Table S1. MIR wavenumbers (cm^{-1}) and preliminary assignments in the range of 400-4000 cm^{-1} for Radix Oryzae Glutinosae (ROG).

IR wavenumbers(cm^{-1})	Assignments
3424.70	ν (O-H, N-H)
2926.68	ν_{as}(-CH_2, -CH_3)
1630.04	ν（C＝O, C＝C）
1603.32	ν（Ar: C＝C, C＝O）, δ(-NH_2)
1513.48	ν（Ar: C＝C）
1420.19	δ(-CH_2, -CH_3), ν(C-N)
1384.47	δ_s(-CH_3)
1278.39	ν_{as}(C-O-C), ν(C-O)
1119.77	ν(C-O-C, C-OH)
1080.19	ν(C-O-C, C-OH)
618.39	δ(O-H, C＝O)

Note: ν: stretching mode; δ: bending mode; s: symmetrical; as: antisymmetrical; Ar: aromatic ring.

Table S2. Assignment of ^{1}H-NMR spectra peaks of ROG.

^{1}H-NMR characteristic signals(ppm)	Metabolite	^{1}H-NMR characteristic signals(ppm)	Metabolite
8.25	Adenosine	3.57	Glycine
7.30	L-phenylalanine	3.37	Taurine
7.15		3.36	
3.93		3.25	Choline
3.25		3.06	GABA
7.13	Histidine	1.83	
6.64	Thymoquinone	2.80	p-cymene
3.00		2.21	
1.97		1.25	
1.13		2.61	Citric acid
6.39	Kaempferol	2.14	Hydroxyproline
6.13		2.09	Proline
5.23	α-glucose	2.03	Fatty acid
3.46		1.34	
4.69	β-Glucose	0.94	
4.02	Fructose	1.80	Lysine
3.85	Maltose	1.61	
3.76	Sucrose	1.75	Arginine
3.63		1.72	Cycloartenol
3.44		0.85	
3.70	Leucine	0.67	
1.00		1.19	Thymol
0.99		1.10	2-ketoisovaleric acid

Table S3. Correlation analysis results of the ROG samples by applying ^{1}H NMR.

Amino/Organic acids	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
S1	1									
S2	0.122	1								
S3	0.168	**0.995***	1							
S4	0.379*	**0.942***	**0.947***	1						
S5	0.739*	0.679*	0.711*	**0.869***	1					
S6	0.763*	0.183	0.233*	0.387*	0.638*	1				
S7	0.115	**0.992***	**0.997***	**0.920***	0.664*	0.192	1			
S8	0.144	**0.964***	**0.976***	**0.881***	0.644*	0.189	**0.982***	1		
S9	0.086	0.255*	0.329*	0.173	0.183	0.168	0.364*	0.443*	1	
S10	0.139	**0.964***	**0.981***	**0.889***	0.657*	0.212	**0.988***	**0.991***	0.493*	1
Carbohydrates	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
S1	1									
S2	**0.913***	1								
S3	**0.853***	**0.984***	1							
S4	**0.861***	**0.986***	**0.992***	1						
S5	**0.879***	**0.990***	**0.985***	**0.993***	1					
S6	**0.906***	**0.955***	**0.909***	**0.935***	**0.954***	1				
S7	**0.920***	**0.993***	**0.972***	**0.979***	**0.990***	**0.962***	1			
S8	**0.944***	**0.884***	**0.858***	**0.838***	**0.843***	0.797*	**0.886***	1		
S9	**0.877***	**0.941***	**0.912***	**0.930***	**0.947***	**0.934***	**0.960***	**0.841***	1	
S10	**0.945***	**0.972***	**0.928***	**0.944***	**0.966***	**0.972***	**0.988***	**0.885***	**0.964***	1
Aromatic substances	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
S1	1									
S2	0.620*	1								
S3	**0.826***	**0.908***	**1**							
S4	0.755*	0.783*	**0.891***	1						
S5	**0.968***	0.728*	**0.895***	**0.810***	1					
S6	**0.803***	0.675*	**0.834***	**0.849***	**0.846***	1				
S7	0.685*	**0.958***	**0.951***	**0.905***	0.775*	0.751*	1			
S8	**0.902***	0.763*	**0.900***	0.773*	**0.936***	0.710*	0.799*	1		
S9	0.701*	**0.957***	**0.955***	**0.876***	0.786*	0.748*	**0.982***	**0.837***	1	
S10	**0.806***	**0.928***	**0.986***	**0.920***	**0.882***	**0.827***	**0.977***	**0.879***	**0.969***	1

[a] Significant correlations (> 0.80) in bold. * P-value < 0.05.

Table S4 Results of determination of the selected elements (mg/kg dry weight) in the ROG samples from ten regions using the ICP-MS method (n=3, mean and standard deviations).

Element	S1 Wuhu Anhui	S2 Meizhou Guangdong	S3 Yulin Guangxi	S4 Xinyang Henan	S5 Huanggang Hubei	S6 Huaihua Hunan	S7 Suqian Jiangsu	S8 Dujiangyan Sichuan	S9 Qujing Yunnan	S10 Quzhou Zhejiang
Co	2.750±	1.213	1.839	1.428	3.869	0.910	1.165	2.140	1.053	1.516

	0.064e	±0.020ab	± 0.037cd	± 0.090abc	± 0.095f	± 0.060a	± 0.062ab	± 0.104d	± 0.042ab	±0.081bc
Be	0.1029	0.1169	0.1098	0.0421	0.2834	0.0251	0.0143	0.0950	0.0328	0.0506
	± 0.0115c	± 0.0226c	± 0.0102c	± 0.0139ab	± 0.0183d	± 0.0147ab	± 0.0020a	± 0.0266c	± 0.0126ab	± 0.0229b
Ba	34.48	26.46	71.04	34.55	86.57	36.79	38.45	50.49	33.68	37.78
	± 2.58b	± 1.41a	± 9.43e	±2.62b	±2.33f	± 1.51c	± 2.51c	±2.90d	± 1.57b	± 1.99c
Sb	0.0419	0.1544	0.0677	0.0665	0.0127	0.0528	0.0425	0.0374	0.0511	0.0549
	±0.0190b	± 0.0315e	± 0.0093d	±0.0024d	± 0.0071a	±0.0076c	±0.0006b	±0.0018b	±0.0035c	± 0.0085c
Fe	6583.2	9024.1	8282.7	3671.2	11151.0	2864.3	2527.8	6451.8	2720.1	3412.858
	±256.6g	± 325.9i	±169.4h	± 126.5e	± 353.6j	±177.8c	±146.8a	±275.9f	±128.2b	± 168.5d
Cr	2.201	2.850	3.395	1.620	6.353	0.6154	0.6730	1.495	0.6323	1.012
	± 0.795d	± 0.334f	± 0.413g	±0.396c	± 0.451h	± 0.0262a	±0.0399a	± 0.027c	±0.0176a	± 0.107b
Mn	281.0	229.4	241.5	121.3	318.7	73.5	102.7	408.3	61.2	142.5
	± 7.2h	±8.4f	± 2.3g	± 8.9d	± 6.5i	±2.9b	±4.3c	±9.6j	±2.9a	±8.6 e
Ni	2.003	1.827	3.185	1.833	6.774	1.121	0.9212	4.260	0.9809	1.662
	± 0.170b	± 0.307b	± 0.485c	±0.210b	± 0.187e	±0.177a	± 0.1095a	±0.478d	±0.0469a	± 0.094b
Zn	72.0	87.5	42.3	57.4	99.2	2.053	1.449	1.767	52.2	67.94 ±4.26 d
	±4.0d	±5.1e	±3.0b	± 3.4c	±6.7f	± 0.304a	± 0.221a	± 0.103a	± 2.0c	
As	11.96	30.18	53.79	20.08	24.26	22.00	17.16	34.17	20.21	27.38 ±1.33ef
	± 0.84a	± 1.63f	± 2.53h	± 0.30bc	± 0.94de	±1.60cd	± 1.01b	±1.43g	±0.88bc	
Cd	0.8253	3.679	0.2540	0.3766	1.244	0.0011	0.0471	1.024	0.2129	0.2133
	± 0.0717b	± 0.160d	± 0.0509a	± 0.0076a	± 0.026c	± 0.0002a	±0.0150a	±0.0639bc	±0.0113a	± 0.0152a
Pb	3.120	21.44	5.335	2.657	11.17	0.0116	0.1742	4.012	1.605	0.0131
	± 0.581c	± 2.09g	± 0.627e	±0.202c	± 0.38f	± 0.0007a	±0.0368a	±0.120d	±0.260b	± 0.0006.a
Cu	43.34	19.41	27.00	26.84	24.79	31.77	35.30	49.02	24.13	50.84 ±3.57f
	± 2.07e	± 1.64a	± 2.20b	± 1.07b	± 0.54b	±1.55c	±1.49d	±0.78f	±1.55b	
Bi	1.691	0.7042	0.4230	0.2369	0.1511	0.3419	0.1301	0.0634	0.0776	0.1509±0.013ab
	±0.129e	±0.0070d	±0.0108c	±0.0056b	±0.0033ab	±0.0181c	±0.0062a	±0.0075a	±0.019a	

Note: n.d.-not detected (below quantification limit)

a–j Values with different letters within a line differ significantly (P< 0.05) using Duncan's test.

Table S5. Correlation matrix for the elemental concentration in the ROG samples (n=10).

Element	**Co**	**Ba**	**Fe**	**Cr**	**Mn**	**Ni**	**Zn**	**As**	**Cd**	**Pb**	**Cu**	**Be**	**Sb**	**Bi**
Co	1.00													
Ba	0.73*	1.00												
Fe	0.73*	0.65*	1.00											
Cr	**0.82***	0.79*	**0.92***	1.00										
Mn	0.73*	0.51	0.76*	0.59	1.00									
Ni	**0.87***	**0.87***	**0.80***	**0.86***	0.77*	1.00								
Zn	0.49	0.18	0.58	0.65	0.19	0.34	1.00							
As	-0.02	0.48	0.40	0.28	0.32	0.31	-0.08	1.00						
Cd	0.14	-0.11	0.64	0.41	0.42	0.22	0.51	0.10	1.00					
Pb	0.24	0.13	0.77*	0.61	0.42	0.36	0.59	0.25	**0.95***	1.00				

Cu	0.10	-0.12	-0.29	-0.38	0.28	-0.03	-0.34	-0.13	-0.36	-0.54	1.00			
Be	**0.88**	0.77	**0.91***	**0.97***	0.68	**0.91***	0.63	0.19	0.44	0.59	-0.24	1.00		
Sb	-0.50	-0.50	0.14	-0.10	-0.13	-0.39	0.24	0.25	0.72	0.66	-0.42	-0.18	1.00	
Bi	0.25	-0.25	0.25	0.10	0.23	-0.14	0.33	-0.31	0.28	0.19	0.09	0.10	0.20	1.00

[a] Significant correlations (> 0.80) in bold. * P-value < 0.05.

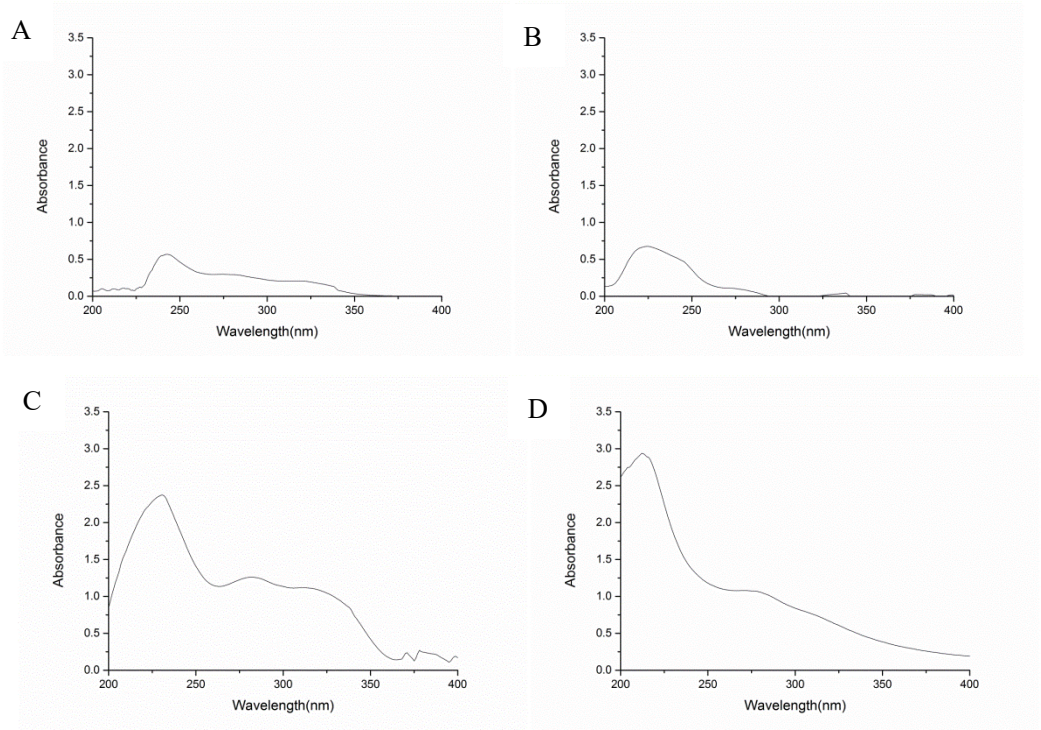

Fig. S1. UV-Vis diagrams of the different extraction solvents: (A) UV-Vis diagram of chloroform (B) UV-Vis diagram of 100% enanol extraction (C)UV-Vis diagram of 50% enanol extraction (D) UV-Vis diagram of water extraction