Supplementary Materials

Identification of Quality Markers in *Schisandra chinensis* (Turcz.) Baill. using UPLC-Q-Extractive Orbitrap/MS, Chemometrics Analysis, and Network Pharmacology

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Supplementary Figures

1. FIGURE S1 TIC overlapping map of QC samples mass spectrometry results. (A) positive ion mode and (B) negative ion mode.

2. FIGURE S2 Representative base peak intensity chromatograms of samples of *S chinensis* derived from UPLC-Q-Extractive Orbitrap/MS. Diagram of samples with different harvesting times in positive (A) and negative (B) modes.

FIGURE S1 TIC overlapping map of QC samples mass spectrometry results. (A) positive ion mode; (B) negative ion mode.

FIGURE S2 Representative base peak intensity chromatograms of samples of *S chinensis* derived from UPLC-Q-Extractive Orbitrap/MS. Diagram of samples with different harvesting times in positive (A) and negative (B) modes.
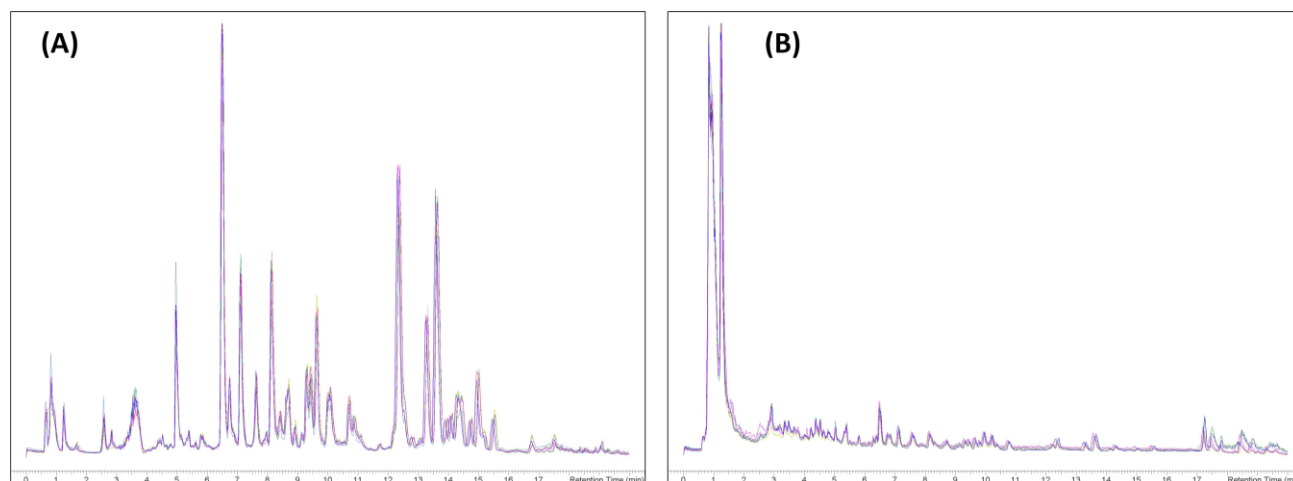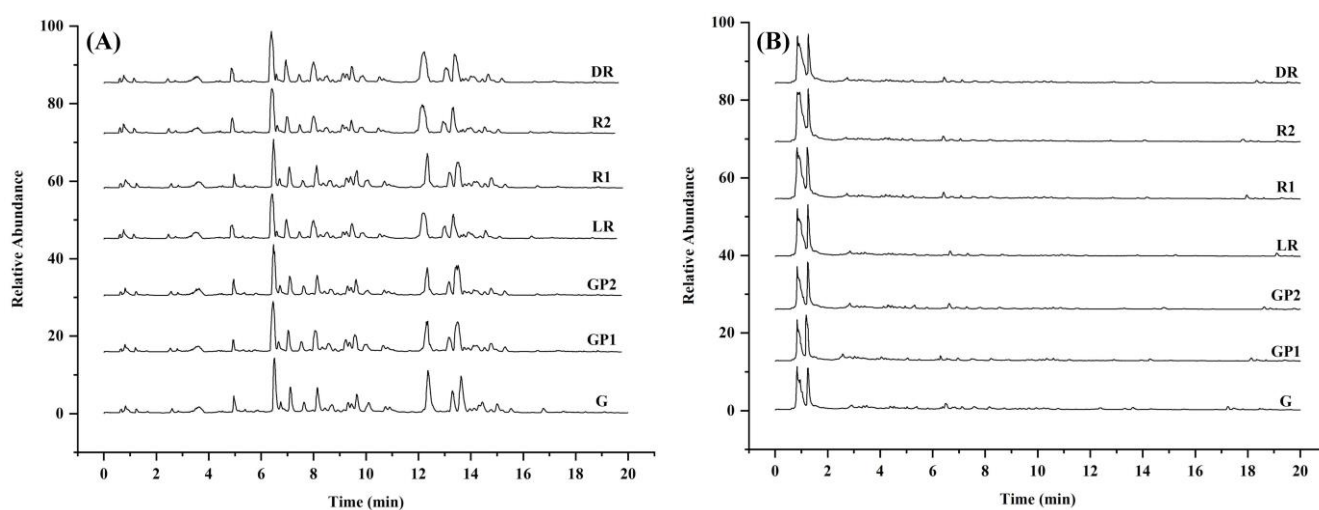
Supplementary Tables

TABLE S1 Collecting information of seven batches of *S. chinensis*

Sample No.	Source	Harvesting time	Reference No.
G	Baoshan Town, Liaoning Province, China	July 21, 2021	DPU-SC2021-0721
GP1	Baoshan Town, Liaoning Province, China	August 1, 2021	DPU-SC2021-0801
GP2	Baoshan Town, Liaoning Province, China	August 12, 2021	DPU-SC2021-0812
LR	Baoshan Town, Liaoning Province, China	August 23, 2021	DPU-SC2021-0823
R1	Baoshan Town, Liaoning Province, China	September 4, 2021	DPU-SC2021-0904
R2	Baoshan Town, Liaoning Province, China	September 15, 2021	DPU-SC2021-0915
DR	Baoshan Town, Liaoning Province, China	September 26, 2021	DPU-SC2021-0926

TABLE S2 Adsorption, distribution, metabolism, and exclusion (ADME) characteristic information of 36 identified compounds from *S. chinensis*

No.	Compound	PubChem CID	MW (g/mol)	GI absorption	OB (%)	DL
1	Phenprobamate	4770	179.2	$+^a$	2.42	0.04
2	Micrandilactone D	101740771	560.6	$-^b$	9.53	0.16
3	Henridilactone D	137347703	544.6	+	23.33	0.30
4	Gomisin H	5317803	418.5	+	7.88	0.62
5	Lancifodilactone D	12080814	526.6	+	29.24	0.16
6	Schisandrol A	23915	432.5	+	7.69	0.66
7	Gomisin D	75130910	530.6	+	7.88	0.59
8	Gomisin J	3001686	388.5	+	8.41	0.54
9	Schisandrol B	634470	416.5	+	28.52	0.78
10	Angeloylgomisin H	26204131	500.6	+	7.51	0.81
11	Tigloylgomisin H	5318766	500.6	+	22.28	0.17
12	Benzoylgomisin Q	14605164	552.6	+	7.5	0.85
13	Gomisin G	14992067	536.6	+	32.68	0.83
14	Angeloylgomisin P	13844273	514.6	+	30.71	0.83
15	Gomisin K$_1$	78385003	402.5	+	8.01	0.58
16	Gomisin F	51003489	514.6	+	7.52	0.83
17	Schisantherin A	151529	536.6	+	7.56	0.81
18	Schisantherin B	6438572	514.6	+	31.99	0.83
19	Schisanhenol	73057	402.5	+	8.02	0.59
20	Gomisin M$_2$	14992068	386.4	+	17.13	0.70
21	Gomisin E	78385000	514.6	+	8.15	0.62
22	Gomisin L$_1$	5317806	386.4	+	9.38	0.71

22	Gomisin L_2	5317807	386.4	+	9.13	0.71
23	Schisandrin A	155256	416.5	+	8.3	0.55
24	Gomisin N	158103	400.5	+	18.53	0.74
25	Schisandrin B	108130	400.5	+	20.16	1.01
26	Schisandrin C	119112	384.4	+	46.27	0.84
27	Benzoylgomisin O	91826818	520.6	+	7.59	0.85
28	Quinic acid	6508	192.2	−	63.53	0.06
29	Citric acid	311	192.1	−	56.22	0.05
30	1-O-caffeoylquinic acid	10155076	354.3	−	22.94	0.80
31	Procyanidin B_1	11250133	578.5	−	67.87	0.66
32	3-O-p-coumaroylquinic acid	9945785	338.3	−	37.63	0.29
33	5-O-p-coumaroylquinic acid	274614191	338.3	−	20.41	0.28
34	Rutin	5280805	610.5	−	3.2	0.68
35	Quercetin-3-O-glucoside	5280804	464.4	−	1.86	0.77
36	Kaempferol-3-O-glucoside	5282102	448.4	−	14.03	0.74

Note: [a] Well-absorbed, polar surface area (PSA) lower than 142 Å^2 and n-octanol/water partition coefficient (log P) between −2.3 and +6.8; [b] poorly-absorbed. Abbreviation: MW, molecular weight (g/mol); GI absorption, gastrointestinal absorption; OB, oral bioavailability; DL, drug-likeness property.

TABLE S3 Characteristic information of 13 potential targets of *S chinensis* for hepatoprotective

No.	Protein Name	Gene Symbol	Uniprot ID
1	Tyrosine-protein kinase ABL1	ABL1	P00519
2	RAC-alpha serine/threonine-protein kinase	AKT1	P31749
3	Serine/threonine-protein kinase ATR	ATR	Q13535
4	Serine/threonine-protein kinase B-raf	BRAF	P15056
5	Prothrombin	F2	P00734
6	Tyrosine-protein kinase JAK2	JAK2	O60674
7	Leucine-rich repeat serine/threonine-protein kinase 2	LRRK2	Q5S007
8	Mitogen-activated protein kinase 14	MAPK14	Q16539
9	Mitogen-activated protein kinase 8	MAPK8	P45983
10	Hepatocyte growth factor receptor	MET	P08581
11	Poly [ADP-ribose] polymerase 1	PARP1	P09874
12	Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform	PIK3CA	P42336
13	Prostaglandin G/H synthase 2	PTGS2	P35354

TABLE S4 Molecular docking of lignans binding with target and their binding energy.

Compound No.	Name	Affinity (kcal/mol)
		PIK3CA (PDBID: 4JPS)
18	Schisantherin B	−8.5
26	Schisandrin C	−8.4
Positive control	DDB	−7.7

TABLE S5 Regression equation, linear range, LOD, LOQ, precision, and repeatability of six analytes

No.	Analyte	Calibration curve	R^2	Linear range (µg/mL)	LOD (µg/mL)	LOQ (µg/mL)	Repeatability (RSD%)	Precision (RSD%)	
								Intra-day	Inter-day
6	Schisandrol A	Y = 40.889X + 231.88	0.9980	34.5 – 230	0.23	1.15	1.95	0.84	1.72
10	Angeloylgomisin H	Y = 30.497X – 78.97	0.9980	10.5 – 52.5	0.35	0.70	2.74	0.57	2.30
17	Schisantherin A	Y = 24.533X – 19.184	0.9990	4 – 40	0.40	1.20	2.12	0.59	1.56
18	Schisantherin B	Y = 22.105X + 14.601	0.9990	4.5 – 31.5	0.45	1.35	1.75	0.49	1.76
23	Schisandrin A	Y = 36.620X – 2.0303	0.9998	1.7 – 25.5	0.17	0.85	1.83	0.52	1.73
26	Schisandrin C	Y = 18.084X - 2.3635	0.9997	3.5 – 14	0.14	0.70	2.25	0.65	2.13