Supplementary materials

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

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Figure S2. ¹³C-NMR spectrum of compound 1 (125 MHz, CD₃OD)



Figure S3. ¹H-NMR spectrum of compound 2 (500 MHz, CDCl₃)



Figure S4. ¹³C-NMR spectrum of compound 2 (125 MHz, CDCl₃)



Figure S5. ¹H-NMR spectrum of compound 3 (500 MHz, Acetone-*d*₆)



Figure S6. ¹³C-NMR spectrum of compound 3 (125 MHz, Acetone-*d*₆)





Figure S7. ¹H-NMR spectrum of compound 4 (500 MHz, Acetone-*d*₆)



Figure S8. ¹³C-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. ¹H-NMR spectrum of compound 5 (500 MHz, CDCl₃)



Figure S12. ¹³C-NMR spectrum of compound 5 (125 MHz, CDCl₃)



Figure S13. ¹H-NMR spectrum of compound 6 (500 MHz, CDCl₃)



Figure S14. ¹³C-NMR spectrum of compound 6 (125 MHz, CDCl₃)



Figure S16. ¹³C-NMR spectrum of compound 7 (125 MHz, CDCl₃)





Figure S18. ¹³C-NMR spectrum of compound 8 (125 MHz, CDCl₃)



Figure S20. ¹³C-NMR spectrum of compound 9 (125 MHz, CDCl₃)



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**.

Compounds K	$K_{\rm SV}$ (x10 ⁵ L·mol ⁻¹)	R ²	$K_{\rm A}({\rm x10^6 \ L\cdot mol^{-1}})$	п	R ²
1 0	0.1845	0.9944	0.5015	0.7268	0.9992
2 0	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	0.5531	0.9999	0.7249	1.0018	0.9967
6 0	0.3645	0.9999	0.6240	0.8154	0.9983
7 0).4797	0.9914	0.6651	0.8836	0.9980
8 0	0.0987	0.9998	0.4667	0.6889	0.9987
9 0	0.0930	0.9804	0.2434	0.6736	0.9998

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

 of xanthine oxidase inhibitors



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 μ M); lane 5, 3 (2 μ M); lane 6, 4 (2 μ M); lane 7, 5 (2 μ M). (B) Lane 1, marker; lane 2, native LDL; lane 3, ox-LDL; lane 4, 2 (1 μ M); lane 5, 3 (1 μ M); lane 6, 4 (1 μ M); lane 7, 5 (1 μ M).

t _R (min)	Formula	Neutral mass (Da)	Observed neutral mass (Da)	Experimental <i>m</i> / <i>z</i> [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)

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

Sequence³

Sequence status¹: Complete. Sequence processing¹: The displayed sequence is further processed into a mature form.

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	20	30	40	50	
MTADELVFFV	NGKKVVEKNA	DPETTLLAYL	RRKLGLRGTK	LGCGEGGCGA	
60	70	80	90	100	
CTVMLSKYDR	LQDKIIHFSA	NACLAPICTL	HHVAVITVEG	IGSTKTRLHP	
110	120	130	140	150	
VQER I AKSHG	SQCGFCTPGI	VMSMYTLLRN	OPEPTVEELE	DAFQGNLCRC	
160	170	180	190	200	
TGYRPILOGE	RTFAKNGGCC	GGNGNNPNCC	MNQKKDHTVT	LSPSLENPEE	
210	220	230	240	250	
EMPLOPTOEP	LEPPELL BLK	DVPPKQLBEE	GERVINIOAS	TLKELLDLKA	
260	270	280	290	300	
OHPEAKI VVG	NTELGIEWKE	KNOLEDWILLC	PAUL PEL NAV	EHGPEGI SEG	
310	320	330	3/0	350	
AACAI SSVEK	TI I EAVAKI P	TOKTEVERGY		DULCENARY OF	
HHCHLOSTEN 960	1LLCHTHNLF 970	200	200	AUD 400	
NUTACOLOD	LUDUEWAGOT			400	
NITIHOFIOD 410	LINEVENAGUI	NL111000000	140	AFO	
410	420	430		40U	
EEILLSIEIP	YSREDEFESA	FKUASHHEDD	TAKYTCGMRV	LEUPGSMUVK	
460	4/U	480	490	500	
ELALCYGGMA	DRITSALKIT	QKQLSKFWNE	KLLQDVCAGL	AEELSLSPDA	
510	520	530	540	550	
PGGMIEFRRT	LTLSFFFKFY	LTVLKKLGKD	SKDKCGKLDP	TYTSATLLFQ	
560	570	580	590	600	
KDPPANI QLF	QEVPNGQSKE	DTVGRPLPHL	AAAMQASGEA	VYCDDIPRYE	
610	620	630	640	650	
NELFLRLVTS	TRAHAKIKSI	DVSEAQKVPG	FVCFLSADDI	PGSNETGLFN	
660	670	680	690	700	
DETVFAKDTV	TCVGHIIGAV	VADTPEHAER	AAHVVKVTYE	DLPAIITIED	
710	700	700			
10	720	730	740	750	
AIKNNSFYGS	FLKI EKGDLK	73U KGFSEADNVV	74U SGELYIGGQD	750 HFYLETHCT I	
ATKNNSFYGS 760	ELKIEKGDLK 770	/3U KGFSEADNVV 780	740 SGELYIGGQD 790	750 HFYLETHCT I 800	
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Status Reviewed - Annotation score: ••••• - Expe

Figure S26. Amino acids sequence of xanthine oxidase from bovine mi	lk.
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Feature table