Table S1 The detailed UPLC linear gradients of serum analysis

Time (min)	Flow rate (ml/min)	A (%)	B (%)	curve
Initial	0.4	5	95	--
0.5	0.4	20	80	6
2.5	0.4	60	40	6
4.0	0.4	66	34	6
5.0	0.4	80	20	6
7.5	0.4	86	14	6
8.0	0.4	99	1	6
9.0	0.4	99	1	6

Table S2 The detailed UPLC linear gradients of urine analysis

Time (min)	Flow rate (ml/min)	A (%)	B (%)	curve
Initial	0.4	1	99	--
2.5	0.4	11	89	6
4.5	0.4	21	79	6
7	0.4	40	60	6
8.5	0.4	99	1	6
9.5	0.4	99	1	6

Table S3 The optimal conditions for MS analysis during the serum/urine data acquisition

	Positive mode (Serum metabolomics)	Negative mode (Serum metabolomics)	Positive mode (Urine metabolomics)	Negative mode (Urine metabolomics)
Source temperature	110℃	110℃	110℃	110℃
Desolvation gas temperature	350℃	350℃	400℃	400℃
Cone gas flow	50L/h	50L/h	50L/h	50L/h
Desolvation gas flow	600L/h	600L/h	800L/h	800L/h
Capillary voltage	2.8kv	2.4kv	3.0kv	2.5kv
Data acquisition rate	0.2s/scan	0.2s/scan	0.2s/scan	V
Inter scan delay	0.1s	0.1s	0.1s	0.1s
Acquisition mode	Centroid	Centroid	Centroid	Centroid
Lock mass	556.2771	554.2615	556.2771	554.2615

Table S4 The 56 chemical components which characterized of SJZD in vivo

NO.	Rt/ min	Identifiend compound	Positive ion(m/z) Indicatied	Error mDa	Negative ion(m/z) Indicatied	Error mDa	Element composition	MW (Da)	Source
1	0.67	Licochalcone A	361.1416	-5	——	——	C21H22O4	338.1518092	Licorice
2	2.14	Umbelliferone	163.0395	-3.1	——	——	C9H6O3	162.0316941	Ginseng
5	2.28	isoliquiritigenin-glucopyranoside	551.1765	0.3	549.16	-4.0	C26H30O13	550.168641	Licorice
6	3.09	Liquiritin	419.1342	-1.6	417.12	-2.0	C21H22O9	418.1263823	Licorice
3	3.12	Glycyrrhizin	257.0814	-0.9	255.07	-2.0	C15H12O4	256.0735589	Licorice
11	3.18	Licochalcone B	287.0919	1.1	285.08	-2.0	C16H14O5	286.0841236	Licorice
32	3.59	20-O- Glucoside ginsenoside Rf	——	——	961.54	2.1	C48H82O19	962.5450304	Ginseng
31	3.68	notoginsenoside R1	——	——	931.53	2.8	C47H80O18	932.5344658	Ginseng
33	3.84	ginsenoside Re	——	——	945.54	0.6	C48H82O18	946.5501158	Ginseng
20	3.85	ginsenoside Rd	947.5579	3	945.54	1.5	C48H82O18	946.5501158	Ginseng
8	3.86	20(S)- ginsenoside Rh2	623.4523	0	——	——	C36H62O8	622.444469	Ginseng
4	3.87	ginsenoside F1	639.4472	-3.1	637.43	-1.0	C36H62O9	638.4393836	Ginseng
10	4.00	7-Methoxycoumarin	177.0552	0.7	——	——	C10H8O3	176.0473441	Licorice
34	4.13	malonyl-ginsenoside Rd	——	——	1031.5	3.2	C51H84O21	1032.55051	Ginseng
12	4.45	Deoxylicorate	455.3525	0.9	——	——	C30H46O3	454.3446953	Licorice
9	4.51	Formononetin	269.0814	1	267.07	-1.0	C16H12O4	268.0735589	Licorice
35	4.58	IV-Atractylenolide	——	——	305.14	0.3	C17H22O5	306.1467238	Macrocephala
14	4.75	16- Methyl oxyacetyl glabrous acid methyl ester	585.4155	-4.4	——	——	C36H56O6	584.4076895	Poria
15	4.77	16- Oxyacetyl poria acid	571.3999	1.7	——	——	C35H54O6	570.3920395	Poria
16	4.84	poricoic acid B	485.3267	-4.3	——	——	C30H44O5	484.3188745	Poria
36	5.05	3β,16α- Dihydroxy lanostene-triene-21-acid	——	——	469.33	2.6	C30H46O4	470.33961	Poria
37	5.08	ferulic acid	——	——	193.05	-3.0	C10H10O4	194.0579088	Licorice
7	5.39	ginsenoside Rf	801.5	2.4	799.48	3.0	C42H72O14	800.492207	Ginseng
38	5.54	ginsenoside Rg1	——	——	799.48	3.0	C42H72O14	800.492207	Ginseng
18	5.88	ginsenoside Ra2	1211.6425	4.5	——	——	C58H98O26	1210.634633	Ginseng
39	6.07	ginsenoside Ra1	——	——	1209.6	-3.0	C58H98O26	1210.634633	Ginseng
40	6.30	20(S)- ginsenoside Rg3	——	——	783.49	4.9	C42H72O13	784.4972924	Ginseng
27	6.58	ginsenoside Ro	957.5059	-2	955.49	-2.0	C48H76O19	956.4980802	Ginseng
21	6.63	ginsenoside Rc	1079.6002	0	1077.6	4.2	C53H90O22	1078.592375	Ginseng
22	6.79	Glabrolide	469.3318	2.2	——	——	C30H44O4	468.3239599	Licorice

23	6.91	malonyl-ginsenoside Rc	1195.6112	3.8	1193.6	4.7	C57H94O26	1194.603333	Ginseng
41	6.96	malonyl-ginsenoside Rb1	——	——	1193.6	-3.0	C57H94O26	1194.603333	Ginseng
42	7.07	ginsenoside Rb2	——	——	1077.6	5.0	C53H90O22	1078.592375	Ginseng
43	7.12	ginsenoside Rb3	——	——	1077.6	2.0	C53H90O22	1078.592375	Ginseng
25	7.97	glycyrrhizic acid	845.3936	1.5	821.4	4.9	C42H62O16	822.4037859	Licorice
44	9.56	poricoic acid D	——	——	513.32	0.8	C31H46O6	514.3294392	Poria
28	9.67	Atractylodes	231.1385	-3.7	——	——	C15H18O2	230.1306798	Macrocephala
45	9.68	Hydroxy albino ester	——	——	247.13	-2.0	C15H20O3	248.1412445	Macrocephala
29	9.77	Licobenzofuran	355.1545	-3.3	353.14	1.0	C21H22O5	354.1467238	Licorice
46	9.91	25- hydroxy -3-Dehydrotumulosic acid	——	——	499.34	-5.0	C31H48O5	500.3501746	Poria
47	10.03	poricoic acid E	——	——	499.31	-1.0	C30H44O6	500.3137891	Poria
19	10.22	ginsenoside Rg2	785.5051	-2	783.49	-5.0	C42H72O13	784.4972924	Ginseng
48	10.36	poricoic acid F	——	——	497.33	2.2	C31H46O5	498.3345246	Poria
49	10.57	Licoricone	——	——	381.13	-5.0	C22H22O6	382.1416384	Licorice
30	10.64	AtractylenolideII	233.1542	-4.5	——	——	C15H20O2	232.1463299	Macrocephala
24	10.88	3β,16α- Dihydroxy lanosteroid-8,24-diene-21-acid	495.345	3.8	471.35	2.3	C30H48O4	472.35526	Poria
50	11.04	Dehydrotumulosic acid	——	——	483.35	1.4	C31H48O4	484.35526	Poria
13	11.13	Isoglabrolide	469.3318	0.8	467.32	-0.0	C30H44O4	468.3239599	Licorice
17	11.24	poricoic acid DM	529.3529	1.5	527.34	2.7	C32H48O6	528.3450893	Poria
52	11.42	poricoic acid C	——	——	481.33	-2.0	C31H46O4	482.33961	Poria
53	11.42	3-epidehydrotumulosic acid	——	——	483.35	1.4	C31H48O4	484.35526	Poria
26	11.59	18β- glycyrrhetinic acid	471.3474	-1.3	469.33	-1.0	C30H46O4	470.33961	Licorice
51	11.63	methylglycyrrhetate	——	——	483.35	0.6	C31H48O4	484.35526	Licorice
54	12.07	3-epi-Dehydropachymic acid	——	——	525.36	-0.0	C33H50O5	526.3658247	Poria
55	12.09	Dehydropachymic acid	——	——	525.36	1.1	C33H50O5	526.3658247	Poria
56	12.59	Glycyrrhetol	——	——	455.35	2.7	C30H48O3	456.3603454	Licorice

Table S5. The prototypical chemical compound peaks we tentatively characterized in vivo by the use of serum pharmacochemistry

NO.	Rt	Expected neutral mass	Ion Mode	Fomula	Calc.Mass	mDa	Name	Origin
1	2.363	162.0316941	H^+	C9H6O3	163.0395	3.4	Umbelliferone	Licorice
2	2.805	550.168641	H^-	C26H30O13	549.1608	-2.0	isoliquiritigenin-glucopyranoside	Licorice
3	2.869	418.1263823	H^-	C21H22O9	417.1186	0.4	Liquiritin	Licorice
4	3.117	256.0735589	H^+	C15H12O4	257.0814	-0.8	Glycyrrhizin	Licorice
5	4.052	268.0735589	H^+	C16H12O4	269.0184	-4.4	Formononetin	Licorice
6	4.864	484.3188745	H^+	C30H44O5	485.3267	3.1	poricoic acid B	Poria
7	6.392	1194.603333	H^-	C57H94O26	1193.5955	-0.8	malonyl-ginsenoside Rb2	Ginseng
8	6.658	1078.592375	H^-	C53H90O22	1077.5845	4.0	ginsenoside Rc	Ginseng
9	6.688	956.4980802	H^-	C48H76O19	955.4903	-2.1	ginsenoside Ro	Ginseng
10	7.231	1078.592375	H^-	C53H90O22	1077.5845	-2.5	ginsenoside Rb2	Ginseng
11	8.028	822.4037859	H^-	C42H62O16	821.396	3.6	Glycyrrhizic acid	Licorice
12	8.037	470.33961	H^+	C30H46O4	471.3474	4.3	Glycyrrhetinic acid	Licorice
13	9.791	230.1306798	H^+	C15H18O2	231.1385	-2.7	Atractylenolide III	Macrocephala
14	9.978	500.3137891	H^-	C30H44O6	499.306	-1.3	Poricoic acid E	Poria
15	10.516	232.1463299	H^+	C15H20O2	233.1542	0.7	2-Atractylenolide	Macrocephala
16	11.13	484.35526	H^-	C31H48O4	483.3474	2.3	Dehydrotumulosic acid	Poria
17	11.411	468.3239599	H^-	C30H44O4	467.3161	-0.7	Isoglabrolide	Licorice
18	11.68	470.33961	H^-	C30H46O4	469.3318	-0.7	3β,16α- Dihydroxy lanostene-triene-21-acid	Poria

Table S6. The metabolized chemical compound peaks we tentatively characterized in vivo by the use of serum pharmacochemistry

NO.	Rt	Expected neutral mass	Ion Mode	Fomula	Calc.Mass	mDa	Name	Origin
1	4.69	444.1056	H^+	C22H20O10	445.1135	1.5	Formononetin 7-O-β-D-Glucuronide	Licorice
2	6.58	594.1585	H^-	C27H30O15	593.1506	2.1	liquiritin-7-O-glucuronide	Licorice
3	7.27	470.3396	H^+	C30H46O4	471.3474	0.2	18-beta-Glycyrrhetinic acid	Licorice
4	9.25	526.3658	H^-	C33H50O5	525.4936	-1.9	Dehydropachymic acid	Poria
5	11.32	486.3709	H^-	C31H49O4	485.3631	1.4	Tumulosic acid	Poria