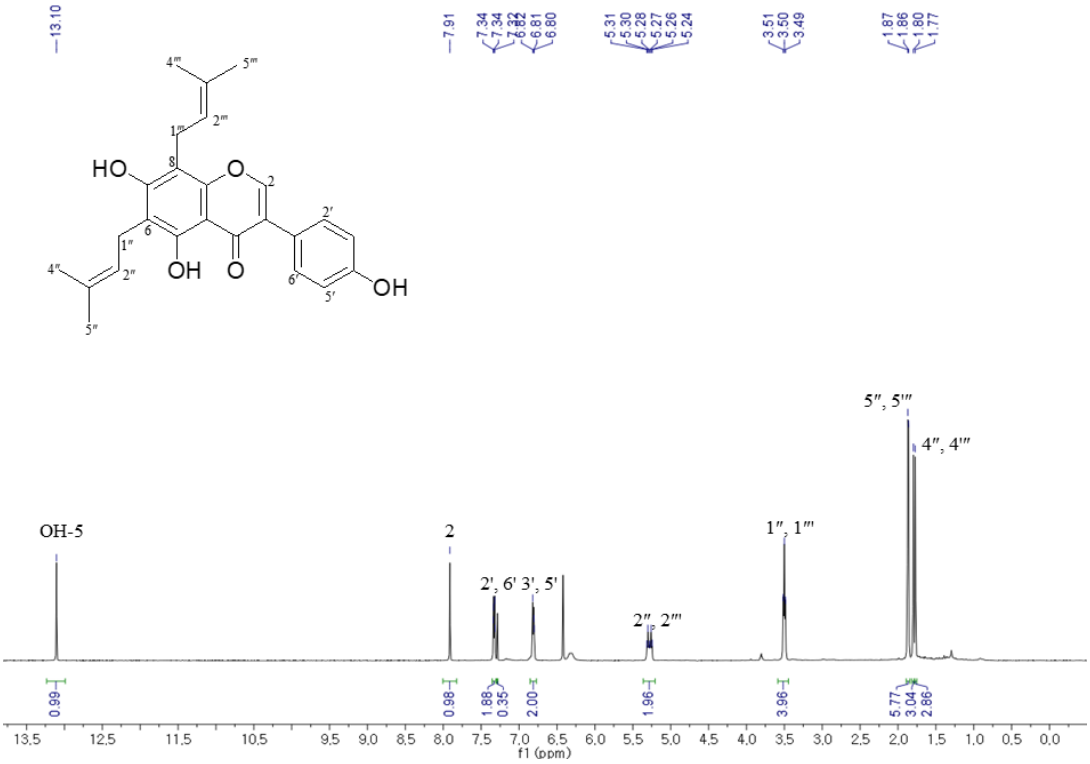

Figure S15. ^{1}H-NMR spectrum of compound **7** (500 MHz, $CDCl_3$)

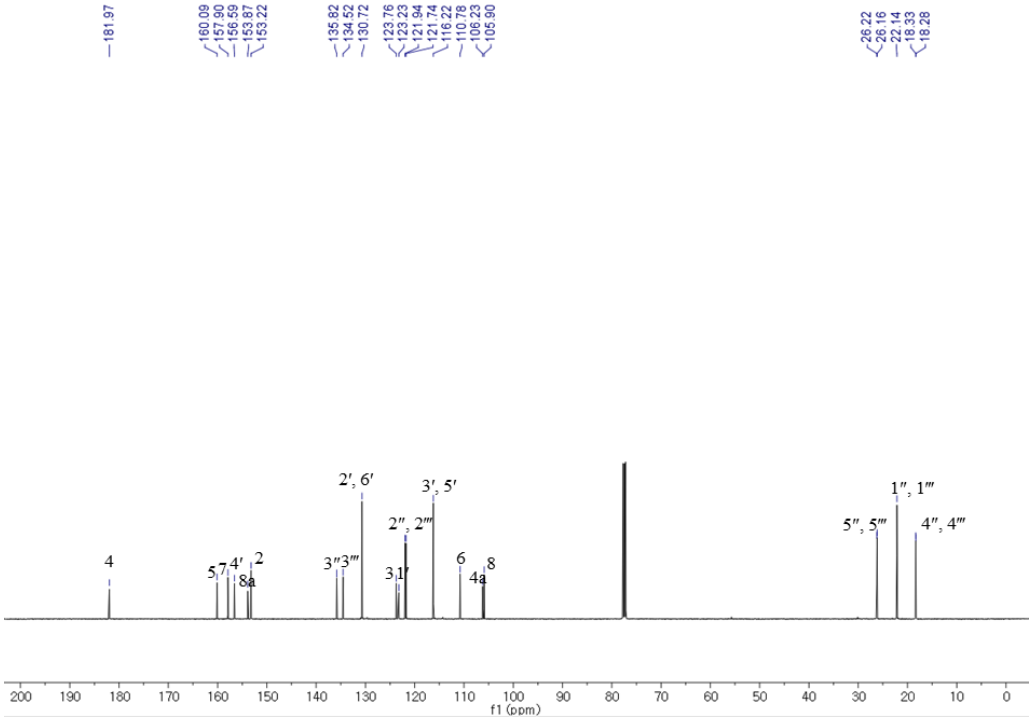

Figure S16. ^{13}C-NMR spectrum of compound **7** (125 MHz, $CDCl_3$)

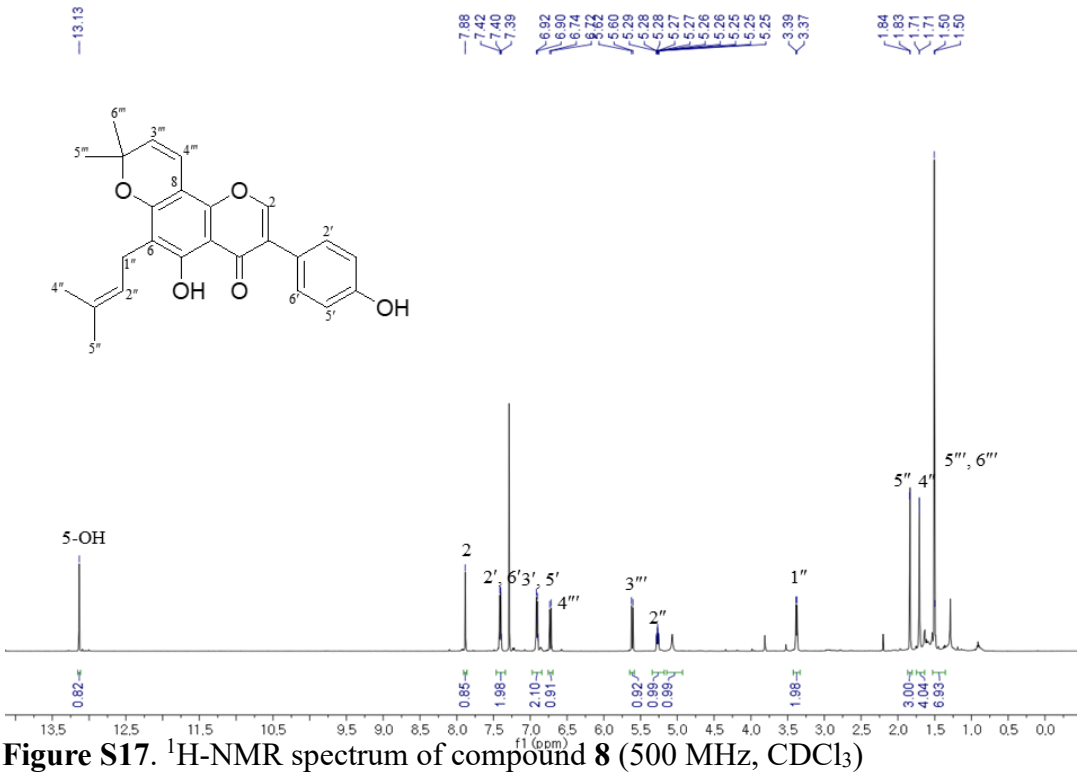

Figure S17. ^{1}H-NMR spectrum of compound **8** (500 MHz, $CDCl_3$)

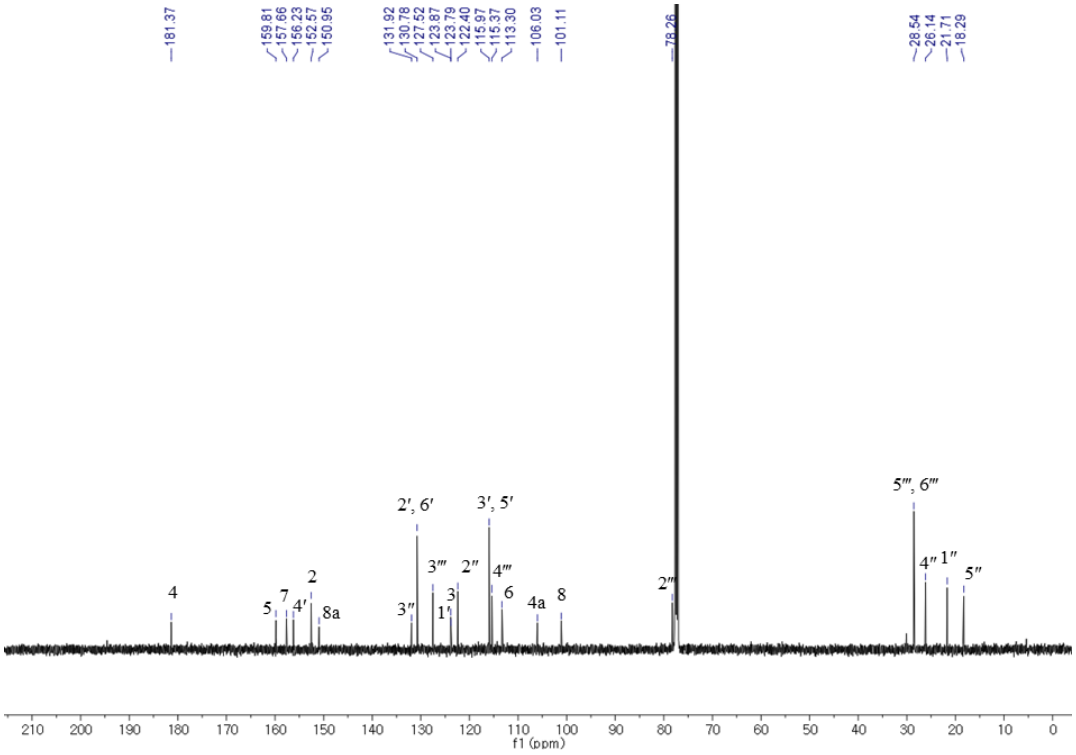

Figure S18. ^{13}C-NMR spectrum of compound **8** (125 MHz, $CDCl_3$)

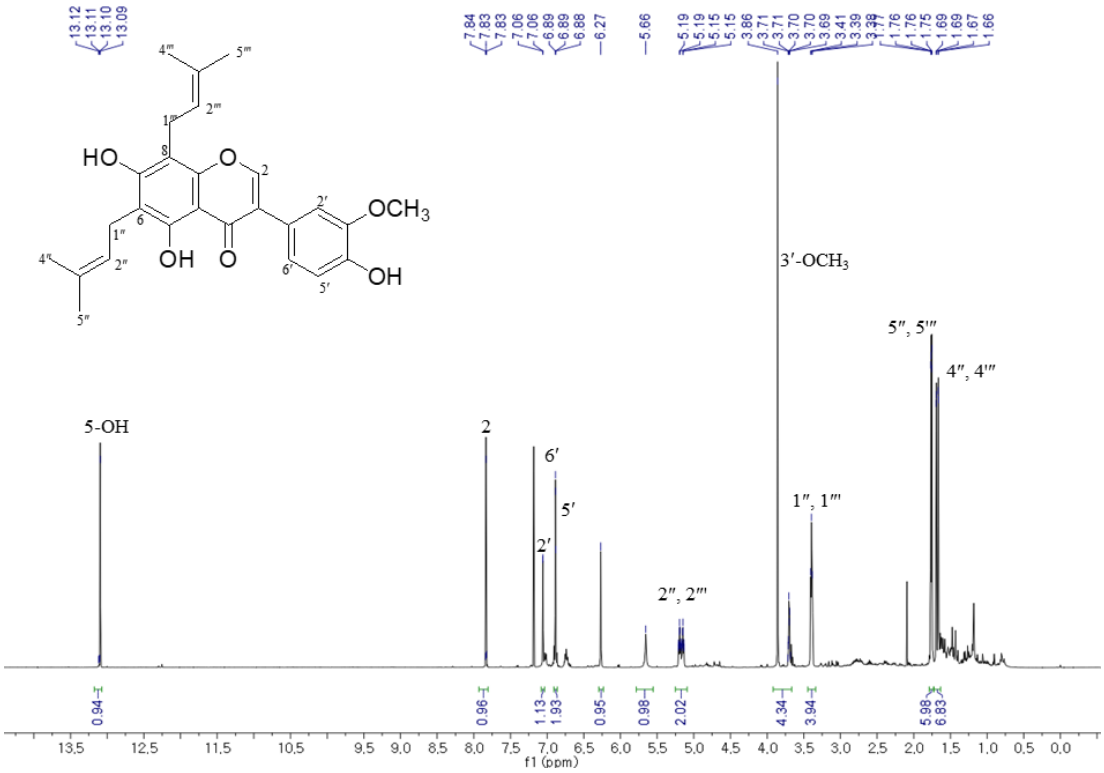

Figure S19. ^{1}H-NMR spectrum of compound **9** (500 MHz, $CDCl_3$)

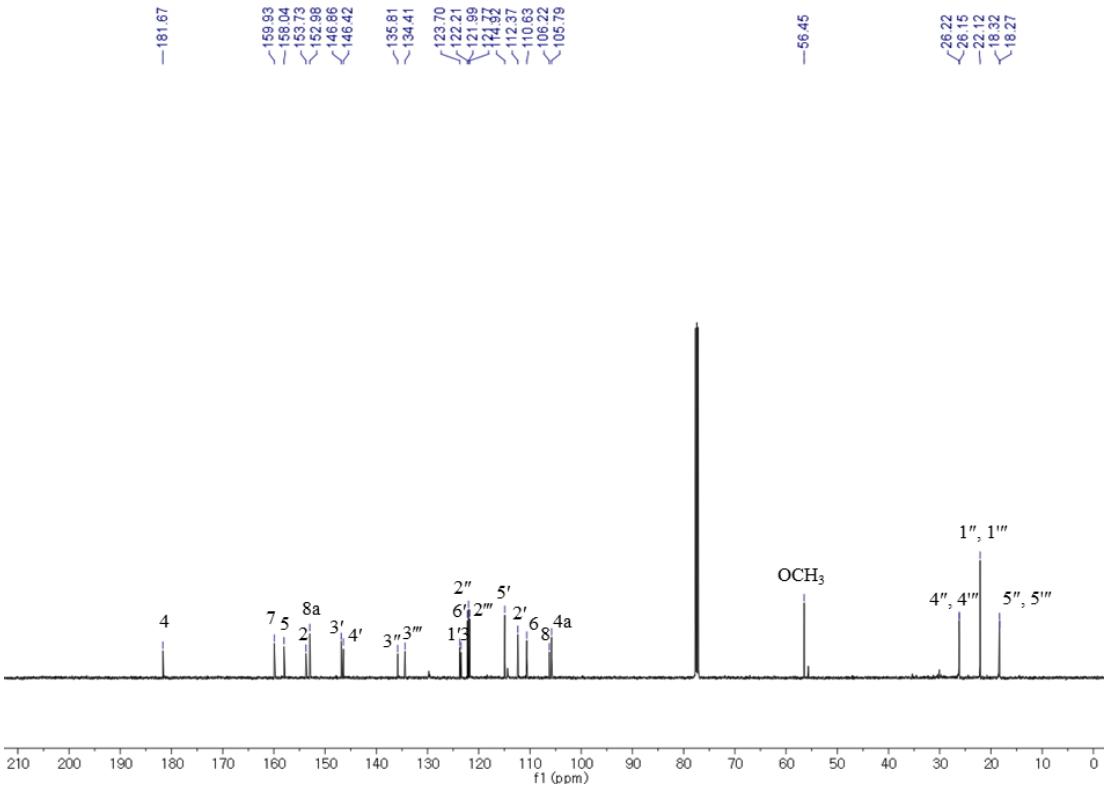

Figure S20. ^{13}C-NMR spectrum of compound **9** (125 MHz, $CDCl_3$)

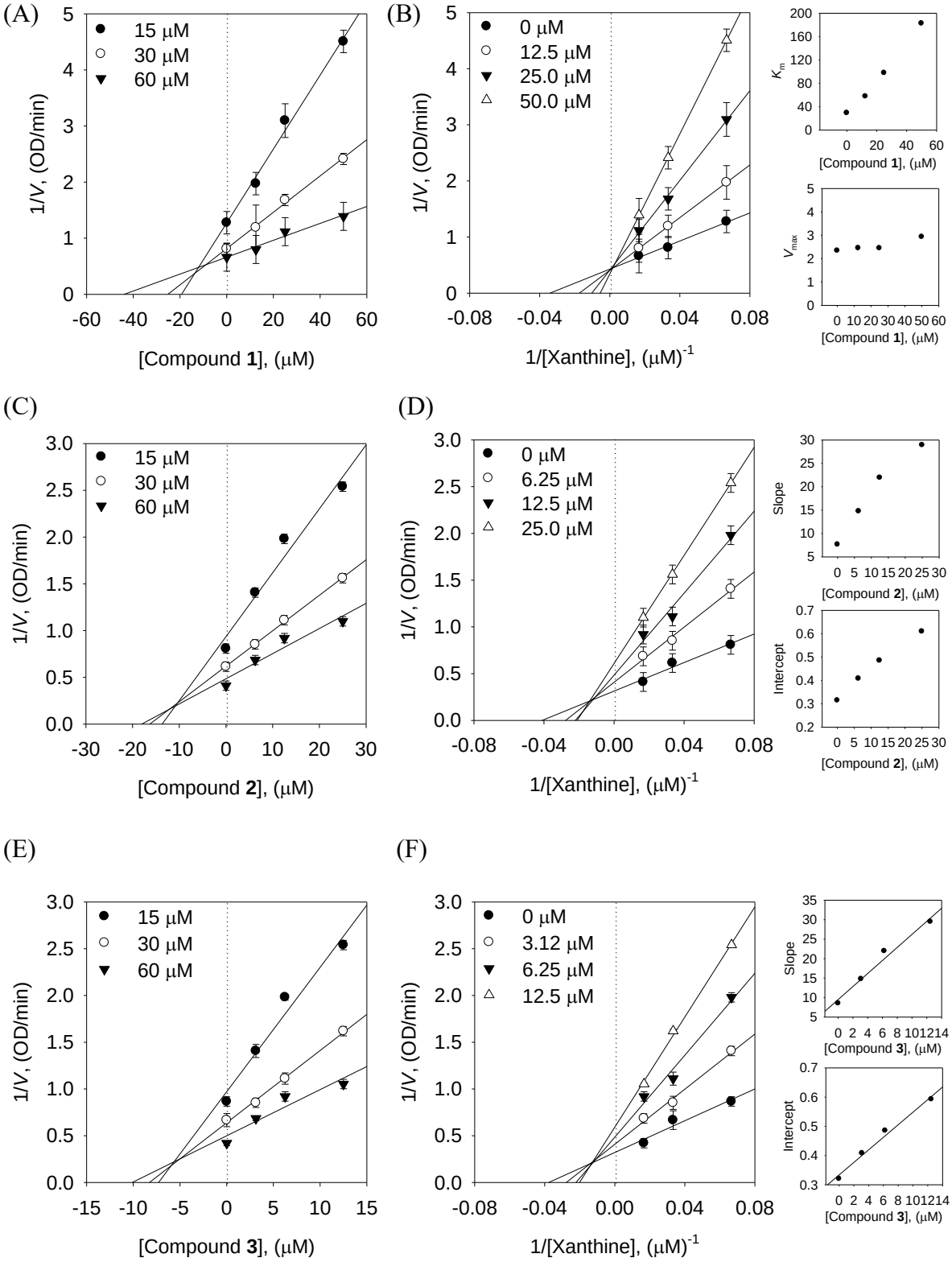

Figure S21. Lineweaver-Burk plots for the XO inhibition of compounds (A) **1**, (C) **2**, (E) **3**. Dixon plots for the XO inhibition of compounds (B) **1**, (D) **2**, (F) **3**.

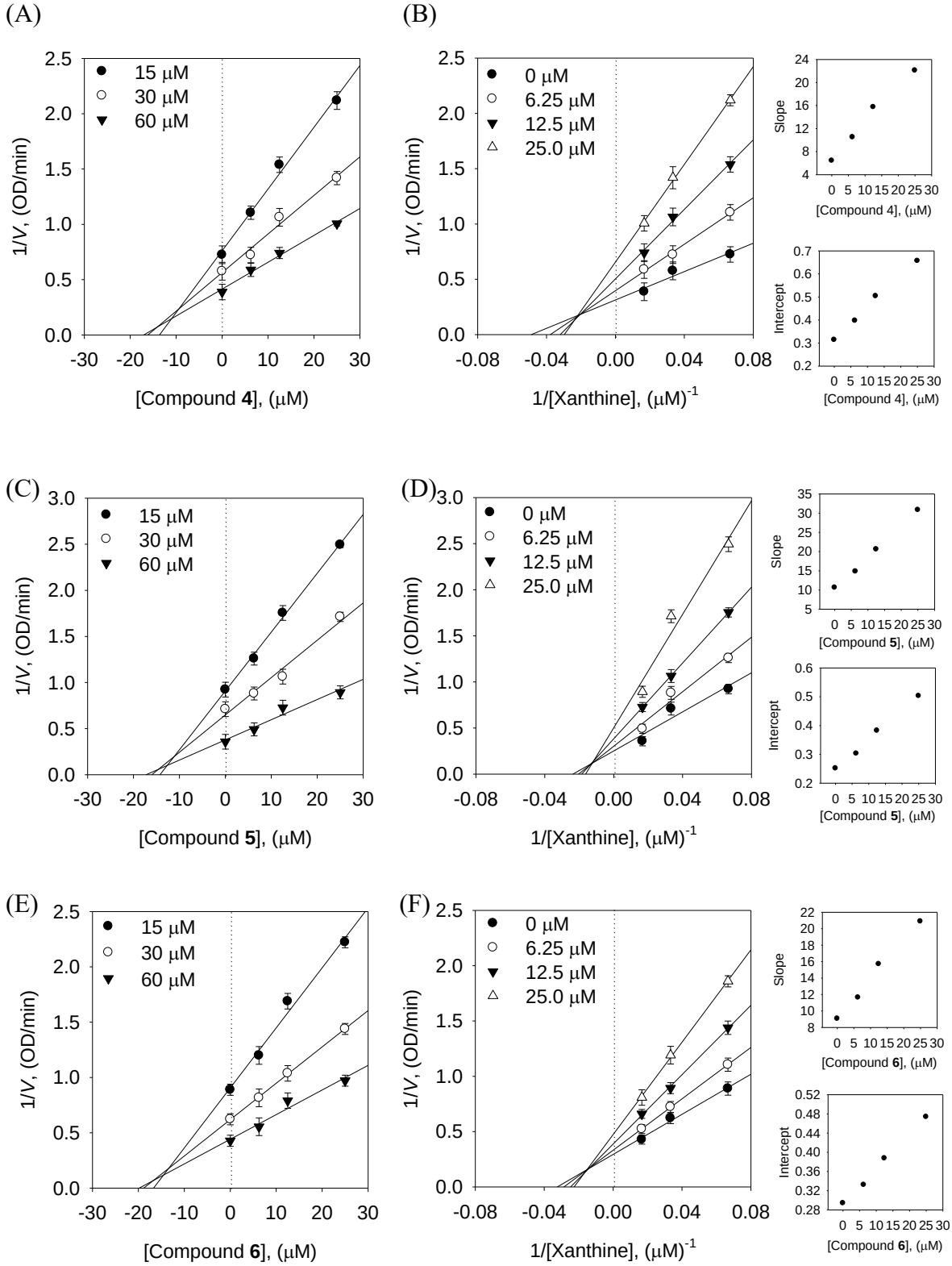

Figure S22. Lineweaver-Burk plots for the XO inhibition of compounds (A) **4**, (C) **5**, (E) **6**. Dixon plots for the XO inhibition of compounds (B) **4**, (D) **5**, (F) **6**.

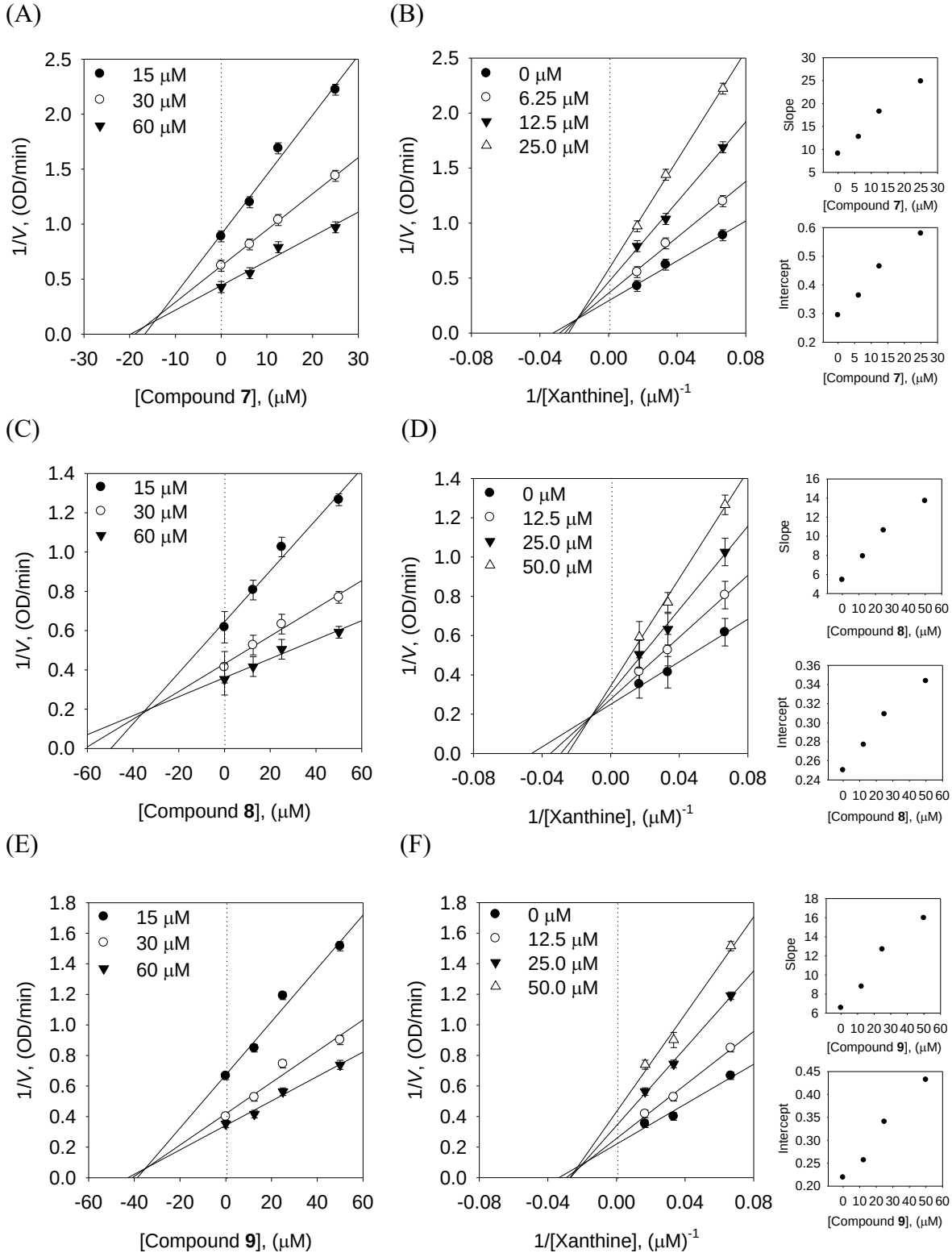

Figure S23. Lineweaver-Burk plots for the XO inhibition of compounds (A) **7**, (C) **8**, (E) **9**. Dixon plots for the XO inhibition of compounds (B) **7**, (D) **8**, (F) **9**.

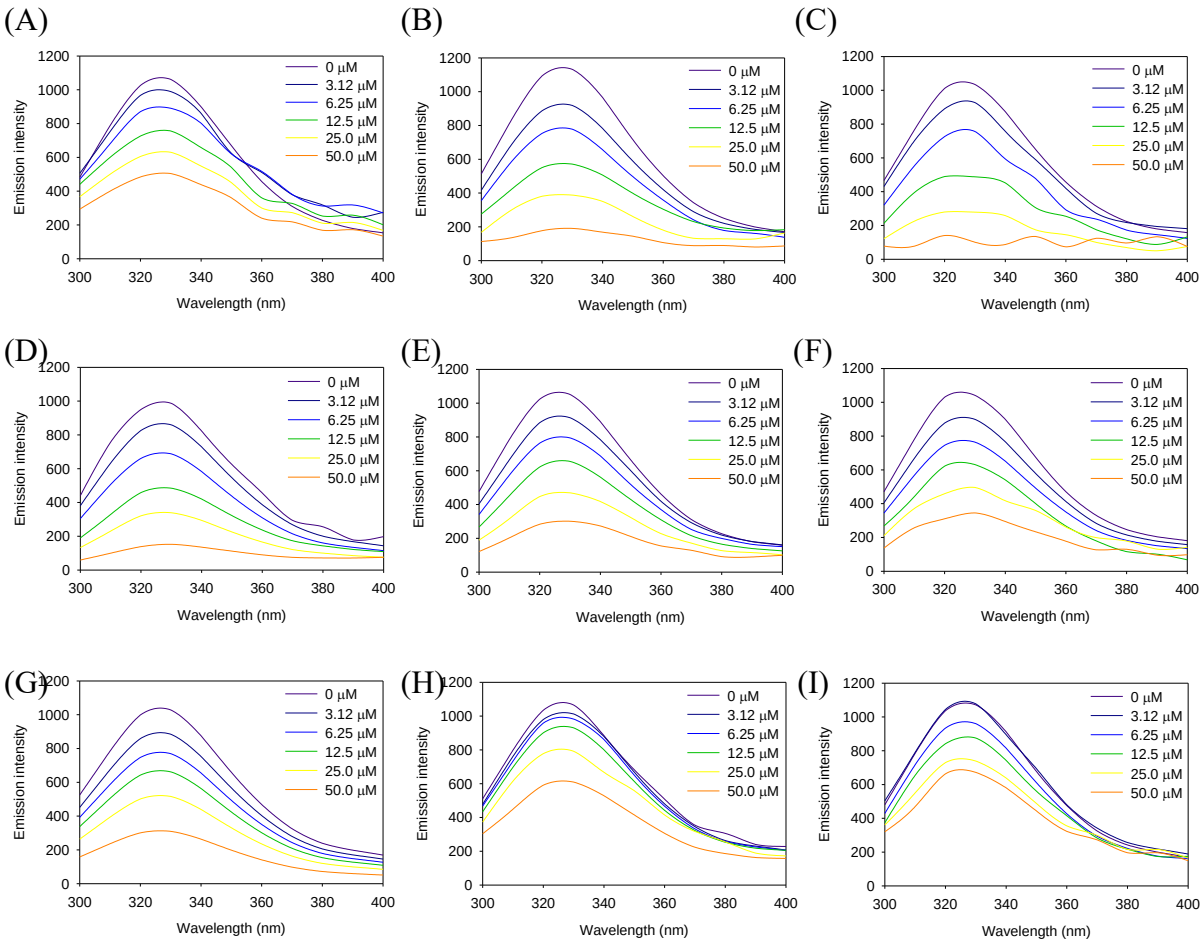

Figure S24. Binding affinity between XO and isoflavones (A) **1**, (B) **2**, (C) **3**, (D) **4**, (E) **5**, (F) **6**, (G) **7**, (H) **8**, and (I) **9**.

Table S1. Evaluation of Stern-Volmer constants depending on fluorescence quenching effects of xanthine oxidase inhibitors

Compounds	K_{SV} (x10^5 L·mol^{-1})	R^2	K_A(x10^6 L·mol^{-1})	*n*	R^2
1	0.1845	0.9944	0.5015	0.7268	0.9992
2	0.7755	0.9991	0.7544	1.0359	0.9984
3	1.2530	0.9998	0.8998	1.4392	0.9964
4	0.9497	0.9999	0.8896	1.4031	0.9961
5	0.5531	0.9999	0.7249	1.0018	0.9967
6	0.3645	0.9999	0.6240	0.8154	0.9983
7	0.4797	0.9914	0.6651	0.8836	0.9980
8	0.0987	0.9998	0.4667	0.6889	0.9987
9	0.0930	0.9804	0.2434	0.6736	0.9998

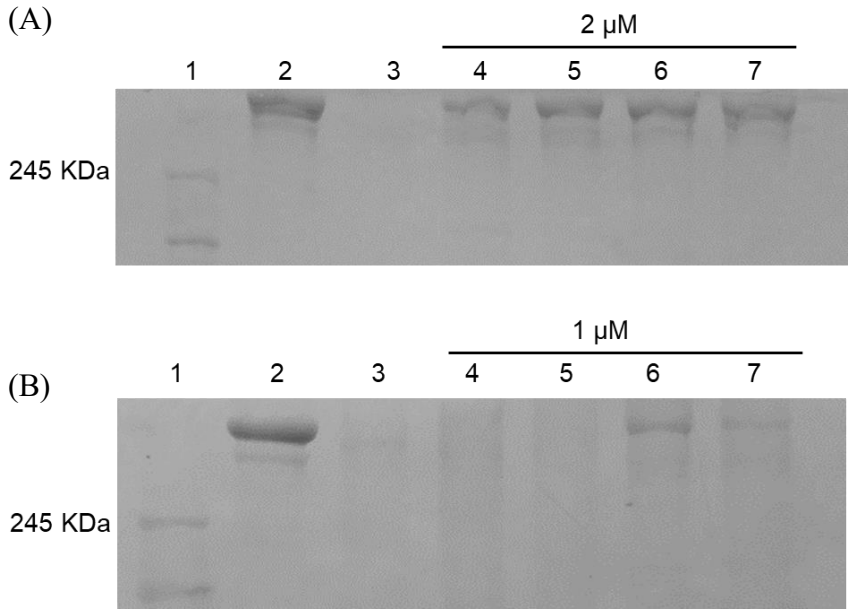

Figure S25. Effects of isoflavones (**2**, **3**, **4**, and **5**) on the ApoB-100 fragmentation. (A) Lane 1, marker; lane 2, native LDL; lane 3, ox-LDL; lane 4, **2** (2 μM); lane 5, **3** (2 μM); lane 6, **4** (2 μM); lane 7, **5** (2 μM). (B) Lane 1, marker; lane 2, native LDL; lane 3, ox-LDL; lane 4, **2** (1 μM); lane 5, **3** (1 μM); lane 6, **4** (1 μM); lane 7, **5** (1 μM).

Table S2. Characterization of isoflavones from methanol extract of *F. philippinensis* by UPLC-ESI-TOF-MS.

t_R (min)	Formula	Neutral mass (Da)	Observed neutral mass (Da)	Experimental *m/z* $[M+H]^+$	Fragmental ion *m/z*	Error (mDa)	Identification
3.51	$C_{15}H_{10}O_5$	270.0528	270.0528	271.06004			genistein (**1**)
4.49	$C_{25}H_{26}O_6$	422.1729	422.1733	423.18057	367, 311	+0.4	5,7,3',4'-tetrahydroxy-2',5'-di(3-methylbut-2-enyl)isoflavone (**4**)
4.76	$C_{25}H_{24}O_6$	420.1573	420.1582	421.16547	365, 283	+0.9	5, 7, 3'-trihydroxy-2'-(3-methylbut-2-enyl)-4',5'-(3,3-dimethylpyrano)isoflavone (**6**)
5.17	$C_{25}H_{26}O_6$	422.1729	422.1733	423.18057	367, 311	+0.4	6,8-diprenylorobol (**3**)
5.31	$C_{26}H_{28}O_6$	436.1886	436.1895	437.19678	381, 311	+0.9	flemingsin (**9**)
5.49	$C_{25}H_{26}O_5$	406.1780	406.1780	407.18525	351, 295		8-γ,γ-dimethylallylwighteone (**7**)
5.82	$C_{25}H_{24}O_6$	420.1573	420.1582	421.16548	365	+0.9	auriculasin (**2**)
6.14	$C_{25}H_{24}O_5$	404.1624	404.1633	405.17058	349	+0.9	osajin (**8**)
6.49	$C_{30}H_{32}O_6$	488.2199	488.2210	489.22831	433, 365	+1.1	flemiphilippinin A (**5**)

Sequence[i]

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Sequence processing[i]: The displayed sequence is further processed into a mature form.

P80457-1 [UniParc] FASTA Add to basket

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Figure S26. Amino acids sequence of xanthine oxidase from bovine milk.