



Figure S2. Principle Component Analysis (PCA) loading plot of metabolites derived from LC/IT-TOF-MS data sets of *Ganoderma lingzhi* at eight developmental stages.

Table S1. Tentatively identified chemical markers at eight developmental stages of *G. lingzhi* analyzed by GC/MS and LC/IT-TOF-MS.

ID ^a	RT ^b (min)	RI ^c Exp.	Tentative identification	\Delta RI	Match correlation	Elemental Formula	Exact Mass	m/z [M-H]-	Mass error \Delta ppm	Mass Fragmentation	ID level ^d	Ref.
1*	5.04	1056	Lactic acid	10	955					147, 73 , 117, 191, 148, 190, 66, 149, 133, 118	2	[1]
2*	5.16	1064	5-Nonanol	N/A	605					56 , 73, 159, 186, 75, 143, 145, 57, 59, 158	3	
3*	6.48	1151	Putrescine	N/A	752					174, 73 , 175, 216, 86, 142, 59, 176, 100, 160	3	
4*	7.62	1227	Ethanolamine	42	876					174 , 73, 175, 147, 100, 86, 176, 59, 130, 133	3	[2]
5*	8.20	1268	Phosphoric acid	14	947					299 , 300, 73, 314, 301, 133, 211, 283, 207, 315	2	[2]
6*	8.21	1270	Glycerol	12	940					73, 147, 205, 117, 103 , 133, 218, 206, 148, 74	2	[2]
7*	8.82	1310	Succinic acid	11	957					147 , 73, 247, 75, 148, 149, 55, 129, 74, 172	2	[1]
8*	11.11	1483	Malic acid	3	944					73 , 147, 233, 245, 133, 148, 189, 75, 190, 74	2	[3]
9*	12.70	1615	Glutamic acid	11	918					246, 73 , 247, 128, 147, 75, 248, 156, 348, 230	2	[3]
10*	13.81	1716	Xylitol	1	868					73 , 147, 103, 205, 307, 129, 319, 204, 189, 148	2	[3]
11*	14.28	1756	Glycerol-3-phosphate	19	956					357 , 299, 147, 358, 315, 300, 211, 445, 370, 359	2	[2]
12*	14.68	1792	Azelaic acid	15	825					116 , 73, 75, 317, 243, 147, 217, 204, 201, 129, 230	2	[1]
13*	14.89	1812	Citric acid	8	793					273 , 147, 363, 347, 274, 375, 465, 211, 305, 364	2	[3]
14*	15.24	1846	Myristic acid	4	878					285, 117 , 73, 75, 129, 286, 145, 55, 131	2	[4]
15*	15.54	1873	Fructose	1	824					219 , 73, 217, 103, 307, 147, 218, 308, 74, 117, 133	2	[3]
16*	16.03	1922	Mannitol	6	959					73 , 319, 205, 147, 217, 103, 320, 307, 321, 117	2	[2]
17*	16.25	1945	Pentadecanoic acid	4	883					299, 117, 73, 75, 132, 129 , 145, 300, 55, 131	2	[2]
18*	17.21	2044	Palmitic acid	6	961					313 , 117, 73, 75, 132, 129, 145, 314, 55, 131	2	[5]
19*	17.57	2082	Myo-Inositol	9	928					305, 73, 217 , 147, 318, 191, 306, 204, 319, 265	2	[3]
20*	17.67	2092	Linoleic acid methyl ester	2	841					67, 81, 95 , 55, 82, 79, 68, 96, 54, 109	2	[5]
21*	18.12	2141	Margaric acid	8	902					327 , 117, 73, 75, 132, 129, 145, 328, 55, 342	2	[1]
22*	18.83	2211	Linoleic acid	1	874					75, 73 , 337, 67, 81, 95, 79, 55, 82, 96	2	[1]
23*	20.26	2388	5-Methyluridine	N/A	719					73, 327, 147, 328, 75, 129, 217 , 103, 149, 74	3	

Table S1. Cont.

24*	21.37	2529	Phthalic acid, bis(2-ethylhexyl) ester	10	881				149, 167, 57, 71, 70, 150, 279, 113, 104, 83	2	[6]	
25*	22.90	2735	Trehalose	9	955				361, 73, 362, 191, 217, 147, 363, 204, 103, 271	2	[3]	
26*	23.18	2774	Chrysophanol	N/A	774				383, 147, 384, 57, 103, 385, 83, 55, 97, 485	3		
27*	23.61	2834	Lignoceric acid	1	810				117, 73, 425, 75, 132, 145, 129, 57, 55, 426	2	[3]	
28*	23.87	2871	Tricosyl alcohol	N/A	784				397, 398, 147, 129, 57, 75, 103, 399, 83, 55	3		
29*	24.54	2968	Lignoceryl alcohol	N/A	790				411, 73, 412, 147, 129, 57, 413, 75, 103, 83	3		
30*	24.62	2984	Eicosamethylcyclodecasiloxane	N/A	767				73, 147, 221, 355, 281, 429, 207, 356, 295, 219	3		
31*	26.64	3228	Ergosterol	4	731				73, 69, 55, 75, 143, 129, 253, 81, 157, 169, 363	2	[7]	
32*	26.83	3246	Stellasterol	N/A	917				75, 255, 69, 343, 55, 81, 73, 107, 105, 229	3		
33**	2.718		Sucrose			C ₁₂ H ₂₂ O ₁₁	342.1162	387.1191	5.4	387 > 341	2	[8]
								[M+HCOO] ⁻				
34**	3.243		Unknown 1					290.0730		290 > 167	4	
35**	4.789		3,12,20-Trihydroxy-7,11,15-trioxolanost-8,16,24-trien-26-oic acid			C ₃₀ H ₄₀ O ₈	528.2723	527.2646	0.8	527 > 509, 465, 421, 317	2	[9]
36**	5.154		Ganodernoid F			C ₃₁ H ₄₄ O ₈	544.3036	543.2933	5.5	543 > 499, 481, 437, 367, 301	2	
37**	5.519		Ganoderic acid I			C ₃₀ H ₄₄ O ₈	532.3036	531.3033	13.2	531 > 513, 469, 401	1	[9]
38**	5.774		Ganoderenic acid C			C ₃₀ H ₄₄ O ₇	516.3087	515.3044	5.8	515 > 497, 481, 453, 435, 383, 193	1	[9]
39**	5.964		Ganoderic acid C2			C ₃₀ H ₄₆ O ₇	518.3244	517.3163	1.6	517 > 499, 481, 455, 437, 303, 287	1	[9-11]
40**	6.741		3,12-Dihydroxy-4,4,14-trimethyl-7,11,15-trioxolanost-8,9,20,22-en-26-oic acid			C ₃₀ H ₄₀ O ₈	528.2723	527.2673	4.4	527 > 525, 509, 483, 465		[10]
41**	7.289		Ganoderic acid C6			C ₃₀ H ₄₂ O ₈	530.2880	529.2809	0.4	529 > 527, 511, 467	1	[9-11]
42**	8.131		Ganoderenic acid B			C ₃₀ H ₄₂ O ₇	514.2931	513.2929	13.8	513>469, 436, 301, 265	2	[9-11]
43**	8.185		Ganoderic acid B			C ₃₀ H ₄₄ O ₇	516.3087	497.2941	6.4	497>453, 438, 409, 303, 287, 249	1	[9-11]
								[M-H ₂ O-H] ⁻				

Table S1. Cont.

44**	8.189	Ganoderenic acid A	C ₃₀ H ₄₂ O ₇	514.2930	513.2930	14.0	513 > 495, 479, 465, 451, 433, 403, 381, 363, 301, 193	2	[9]
45**	8.244	Ganoderic acid K	C ₃₂ H ₄₆ O ₉	574.3142	555.3039	13.7	499 > 481, 451, 437, 421, 367	1	[9–11]
					[M-H ₂ O-H] ⁻				
46**	9.093	Ganoderenic acid K	C ₃₂ H ₄₄ O ₉	572.2985	571.2916	0.5	553 > 538, 511, 494, 467, 449, 303	2	[9]
47**	9.409	3,7-Dihydroxy-11,15,23-trioxolanost-8,16-dien-26-oic acid	C ₃₀ H ₄₂ O ₇	514.2930	513.2860	0.4	513 > 495, 479, 433, 301, 193	2	[9]
48**	9.734	12-Acetoxy-3-hydroxy-7,11,15,23-tetraoxolanost-8,20-dien-26-oic acid	C ₃₂ H ₄₂ O ₉	570.2829	569.2869	19.8	513 > 495, 451, 433, 301, 193	2	[9]
49**	9.775	Ganoderic acid H	C ₃₂ H ₄₄ O ₉	572.2985	571.2887	4.5	571 > 553 > 511, 467	1	[9–11]
50**	10.493	Ganoderic acid A	C ₃₀ H ₄₄ O ₇	516.3087	515.2978	4.5	515 > 497, 435, 301	1	[9–11]
51**	11.284	12-Hydroxy-3,7,11,15,23-pentaoxo-lanost-8-en-26-oic acid	C ₃₀ H ₄₀ O ₈	528.2723	527.2687	20.1	527 > 509	2	[11]
52**	11.670	12-Acetoxy-3-hydroxy-7,11,15-trioxolanost-8,16,24-trien-26-oic acid	C ₃₂ H ₄₂ O ₈	554.2880	553.2745	11.2	553 > 511, 494, 467, 449, 301, 263	2	[9]
53**	11.703	7,12-Dihydroxy-3,11,15,23-tetraoxo-lanost-8,20-dien-26-oic acid	C ₃₀ H ₄₀ O ₈	528.2723	527.2721	13.5	527 > 509	3	[9]
54**	12.148	Ganoderenic acid D	C ₃₀ H ₄₀ O ₇	512.2774	511.2701	7.24	511 > 495, 478, 449, 434, 405, 285, 261	1	[9–11]
55**	12.494	12-Acetoxy-7-hydroxy-3,11,15-trioxolanost-8,16,24-trien-26-oic acid	C ₃₂ H ₄₂ O ₈	554.2880	553.2753	12.1	511 > 493, 449, 434	2	[9]
56**	12.928	Ganolucidic acid A	C ₃₀ H ₄₄ O ₆	500.3138	499.3065	5.2	499 > 482, 437, 419, 285, 269, 213	2	[9]
57**	13.342	12-Acetoxy-7-hydroxy-3,11,15-trioxolanost-8,20-dien-26-oic acid	C ₃₂ H ₄₂ O ₉	570.2829	569.2725	5.4	569 > 551 > 277	2	[9]
58**	13.514	12-Acetoxy-3,7,11,15,23-pentaoxolanost-8,20-dien-26-oic acid	C ₃₂ H ₄₀ O ₉	568.2672	567.2600	16.7	549 > 507, 463	2	[9]

Table S1. Cont.

59**	14.548	Ganoderenic acid F	C ₃₀ H ₃₈ O ₇	510.2618	509.2656	21.8	509 > 491, 473, 465, 301, 261, 247, 217, 175	2	[9]
60**	14.694	Unknown 2			533.3317		533 > 487, 469		
61**	14.913	Unknown 3			535.3326		535 > 489, 371		
62**	15.158	Unknown 4			535.3543		535 > 445, 419		
63**	16.761	Unknown 5			553.2384		533 > 531, 487		
64**	18.024	Unknown 6			483.2261		483 > 465, 439, 421, 287, 233		
65**	18.415	Unknown 7			483.2673		483 > 465, 421		
66**	19.336	Unknown 8			476.2464		476 > 279		
67**	19.975	Unknown 9			341.1687		341 > 320, 297, 279, 159		
68**	22.089	Unknown 10			295.2411		295 > 277, 195, 171, 113		
69**	22.560	Unknown 11			293.1830		293 > 275, 249, 197, 185		
70**	22.931	Unknown 12			527.3350		527 > 525, 485, 467		
71**	23.007	Unknown 13			311.1089		311 > 182		
72**	25.556	Unknown 14			475.2102		475 > 431		
73**	25.801	Unknown 15			475.2904		475 > 431		
74**	29.860	Unknown 16			355.2920		355 > 309		

^aMetabolites were selected according to VIP > 1.0 and p-value < 0.05 in PLS-DA (*analyzed by GC/MS, **analyzed by LC/IT-TOF-MS); ^bRetention time (RT) were corrected by data pre-processing software; ^cRetention index (RI) metabolites analyzed by GC/MS were normalized with n-alkanes; ^dThe level of metabolite identification according to Metabolomics Standards Initiative [12]; ^eThe structure were deduced from previous reports

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