Electronic Supplementary Material (ESI) for RSC Advances.

Metabolic profile analysis of *Zhi-zi-chi* decoction in feces of normal and chronic unpredictable mild stress-induced depression rats based on UHPLC–ESI–Q–TOF–MS/MS and multiple analytical strategies

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# These authors contributed equally to this work.

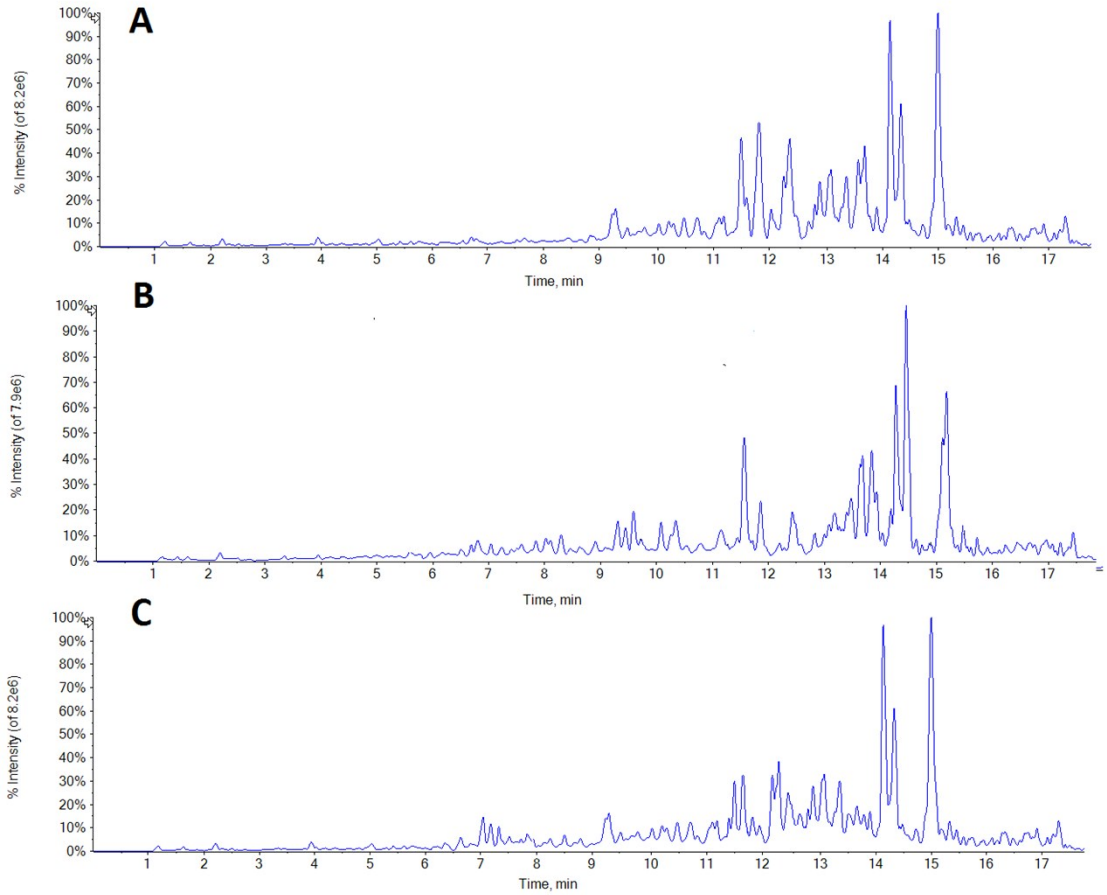

Fig. S1 Typical UHPLC-ESI-Q-TOF-MS/MS chromatograms. UHPLC-ESI-Q-TOF-MS/MS chromatograms total ion chromatograms (TICs) of control rat feces (A), normal+ZZCD rat feces (B) and CUMS+ZZCD (C) in positive mode.

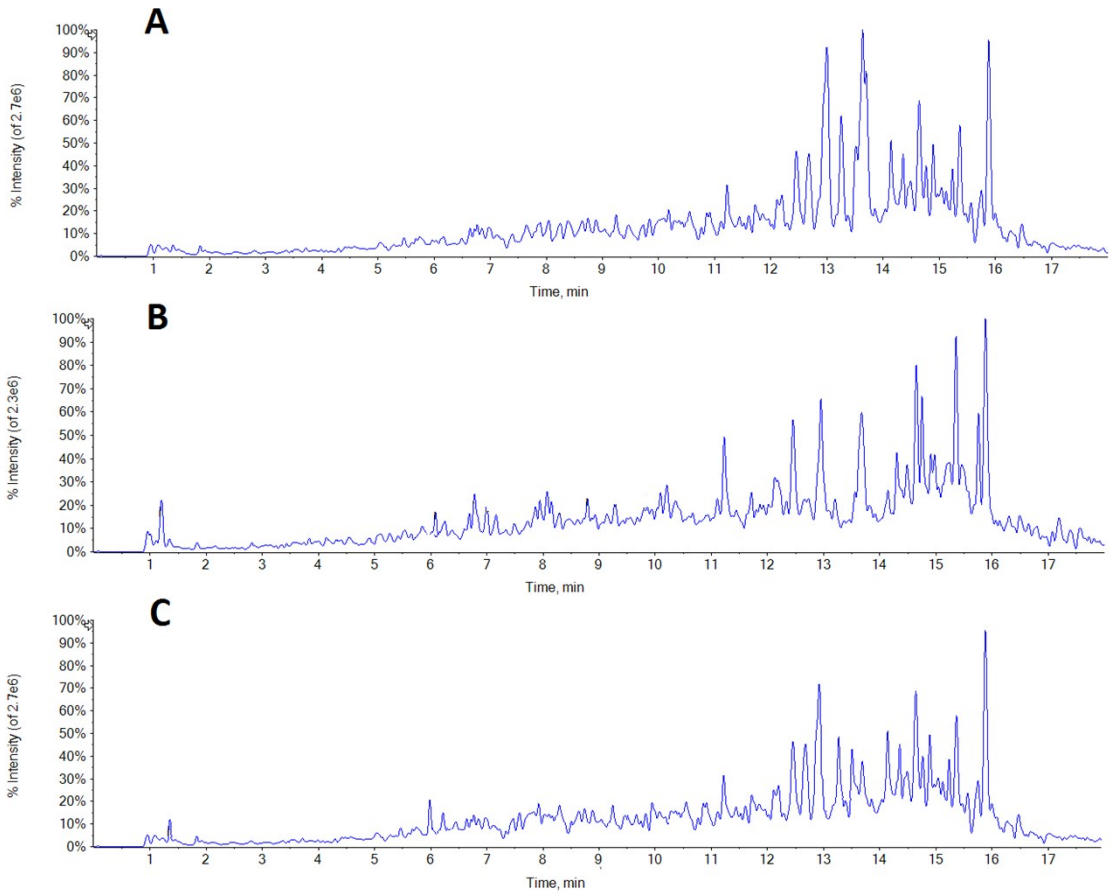

Fig. S2 Typical UHPLC-ESI-Q-TOF-MS/MS chromatograms. UHPLC-ESI-Q-TOF-MS/MS chromatograms total ion chromatograms (TICs) of control rat feces (A), normal+ZZCD rat feces (B) and CUMS+ZZCD rat feces (C) in negative mode.

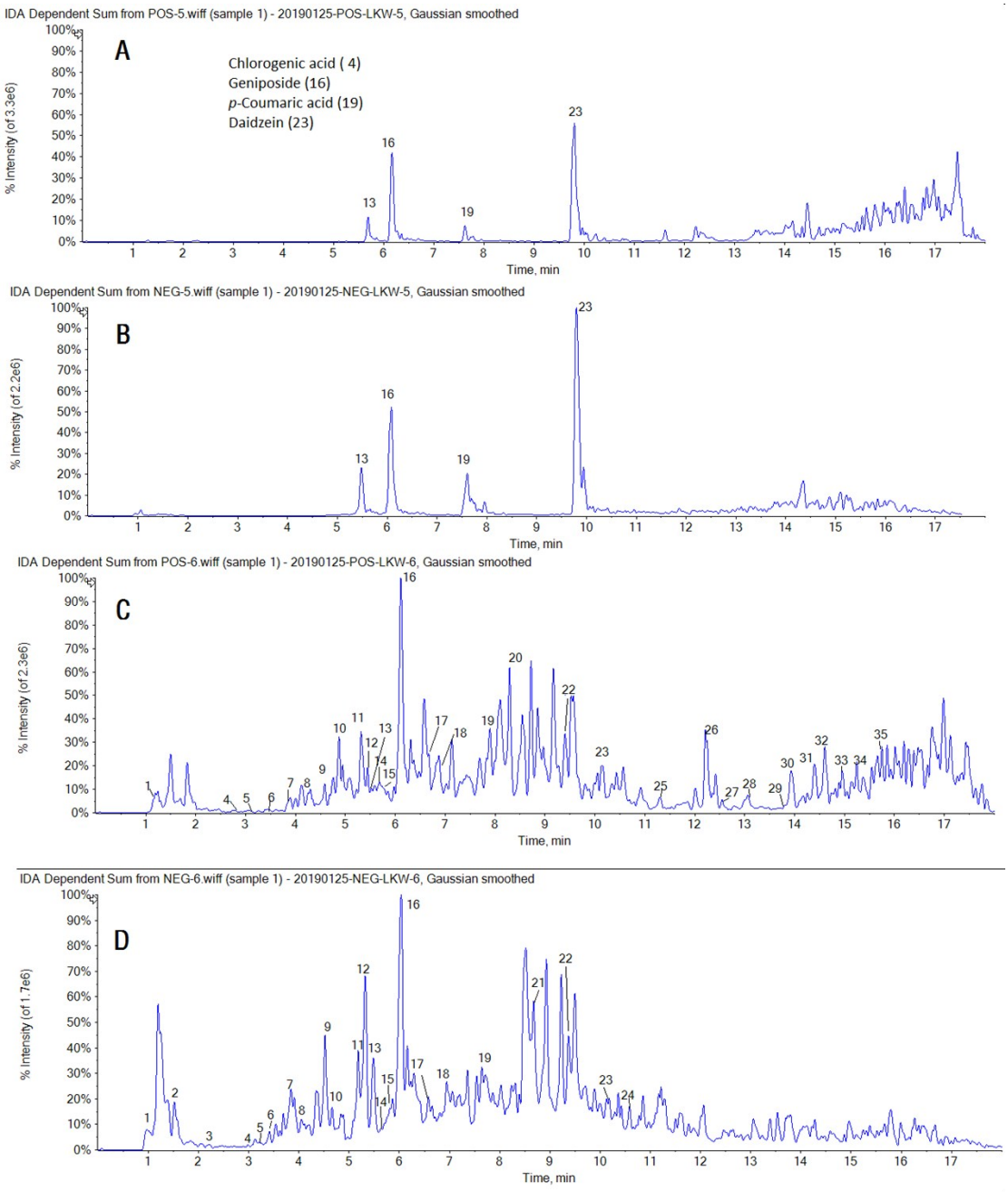

Fig. S3 Typical UHPLC-ESI-Q-TOF-MS/MS chromatograms.UHPLC-ESI-Q-TOF-MS/MSchromatograms total ion chromatograms (TICs) of four standard compounds in positive mode (A) and negative mode (B); TICs of ZZCD in positive mode (C) and negative mode (D).

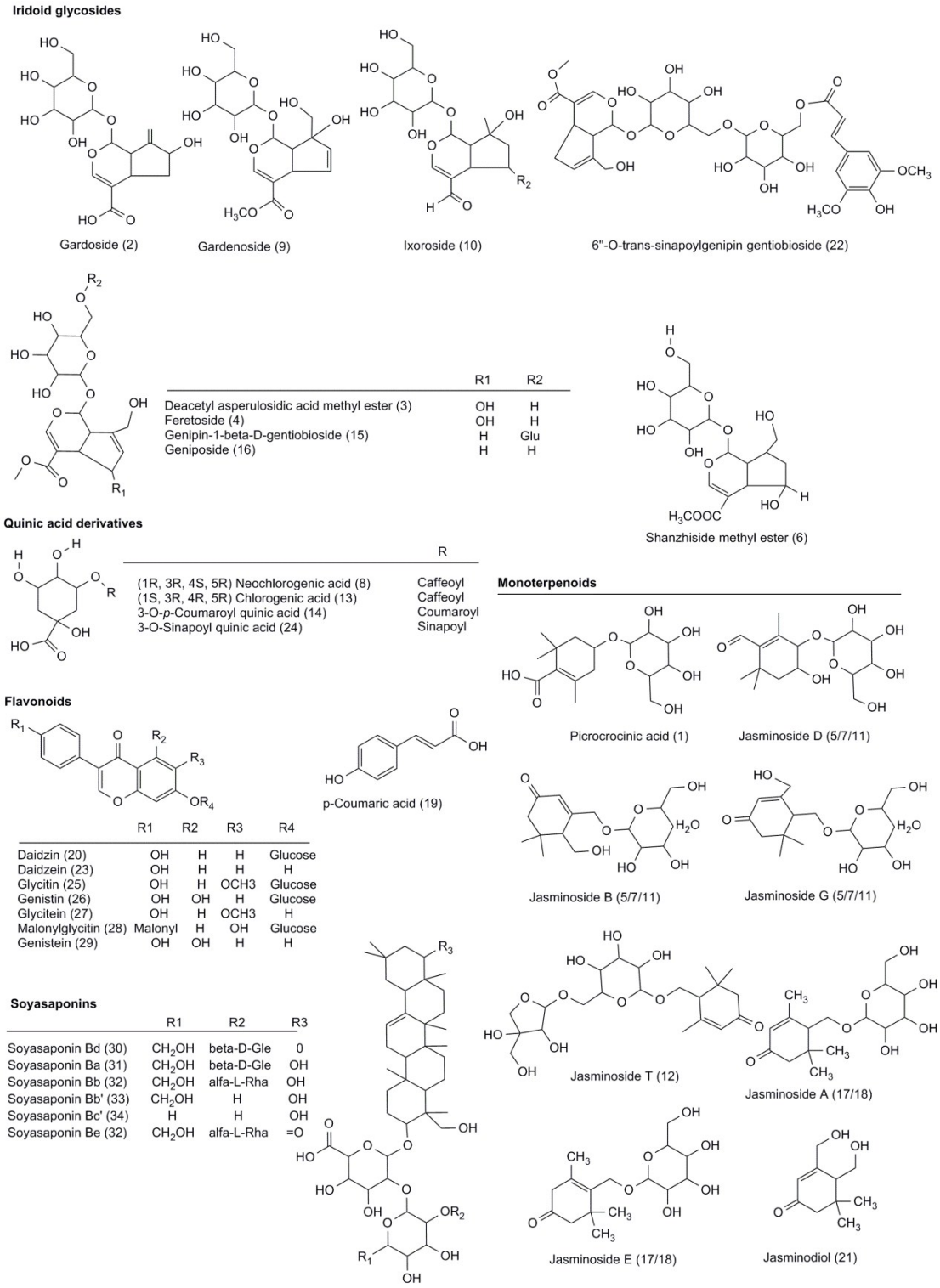

Fig. S4. Molecular structural formulas of prototype constituents of *ZZCD* in rat feces.

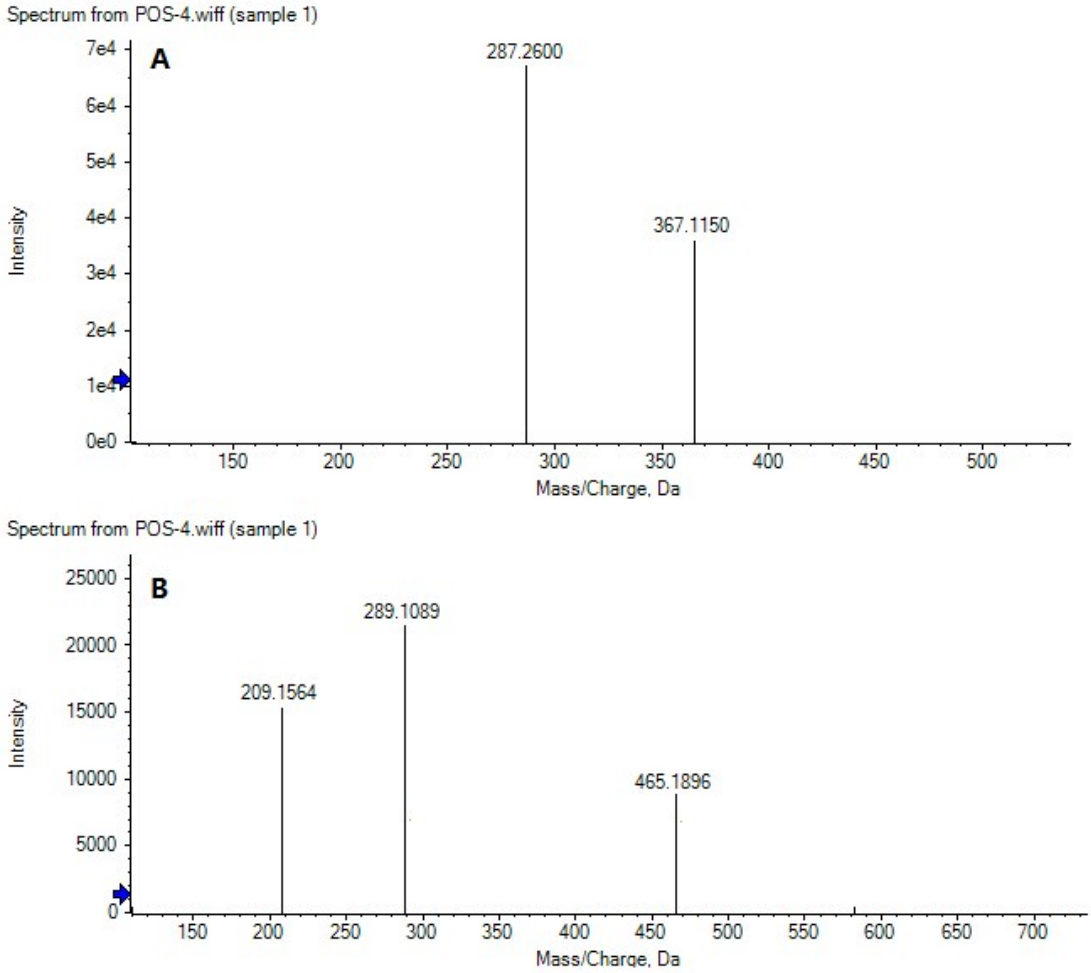

Fig. S5. MS/MS spectra of M11 (A) and M17 (B).

Table S1. Identification of prototype constituents of *ZZC*D in feces of rat model of depression by UHPLC-Q-TOF-MS/MS

No.	t_R(min)	$[M+Na]^+$ *m/z* Detected	ppm	$[M-H]^-$ *m/z* Detected	ppm	MW(Da)	Formula	MS/MS ESI+	ESI-	Identification	Source
1	1.006	369.1512	-2.1	381.1308☆	-3.4	346.1628	$C_{16}H_{26}O_8$	207[M + Na-162] $^+$ 177 [M + Na-162-2CH_3] $^+$ 189 [M + Na-162-H_2O] $^+$ 163 [M + Na-162-CO_2] $^+$	345[M-H] $^-$	Picrocrocinic acid (M)	*ZZ*
2	2.170	-	-	373.1142 409.0911☆	0.5 1.0	374.1213	$C_{16}H_{22}O_{10}$	-	167[M-H- CO_2-$C_6H_{10}O_5$] $^-$ 149[M-H- CO_2.$C_6H_{12}O_6$] $^-$ 123[M-H-$C_6H_{10}O_5$-$C_3H_4O_3$] $^-$	Gardoside (I)	*ZZ*
3	2.813			403.1262	4.0	404.1319	$C_{17}H_{24}O_{11}$	265 [M + Na-162] $^+$ 247 [M + Na-162-H_2O] $^+$	241 [M-H-162] $^-$	Deacetylasperulosidic acid methyl ester (I)	*ZZ*
4	3.094	427.1227	3.8	439.1021☆	1.8	404.1319	$C_{17}H_{24}O_{11}$	265 [M + Na-162] $^+$ 247 [M + Na-162-H_2O] $^+$	241 [M-H-162] $^-$	Feretoside (I)	*ZZ*
5	3.402	369.1521	-0.3	381.1308☆	3.7	346.1628	$C_{16}H_{26}O_8$	-	381 [M + Cl] $^-$ 327 [M-H-H_2O] $^-$ 165 [M-H-H_2O- 162] $^-$ 331 [M-H-CH_2] $^-$ 289 [M-H-C_4H_8] $^-$ 247 [M-H-C_4H_8-C_2H_2O] $^-$ 127 [M-H-C_4H_8-162] $^-$	Jasminoside B/D/G (M)	*ZZ*
6	3.834	407.1543	-1.2	405.1415	-0.8	406.1475	$C_{17}H_{26}O_{11}$		405[M-H] $^-$ 225[M-H-$C_6H_{10}O_5$-H_2O] $^-$ 123[M-H-$C_6H_{10}O_5$-$C_4H_6O_3$] $^-$ 101[M-H-$C_6H_{10}O_5$-$C_7H_{10}O_3$] $^-$	Shanzhiside methyl ester (I)	*ZZ*
7	4.147	369.1517	-0.8	381.1321☆	-0.3	346.1628	$C_{16}H_{26}O_8$	-	381 [M + Cl] $^-$ 327 [M-H-H_2O] $^-$ 165 [M-H-H_2O- 162] $^-$ 331 [M-H-CH_2] $^-$ 289 [M-H-C_4H_8] $^-$ 247 [M-H-C_4H_8-C_2H_2O] $^-$ 127 [M-H-C_4H_8-162] $^-$	Jasminoside B/D/G (M)	*ZZ*
8	1.347	377.0837	-1.6	353.0877	-0.3	354.0951	$C_{16}H_{18}O_9$	-	191 [M-H-caffeoyl] $^-$ 179 [M-H-$C_7H_{10}O_5$] $^-$	Neochlorogenic acid (QA)	*ZZ*
9	4.551	427.1225	3.3	403.1231	-3.7	404.1319	$C_{17}H_{24}O_{11}$	265 [M + Na-162] $^+$ 247 [M + Na-162-H2O] $^+$	403[M-H] $^-$ 241[M-H-$C_6H_{10}O_5$] $^-$ 223[M-H-$C_6H_{12}O_6$] $^-$	Gardenoside (I)	*ZZ*
10	4.711	383.1312	0.14	359.1365 395.1132☆	4.7 4.6	360.142	$C_{16}H_{24}O_9$	-	197 [M-H-162] $^-$ 179 [M-H-162-H_2O] $^-$ 151 [M-H-162-H_2O-CO] $^-$ 161 [M-H-162-2H_2O] $^-$ 125 [M-H-162-$C_3H_4O_2$] $^-$ 107 [M-H-162-$C_3H_4O_2$-H_2O] $^-$	Ixoroside (I)	*ZZ*
11	4.901	369.1523	0.8	381.1253☆	8.4	346.1628	$C_{16}H_{26}O_8$	-	381 [M + Cl] $^-$ 327 [M-H-H_2O] $^-$ 165 [M-H-H_2O- 162] $^-$ 331 [M-H-CH_2] $^-$ 289 [M-H-C_4H_8] $^-$ 247 [M-H-C_4H_8-C_2H_2O] $^-$ 127 [M-H-C_4H_8-162] $^-$	Jasminoside B/D/G (M)	*ZZ*
12	5.270	485.1995	-0.34	497.1776☆	-3.8	462.2101	$C_{21}H_{34}O_{11}$	-	461 [M-H] $^-$ 311 [M-H-$C_{10}H_{14}O$] $^-$ 293 [M-H-$C_{10}H_{14}O$-H_2O] $^-$	Jasminoside T (M)	*ZZ*
13	5.482	377.0839	-1.1	353.0891	3.7	354.0951	$C_{16}H_{18}O_9$	-	191 [M-H-caffeoyl] $^-$ 335 [M-H-H_2O] $^-$	Chlorogenic acid ^{s} (QA) ^{s}	*ZZ*
14	5.656	361.0898	1.1	337.0907	-1.7	338.1002	$C_{16}H_{18}O_8$		337 [M-H] $^-$ 191 [M-H- Coumaroyl] $^-$ 173 [M-H- Coumaroyl-H_2O] $^-$	3-O-p-Coumaroyl quinic acid (QA)	*ZZ*
15	5.852	573.1783	1.21	585.1562☆ 549.1828	-5.1 0.5	550.1898	$C_{23}H_{34}O_{15}$	-	549[M-H] $^-$ 225[M-H-2$C_6H_{10}O_5$] $^-$ 207[M-H-$C_6H_{12}O_6$-$C_6H_{10}O_5$] $^-$ 123[M-H-2$C_6H_{10}O_5$-$C_4H_6O_3$] $^-$ 101[M-H-2$C_6H_{10}O_5$-$C_7H_8O_2$] $^-$	Genipin-1-β-D-gentiobioside (I)	*ZZ*

No.	t_R(min)	$[M+Na]^+$ *m/z* Detected	ppm	$[M-H]^-$ *m/z* Detected	ppm	MW(Da)	Formula	MS/MS ESI+	ESI-	Identification	Source
16	6.131	411.1245	4.06	387.1289	-2.1	388.1369	$C_{17}H_{24}O_{10}$	-	387$[M-H]^-$ 225$[M-H-C_6H_{10}O_5]^-$ 207$[M-H-C_6H_{12}O_6]^-$ 147$[M-H-C_6H_{12}O_6-C_2H_4O_2]^-$ 123$[M-H-C_6H_{10}O_5-C_4H_6O_3]^-$ 101$[M-H-C_6H_{10}O_5-C_7H_8O_2]^-$	Geniposide [S](I)	*ZZ*
17	6.781	353.1581	-2.9	329.1611	1.5	330.1679	$C_{16}H_{26}O_7$	331$[M+H]^+$ 169$[M+H-C_6H_{10}O_5]^+$ 151$[M+H-C_6H_{12}O_6]^+$	-	Jasminoside A/E (M)	*ZZ*
18	6.999	353.1567	-1.0	389.1815* 365.1381☆	-0.5 2.2	330.1679	$C_{16}H_{26}O_7$	331$[M+H]^+$ 169$[M+H-C_6H_{10}O_5]^+$ 151$[M+H-C_6H_{12}O_6]^+$	-	Jasminoside A/E (M)	*ZZ*
19	7.601	165.0551◦	2.9	163.0402	0.6	164.0473	$C_9H_8O_3$	-	163 $[M-H]^-$ 119 $[M-H-CO_2]^-$	p-Coumaric acid [S] (OA)	*ZZ*
20	8.187	439.0996 417.1198	0.8 4.3			416.1107	$C_{21}H_{20}O_9$	417$[M+H]^+$ 255$[M+H-C_6H_{10}O_5]^+$ 199$[M+H-C_6H_{10}O_5-2CO]^+$		Daidzin (F)	*DDC*
21	8.621	-	-	183.1019	-4.4	184.1099	$C_{10}H_{16}O_3$	-	183$[M-H]^-$ 165$[M-H-H_2O]^-$ 147$[M-H-2H_2O]^-$	Jasminodiol (M)	*ZZ*
22	9.444	779.2375 795.2114[§]	0.77 0.71	755.2409 791.2167☆	0.7 -0.5	756.2477	$C_{34}H_{44}O_{19}$	-	367 $[M-H-C_{11}H_{14}O_5-162]^-$ 173 $[M-H-C_{11}H_{14}O_5-162]^-$ 162-MeOH$]^-$ 161 $[M-H-C_{11}H_{14}O_5-162-162-CO_2]^-$	6''-O-trans-sinapoylgenipin gentiobioside (I)	*ZZ*
23	10.273	255.0689	1.23	253.0502	-1.6	254.0579	$C_{15}H_{10}O_4$	255$[M+H]^+$ 227$[M+H-CO]^+$ 199$[M+H-2CO]^+$ 137$[M+H-C_8H_6O]^+$		Daidzein (F) [S]	*DDC*
24	10.664			397.1132	-2.0	398.1213	$C_{18}H_{22}O_{10}$		191 [M-H- Sinapoyl]$^-$	3-*O*-Sinapoyl quinic acid (QA)	*ZZ*
25	11.443	447.1265◦	-4.6			446.1213	$C_{22}H_{22}O_{10}$	447$[M+H]^+$ 285$[M+H-C_6H_{10}O_5]^+$ 270$[M+H-C_6H_{10}O_5-CH_3]^+$		Glycitin (F)	*DDC*
26	12.191	433.1135◦	1.3			432.1057	$C_{21}H_{20}O_{10}$	433$[M+H]^+$ 241$[M+H-C_6H_{10}O_5]^+$		Genistin (F)	*DDC*
27	12.575	285.0749◦	-2.98			284.0685	$C_{16}H_{12}O_5$	285$[M+H]^+$ 270$[M+H-CH_3]^+$ 242$[M+H-CH_3-CO]^+$ 257$[M+H-CO]^+$ 229$[M+H-2CO]^+$ 167$[M+H-C_8H_6O]^+$		Glycitein (F)	*DDC*
28	13.182	533.1292◦	0.4			532.1217	$C_{25}H_{24}O_{13}$	533$[M+H]^+$ 285$[M+H-C_3H_2O_3-C_6H_{10}O_5]^+$		Malonylglycitin (F)	*DDC*
29	13.835	271.0612◦	4.1			270.0528	$C_{15}H_{10}O_5$	241$[M+H]^+$ 253$[M+H-H_2O]^+$ 243$[M+H-CO]^+$ 215$[M+H-2CO]^+$ 153$[M+H-C_8H_6O]^+$		Genistein (F)	*DDC*
30	13.930	957.5085◦	3.3			956.4981	$C_{48}H_{76}O_{19}$	957$[M+H]^+$ 795$[M+H-C_6H_{10}O_5]^+$ 633$[M+H-2C_6H_{10}O_5]^+$ 615$[M+H-C_6H_{10}O_5-C_6H_{12}O_6]^+$ 597$[M+H-C_6H_{10}O_5-C_6H_{12}O_6-H_2O]^+$ 457$[M+H-2C_6H_{10}O_5-C_6H_8O_6]^+$ 439$[M+H-2C_6H_{10}O_5-C_6H_{10}O_7]^+$ 421$[M+H-2C_6H_{10}O_5-C_6H_{10}O_7-H_2O]^+$		Soyasaponin Bd (S)	*DDC*
31	14.387	959.5223◦	1.3			958.5137	$C_{48}H_{78}O_{19}$	959$[M+H]^+$ 797$[M+H-C_6H_{10}O_5]^+$ 635$[M+H-2C_6H_{10}O_5]^+$ 617$[M+H-C_6H_{10}O_5-C_6H_{12}O_6]^+$ 599$[M+H-C_6H_{10}O_5-C_6H_{12}O_6-H_2O]^+$ 581$[M+H-C_6H_{10}O_5-C_6H_{12}O_6-2H_2O]^+$		Soyasaponin Ba (S)	*DDC*

No.	t_R(min)	$[M+Na]^+$ *m/z* Detected	ppm	$[M-H]^-$ *m/z* Detected	ppm	MW(Da)	Formula	MS/MS ESI+	ESI-	Identification	Source
32	14.640	943.5301°	4.3			942.5188	$C_{48}H_{78}O_{18}$	459[M+H-2$C_6H_{10}O_5$-$C_6H_8O_6$]$^+$ 441[M+H-2 $C_6H_{10}O_5$-$C_6H_{10}O_7$]$^+$ 423[M+H-2 $C_6H_{10}O_5$- $C_6H_{10}O_7$-H_2O]$^+$ 405[M+H-2 $C_6H_{10}O_5$- $C_6H_{10}O_7$-2H_2O]$^+$ 943[M+H]$^+$ 797[M+H-$C_6H_{10}O_4$]$^+$ 617[M+H- $C_6H_{10}O_4$-$C_6H_{12}O_6$]$^+$ 599[M+H- $C_6H_{10}O_4$- $C_6H_{12}O_6$-H_2O]$^+$ 581[M+H- $C_6H_{10}O_4$- $C_6H_{12}O_6$-2H_2O]$^+$ 459[M+H- $C_6H_{10}O_4$-$C_6H_{10}O_5$-$C_6H_8O_6$]$^+$ 441[M+H- $C_6H_{10}O_4$-$C_6H_{10}O_5$-$C_6H_{10}O_7$]$^+$ 423[[M+H- $C_6H_{10}O_4$- $C_6H_{10}O_5$-$C_6H_{10}O_7$-H_2O]$^+$		Soyasaponin Bb (S)	*DDC*
33	14.979	797.4673°	-1.11			796.4609	$C_{42}H_{68}O_{14}$	797[M+H]$^+$ 635[M+H-$C_6H_{10}O_5$]$^+$ 617[M+H-$C_6H_{12}O_6$]$^+$ 599[M+H- $C_6H_{12}O_6$-H_2O]$^+$ 581[M+H- $C_6H_{12}O_6$-2H_2O]$^+$ 423[M+H- $C_6H_{10}O_5$-$C_6H_{10}O_7$-H_2O]$^+$ 405[M+H- $C_6H_{10}O_5$- $C_6H_{10}O_7$-2H_2O]$^+$		Soyasaponin Bb' (S)	*DDC*
34	15.212	767.4571°	-0.68			766.4503	$C_{41}H_{66}O_{13}$	767[M+H]$^+$ 635[M+H-$C_5H_8O_4$]$^+$ 617[M+H-$C_6H_{10}O_5$]$^+$ 423[M+H- $C_5H_8O_4$-$C_6H_{10}O_7$-H_2O]$^+$ 405[M+H- $C_5H_8O_4$- $C_6H_{10}O_7$-2H_2O]$^+$		Soyasaponin Bc' (S)	*DDC*
35	15.682	941.5095°	-1.0			940.5032	$C_{48}H_{76}O_{18}$	941[M+H]$^+$ 795[M+H-$C_6H_{10}O_4$]$^+$ 457[M+H- $C_6H_{10}O_4$-$C_6H_{10}O_5$-$C_6H_8O_6$]$^+$ 439[M+H-$C_6H_{10}O_4$-$C_6H_{10}O_5$-$C_6H_{10}O_7$]$^+$ 421[[M+H-$C_6H_{10}O_4$-$C_6H_{10}O_5$-$C_6H_{10}O_7$-H2O]$^+$		Soyasaponin Be (S)	*DDC*

I: iridoid glycosides; M: monoterpenoids; F: flavonoids; QA: Quinic acid derivatives; OA: organic acids; S: Soyasaponins.

° $[M+H]^+$, § $[M+K]^+$, ☆ $[M+Cl]^-$, * $[M+CH_3COO]^-$

ˢConfirmed with standard compound

Table S2. Identification of metabolites of *ZZCD* in feces of rat model of depression by UHPLC-Q-TOF-MS/MS

No.	t_R(min)	$[M+H]^+$ m/z		$[M-H]^-$ m/z		MW(Da)	Formula	MS/MS		Identification
		Detected	ppm	Detected	ppm			ESI+	ESI-	
M1	1.104	389.1432	-2.6	387.1311	3.7	388.1369	$C_{17}H_{24}O_{10}$	213[M+H-$C_6H_8O_6$]$^+$ 181[M+H-$C_6H_8O_6$-CH_3O]$^+$ 163[M+H-$C_6H_8O_6$-CH_4O-H_2O]$^+$ 135[M+H-$C_6H_8O_6$-CH_4O-H_2O-CO]$^+$ 105[M+H-$C_6H_8O_6$-CH_3O-H_2O-CO-CH_2O]$^+$	211[M-H-$C_6H_8O_6$]$^-$ 133[M-H-$C_6H_8O_6$-CH_3O-H_2O-CO]$^-$	Ring-opened metabolite of genipin-O-glucuronide 3-hydroxyl-1-deoxygenipin-10-β-D-glucuronide (I)
M2	1.838	-	-	169.0135	-4.7	170.0215	$C_7H_6O_5$	-	151[M-H-H_2O]$^-$ 125[M-H-CO_2]$^-$	2,3,5-trihydroxybenzoic acid (OA)
M3	2.776	-	-	241.0721	1.4	242.0790	$C_{11}H_{14}O_6$	-	241[M-H]$^-$ 209[M-H-CH_3OH]$^-$ 163[M-H-$C_2H_4O_2$-H_2O]$^-$ 101[M-H-C7H_8O_3]$^-$ 69[M-H-$C_7H_8O_5$]$^-$	Hydroxylation of genipin(I)
M4	2.914	-	-	232.9757	-1.7	233.9834	$C_7H_6O_7S$	-	153[M-H-80]$^-$ 109[M-H-80-CO_2]$^-$	Gentisic acid-O-sulfate (OA)
M5	3.612	-	-	181.0515	4.79	182.0579	$C_9H_{10}O_4$	-	137[M-H-CO_2]$^-$ 119[M-H-CO_2-H_2O]$^-$	Dihydrocaffeic acid (OA)
M6	4.315	-	-	359.1353	1.4	360.142	$C_{16}H_{24}O_9$	-	341[M-H-H_2O]$^-$ 183[M-H-GluA]$^-$ 165[M-H-GluA-H_2O]$^-$	Ring-opened and methyl formate removal derivative of genipin-O-glucuronide (I)
M7	5.499	-	-	375.1285	-2.9	376.13695	$C1_6H_{24}O_{10}$		329[M-H-HCOOH]$^-$ 213[M-H-$C_6H_{10}O_5$]$^-$ 195[M-H-$C_6H_{10}O_5$-H_2O]$^-$ 167[M-H-$C_6H_{10}O_5$-HCOOH]$^-$ 125[M-H-$C_6H_{10}O_5$-$C_3H_4O_3$]$^-$ 69[M-H-$C_{12}H_{18}O_9$]$^-$	Loss of CH_2 and cleavage of geniposide (I)
M8	6.606	425.1046°	-2.0	437.0863☆	1.6	402.1162	$C_{17}H_{22}O_{11}$	403[M+H]$^+$ 227[M+H-162]$^+$	225[M-H-GluA]$^-$ 207[M-H-GluA-H_2O]$^-$ 193[M-H-GluA-H_2O-CH]$^-$ 175[M-H-GluA-H_2O-CH_3O]$^-$ 123[M-H-80-162-$C_4H_6O_3$]$^-$ 101[M-H-80-162-$C_7H_8O_2$]$^-$	Genipin-O-glucuronide (I)
M9	7.364	425.1053°	-0.3	437.0854☆	-0.5	402.1162	$C_{17}H_{22}O_{11}$	403[M+H]$^+$ 227[M+H-162]$^+$	225[M-H-GluA]$^-$ 207[M-H-GluA-H_2O]$^-$ 193[M-H-GluA-H_2O-CH]$^-$ 175[M-H-GluA-H_2O-CH_3O]$^-$ 123[M-H-80-162-$C_4H_6O_3$]$^-$ 101[M-H-80-162-$C_7H_8O_2$]$^-$	Genipin-O-glucuronide (I)
M10	7.727	367.1150	-	-	-	-	-	367[M+H]$^+$ 287[M+H-80]$^+$	-	M- O-sulfate (unidentified) (O)
M11	8.005	431.0963	-2.3	-	-	430.0900	$C_{21}H_{18}O_{10}$	431 [M+H]$^+$ 255[M–Glu A +H]$^+$ 227 [M–Glu A-CO+H]$^+$ 199[M+H-2CO]$^+$ 137[M+H-C_8H_6O]$^+$	-	Daidzein-O-glucuronide (F)
M12	8.150	-	-	305.0322	-4.6	306.0409	$C_{11}H_{14}O_8S$	-	225[M-H-80]$^-$ 207[M-H-80-H_2O]$^-$ 193[M-H-80-H_2O-CH]$^-$ 175[M-H-80-H_2O-CH_3O]$^-$ 123[M-H-80-$C_4H_6O_3$]$^-$ 101[M-H-80-$C_7H_8O_2$]$^-$	Genipin-O-sulfate (I)
M13	8.289	-	-	263.0592	-0.8	264.0668	$C_{10}H_{16}O_6S$	-	183[M-H-80]$^-$	Jasminodiol-O-sulfate (M)
M14	8.621	461.1065	-2.9	-	-	460.1006	$C_{22}H_{20}O_{11}$	285[M+H-$C_6H_8O_6$]$^+$ 270[M+H-$C_6H_8O_6$-CH_3]$^+$; 242[M+H-$C_6H_8O_6$-CH_3-CO]$^+$ 225[M+H-$C_6H_8O_6$-CH_3-CO-OH]$^+$	-	Glycitein-O-glucuronide (F)

No.	t_R(min)	[M+H]$^+$ m/z		[M-H]$^-$ m/z		MW(Da)	Formula	MS/MS		Identification
		Detected	ppm	Detected	ppm			ESI+	ESI-	
M15	8.905	-	-	467.0873	1.74	468.0938	$C_{17}H_{24}O_{13}S$	197[M+H-$C_6H_8O_6$-CH_3-2CO-OH]$^+$	387[M-H-SO_3]$^-$ 225[M-H-SO_3-$C_6H_{10}O_5$]$^-$ 207[M-H-SO_3-$C_6H_{10}O_5$-H_2O]$^-$ 101[M-H-$C_{13}H_{18}O_{10}S$]$^-$ 96[M-H-$C_{17}H_{23}O_9$]$^-$	Glycitein -O -Sulfate (F)
M16	9.104	465.1896	-	-	-	-	-	289[M+H-176]$^+$ 209[M+H-176-80]$^+$	-	M-O-sulfate-glucuronide (unidentified) (O)
M17	9.142	367.1371°	2.1	343.1387	-3.2	344.1471	$C_{16}H_{24}O_8$	345 [M+H]$^+$	343[M-H]$^-$ 167[M-H-GluA]$^-$	Ring-opened and reduced products of genipin-O-glucuronide (I)
M18	9.854	345.1549 367.1357°	1.5 -1.7	343.188	-3.0	344.1471	$C_{16}H_{24}O_8$	-	343[M-H]$^-$ 167[M-H-GluA]$^-$	Ring-opened and reduced products of genipin-O-glucuronide (I)
M19	11.154	469.0748° 447.0903	1.4 -4.2	-	-	446.0849	$C_{21}H_{18}O_{11}$	447 [M+H]$^+$, 293 [M–Glu A+Na]$^+$, 271 [M–Glu A +H]$^+$	-	Genistein-O-glucuronide (F)
M20	14.721	635.4163	1.48	-	-	634.8510	$C_{36}H_{58}O_9$	441 [M-GluA –OH]$^+$ 423 [M- GluA -OH-H_2O]$^+$	-	Soyasapogenol B-O- glucuronide
M21	15.425	539.3392	-1.64			538.7840	$C_{36}H_{58}O_6S$	441 [M-SO_3H -OH]$^+$ 423 [M- GluA -OH-H_2O]$^+$		Soyasapogenol B-O-sulfate

I: iridoid glycosides-related metabolites; M: monoterpenoids-related metabolites; F: flavonoids-related metabolites; OA: organic acids-related metabolites; S: Soyasaponins-related metabolites; O: other metabolites.

° [M+Na]$^+$, ☆[M+Cl]$^-$