Electronic Supplementary Information

Metabolites identification and pharmacokinetic study of *Lamiophlomis rotata* in rats

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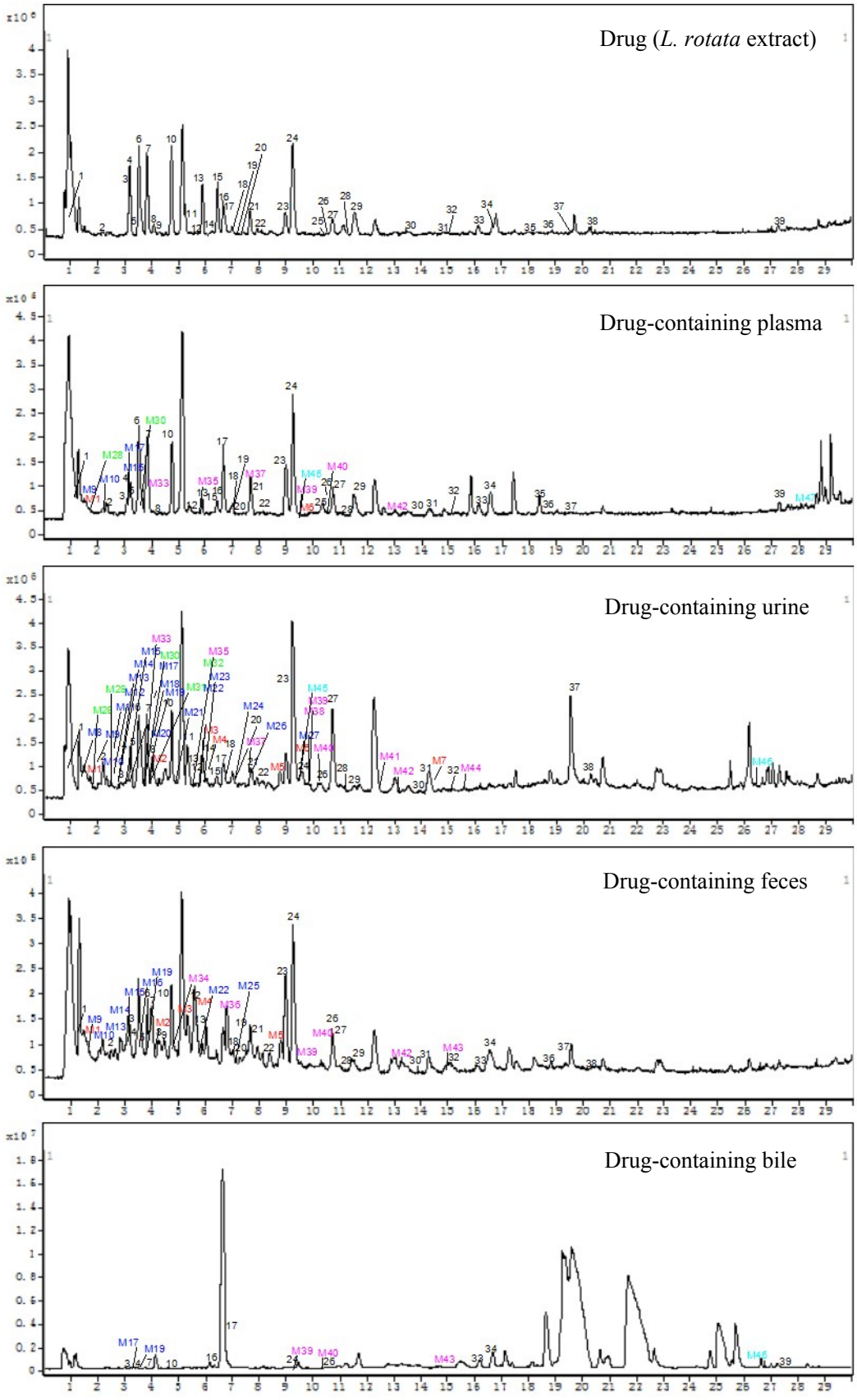

Fig. S1. TIC of *L. rotata* extract and metabolic fingerprints of biological samples after oral administration of *L. rotata* extract in negative mode.

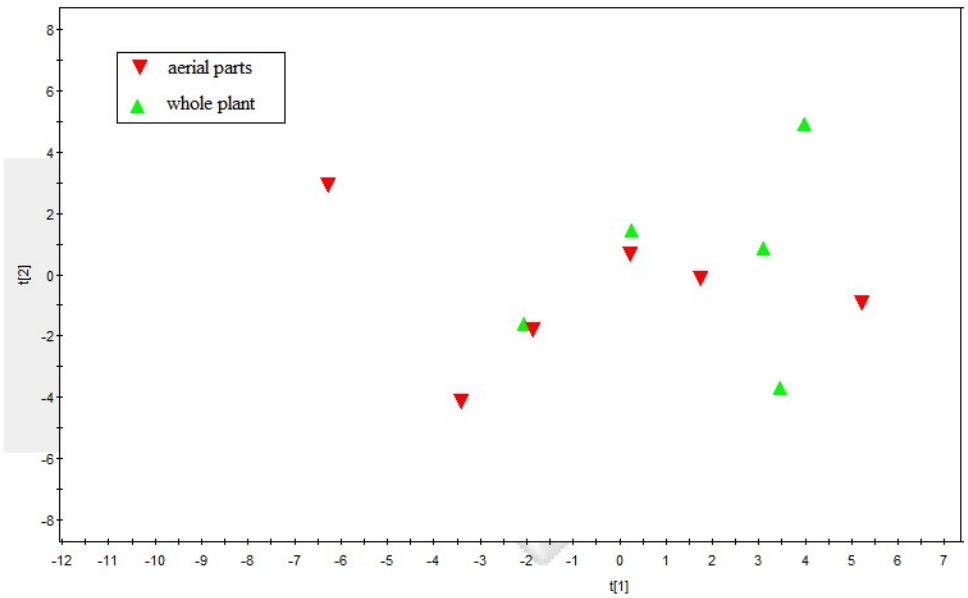

Fig. S2. Partial least squares analysis for fingerprint chromatograms of drug-containing plasma of two groups' rats after oral administration of the aerial parts and the whole plant of *L. rotata*.

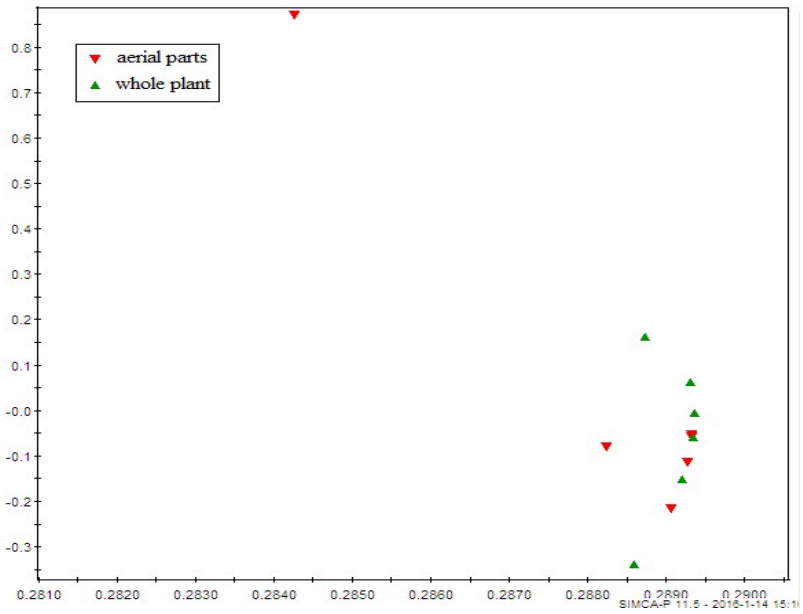

Fig. S3. Partial least squares analysis for fingerprint chromatograms of in vivo metabolites in drug-containing plasma of two groups' rats after oral administration of the aerial parts and the whole plant of *L. rotata*.

Table S1 Identification of the prototype constituents from *L. rotata* in biological samples by UPLC/Q-TOF-MS

Peak no.	RT (min)	Formula	Selected ion	Identification	Class	Source			
						P	U	F	B
1	0.908	$C_{12}H_{22}O_{11}$	$[M+H]^+$	2-D-glucopyranoside-(2→1)-2-D-glucopyranoside	G	√	√	√	
2	2.183	$C_{17}H_{26}O_{13}$	$[M+HCOO]^-$	phlomiol	I	√	√	√	
3	3.116	$C_{17}H_{24}O_{11}$	$[M+HCOO]^-$	phlorigidoside C	I	√	√	√	√
4	3.205	$C_{17}H_{26}O_{12}$	$[M+HCOO]^-$	lamalbid	I	√	√	√	√
5	3.590	$C_{20}H_{30}O_{12}$	$[M-H]^-$	decaffeoylverbascoside	I	√	√	√	
6	3.631	$C_{17}H_{26}O_{11}$	$[M+HCOO]^-$	shanzhiside methyl ester	I	√	√	√	
7	3.843	$C_{17}H_{24}O_{12}$	$[M+H]^+$	sesamoside	I	√	√	√	√
8	4.089	$C_{21}H_{28}O_{13}$	$[M-H]^-$	cistanoside F	PG	√	√	√	
9	4.540	$C_7H_6O_3$	$[M-H]^-$	4-hydroxybenzoic acid	P			√	
10	4.752	$C_{17}H_{26}O_{11}$	$[M+HCOO]^-$	5-hydroxyloganin	I	√	√	√	√
11	5.603	$C_{10}H_{20}O_6$	$[M+HCOO]^-$	(2R,5R)-2-butoxy-2,5-bis(hydroxymethyl) tetrahydrofuran-3,4-diol	G		√		
12	5.661	$C_{14}H_{20}O_8$	$[M-H]^-$	vanillyl-β-D-glucopyranside	G	√	√	√	
13	5.847	$C_{19}H_{28}O_{12}$	$[M+HCOO]^-$	6-O-acetylshanzhiside methyl ester	I	√	√	√	
14	6.207	$C_{21}H_{32}O_{12}$	$[M+HCOO]^-$	cistanoside E	PG		√		
15*	6.306	$C_7H_6O_3$	$[M+H]^+$	3,4-dihydroxybenzaldehyde	P	√	√		
16*	6.457	$C_{17}H_{24}O_{11}$	$[M+HCOO]^-$	7,8-dehydropenstemoside	I	√			√
17	6.633	$C_{17}H_{24}O_{10}$	$[M+HCOO]^-$	7,8-dehydropenstemonoside	I	√	√		√
18	6.698	$C_{17}H_{25}ClO_{11}$	$[M+H]^+$	chlorotuberoside	I	√	√	√	
19*	6.986	$C_{17}H_{26}O_{10}$	$[M+HCOO]^-$	7-epi-loganin	I	√		√	
20*	7.018	$C_{17}H_{24}O_{10}$	$[M+H]^+$	7-dehydroxy-zaluzioside	I	√	√	√	
21	7.672	$C_{17}H_{26}O_{10}$	$[M+H]^+$	loganin	I	√	√	√	
22	8.056	$C_{29}H_{36}O_{16}$	$[M-H]^-$	campneoside II	PG	√	√	√	
23	9.008	$C_{16}H_{28}O_7$	$[M+HCOO]^-$	(2Z)-2,6-dimethyl-6-hydroxyocta-2,7-dienyl-O-b-D-glucopyranoside	G	√	√	√	
24	9.250	$C_{19}H_{28}O_{12}$	$[M+HCOO]^-$	8-O-acetylshanzhiside methyl ester (barlerin)	I	√	√	√	√
25	10.652	$C_{22}H_{14}O_7$	$[M+HCOO]^-$	4'-(p-carbonylphenyl)-luteolin	F	√			
26	10.657	$C_{26}H_{28}O_{15}$	$[M-H]^-$	luteolin-7-O-β-D-apiofuranosyl (1→6)-β-D-glucopyranoside	F	√	√	√	√
27	10.755	$C_{34}H_{44}O_{19}$	$[M-H]^-$	forsythoside B	PG	√	√	√	
28	11.141	$C_{30}H_{38}O_{16}$	$[M-H]^-$	betonyoside A	PG	√	√	√	
29	11.581	$C_{21}H_{20}O_{11}$	$[M+H]^+$	luteolin-7-β-D-glucopyranside	F	√	√	√	
30*	13.986	$C_{26}H_{28}O_{14}$	$[M-H]^-$	apigenin 7-O-β-D-apiofuranosyl (1→6)-β-D-glucopyranoside	F	√	√	√	
31	14.256	$C_{29}H_{36}O_{15}$	$[M-H]^-$	verbascoside	PG	√	√	√	
32	15.05	$C_{21}H_{20}O_{10}$	$[M+H]^+$	apigenin-7-O-β-D-glucopyranoside	F	√	√	√	
33	16.143	$C_{23}H_{22}O_{12}$	$[M-H]^-$	eugenyl-β-D-glucopyranoside	F	√		√	√

34	16.681	$C_{17}H_{26}O_9$	$[M+H]^+$	8-epi-7-deoxyloganin	I	√		√	√
35	18.340	$C_{15}H_{10}O_5$	$[M-H]^-$	salviifoside A	F	√			
36*	18.808	$C_{21}H_{32}O_{10}$	$[M+H]^+$	6β-n-butoxy-7,8-dehydropenstemonoside	I	√		√	
37	19.617	$C_{15}H_{10}O_6$	$[M+H]^+$	luteolin	F	√	√	√	
38	20.156	$C_{16}H_{28}O_6$	$[M+HCOO]^-$	(+/-)-α-terpineol-β-D-O-glucopyranoside	G		√	√	
39*	27.576	$C_{29}H_{46}O_4$	$[M+H]^+$	notohamosin B	N	√			√

I – iridoids, F – flavanoids, PG – phenylethanoid glycosides, N – nortriterpenoid, P – phenolic compounds and G – glycoside compounds;

P-plasma, U-urine, F-feces and B-bile.

* Means that compounds were tentatively identified by the MS spectra by lack of reference compounds.

Table S2 Regression data and LLOQs of the six analytes.

Compound	Regression equation	Correlation coefficient (*r*)	LLOQ (ng/mL)
acetylshanzhiside methyl ester	y=69.2471x-0.0236	0.9936	4.00
8-O-acetylshanzhiside methyl ester	y=10.2167x-0.0045	0.9963	4.00
lamalbid	y=98.5013x-0.0087	0.9958	1.00
verbascoside	y=334.0191x+0.0146	0.9955	4.00
forsythoside B	y=55.2983x+0.0794	0.9963	3.50
luteolin-7-O-β-D -glucopyranoside	y=139.0578x-0.0978	0.9952	0.40