

**Identification of the metabolites produced following *Iris tectorum* Maxim oral administration
and a network pharmacology-based analysis of their potential pharmacological properties**

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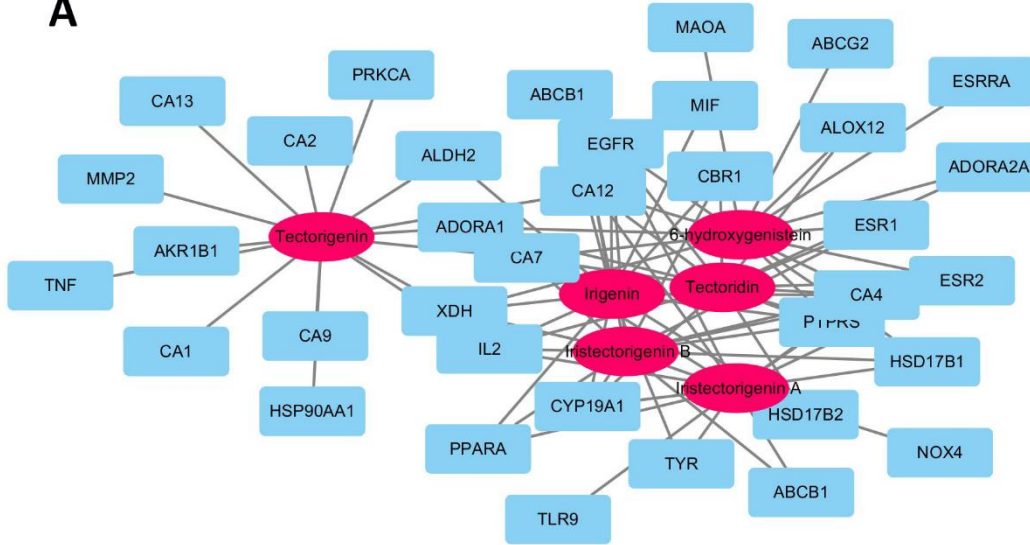
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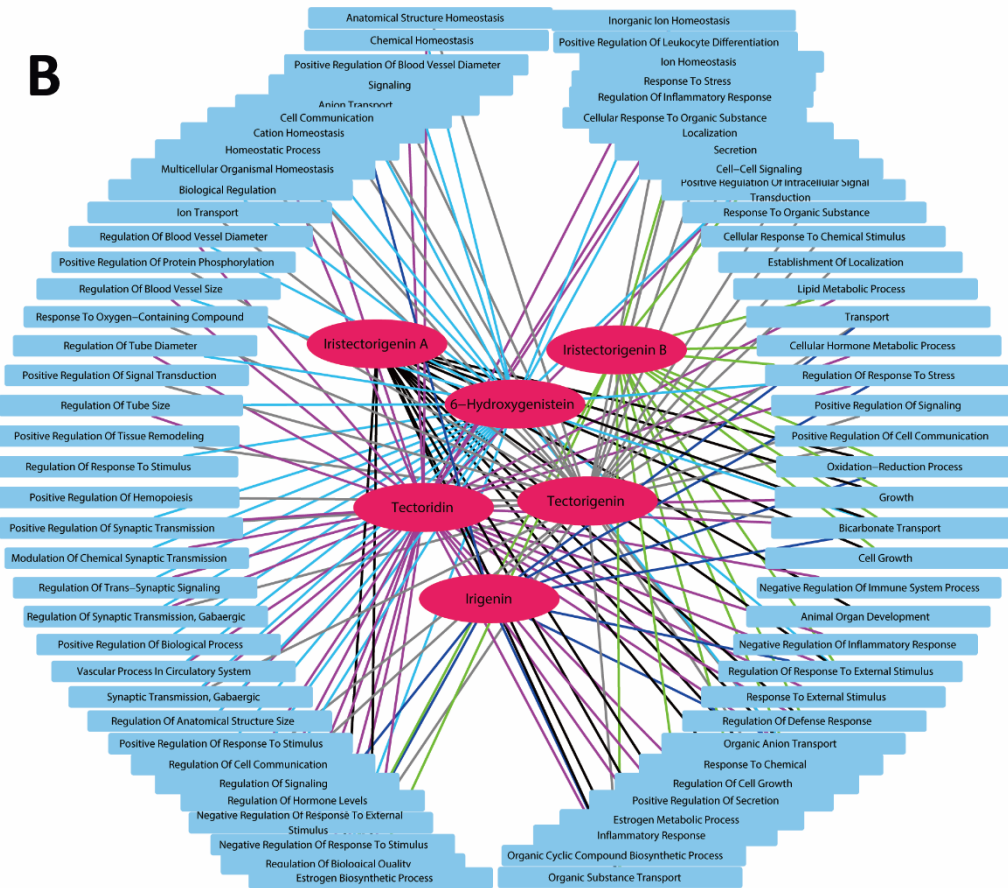
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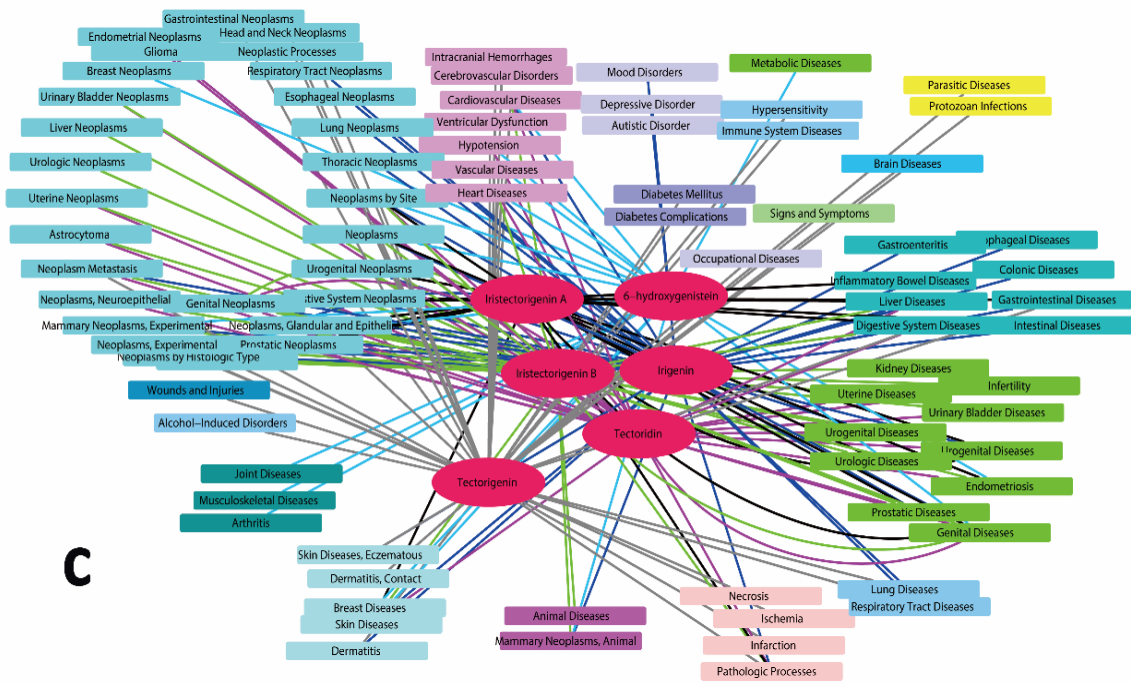
Supplementary Data

A



B





C

Figure S1. The network for systems pharmacology analysis (A) Compound-target network of candidate compounds, (B) Classification human targets of candidate compounds with their biological processes, (C) Compound-disease network of candidate compounds

Table S1 The data of collected urine, feces and bile samples

	0-12h	12-24h	24-36h
Feces	5.03g	2.06g	2.60g
Urine	21.9mL	15.4mL	18.7mL
Bile	4.1mL	8.2mL	-

Table S2 34 metabolites in feces and urine identified in the positive mode

Peak No.	t_R (min)	Theoretical mass	Molecular formula	Error (ppm)	Observed mass	MS/MS fragments	Proposed structure	Source	12h	24h	36h
M1	12.68	416.1107	C ₂₁ H ₂₀ O ₉	1.94	417.1172	255.0632(100)	Daidzin*	U	√	√	√
M2	14.08	460.1006	C ₂₂ H ₂₀ O ₁₁	-0.13	461.1079	285.0751(100)	Glycitein glucuronide	U	√	√	√
M3	15.53	430.0900	C ₂₁ H ₁₈ O ₁₀	1.80	431.0965	255.0642(100)	Daidzein glucuronide	U	√	√	√
M4	16.01	462.1162	C ₂₂ H ₂₂ O ₁₁	-1.76	463.1243	301.0715(100), 286.0466(50)	Tectoridin*	U	√	√	√
								F	√	√	√
M5	16.52	492.1268	C ₂₃ H ₂₄ O ₁₂	-0.10	493.1341	331.0799(100), 316.0556(30)	Iristectorin	F	√	√	√
M6	16.94	446.0849	C ₂₁ H ₁₈ O ₁₁	2.66	447.0910	271.0581(100)	Genistein glucuronide	U	√	√	√
M7	17.09	462.1162	C ₂₂ H ₂₂ O ₁₁	0.19	463.1234	301.0687(100), 286.0473(50)	Tectorigenin-4'-O-β-D-glucoside	U	√	√	√
								F	√	×	×
M8	17.34	476.0955	C ₂₂ H ₂₀ O ₁₂	2.42	477.1016	301.0723(100), 286.0486(40)	Tectorigenin glucuronide	U	√	√	√
M9	17.49	492.1268	C ₂₃ H ₂₄ O ₁₂	-4.36	493.1362	331.0823(100), 316.0581(40)	Iristectorin	F	√	√	√
M10	17.79	476.0955	C ₂₂ H ₂₀ O ₁₂	1.16	477.1022	301.0702(100), 286.0442(40)	Tectorigenin glucuronide	F	×	×	√
M11	18.27	506.1060	C ₂₃ H ₂₂ O ₁₃	-2.53	507.1146	331.0814(100), 316.0577(30)	Iristectorigenin glucuronide	U	√	√	√
M12	18.75	476.0955	C ₂₂ H ₂₀ O ₁₂	1.16	477.1022	301.0723(100), 286.0485(40)	Tectorigenin glucuronide	U	√	√	√
M13	19.53	506.1060	C ₂₃ H ₂₂ O ₁₃	2.41	507.1121	331.0802(100), 316.0575(30)	Iristectorigenin glucuronide	U	√	√	√
M14	19.79	536.1166	C ₂₄ H ₂₄ O ₁₄	-1.34	537.1246	361.0918(100), 346.0674(10)	Irogenin glucuronide	U	√	√	√
M15	20.50	506.1060	C ₂₃ H ₂₂ O ₁₃	-2.73	507.1147	331.0819(100), 316.0574(30)	Iristectorigenin glucuronide	U	√	√	√
M16	21.01	506.1060	C ₂₃ H ₂₂ O ₁₃	-1.74	507.1142	331.0855(100), 316.0616(30)	Iristectorigenin glucuronide	U	√	√	√
M17	24.42	300.0634	C ₁₆ H ₁₂ O ₆	-3.12	301.0716	301.0712(30), 286.0478(100)	Tectorigenin*	U	√	√	√
								F	√	×	√
M18	25.13	300.0634	C ₁₆ H ₁₂ O ₆	-1.78	301.0712	301.0712(25), 286.0478(100)	Isotectorigenin	U	√	√	√
								F	√	√	√

M19	25.72	330.0740	C ₁₇ H ₁₄ O ₇	-3.85	331.0825	331.0804(30), 316.0569(100) 301.0339(10)	Iristectorigenin A	U F	√ √	√ √	√ √
M20	26.38	360.0845	C ₁₈ H ₁₆ O ₈	-3.63	361.0931	361.0918(90), 346.0694(70) 331.0449(100), 328.0576(40) 313.0356(35), 310.0476(50) 303.0498(40), 301.0269(40)	Irigenin	U	√	√	√
M21	26.50	330.0740	C ₁₇ H ₁₄ O ₇	-0.21	331.0813	331.0827(40), 316.0600(100) 301.0366(15)	Iristectorigenin B	U F	√ √	√ √	√ √
M22	30.39	344.0896	C ₁₈ H ₁₆ O ₇	-4.42	345.0984	345.0965(90), 330.0746(100) 315.0510(30), 312.0586(30) 287.0529(30), 284.0675(25)	Methyl iristectorigenin	U	√	√	√
M23	31.79	380.0202	C ₁₆ H ₁₂ O ₉ S	-1.37	381.0280	301.0711(90), 286.0451(100)	Tectorigenin sulfate	F	√	√	×
M24	32.38	380.0202	C ₁₆ H ₁₂ O ₉ S	4.94	381.0256	301.0732(95), 286.0457(100)	Tectorigenin sulfate	F	√	√	×
M25	32.68	380.0202	C ₁₆ H ₁₂ O ₉ S	4.68	381.0257	301.0732(100), 286.0457(95)	Isotectorigenin sulfate	F	√	×	×
M26	33.05	380.0202	C ₁₆ H ₁₂ O ₉ S	3.63	381.0261	301.0716(100), 286.0470(95)	Isotectorigenin sulfate	U F	√ √	√ ×	√ √
M27	33.53	410.0308	C ₁₇ H ₁₄ O ₁₀ S	-0.14	411.0381	331.0819(100), 316.0579(99) 301.0329(20)	Iristectorigenin sulfate	F	×	√	×
M28	34.09	410.0308	C ₁₇ H ₁₄ O ₁₀ S	-3.31	411.0394	331.0811(100), 316.0599(95) 301.0361(5)	Iristectorigenin sulfate	F	√	√	×
M29	34.61	410.0308	C ₁₇ H ₁₄ O ₁₀ S	2.3	411.0371	331.0825(100), 316.0589(99) 301.0379(10)	Iristectorigenin sulfate	U F	√ √	×	×
M30	34.61	314.0790	C ₁₇ H ₁₄ O ₆	-1.23	315.0867	315.0866(30), 300.0629(100) 285.0390(5)		U	√	√	√

M31	34.83	440.0413	C ₁₈ H ₁₆ O ₁₁ S	-1.80	441.0494	361.0915(100), 346.0702(50) 331.0401(30), 310.0431(20) 301.0713(20)	Irigenin sulfate	F	×	√	√
M32	35.24	396.0151	C ₁₆ H ₁₂ O ₁₀ S	-3.80	397.0239	317.0662(100), 302.0423(80)	Irilin D sulfate	U	√	×	×
M33	35.27	440.0413	C ₁₈ H ₁₆ O ₁₁ S	4.34	441.0467	361.0915(100), 346.0702(50) 331.0401(30), 310.0431(20) 301.0713(20)	Irigenin sulfate	F	√	√	×
M34	35.80	440.0413	C ₁₈ H ₁₆ O ₁₁ S	-3.84	441.0503	361.0927(100), 346.0710(50) 331.0437(25), 328.0601(25) 313.0319(20), 310.0438(20) 301.0685(20)	Irigenin sulfate	U F	√ √	√ √	√ ×

Urine-U, Feces-F, "*" represent for reference standards

Table S3 17 metabolites in bile identified in the positive mode

Peak No.	t_R (min)	Theoretical mass	Molecular formula	Error (ppm)	Observed mass	MS/MS fragments	Proposed structure	12h	24h
M35	7.92	587.0958	C ₂₃ H ₂₅ NO ₁₅ S	-2.27	588.1031	463.0898(100), 412.0722(10) 287.0536(25)	Taurine and glucuronide conjugate of 6-hydroxygenistein	√	×
M36	10.42	537.1133	C ₂₃ H ₂₃ NO ₁₄	-2.74	538.1206	463.0862(100), 287.0562(25)	Glycine and glucuronide conjugate of 6-hydroxygenistein	√	×
M37	10.66	612.1538	C ₃₆ H ₂₄ N ₂ O ₈	-0.91	613.1611	538.1367(5), 484.1171(60) 409.0855(5), 355.0742(100) 231.0489(10)	Unknown structure	√	×
M38	11.79	609.1350	C ₂₆ H ₂₇ NO ₁₆	-3.35	610.1423	463.0863(100), 287.0554(15)	Glutamic acid and glucuronide conjugate of 6-hydroxygenistein	√	×
M39	17.03	556.0551	C ₂₂ H ₂₀ SO ₁₅	-5.09	557.0624	381.0281(100), 301.0707(40)	Glucuronide and sulphate conjugate of tectorigenin	√	√
M40	17.65	712.1508	C ₃₀ H ₃₂ O ₂₀	-2.99	713.1581	537.1260(30), 361.0924(100)	Double glucuronide conjugate of irigenin	√	×
M41	17.78	682.1409	C ₂₉ H ₃₀ O ₁₉	-4.10	683.1482	507.1151(60), 331.0824(100)	Double glucuronide conjugate of iristectorigenin	√	√
M42	18.40	510.1026	C ₂₅ H ₂₀ NO ₁₁	1.98	511.1099	303.0508(30), 225.0400(100)	Unidentified	√	×
M43	18.65	586.0651	C ₂₃ H ₂₂ SO ₁₆	-3.87	587.0724	411.0391(100), 331.0821(80)	Glucuronide and sulphate conjugate of iristectorigenin	√	√
M44	18.90	643.1555	C ₃₀ H ₂₉ NO ₁₅	-2.81	644.1628	463.0893(55), 287.0559(100)	Tyrosine and glucuronide conjugate of 6-hydroxygenistein	√	×
M45	19.03	616.0740	C ₂₄ H ₂₄ SO ₁₇	-0.98	617.0813	441.0496(45), 361.0922(100)	Glucuronide and sulphate conjugate of irigenin	√	√

M46	20.28	579.1600	C ₂₆ H ₂₉ NO ₁₄	-2.1	580.1673	463.0869(25), 287.0552(100)	Valine and glucuronide conjugate of 6-hydroxygenistein	√	×
M47	20.53	478.1121	C ₂₂ H ₂₂ O ₁₂	-2.09	479.1194	303.0878(100), 285.0760(30) 257.0808(90), 167.0337(45)	Glucuronide conjugate of unidentified aglycone	√	√
M48	20.65	490.1115	C ₂₃ H ₂₂ O ₁₂	-0.81	491.1188	316.0897(20), 315.0877(100)	Glucuronide conjugate of irisolidone	√	×
M49	22.52	492.0919	C ₂₂ H ₂₀ O ₁₃	-3.31	493.0992	318.0684(15), 317.0655(100)	Glucuronide conjugate of unidentified aglycone	√	×
M50	23.02	448.1024	C ₂₁ H ₂₀ O ₁₁	-4.16	449.1097	273.0769(100), 274.0808(15)	Glucuronide conjugate of unidentified aglycone	√	×
M51	24.77	666.1729	C ₃₂ H ₃₀ N ₂ O ₁₄	-4.83	667.1802	463.0858(100), 287.0519(95)	Tryptophan and glucuronide conjugate of 6-hydroxygenistein	√	×

