

1 **Supplementary materials**

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3 **Supplementary Table 1. The catalog number and purity of standards.**

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NO.	Compound name	Catalog No.	Purity
1	Ginsenoside Rb1	41753-43-9	99.32% (HPLC)
2	Ginsenoside Rg1	22427-39-0	98.65% (HPLC)
3	Ginsenoside Re	52286-59-6	99.26% (HPLC)
4	Ophiopogonin D	945619-74-9	99.80% (HPLC)
5	Ophiopogonin D'	65604-80-0	99.71% (HPLC)

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Supplementary Table 2. Detail information of material medica from Shenmai injection

No	Herb	Ingredient	Formula	CAS NO.
1	HS	Arachic acid	C ₂₀ H ₄₀ O ₂	506-30-9
2	HS	beta-caryophyllene	C ₁₅ H ₂₄	87-44-5
3	HS	alloaromadendrene	C ₁₅ H ₂₄	25246-27-9
4	HS	palmitic acid	C ₁₆ H ₃₂ O ₂	57-10-3
5	HS	alpha-Guaiene	C ₁₅ H ₂₄	3691-12-1
6	HS	()-Aromadendrene	C ₁₅ H ₂₄	489-39-4
7	HS	beta-sitosterol	C ₂₉ H ₅₀ O	83-46-5
8	HS	Nonacosane	C ₂₉ H ₆₀	630-03-5
9	HS	delta-amorphene	C ₁₅ H ₂₄	16729-01-4
10	HS	58924_FLUKA	C ₁₅ H ₂₄	1135-66-6
11	HS	Cedrol	C ₁₅ H ₂₆ O	77-53-2
12	HS	beta-elemene	C ₁₅ H ₂₄	33880-83-0
13	HS	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	C ₁₅ H ₂₄	30824-67-0
14	HS	myristic acid	C ₁₄ H ₂₈ O ₂	544-63-8
15	HS	PENTADECYLIC ACID	C ₁₅ H ₃₀ O ₂	1002-84-2
16	HS	HEXACOSANE	C ₂₆ H ₅₄	630-01-3
17	HS	Octacosane	C ₂₈ H ₅₈	630-02-4
18	HS	Daturic acid	C ₁₇ H ₃₄ O ₂	506-12-7
19	HS	Piperonal	C ₈ H ₆ O ₃	120-57-0
20	HS	zoomaric acid	C ₁₆ H ₃₀ O ₂	373-49-9
21	HS	Tetracosane	C ₂₄ H ₅₀	211-474-5
22	HS	panaxynol	C ₁₇ H ₂₄ O	21852-80-2
23	HS	DNOP	C ₂₄ H ₃₈ O ₄	117-84-0
24	HS	HEPTACOSANE	C ₂₇ H ₅₆	593-49-7
25	HS	(6Z,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracosane	C ₃₀ H ₅₀	7683-64-9
26	HS	Vetol	C ₆ H ₆ O ₃	118-71-8
27	HS	spathulenol	C ₁₅ H ₂₄ O	6750-60-3
28	HS	Coumaran	C ₈ H ₈ O	496-16-2
29	HS	ginsenoside-Rh1	C ₃₆ H ₆₂ O ₉	63223-86-9
30	HS	ginsenoside-Rh1_qt	C ₃₆ H ₆₂ O ₉	80952-71-2
31	HS	20(S)-Ginsenoside-Rh1_qt	C ₄₂ H ₇₂ O ₁₃	80952-72-3
32	HS	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	C ₃₀ H ₅₂ O ₄	34080-08-5

33	HS	20(R)-ginsenoside Rg2	C ₄₂ H ₇₂ O ₁₃	80952-72-3
34	HS	ginsenoside Rb1	C ₅₄ H ₉₂ O ₂₃	41753-43-9
35	HS	(3R,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	C ₅₄ H ₉₂ O ₂₃	41753-43-9
36	HS	ginsenoside-Rb2	C ₅₃ H ₉₀ O ₂₂	11021-13-9
37	HS	(3S,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	C ₃₀ H ₅₂ O ₃	30636-90-9
38	HS	ginsenoside-Rc	C ₅₃ H ₉₀ O ₂₂	11021-14-0
39	HS	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,1	C ₄₈ H ₈₂ O ₁₈	52705-93-8
40	HS	Ginsenoside Re	C ₄₈ H ₈₂ O ₁₈	52286-59-6
41	HS	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	C ₃₀ H ₅₂ O ₄	1453-93-6
42	HS	Sanchinoside C1	C ₄₂ H ₇₂ O ₁₄	22427-39-0
43	HS	ginsenoside rh2	C ₃₆ H ₆₂ O ₈	78214-33-2
44	HS	notoginsenoside R2	C ₄₁ H ₇₀ O ₁₃	80418-25-3
45	HS	notoginsenoside R2_qt	C ₄₁ H ₇₀ O ₁₃	80418-25-3
46	HS	β-guaiene	C ₁₅ H ₂₄	88-84-6
47	HS	(2R,3R,4S,5S,6R)-2-[[[(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-3,12-dihydroxy-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-6-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol	C ₃₆ H ₆₂ O ₉	63223-86-9
48	HS	panaxydol	C ₁₇ H ₂₄ O ₂	72800-72-7
49	HS	NSC692928	C ₁₇ H ₂₄ O	81203-57-8
50	HS	ginsenoside rf	C ₄₂ H ₇₂ O ₁₄	52286-58-5
51	HS	β-cedrene	C ₁₅ H ₂₄	546-28-1
52	HS	(butylsulfonyl)ethynylbenzene	C ₁₂ H ₁₄ O ₂ S	NA

53	HS	1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(isopropyl)-cyclohexane	NA	NA
54	HS	Agidol 7	C ₂₅ H ₃₆ O ₂	88-24-4
55	HS	20(S)-ginsenoside Rg3	C ₄₂ H ₇₂ O ₁₃	14197-60-5
56	HS	20(S)-ginsenoside Rg3_qt	C ₄₂ H ₇₂ O ₁₃	14197-60-5
57	HS	ginsenoside R0	C ₄₈ H ₇₆ O ₁₉	34367-04-9
58	HS	ginsenoside R0_qt	C ₄₈ H ₇₆ O ₁₉	34367-04-9
59	HS	ginsenoside Rg2	C ₄₂ H ₇₂ O ₁₃	52286-74-5
60	HS	ginsenoside Rg2_qt	C ₄₂ H ₇₂ O ₁₃	52286-74-5
61	HS	ginsenoside Rg3	C ₄₂ H ₇₂ O ₁₃	14197-60-5
62	HS	ginsenoside Rg3_qt	C ₄₂ H ₇₂ O ₁₃	14197-60-5
63	HS	ginsenoside Rh4	C ₃₆ H ₆₀ O ₈	174721-08-5
64	HS	ginsenoside Rh4_qt	C ₃₆ H ₆₀ O ₈	174721-08-5
65	HS	ginsenoside Rs1	C ₅₅ H ₉₂ O ₂₃	87733-67-3
66	HS	ginsenoside Rs1_qt	C ₅₅ H ₉₂ O ₂₃	87733-67-3
67	HS	globulol	C ₁₅ H ₂₆ O	489-41-8
68	HS	O-isoprenyl benzophenone	C ₁₈ H ₁₈ O	NA
69	HS	p-tert-Butylanisole	C ₁₁ H ₁₆ O	5396-38-3
70	HS	(3R,9R,10R)-heptadec-1-en-4,6-diyne-3,9,10-triol	C ₁₇ H ₂₆ O ₃	87005-03-6
71	HS	(4aR,9aS)-2,9,9-trimethyl-5-methylene-4,4a,6,7,8,9a-hexahydro-3H-benzo[7]annulene	C ₁₅ H ₂₄	469-92-1
72	HS	CLOVENE	C ₁₅ H ₂₄	469-92-1
73	MD	1-Isopropyl-4-Methylcyclohex-3-Enol,4-Terpineol	C ₁₀ H ₁₈ O	562-74-3
74	MD	2'-Hydroxymethylpogonone A	C ₁₉ H ₁₆ O ₇	N/A
75	MD	3,7-Dimethylocta-1,6-Dien-3-Ol,Linalol,Linalool	C ₁₀ H ₁₈ O	78-70-6
76	MD	5,7,2'-Trihydroxy-6-Methyl-3-(3',4'-Methylenedioxybenzyl) Chromone	C ₁₈ H ₁₄ O ₇	N/A
77	MD	5,7-Dihydroxy-6,8-Dimethyl-3-(4'-Hydroxy-3'-Methoxybenzyl)Chroman-4-One	C ₁₉ H ₂₀ O ₆	N/A
78	MD	5-Hydroxy-7,8-Dimethoxy-6-Methyl-3-(3',4'-Dihydroxybenzyl) Chroman-4-One	C ₁₉ H ₂₀ O ₇	
79	MD	6-Aldehydo-Isoophiopogone A	C ₁₉ H ₁₄ O ₇	112500-90-0
80	MD	6-Aldehydo-Isoophiopogone B	C ₁₉ H ₁₆ O ₆	N/A
81	MD	Adenosine,Adenine Nucleoside Alexandrin,Daucosterol,Caproic Acid,Eletheroside	C ₁₀ H ₁₃ N ₅ O ₄	58-61-7
82	MD	A,Sitogluside,Strumaroside,Î'-Sitosterol-Î'-D-Glucoside	C ₃₅ H ₆₀ O ₆	474-58-8
83	MD	Borneol-2-O-Î'-L-Arabinofuranosyl(1â†'6)-Î'-D-Glucopyranoside	C ₂₁ H ₃₆ O ₁₀	N/A
84	MD	Borneol-2-O-Î'-D-Apiofuranosyl(1â†'6)-Î'-D-Glucopyranoside	C ₂₁ H ₃₆ O ₁₀	N/A
85	MD	Camphor	C ₁₀ H ₁₆ O	76-22-2

86	MD	Cyperene	C ₁₅ H ₂₄	2387-78-2
87	MD	Glycerol	C ₃ H ₈ O ₃	56-81-5
88	MD	Guaiol	C ₁₅ H ₂₆ O	489-86-1
89	MD	Alpha-Humulene, Humulene, Î ⁺ -Humulene	C ₁₅ H ₂₄	6753-98-6
90	MD	Î ⁺ -Cyperene	C ₁₅ H ₂₄	2387-78-2
91	MD	Î ⁺ -Patchoulene	C ₁₅ H ₂₄	514-51-2
92	MD	Isoophiopogonone A	C ₁₈ H ₁₆ O ₆	N/A
93	MD	Jasmololone	C ₁₁ H ₁₆ O ₂	93221-50-2
94	MD	Jasmololone1	C ₁₁ H ₁₆ O ₂	54383-66-3
95	MD	Longifolene	C ₁₅ H ₂₄	475-20-7
96	MD	Methyl Ophiopogonanone A	C ₁₉ H ₁₈ O ₆	74805-92-8
97	MD	Methyl Ophiopogonanone B	C ₁₉ H ₂₀ O ₅	74805-91-7
98	MD	N-(Trans-P-Coumaroyl) Tyramine	C ₁₇ H ₁₇ NO ₃	36417-86-4
99	MD	N-[Î ⁺ -Hydroxy-Î ⁺ -(4-Hydroxyphenyl)]Ethyl-4-Hydroxy Cinnamide	C ₁₇ H ₁₇ NO ₄	N/A
100	MD	N-Trans-Feruloyltyramine	C ₁₈ H ₁₉ NO ₄	66648-43-9
101	MD	Oleanolic Acid	C ₃₀ H ₄₈ O ₃	508-02-1
102	MD	Ophiogenin-3-O-Î ⁺ -L-Rhamnopyranosyl(1â†'2)-Î ⁺ -D-Glucopyranoside	C ₃₉ H ₆₂ O ₁₄	N/A
103	MD	Ophiopogon A	C ₄₄ H ₇₀ O ₁₈	288143-27-1
104	MD	Ophiopogonanone A	C ₁₈ H ₁₆ O ₆	75239-63-3
105	MD	Ophiopogonanone B	C ₁₈ H ₁₈ O ₅	N/A
106	MD	Ophiopogonanone C	C ₁₉ H ₁₆ O ₇	477336-75-7
107	MD	Ophiopogonanone D	C ₂₀ H ₁₈ O ₇	N/A
108	MD	Ophiopogonanone E	C ₁₉ H ₂₀ O ₇	N/A
109	MD	Ophiopogonanone F	C ₂₀ H ₂₂ O ₇	N/A
110	MD	Ophiopogonin A	C ₄₁ H ₆₄ O ₁₃	11054-24-3
111	MD	Ophiopogonin B	C ₃₉ H ₆₂ O ₁₂	38971-41-4
112	MD	Ophiopogonin C'	C ₃₉ H ₆₂ O ₁₂	19057-67-1
113	MD	Ophiopogonin D	C ₄₄ H ₇₀ O ₁₆	945619-74-9
114	MD	Ophiopogonin D'	C ₄₄ H ₇₀ O ₁₆	65604-80-0
115	MD	Ophiopogonone C	C ₁₉ H ₁₄ O ₇	N/A
116	MD	Ophiopogonoside A	C ₂₁ H ₃₈ O ₈	N/A
117	MD	Ruscogenin	C ₂₇ H ₄₂ O ₄	472-11-7
118	MD	Ruscogenin 1-O-Sulfate	C ₂₇ H ₄₂ O ₇ S	N/A
119	MD	Stigmasterol	C ₂₉ H ₄₈ O	481-16-3

Abbreviations: HS, Hongshen; MD, Maidong; N/A, not available.

Supplementary Table 3. Compound-related targets, disease-related targets, potential therapeutic targets

No.	770 compounds-related targets	610 AP-related targets	59 potential therapeutic targets
1	PPARA	REG3A	CA2
2	PPARD	KIT	ADH1C
3	FABP2	CX3CL1	VDR
4	FFAR1	BIRC5	NR1H4
5	HSD11B1	MTNR1B	NOS2
6	SLC22A6	LMNA	HMOX1
7	FABP4	TNF	PTGS2
8	FABP5	LMF1	JAK2
9	AR	BSCL2	TYMS
10	VDR	NSMCE2	FABP1
11	POLB	GPIHBP1	TERT
12	GPBAR1	AGPAT2	FABP4
13	AKR1B10	SPINK1	TLR9
14	FABP3	CD14	DPP4
15	CDC25A	TLR4	HSPA1A
16	NR1H4	IL1A	MMP9
17	KDM2A	IL10	MMP2
18	PHF8	IL1B	MMP1
19	KDM5C	CCL2	BRAF
20	UGT2B7	CFTR	ALDH2
21	CYP19A1	PRSS1	MMP3
22	SERPINA6	IL6	MMP8
23	SHBG	MIR216A	MMP7
24	HSD17B3	HSPA1B	TNF
25	G6PD	ADH1B	MIF
26	GABBR1	PTGS2	SHH
27	PTGFR	HSPA2	KIT
28	GABRA2	HSPA1A	MET
29	GABRB2	IL1RN	CTSB
30	GABRG2	TP53INP1	CFTR
31	PTGER2	CARD9	VEGFA
32	HSD11B2	HMOX1	STAT3
33	HAO1	ALDH2	MME
34	NPC1L1	IL33	FGFR1
35	CA2	TNFAIP3	SELE
36	CA1	VMP1	MTNR1B
37	PLG	TLR2	SERPINE1
38	GSTK1	TGFB1	BCL2
39	LTA4H	RIPK3	RIPK2

40	CDC45	TAC1	FOXO1
41	PTPRC	STAT3	KCNA3
42	FNTA	MIR375	COMT
43	FNTB	SNAP25	F3
44	CACNA2D1	SMAD7	MPO
45	PSEN2	PLA2G7	IL6
46	PSENE1	GALR3	PLA2G2A
47	NCSTN	OR10A4	REN
48	APH1A	MPRIP	PRKCA
49	PSEN1	MBL3P	ACE
50	APH1B	GAL	FABP2
51	CHRNA7	TLR9	PTPRC
52	PLA2G10	PROCR	ICAM1
53	FOLH1	TREM1	ITGB2
54	SAE1	TLR6	GCG
55	UBA2	PARD3	FLT1
56	GRM5	TIGAR	PLA2G7
57	FDFT1	NR1H4	AGPAT2
58	EPHX2	MAGI2	ERBB2
59	PTGES	AIM2	P2RX7
60	CNR2	GALR2	
61	FAAH	KMO	
62	TRPV1	TYMS	
63	PTPN1	AGT	
64	NR0B2	F5	
65	PPARG	FCGR3A	
66	RXRA	FCGR3B	
67	CYP26A1	FGFR1	
68	CYP26B1	FUT2	
69	RARG	GSTM1	
70	RARB	GSTT1	
71	RARA	ACE	
72	TERT	ERBB2	
73	FABP1	EGF	
74	FFAR4	APOE	
75	RXRG	BCL2	
76	ALOX15	BCL3	
77	ALOX12	CAT	
78	PTGER4	CPB1	
79	RXRB	CTSB	
80	SLC16A1	DECR1	
81	GLRA1	EDN1	
82	ABCC1	ICAM1	
83	ABCB1	CXCL8	

84	HMGCR	JAK2	
85	TBXA2R	SERPINA1	
86	PLA2G4A	PLA2G2A	
87	SCD	PRH2	
88	HTR2B	PRSS3	
89	RORB	PTHLH	
90	MAPK1	PTPRC	
91	RORA	RAC1	
92	HNF4A	REN	
93	CXCR3	SERPINE1	
94	NR1I3	P2RX7	
95	NR1H3	LTA	
96	RORC	MBL2	
97	CYP51A1	MEFV	
98	CYP17A1	MPO	
99	SREBF2	MTHFR	
100	ESR1	MYO9B	
101	ESR2	NFKB1	
102	CYP2C19	NFKBIA	
103	SLC6A2	S100A9	
104	ACHE	HMGCL	
105	BCHE	MME	
106	SLC6A4	Reg3b	
107	CHRM2	Knq2	
108	NR1H2	Reg3g	
109	DHCR7	PRSS2	
110	PTGER1	KRAS	
111	TBXAS1	CDKN2A	
112	CES2	TERT	
113	SQLE	CTRC	
114	PTPN6	SAA1	
115	PTPN2	CST3	
116	NOS2	CRP	
117	GLI2	CLDN2	
118	GLI1	Nlrp3	
119	CTSD	KCNA3	
120	SRD5A1	CALCA	
121	SRD5A2	ABO	
122	NR3C2	HLA-DRB1	
123	NR3C1	Tacr1	
124	PGR	HMGB1	
125	SIGMAR1	SPP1	
126	NR1I2	MMP9	
127	CDC25B	GSTP1	

128	POLA1	Pparg	
129	SHH	RETN	
130	TRPM8	LCN2	
131	CA4	LEP	
132	IDO1	IFNG	
133	TRPA1	TIMP1	
134	SLC22A12	Mapk14	
135	IMPDH2	ANGPT2	
136	PTGDR2	F3	
137	RBP4	SBDS	
138	ADRA2B	ADIPOQ	
139	MAPK14	Rela	
140	PTGDR	HAMP	
141	BCL2L1	CD44	
142	CMA1	S100A8	
143	CTSG	IL18	
144	MDM2	ELANE	
145	EDNRA	Adcyap1	
146	PTGER3	AGER	
147	KEAP1	LPL	
148	PTGES2	Fasl	
149	AKR1C3	PLAUR	
150	OXER1	MMP2	
151	AKR1C1	IL2RA	
152	ITGAL	IL17A	
153	ICAM1	VEGFA	
154	ITGB2	MIR21	
155	SPHK2	CD163	
156	GCG	Cxcr2	
157	ERN1	SRP54	
158	EPHX1	MIF	
159	MKNK1	CEL	
160	PTGS1	MIR146A	
161	PREP	COMT	
162	TOP1	DNAJC21	
163	LTB4R	CHI3L1	
164	PDE4D	PTX3	
165	CNR1	TNFSF13B	
166	PTGS2	GDF15	
167	PTPRF	CD274	
168	ALOX5	Myd88	
169	PLA2G1B	PON1	
170	PTGIR	CTLA4	
171	CD81	Ghrl	

172	PRKCH	FOXP3	
173	ACP1	Nfe2l2	
174	ADORA3	CYP1A1	
175	PTPN11	Notch1	
176	MAPK3	TNFSF10	
177	TOP2A	Tnfrsf1a	
178	BACE1	NOS2	
179	SLC6A3	UBR1	
180	PIM2	Egfr	
181	ENPP2	ALB	
182	THRA	MMP8	
183	THRB	FLT1	
184	MCL1	MIR155	
185	BCL2	Gsk3b	
186	OPRM1	VDR	
187	OPRD1	CXCL10	
188	OPRK1	ADAMTS13	
189	PGGT1B	Trpv1	
190	PER2	NRAS	
191	EIF2AK1	SELP	
192	PABPC1	TIMP2	
193	CASR	Mtor	
194	ICMT	IL21	
195	HRH3	Fas	
196	GCGR	AVP	
197	CHRM1	F2rl1	
198	CHRM3	Chrna7	
199	ABHD6	MIR29A	
200	PTPN22	Trpa1	
201	MGLL	Il22	
202	CHRM4	IL1RL1	
203	CHRM5	FABP1	
204	SMO	IL23R	
205	ACACB	Ctnnb1	
206	C5AR1	Cxcr3	
207	GRM2	HGF	
208	PRKCD	CYP2E1	
209	TSPO	FGF21	
210	PRKCA	CD4	
211	SLC2A1	MIR126	
212	SLC2A3	Egr1	
213	SLC2A2	NEWENTRY	
214	CRHR1	Alox5	
215	PDE10A	Ccr2	

216	OXTR	TLR3	
217	F2R	Ppargc1a	
218	CAPN1	MIR34A	
219	ABL1	HSPA4	
220	AVPR1A	Mapk3	
221	AVPR1B	Mapk1	
222	KCNK2	PROC	
223	NOD1	Agtr1a	
224	NOD2	BRAF	
225	CDK5R1	Socs3	
226	CDK5	Oprm1	
227	DYRK1A	PDGFB	
228	C3AR1	Lbp	
229	MAPK11	Ngf	
230	FLT1	SOD1	
231	PDGFRB	Nupr1	
232	KIT	Atf3	
233	PDE2A	Ace2	
234	CTSK	TNFRSF9	
235	CTSL	Ahr	
236	CTSB	AHSG	
237	PDE1B	DPP4	
238	CASP3	APOA5	
239	CASP6	Pik3cg	
240	CASP7	MMP7	
241	CYP24A1	SELE	
242	CCR8	Ikbkb	
243	CASP1	ANGPT1	
244	DCK	Reg1a	
245	FKBP1A	Bdkrb2	
246	AGTR1	CXCL16	
247	MDM4	THPO	
248	CYP11B1	MUC1	
249	P2RY12	MMP1	
250	PTAFR	Txn1	
251	CYP11B2	MMP3	
252	CTSS	FOXO1	
253	BRD4	ENG	
254	BRD2	ITGB2	
255	BRD3	CD38	
256	HTR1A	Ido1	
257	AKT1	KRT18	
258	ALOX5AP	DEFB1	
259	LCK	Mir21a	

260	PIK3CD	Mapk8
261	MTNR1A	Ppara
262	MTNR1B	TNFSF12
263	GABRB3	GAS6
264	GABRA1	Aqp1
265	PARP1	Adra2a
266	IDH1	ICOS
267	TRPV4	Faslg
268	PORCN	Hspb1
269	PDE5A	HLA-DQB1
270	HCRTR2	Mir214
271	HCRTR1	Glp1r
272	DNM1	SOD2
273	CETP	Cdh1
274	DAO	Cdkn1a
275	DBH	MIR551B
276	SCN4A	SHH
277	HTR2A	Tnfrsf1b
278	STAT3	Casp3
279	IL2	CDX2
280	HSP90AA1	APOA2
281	VEGFA	FABP4
282	FGF1	Atg7
283	FGF2	Ucp2
284	HPSE	FABP2
285	ATP1A1	Traf6
286	SLC5A2	CPA1
287	SLC5A1	GPT
288	HDAC6	Postn
289	HDAC1	Cxcr4
290	HDAC4	Cacna1c
291	SLC28A2	Hspa5
292	F7	MASP2
293	REN	Stat1
294	LGALS4	Lepr
295	LGALS8	Vip
296	PIM1	MIR24-1
297	MTOR	BRCA2
298	CCR1	Cx3cr1
299	SLC18A3	MET
300	F2	Casp1
301	TYMS	Irf5
302	ATP12A	Ptpn1
303	P2RX3	Ifnar1

304	TTL	PPY	
305	MMP3	Sox9	
306	MMP1	PRKCA	
307	MMP2	FGL2	
308	MMP7	Cd276	
309	CYP2C9	HLA-DQA1	
310	ALK	LGALS1	
311	GPR55	TF	
312	GPR18	Cd40lg	
313	GSK3B	HSF1	
314	GSK3A	CHGA	
315	SORD	TNFRSF10B	
316	LIMK1	Prkcd	
317	AURKA	Smad2	
318	PIK3CA	Trpv4	
319	COL4A3BP	A2M	
320	CCNB3	Hc	
321	CDK1	GCH1	
322	CCNB1	Thbs1	
323	CCNB2	TGFA	
324	MAPK8	TNFRSF10A	
325	CHEK1	Cxcl12	
326	PDK1	Gjb1	
327	LGALS3	MGP	
328	JAK3	Ednra	
329	KDR	Xdh	
330	CYP27B1	S100A12	
331	INSR	PYY	
332	PDE4B	Ikbkg	
333	PIK3CB	GREM1	
334	PIK3CG	Pecam1	
335	SCN9A	SST	
336	DRD1	Trpc3	
337	DRD2	Capn1	
338	DRD3	Nod2	
339	PPP1CC	SH2B3	
340	PPP2CA	Cck	
341	CYP2D6	Cacna1b	
342	CYP3A4	Fgf10	
343	CAPN2	Bhlha15	
344	CCNC	Gnaq	
345	CDK8	Agtr1b	
346	PCSK7	Ly6c1	
347	PYGL	YAP1	

348	JAK1	Lum	
349	JAK2	Stat6	
350	CALCRL	APOC3	
351	PTK6	CBS	
352	IL6ST	GCG	
353	MET	Ticam1	
354	CCNT1	LIPC	
355	CCR2	IFNA1	
356	PGC	Cnr2	
357	CHEK2	Ccn2	
358	CTSE	Cav1	
359	PGA5	Atg5	
360	ADORA1	RACK1	
361	ADORA2A	GGT1	
362	ADORA2B	PROS1	
363	TACR2	Col1a1	
364	IGF1R	UMOD	
365	PFKFB3	Sqstm1	
366	S1PR1	IL24	
367	MAP2K1	KRT8	
368	BCL2A1	Dusp1	
369	ADK	Prkcz	
370	MAP3K14	Extl3	
371	KDM5A	Itgal	
372	EGFR	Clu	
373	SCN5A	Ephx2	
374	GRM1	APOC2	
375	PDE7A	SKI	
376	NTRK1	Tnfrsf18	
377	ASAHI	Mapkapk2	
378	CA12	Cth	
379	CA9	Nqo1	
380	PLA2G7	Mas1	
381	FGFR1	Cckar	
382	PIM3	RNLS	
383	ALPL	Aqp5	
384	TYK2	IRF2	
385	SYK	Il15	
386	S1PR3	MIR193B	
387	AGPAT2	JAM3	
388	ERBB2	PNLIP	
389	KARS	Ifitm3	
390	CDK2	Ctsc	
391	CCNA1	Atp2a1	

392	CCNA2	Vamp8	
393	CCR9	Btc	
394	CXCR2	Tacr2	
395	CXCR1	Napa	
396	GABRA5	Vasp	
397	MAP3K5	Mir9-1	
398	GRIN2A	RHOA	
399	GRIN1	Mir542	
400	F10	STIM1	
401	GRIA2	CD24	
402	DUT	TLR7	
403	CPT1A	Bace1	
404	LYPLA2	CA2	
405	P2RX7	IL1R1	
406	MPO	ZEB2	
407	ESRRG	ADH1C	
408	HTR6	Chuk	
409	HTR2C	Alpl	
410	SIRT2	STING1	
411	CFTR	ABCB4	
412	TACR3	Map3k14	
413	GABBR2	CLDN4	
414	MAPT	Mdk	
415	CCKBR	AZGP1	
416	GLRA2	Pak1	
417	JUN	Kenma1	
418	PPM1A	Hspd1	
419	PTPA	Itrp2	
420	CES1	RIPK2	
421	CDC25C	Tgfbr2	
422	EPHB4	Map3k8	
423	INCENP	TNFAIP6	
424	AURKB	SCARB2	
425	TTK	Nfatc3	
426	ITK	MMUT	
427	PRKCB	Thbs2	
428	GABRA3	Eif4e	
429	PDPK1	Pdgfra	
430	TKT	Rcan1	
431	CCR3	Ptpn11	
432	CCND1	Hdac2	
433	CDK4	Ptafr	
434	CCNE2	IGHE	
435	CCNE1	Irak4	

436	RET	TNFRSF10C
437	MMP9	GOLGA2
438	GRB2	Ocln
439	MKNK2	Capn2
440	FLT3	Rab7
441	DHFR	Cast
442	AKR1B1	TNFRSF10D
443	MAOB	Piezo1
444	ABCB11	SLC7A7
445	CFD	Gnai2
446	PRF1	Ryr1
447	MAPK9	Jak3
448	CDK6	Fgf7
449	PAK1	MIR127
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451	IL6	Ramp1
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453	APP	MMAB
454	MAST3	Cxcl9
455	PDE3A	Itgam
456	PDE3B	Mir22
457	GCK	Vipr1
458	KCNA3	Mtnr1a
459	LIMK2	Ggps1
460	FASN	Reg2
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462	CDK9	MMADHC
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470	KCNH2	Hyou1
471	KCNN4	Eif2b1
472	CCR5	MCEE
473	MC4R	ARPIN
474	G6PC	Fntb
475	HTR7	Mir217
476	DRD4	Eppk1
477	ADRA2A	Kpna2
478	HTR1B	Mir135a
479	ADRA2C	Hbp1

480	HRH2	Mir194-1	
481	HTR1D	Mir181b1	
482	ADRA1D	Mir194-2	
483	ADRA1A	MTPA	
484	HSD17B2	GNB1	
485	CHRNA4	TAL1	
486	CHRN2	CPT2	
487	KAT2B	AIR	
488	CALM1	RBM15	
489	ADH1A	ABL2	
490	AOC3	LPIN1	
491	HIF1A	DNMT3A	
492	UPP1	HADHA	
493	GYS1	PAP	
494	HRAS	RANBP2	
495	HSD17B1	GATA2	
496	PLA2G2A	MLF1	
497	SELE	LPP	
498	NR4A2	CHIC2	
499	CBFB	RAP1GDS1	
500	SLC5A4	ACSL6	
501	CDK7	IRF1	
502	PLK4	NPM1	
503	STK16	NSD1	
504	CLK4	DEK	
505	CLK1	MYB	
506	CLK2	ALL2	
507	CLK3	BLACE	
508	CDK3	STAR	
509	CDK16	NBN	
510	MAPK15	BAALC	
511	CDK18	LALL	
512	MAPK7	PAX5	
513	DYRK1B	TAL2	
514	CDK17	ALAD	
515	PTK2	SET	
516	CSNK1A1	NUP214	
517	IRAK4	AF10	
518	MAPK10	ALL1	
519	ADH1C	LMO1	
520	TRPV3	LMO2	
521	HMOX1	UNC93B1	
522	KCNA5	NUMA1	
523	LRRK2	PICALM	

524	TNNC1	ZBTB16	
525	TNNT2	HMBS	
526	TNNI3	ETV6	
527	HRH4	KRAS,	
528	TLR9	TBK1	
529	GRIK1	MRD42	
530	GRIK2	NAK	
531	DPP4	FTDALS4	
532	HSPA8	IIAE8	
533	HSPA5	CLCR	
534	ADA	TCL5	
535	AHCY	SCL	
536	GAPDH	TRY2	
537	EHMT1	TEL	
538	EHMT2	THC5	
539	SETD7	IAE4	
540	AMD1	KRAS2	
541	SRM	RASK2	
542	PDCD4	NSCFC2	
543	SRC	RALD	
544	SLC29A1	OES	
545	PNP	SPEN	
546	SETD2	OTT	
547	CARM1	ABLL	
548	PRMT1	ARG	
549	DOT1L	TBR5	
550	GRK1	HESJAS	
551	P2RY1	PBGD	
552	P2RY11	UPS	
553	MTAP	ZNF145	
554	ROCK2	PLZF	
555	PRKACA	NUP358	
556	FBP1	ANE1	
557	SMS	IIAE3	
558	CDA	CALM	
559	FHIT	CLTH	
560	QARS	LAP	
561	KMT2A	DCML	
562	SUV39H1	MONOMAC	
563	DNMT1	IMD21	
564	INMT	ABCC7	
565	SMYD2	CF	
566	EZH2	MRP7	
567	EZH1	IIAE1	

568	SETDB1	ALADH	
569	PNMT	PBGS	
570	DNMT3B	D9S46E	
571	MAPKAPK2	CAN	
572	HSPA1A	CAIN	
573	RARS	IIAE9	
574	OGA	BSAP	
575	CCND1	ALL3	
576	GBA	CD10	
577	GAA	CALLA	
578	FUCA1	NEP	
579	CA14	CMT2T	
580	MARS	SCA43	
581	PRMT7	BTL	
582	PARG	RBTN1	
583	IARS	RHOM1	
584	TYR	NBS1	
585	BRAF	RBTN1	
586	WEE1	RHOM2	
587	CDK5R1	TTG2	
588	ALDH2	MAR	
589	ESRRA	THCYT3	
590	ESRRB	MRD58	
591	PRKCZ	TRY1	
592	RPS6KB1	D6S231E	
593	BMP1	PBT	
594	DUSP3	MASTC	
595	MMP8	PSTI	
596	CA7	PCTT	
597	CA6	TATI	
598	CA5A	TCP	
599	HPGDS	IIAE2	
600	PDE4C	FACL6	
601	ADAM17	ACS2	
602	GRK2	TCS1	
603	MMP13	EST2	
604	TNF	DKCA2	
605	ANPEP	DKCB4	
606	MMP14	PFBMFT1	
607	TRAP1	CMM9	
608	HSP90B1	ARA267	
609	HTR3A	STO	
610	HSP90AB1	SOTOS1	
611	VCP		

612	ADAM10		
613	CA13		
614	CA5B		
615	MIF		
616	EPHA2		
617	MMP16		
618	AKT2		
619	EPHB2		
620	EPHA5		
621	EPHA4		
622	EPHA8		
623	MMP12		
624	EPHA7		
625	EPHB3		
626	DYRK2		
627	DNASE1L3		
628	EGLN1		
629	NOX4		
630	IKBKB		
631	TNNC1		
632	NQO1		
633	SIRT1		
634	KDM3A		
635	KDM5B		
636	KDM4D		
637	KDM4C		
638	MME		
639	MAP3K9		
640	BTK		
641	ECE1		
642	IGFBP3		
643	DHODH		
644	MMP10		
645	PSEN2		
646	NCSTN		
647	AMPD3		
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649	FYN		
650	YES1		
651	BLK		
652	CSK		
653	BMX		
654	LYN		
655	TXK		

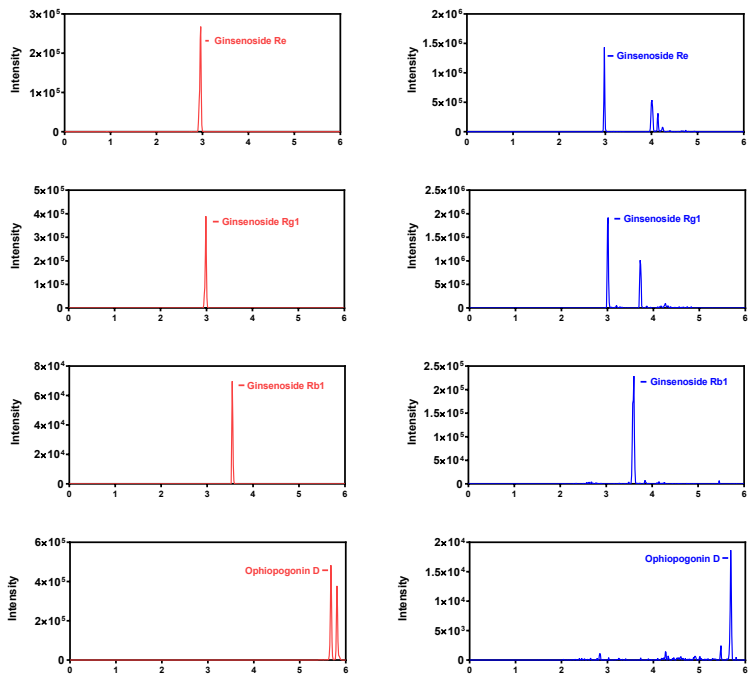
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663	TTR		
664	SERPINE1		
665	NQO2		
666	RIPK2		
667	HSD17B14		
668	HDAC2		
669	HDAC8		
670	FOXO1		
671	ABCG2		
672	TAS2R31		
673	NFE2L2		
674	KLK2		
675	CBR1		
676	MT-ND4		
677	RAF1		
678	FOS JUN		
679	PLK1		
680	BACE2		
681	CA3		
682	COMT		
683	PAK4		
684	SLC9A1		
685	TGFBR1		
686	ACVR1		
687	TGM2		
688	KLK1		
689	GNRHR		
690	NCOR2 HDAC3		
691	FCER2		
692	PLAA		
693	PRKDC		
694	PGF		
695	TYMP		
696	ADAMTS5		
697	ADAMTS4		
698	ADAMTS1		
699	ROCK1		

700	EIF2AK3		
701	GAK		
702	F9		
703	LIPE		
704	MAP4K4		
705	LNPEP		
706	F3		
707	MAP3K8		
708	RPS6KA3		
709	CCNE2		
710	DYRK3		
711	ASF1A		
712	DBF4		
713	ADCY5		
714	EZR		
715	HDAC5		
716	HDAC7		
717	HDAC9		
718	MPEG1		
719	CHRNA3		
720	CHRNA4		
721	ABCC9		
722	KCNJ11		
723	CSNK2A1		
724	CSNK1D		
725	CSNK1E		
726	KCNE1		
727	KCNQ1		
728	F2RL3		
729	PRKCG		
730	NOS1		
731	ADAM9		
732	ATP4B		
733	ATP4A		
734	MELK		
735	TNKS2		
736	TNKS		
737	CDK1 CCNB1		
738	TUBB3		
739	OXSRI		
740	PIK3C2G		
741	YWHAG		
742	TRPM6		
743	PIP4K2C		

744	PIP5K1C		
745	MAP2K3		
746	CSNK1G1		
747	PLA2G5		
748	MMP15		
749	MMP26		
750	PPM1B		
751	PPP2R5A		
752	DBF4		
753	EIF2AK2		
754	HCK		
755	MMP25		
756	ALPG		
757	GRM4		
758	LIG1		
759	KCNMA1		
760	TUBB1		
761	CDK2		
762	PLA2G2C		
763	AXL		
764	MERTK		
765	KLK3		
766	VHL		
767	RASGRP3		
768	ACE		
769	DGAT1		
770	ACPP		

Abbreviations: AP, acute pancreatitis.

Supplementary Figure 1



Supplementary figure 1 Extraction of ion chromatogram (EIC) of four components.