

Figure S1 Drug treatment and sample collection schedules.

Table S1 The differential metabolites between puerarin treatment groups and PTSD groups in negative and positive ion modes (n=6/group)

ID	Name_description	FC	log2FC	P value	VIP	Regulation
Com_2934_pos	4-cyclopropyl-6-(methylthio)-2-pyrazin-2-ylpyrimidine-5-carbonitrile	18.28	4.19	1.92E-08	3.95	Up
Com_365_pos	L-(-)-Methionine	5.61	2.49	5.21E-05	2.25	Up
Com_3159_pos	Daidzein	4.99	2.32	2.51E-03	2.00	Up
Com_2799_pos	2-(acetylamino)-3-[4-(acetylamino)phenyl]acrylic acid	4.62	2.21	5.16E-06	2.09	Up
Com_4003_pos	Glycitein	4.45	2.15	8.67E-03	2.24	Up
Com_2513_pos	4-morpholinobenzoic acid	3.43	1.78	6.13E-05	1.72	Up
Com_655_pos	Kojic acid	3.21	1.68	4.94E-05	1.58	Up
Com_8147_pos	PB-22 N-(4-Hydroxypentyl)-3-carboxyindole metabolite	3.19	1.68	9.94E-05	1.57	Up
Com_1476_pos	DL-2-(acetylamino)-3-phenylpropanoic acid	2.96	1.56	6.13E-05	1.51	Up
Com_4650_pos	Acetylcholine	2.92	1.55	5.26E-07	1.47	Up
Com_7558_pos	ethyl 4-hydroxy-2-[(4-methoxyphenoxy)methyl]pyrimidine-5-carboxylate	2.52	1.34	1.62E-03	1.30	Up
Com_1753_pos	5-Methylcytosine	2.40	1.26	5.66E-03	1.30	Up
Com_346_pos	Methionine	2.36	1.24	6.66E-06	1.17	Up
Com_3519_pos	Miquelianin	2.34	1.23	4.63E-05	1.14	Up
Com_552_pos	Glycyl-L-Proline	2.33	1.22	4.15E-06	1.16	Up
Com_1586_pos	D-(+)-Maltose	2.32	1.21	8.63E-03	1.23	Up
Com_5564_pos	2-[5-(2-hydroxypropyl)oxolan-2-yl]propanoic acid	2.21	1.14	6.92E-05	1.10	Up
Com_2582_pos	(R)-Equol	2.16	1.11	1.85E-02	1.00	Up
Com_4510_pos	PC (5:0/13:1)	2.15	1.11	8.15E-03	1.07	Up
Com_7238_pos	2-(3,4-dimethoxyphenyl)ethanamine	2.13	1.09	4.35E-07	1.04	Up
Com_1117_pos	Trigonelline	2.08	1.06	1.67E-03	1.00	Up
Com_4867_pos	Pyridoxamine	2.06	1.04	1.08E-04	1.01	Up
Com_122_neg	3-Hydroxy-3-methylglutaric acid	12.93	3.69	1.18E-02	3.39	Up
Com_1693_neg	3-[4-(tert-butyl)anilino]-2-(3-thienylcarbonyl)acrylonitrile	5.57	2.48	4.37E-02	2.24	Up
Com_4247_neg	2-[2-(3,4-dichlorophenyl)acetyl]-N-propylhydrazine-1-carbothioamide	5.55	2.47	8.18E-03	1.94	Up
Com_248_neg	acetoacetate	4.64	2.21	1.26E-04	1.97	Up
Com_187_neg	DI-3-Hydroxynorvaline	4.57	2.19	9.32E-05	1.91	Up
Com_186_neg	DI-Proline	4.57	2.19	8.56E-05	1.91	Up
Com_3726_neg	N-(1,1-Dioxotetrahydro-1H-1λ6-thiophen-3-yl)-4-methoxybenzamide	4.41	2.14	1.52E-05	2.05	Up
Com_2449_neg	N-Acetyl-L-phenylalanine	4.03	2.01	6.49E-05	1.89	Up
Com_1230_neg	2,3-Dihydroxybenzoic Acid	3.50	1.81	3.44E-04	1.58	Up
Com_70_neg	D(-)-Threose	3.44	1.78	2.22E-04	1.68	Up
Com_46_neg	D-(+)-Mannose	3.32	1.73	1.22E-04	1.61	Up
Com_157_neg	Acrylic acid	3.16	1.66	4.66E-05	1.52	Up
Com_2453_neg	N-Acetyl-DL-tryptophan	2.65	1.41	5.70E-03	1.29	Up
Com_282_neg	Dimethyl fumarate	2.63	1.39	2.82E-04	1.29	Up
Com_1028_neg	PI (18:1/18:2)	2.49	1.31	3.38E-03	1.19	Up
Com_2471_neg	DI-Indole-3-lactic acid	2.47	1.30	2.28E-04	1.19	Up
Com_3946_neg	Esculin	2.46	1.30	1.91E-03	1.15	Up
Com_1446_neg	Glu-Gln	2.45	1.29	2.59E-03	1.15	Up
Com_1668_neg	LPC 20:5	2.45	1.29	7.99E-04	1.15	Up

Table S1 (continued)

Table S1 (continued)

ID	Name_description	FC	log2FC	P value	VIP	Regulation
Com_330_neg	L-Histidine	2.35	1.23	1.00E-02	1.25	Up
Com_55_neg	LPC 18:2	2.29	1.20	1.38E-03	1.05	Up
Com_3870_neg	Adipic acid	2.25	1.17	2.60E-05	1.06	Up
Com_786_pos	α -Eleostearic acid	0.52	-0.94	3.86E-02	1.27	Down
Com_2071_pos	octadec-9-ynoic acid	0.51	-0.97	1.93E-02	1.15	Down
Com_1184_pos	10E,12Z-Octadecadienoic acid	0.49	-1.03	1.57E-02	1.20	Down
Com_3102_pos	LPC 14:1	0.48	-1.07	3.34E-04	1.04	Down
Com_1886_pos	ACar 20:2	0.48	-1.07	5.26E-04	1.04	Down
Com_6479_pos	Pleuromutilin	0.47	-1.10	4.63E-04	1.03	Down
Com_1685_pos	ACar 20:1	0.47	-1.10	2.66E-04	1.02	Down
Com_5395_pos	5-Methyl-dl-tryptophan	0.46	-1.12	5.78E-03	1.13	Down
Com_5622_pos	2-morpholino-1-phenyl-1-ethanol	0.46	-1.12	4.73E-05	1.06	Down
Com_188_pos	Glycocholic acid	0.45	-1.17	4.41E-02	1.12	Down
Com_7779_pos	Lysopg 18:1	0.43	-1.21	4.41E-02	1.36	Down
Com_209_pos	Deoxycholic Acid	0.43	-1.21	1.35E-02	1.09	Down
Com_407_pos	15-Deoxy- Δ 12,14-prostaglandin A1	0.43	-1.22	1.99E-02	1.44	Down
Com_3585_pos	Coenzyme Q2	0.43	-1.23	7.46E-06	1.15	Down
Com_1606_pos	Oleic acid	0.43	-1.23	1.39E-02	1.50	Down
Com_2280_pos	5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one	0.42	-1.24	2.84E-02	1.22	Down
Com_1721_pos	Decanoylcarnitine	0.41	-1.27	1.17E-03	1.27	Down
Com_3865_pos	Guggulsterone	0.41	-1.28	2.04E-02	1.62	Down
Com_1604_pos	Hexanoylcarnitine	0.40	-1.31	3.66E-03	1.36	Down
Com_6545_pos	Propionyl-L-carnitine	0.40	-1.31	3.66E-02	1.05	Down
Com_6127_pos	N-Arachidonoyl-L-serine	0.40	-1.33	3.41E-03	1.39	Down
Com_5562_pos	Kanamycin	0.40	-1.33	3.62E-03	1.36	Down
Com_8440_pos	1-(2-furyl)pentane-1,4-dione	0.40	-1.33	3.44E-04	1.24	Down
Com_5623_pos	13,14-dihydro-15-keto-PGD2	0.40	-1.34	1.19E-02	1.23	Down
Com_871_pos	1,2-dihydroxyheptadec-16-yn-4-yl acetate	0.39	-1.35	6.81E-05	1.29	Down
Com_1801_pos	ACar 17:0	0.38	-1.40	2.00E-05	1.33	Down
Com_6872_pos	7 α -Hydroxytestosterone	0.37	-1.43	4.23E-02	1.10	Down
Com_1395_pos	11 β -Hydroxyandrosterone	0.37	-1.43	2.34E-02	1.18	Down
Com_57_pos	16(R)-HETE	0.37	-1.44	1.16E-02	1.61	Down
Com_1261_pos	9,10-Dihome	0.37	-1.45	3.22E-03	1.25	Down
Com_946_pos	ACar 20:4	0.37	-1.45	8.13E-06	1.37	Down
Com_1734_pos	ACar 13:0	0.36	-1.46	2.89E-04	1.40	Down
Com_2051_pos	ACar 12:1	0.36	-1.46	7.17E-04	1.45	Down
Com_2348_pos	Styrene	0.36	-1.49	3.36E-03	1.51	Down
Com_3535_pos	3-Methoxybenzaldehyde	0.35	-1.51	2.96E-04	1.38	Down
Com_5114_pos	ACar 15:1	0.35	-1.51	2.10E-05	1.40	Down
Com_2048_pos	ACar 18:3	0.35	-1.53	1.37E-05	1.44	Down
Com_20_pos	Allocholic acid	0.35	-1.53	3.00E-02	2.39	Down

Table S1 (continued)

Table S1 (continued)

ID	Name_description	FC	log2FC	P value	VIP	Regulation
Com_2139_pos	5 α -Dihydrotestosterone	0.34	-1.54	1.93E-02	1.52	Down
Com_3800_pos	T-2 Triol	0.34	-1.54	1.00E-03	1.54	Down
Com_4339_pos	Indole-3-butyric acid	0.34	-1.55	1.53E-05	1.48	Down
Com_9028_pos	Biotin	0.34	-1.57	9.29E-05	1.45	Down
Com_7820_pos	Phenylpyruvic Acid	0.34	-1.58	3.90E-06	1.48	Down
Com_2003_pos	Ecgonine methyl ester	0.33	-1.60	3.09E-05	1.49	Down
Com_281_pos	ACar 18:2	0.33	-1.61	2.52E-05	1.50	Down
Com_3601_pos	1-[2-(2,5-dimethyl-1H-pyrrol-1-yl)-4-nitrophenyl]-1H-imidazole	0.32	-1.62	6.56E-03	1.57	Down
Com_1891_pos	N-[2-[(2-furylmethyl)thio]ethyl]-2-[(3-methoxyphenyl)thio]acetamide	0.32	-1.63	1.47E-02	1.97	Down
Com_1941_pos	ACar 15:0	0.31	-1.67	8.92E-05	1.62	Down
Com_16_pos	Eicosapentaenoic acid	0.31	-1.67	6.43E-03	1.77	Down
Com_8123_pos	5,7-dihydroxy-3-(4-methoxyphenyl)-4H-chromen-4-one	0.31	-1.69	2.20E-02	1.44	Down
Com_5310_pos	DI-Tropic acid	0.31	-1.70	1.80E-04	1.56	Down
Com_2502_pos	ACar 20:3	0.31	-1.71	5.81E-06	1.61	Down
Com_1602_pos	2-Arachidonoyl glycerol	0.30	-1.73	4.60E-06	1.63	Down
Com_657_pos	ACar 14:1	0.30	-1.74	8.41E-06	1.65	Down
Com_2443_pos	Dehydroepiandrosterone (DHEA)	0.30	-1.76	8.44E-04	1.65	Down
Com_2870_pos	N-Acetylvaline	0.29	-1.77	1.87E-07	1.67	Down
Com_4136_pos	Ecgonine	0.29	-1.77	1.62E-03	1.60	Down
Com_1934_pos	3-Succinoylpyridine	0.28	-1.84	9.91E-07	1.73	Down
Com_122_pos	Palmitoylcarnitine	0.27	-1.89	1.27E-08	1.77	Down
Com_7670_pos	Artemisinin	0.27	-1.89	1.72E-04	1.72	Down
Com_1294_pos	Testosterone	0.27	-1.91	6.34E-03	1.62	Down
Com_1761_pos	5-(2,5-dihydroxyhexyl)oxolan-2-one	0.26	-1.93	1.67E-04	1.74	Down
Com_4424_pos	ACar 19:1	0.26	-1.96	8.83E-05	1.92	Down
Com_3824_pos	N-(2-morpholinophenyl)-2-furamide	0.25	-1.98	2.27E-03	1.73	Down
Com_2483_pos	Medroxyprogesterone	0.25	-2.01	3.94E-02	1.62	Down
Com_4342_pos	Cyclobutyl fentanyl-d5	0.25	-2.03	1.98E-04	1.97	Down
Com_5834_pos	[4-(7-chloroquinolin-4-yl)piperazino](phenyl)methanone	0.25	-2.03	1.46E-03	2.01	Down
Com_7850_pos	ethyl 4-((3-[5-(trifluoromethyl)-2-pyridyl]prop-2-ynyl)oxy)benzoate	0.24	-2.03	1.69E-04	2.01	Down
Com_155_pos	ACar 18:1	0.24	-2.04	8.54E-06	1.94	Down
Com_1788_pos	11-Deoxy prostaglandin F1 α	0.24	-2.09	4.16E-02	1.73	Down
Com_6386_pos	4-hydroxy-5,8-dimethylquinoline-3-carboxylic acid	0.23	-2.12	7.44E-03	1.74	Down
Com_423_pos	ACar 16:1	0.22	-2.17	1.71E-04	2.14	Down
Com_6167_pos	N1-isopropyl-2-(1H-2-pyrrolylcarbonyl)-1-hydrazinecarboxamide	0.22	-2.20	2.19E-04	2.10	Down
Com_837_pos	Pyrogallol	0.21	-2.24	9.05E-05	2.03	Down
Com_571_pos	3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazol-5-ol	0.20	-2.35	1.28E-03	2.06	Down
Com_3806_pos	Meperidine-d5	0.18	-2.48	4.89E-03	2.89	Down
Com_842_pos	2,4-dihydroxyheptadec-16-en-1-yl acetate	0.17	-2.56	2.23E-04	2.49	Down
Com_604_pos	all-cis-4,7,10,13,16-Docosapentaenoic acid	0.15	-2.73	2.02E-03	2.89	Down
Com_5312_pos	5,6-dimethoxy-2-(2-methoxyphenyl)-4H-chromen-4-one	0.14	-2.83	2.08E-04	2.65	Down

Table S1 (continued)

Table S1 (continued)

ID	Name_description	FC	log2FC	P value	VIP	Regulation
Com_635_pos	PC (4:0/18:5)	0.13	-2.95	2.35E-03	3.03	Down
Com_2681_pos	LPE 20:5	0.08	-3.68	2.96E-04	3.27	Down
Com_638_neg	FAHFA (18:2/20:3)	0.50	-1.01	8.72E-03	1.05	Down
Com_1268_neg	FAHFA (14:0/22:3)	0.47	-1.09	2.70E-02	1.10	Down
Com_94_neg	11(Z),14(Z)-Eicosadienoic acid	0.47	-1.09	8.77E-04	1.02	Down
Com_1140_neg	FAHFA (18:2/20:4)	0.47	-1.10	3.96E-02	1.35	Down
Com_145_neg	FAHFA (18:1/22:3)	0.46	-1.11	4.91E-03	1.10	Down
Com_24_neg	Lauric acid ethyl ester	0.46	-1.12	4.41E-02	1.44	Down
Com_3_neg	Elaidic acid	0.46	-1.14	4.02E-03	1.12	Down
Com_56_neg	8Z,11Z,14Z-Eicosatrienoic acid	0.45	-1.17	2.35E-04	1.07	Down
Com_3279_neg	11-Deoxy prostaglandin F2 β	0.44	-1.17	1.41E-02	1.04	Down
Com_22_neg	Docosahexaenoic acid	0.43	-1.21	1.01E-04	1.10	Down
Com_3836_neg	(\pm)-Abscisic acid	0.42	-1.26	5.33E-03	1.06	Down
Com_1274_neg	FAHFA (22:4/22:3)	0.40	-1.34	6.25E-04	1.23	Down
Com_710_neg	FAHFA (22:6/22:3)	0.39	-1.35	9.19E-05	1.24	Down
Com_646_neg	Pregnenolone	0.39	-1.37	1.74E-02	1.57	Down
Com_2564_neg	Cis-11,14,17-Eicosatrienoic Acid (C20:3)	0.38	-1.39	3.24E-04	1.27	Down
Com_1841_neg	FAHFA (22:5/22:3)	0.37	-1.44	1.00E-03	1.42	Down
Com_3674_neg	(3 β ,5 ξ ,9 ξ)-3,23-Dihydroxy-1-oxoolean-12-en-28-oic acid	0.34	-1.56	1.77E-03	1.40	Down
Com_1088_neg	FAHFA (18:1/20:3)	0.33	-1.59	1.50E-02	2.06	Down
Com_900_neg	FAHFA (16:0/18:2)	0.32	-1.62	6.55E-03	1.73	Down
Com_1142_neg	8,15-Dihete	0.32	-1.65	9.33E-03	1.61	Down
Com_1863_neg	Deoxycorticosterone 21-glucoside	0.26	-1.94	1.09E-02	1.84	Down
Com_18_neg	11,12-Epoxy-(5Z,8Z,11Z)-icosatrienoic acid	0.25	-2.02	1.22E-02	1.80	Down
Com_1188_neg	Hydrocortisone 17-valerate	0.22	-2.18	1.03E-02	2.13	Down
Com_2295_neg	(3 β ,9 α)-3-(β -D-Glucopyranosyloxy)-14-hydroxycard-20(22)-enolide	0.21	-2.22	3.42E-02	2.16	Down
Com_650_neg	Deoxycholic acid	0.19	-2.42	5.80E-03	2.29	Down
Com_1022_neg	Ginkgoic acid	0.17	-2.57	6.07E-04	2.13	Down
Com_617_neg	PC (2:0/18:3)	0.14	-2.87	2.82E-03	2.85	Down
Com_2170_neg	FAHFA (22:6/22:5)	0.13	-2.99	9.43E-06	2.72	Down
Com_89_neg	7-Ketodeoxycholic acid	0.08	-3.72	1.40E-03	3.70	Down

PTSD, post-traumatic stress disorder. FC, fold change. VIP, variable importance in the projection.

Table S2 The differential metabolites between PTSD groups and control groups in negative and positive ion modes (n = 6/group)

ID	Name_des	FC	log2FC	Pvalue	VIP	Regulation
Com_6872_pos	7 α -Hydroxytestosterone	3.42	1.77	1.29E-02	2.72	up
Com_3824_pos	N-(2-morpholinophenyl)-2-furamide	3.28	1.71	5.18E-03	2.75	up
Com_571_pos	3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazol-5-ol	3.19	1.67	9.85E-03	2.64	up
Com_2280_pos	5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one	3.16	1.66	5.41E-03	2.76	up
Com_1934_pos	3-Succinoylpyridine	2.83	1.50	9.03E-04	2.68	up
Com_1891_pos	N-{2-[(2-furylmethyl)thio]ethyl}-2-[(3-methoxyphenyl)thio]acetamide	2.71	1.44	5.24E-03	2.58	up
Com_5536_pos	Nicotinic Acid	2.57	1.36	4.33E-03	2.16	up
Com_7084_pos	Asp-glu	2.56	1.36	2.25E-03	2.41	up
Com_1761_pos	5-(2,5-dihydroxyhexyl)oxolan-2-one	2.46	1.30	2.00E-03	2.12	up
Com_596_pos	5-Aminosalicylic Acid	2.41	1.27	1.09E-02	2.49	up
Com_639_pos	methyl isoquinoline-3-carboxylate	2.30	1.20	7.47E-03	1.94	up
Com_481_pos	1,4-Dihydro-1-Methyl-4-Oxo-3-Pyridinecarboxamide	2.20	1.14	2.10E-02	2.14	up
Com_7558_pos	ethyl 4-hydroxy-2-[(4-methoxyphenoxy)methyl]pyrimidine-5-carboxylate	2.15	1.11	1.10E-02	1.92	up
Com_642_pos	Hippuric acid	2.14	1.10	2.03E-03	1.87	up
Com_5958_pos	1,7-bis(3,4-dihydroxyphenyl)heptan-3-one	2.09	1.06	7.52E-05	1.80	up
Com_6167_pos	N1-isopropyl-2-(1H-2-pyrrolylcarbonyl)-1-hydrazinecarboxamide	1.99	0.99	2.39E-02	1.63	up
Com_5310_pos	DI-Tropic acid	1.65	0.72	3.19E-02	1.14	up
Com_7316_pos	Pilocarpine	1.62	0.69	1.23E-02	1.23	up
Com_6885_pos	4-(2,3-dihydro-1,4-benzodioxin-6-yl)butanoic acid	1.58	0.66	1.55E-02	1.17	up
Com_421_pos	Indole-3-acetic acid	1.56	0.64	1.19E-02	1.10	up
Com_7311_pos	4-methoxy-6-(prop-2-en-1-yl)-2H-1,3-benzodioxole	1.56	0.64	2.32E-03	1.13	up
Com_8440_pos	1-(2-furyl)pentane-1,4-dione	1.56	0.64	3.33E-02	1.07	up
Com_1670_pos	3-(3,4,5-trimethoxyphenyl)propanoic acid	1.54	0.62	3.05E-03	1.06	up
Com_2283_neg	Lysopc 17:0	2.23	1.16	2.68E-02	2.17	up
Com_282_neg	Dimethyl fumarate	2.19	1.13	3.32E-02	2.59	up
Com_3870_neg	Adipic acid	2.18	1.12	2.38E-05	2.23	up
Com_3836_neg	(\pm)-Abscisic acid	2.08	1.06	1.55E-02	1.85	up
Com_1230_neg	2,3-Dihydroxybenzoic Acid	2.04	1.03	1.53E-02	2.16	up
Com_702_neg	4-Oxoproline	2.02	1.01	1.99E-02	1.82	up
Com_322_neg	LPA 18:0	1.90	0.93	2.94E-02	1.62	up
Com_3171_neg	Aflatoxin G2	1.88	0.91	5.21E-04	1.84	up
Com_3390_neg	12-Hydroxydodecanoic acid	1.74	0.80	2.70E-02	1.50	up
Com_248_neg	acetoacetate	1.65	0.72	4.47E-02	1.33	up
Com_3355_neg	Lysopc 16:1	1.64	0.71	1.29E-03	1.47	up

Table S2 (continued)

Table S2 (continued)

ID	Name_des	FC	log2FC	Pvalue	VIP	Regulation
Com_1533_neg	4-Methylphenol	1.63	0.70	1.91E-02	1.47	up
Com_46_neg	D-(+)-Mannose	1.58	0.66	3.85E-02	1.26	up
Com_466_neg	LPA 16:1	1.57	0.65	1.05E-02	1.22	up
Com_157_neg	Acrylic acid	1.56	0.64	4.78E-02	1.31	up
Com_256_neg	PI (16:0/20:4)	1.54	0.62	3.70E-02	1.11	up
Com_5395_pos	5-Methyl-dl-tryptophan	0.66	-0.60	1.59E-02	1.05	down
Com_464_pos	Threonine	0.66	-0.60	4.35E-04	1.01	down
Com_875_pos	2-Pyridylacetic acid	0.65	-0.61	1.61E-02	1.12	down
Com_1476_pos	DL-2-(acetylamino)-3-phenylpropanoic acid	0.65	-0.62	2.70E-02	1.03	down
Com_5597_pos	ethyl 4-methyl-2-(1H-pyrrol-1-yl)-1,3-thiazole-5-carboxylate	0.64	-0.64	2.51E-03	1.08	down
Com_2474_pos	Spermidine	0.64	-0.65	2.16E-02	1.15	down
Com_4713_pos	glutathione	0.62	-0.68	2.65E-02	1.09	down
Com_212_pos	DL-Lysine	0.62	-0.69	2.53E-03	1.22	down
Com_5335_pos	Lysopc 14:0	0.61	-0.71	4.93E-02	1.12	down
Com_8339_pos	3,4-dihydroxy-4-(4-methoxyphenyl)-1,2,3,4-tetrahydroquinolin-2-one	0.58	-0.79	4.08E-02	1.33	down
Com_5367_pos	Deisopropylatrazine	0.58	-0.79	4.64E-02	1.23	down
Com_7334_pos	N2,N2-Dimethylguanosine	0.57	-0.80	3.78E-02	1.20	down
Com_6180_pos	4-bromo-3-[[[(methylamino)carbonyl]oxy]imino]methyl]-1H-pyrazole	0.50	-0.99	4.11E-02	1.43	down
Com_1879_pos	N-Acetyl-D-phenylalanine	0.48	-1.05	2.95E-02	2.17	down
Com_5435_pos	Gly-Phe	0.44	-1.19	4.01E-02	1.65	down
Com_1017_pos	1-Methylnicotinamide	0.19	-2.38	3.51E-03	3.85	down
Com_1020_pos	6-Methylnicotinamide	0.18	-2.48	9.47E-04	4.06	down
Com_3159_pos	Daidzein	0.17	-2.57	1.17E-02	3.49	down
Com_1881_neg	Bilirubin	0.65	-0.63	1.36E-02	1.23	down
Com_623_neg	L-Cysteine-S-sulfate	0.63	-0.67	1.92E-02	1.47	down
Com_994_neg	Delta-Tridecalactone	0.62	-0.68	3.87E-02	1.49	down
Com_42_neg	PI (18:0/20:4)	0.59	-0.75	1.79E-04	1.51	down
Com_330_neg	L-Histidine	0.44	-1.17	1.83E-02	2.44	down
Com_3726_neg	N-(1,1-Dioxotetrahydro-1H-1λ6-thiophen-3-yl)-4-methoxybenzamide	0.40	-1.34	2.58E-02	2.29	down

PTSD, post-traumatic stress disorder. FC, fold change. VIP, variable importance in the projection.

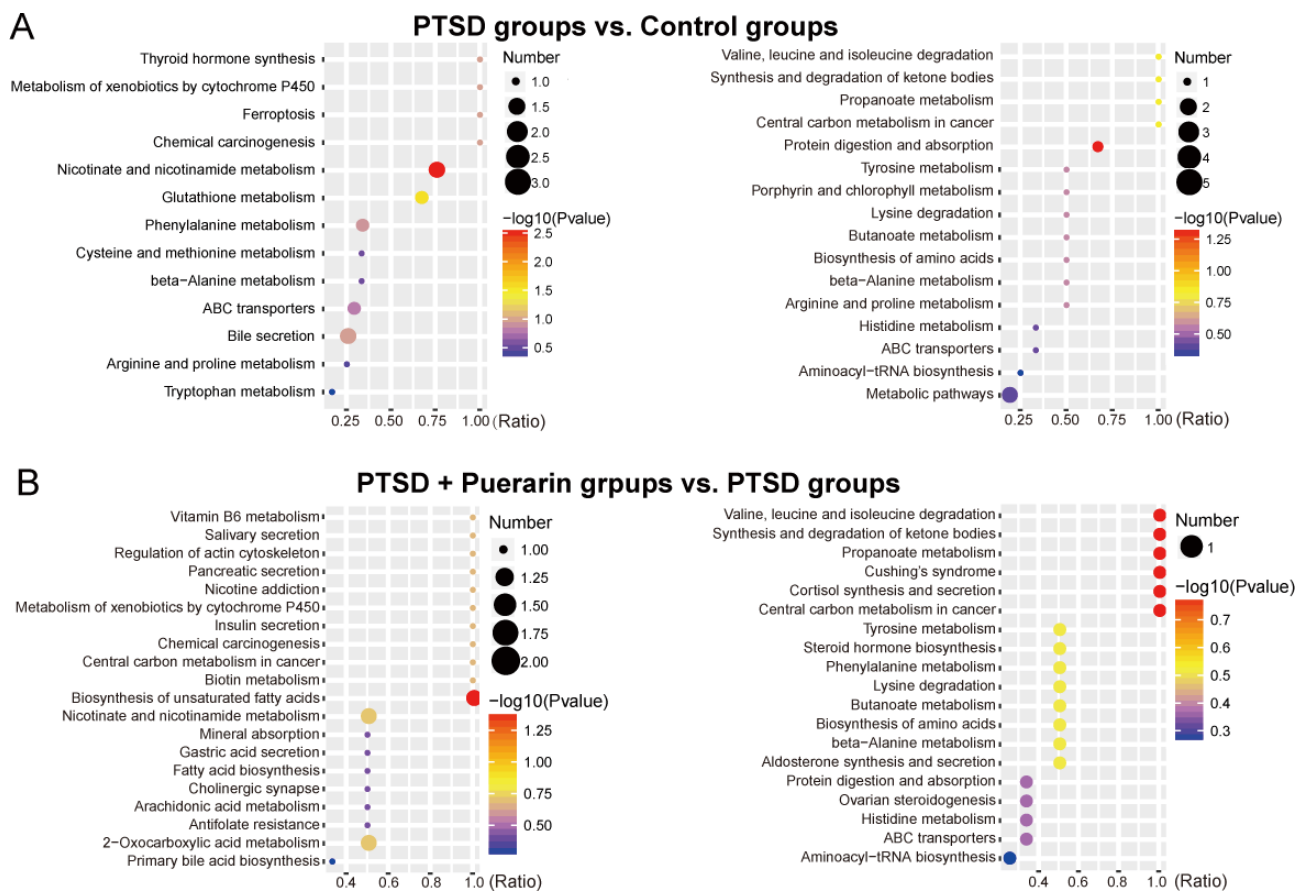


Figure S2 KEGG enrichment of differential metabolites of PTSD group *vs.* control group (A) and puerarin treatment group *vs.* PTSD group (B). The size of the spots represents the number of metabolites enriched in the representative KEGG pathway. The colors of the spots represent $-\log_{10}(P \text{ value})$. PTSD, post-traumatic stress disorder; KEEG, Kyoto Encyclopedia of Genes and Genomes.