

**Study on the active constituents and molecular mechanism of Zhishi Xiebai
Guizhi decoction (ZXGD) in the treatment of CHD based on UPLC-UESI-Q
Exactive Focus, gene expression profiling, network pharmacology and
experimental validation**

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Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
1	lauric acid	+	9.37E+04	0.19	C12H24O2	201.1849	201.1849	-0.25	Trichosanthis fructus
2	pentadecanoic acid	+	4.55E+05	0.87	C15H30O2	243.2319	243.232	0.68	Trichosanthis fructus
3	lysine	+	1.59E+07	0.9	C6H14N2O2	147.1128	147.1127	-0.36	Trichosanthis fructus
4	aspartic acid	+	4.34E+07	0.94	C4H7NO4	134.0448	134.0447	-0.88	Trichosanthis fructus/Allii macrostemonis bulbus
5	histidine	+	3.16E+07	0.94	C6H9N3O2	156.0768	156.0766	-0.97	Trichosanthis fructus
6	galactonic acid- γ -lactone	+	1.58E+07	0.97	C6H10O6	179.055	179.0547	-1.89	Trichosanthis fructus
7	glutamic acid	+	4.04E+07	0.97	C5H9NO4	148.0604	148.0602	-1.27	Trichosanthis fructus
8	L-threonine	+	1.44E+06	0.97	C4H9NO3	120.0655	120.0656	0.58	Trichosanthis fructus/Allii macrostemonis bulbus
9	L-rhamnose monohydrate	+	1.80E+07	0.97	C6H12O5	165.0758	165.0756	-1.05	Magnoliae officinalis cortex
10	allose	-	1.76E+08	0.98	C6H12O6	179.0561	179.0554	-3.77	Magnoliae officinalis cortex

11	glucose	-	1.76E+08	0.98	C6H12O6	179.0561	179.0554	-3.77	Magnoliae officinalis cortex/Allii macrostemonis bulbus
12	3,4-Dihydroxybenzaldehyde	+	5.64E+06	0.99	C7H6O3	139.039	139.0388	-0.98	Cinnamomi ramulus
13	p-Hydroxybenzoic acid	+	5.64E+06	0.99	C7H6O3	139.039	139.0388	-0.98	Allii macrostemonis bulbus
14	methyl-β-D-fructofuranoside	-	1.08E+06	1	C7H14O6	193.0718	193.0712	-2.83	Allii macrostemonis bulbus
15	quinic acid	-	9.82E+08	1	C7H12O6	191.0561	191.0555	-3.21	Aurantii fructus immaturus
16	6-isoinosine	-	2.90E+06	1.03	C10H12N4O5	267.0735	267.0723	-4.36	Trichosanthis fructus
17	cytidine	+	1.92E+07	1.04	C9H13N3O5	244.0928	244.0925	-1.3	Trichosanthis fructus
18	scopoletin	+	2.76E+06	1.04	C10H8O4	193.0495	193.0496	0.19	Aurantii fructus immaturus
19	adenine	+	3.60E+07	1.06	C5H5N5	136.0618	136.062	1.89	Trichosanthis fructus

Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
20	3-Hydroxy-ben-zaldehyde	+	1.84E+07	1.06	C7H6O2	123.0441	123.044	-0.13	Cinnamomi ramulus

21	benzoic Acid	+	1.84E+07	1.06	C6H5COOH	123.0441	123.044	-0.13	Cinnamomi ramulus/Aurantii fructus immaturus
22	magnosprengerine	+	2.56E+07	1.06	C11H17NO2	196.1332	196.1331	-0.7	Magnoliae officinalis cortex
23	synephrine	+	3.42E+08	1.06	C9H13NO2	168.1019	168.1017	-1.16	Aurantii fructus immaturus
24	heptadecanoic acid	+	9.06E+06	1.09	C17H34O2	271.2632	271.2625	-2.28	Trichosanthis fructus/Cinnamomi ramulus
25	isovanillic Acid	+	1.06E+06	1.09	C8H8O4	169.0495	169.0496	0.12	Trichosanthis fructus/Cinnamomi ramulus/Magnoliae officinalis cortex
26	quercitrin	-	5.28E+05	1.1	C21H20O11	447.0933	447.0952	4.26	Trichosanthis fructus/Magnoliae officinalis cortex
27	DL-methionine	+	2.26E+06	1.24	C5H11NO2S	150.0583	150.0585	1.05	Trichosanthis fructus
28	capric acid	+	6.54E+05	1.26	C10H20O2	173.1536	173.1534	-1.06	Trichosanthis fructus
29	nicotinic acid	+	9.29E+06	1.26	C6H5NO2	124.0393	124.0394	0.67	Trichosanthis fructus
30	nonanoic acid	+	7.73E+05	1.36	C9H18O2	159.138	159.1379	-0.23	Trichosanthis fructus
31	pyroglutamic acid	+	7.95E+07	1.39	C5H7NO3	130.0499	130.05	0.67	Trichosanthis fructus
32	octanoic acid	+	1.59E+05	1.39	C8H16O2	145.1223	145.1222	-0.5	Trichosanthis fructus

33	hypoxanthine	+	6.69E+06	1.41	C5H4N4O	137.0458	137.0458	-0.1	Trichosanthis fructus
34	4-hydroxynicotinic acid	+	6.04E+06	1.47	C6H5NO3	140.0342	140.0342	-0.18	Trichosanthis fructus
35	phlorin	-	4.95E+07	1.48	C12H16O8	287.0772	287.0777	1.7	Aurantii fructus immaturus
36	terpinen-4-ol	+	5.07E+05	1.51	C10H18O	155.143	155.1431	0.17	Cinnamomi ramulus
37	uridine	-	3.85E+07	1.55	C9H12N2O6	243.0623	243.0624	0.42	Magnoliae officinalis cortex
38	myristic acid	+	8.11E+04	1.67	C14H28O2	229.2162	229.2164	0.96	Trichosanthis fructus

Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
39	tyrosine	+	6.17E+07	1.75	C9H11NO3	182.0812	182.0812	0.04	Trichosanthis fructus
40	leucine	+	1.04E+08	1.75	C6H13NO2	132.1019	132.102	0.37	Trichosanthis fructus
41	N-methyltyramine	+	1.37E+08	2.03	C9H13NO	152.107	152.107	0.03	Aurantii fructus immaturus
42	adenosine	+	1.30E+08	2.18	C10H13N5O4	268.104	268.1038	-1.01	Trichosanthis fructus
43	guanosine	+	4.40E+07	2.46	C10H13N5O5	284.099	284.0989	-0.15	Allii macrostemonis bulbus

44	Phenylalanine	+	1.46E+08	3.03	C9H11NO2	166.0863	166.0862	-0.47	Trichosanthis fructus
45	Thymidine	-	4.32E+06	3.43	C10H14N2O5	241.083	241.0831	0.33	Allii macrostemonis bulbus
46	quercetin-3-O-β-rutinoside	+	1.27E+06	3.72	C27H30O16	611.1607	611.1577	-4.82	Trichosanthis fructus
47	Protocatechuicacid	-	1.06E+07	4.12	C7H6O4	153.0193	153.0186	-4.97	Cinnamomi ramulus
48	benzyl benzoate	+	1.34E+06	4.29	C14H12O2	213.091	213.0909	-0.46	Cinnamomi ramulus
49	magnolianone	+	2.46E+05	4.36	C19H22O6	347.1489	347.1492	0.84	Magnoliae officinalis cortex
50	Meranzin hydrate	+	3.23E+04	4.36	C15H18O5	279.1227	279.1217	-3.68	Aurantii fructus immaturus
51	4-(beta-D-glucopyranosyloxy)-3-methoxybenzoic acid	-	1.15E+07	4.45	C14H18O9	329.0878	329.0883	1.45	Trichosanthis fructus
52	syringin	+	1.02E+05	4.8	C17H24O9	373.1493	373.1477	-4.38	Magnoliae officinalis cortex
53	indole-3-aldehyde	+	4.06E+06	5	C9H7NO	146.06	146.0601	0.13	Magnoliae officinalis cortex
54	tryptophan	+	3.48E+07	5.02	C11H12N2O2	205.0972	205.0971	-0.28	Allii macrostemonis bulbus
55	ethyl-3-methyl-4, 5, 6, 7-tetrahydro-1H-indole-2-carboxylate	+	1.31E+06	5.07	C12H17NO2	208.1332	208.1332	0.14	Trichosanthis fructus
56	syringic acid	-	1.43E+06	5.69	C9H10O5	197.0456	197.0452	-1.56	Cinnamomi ramulus/Magnoliae officinalis

cortex

57	N-p-coumaroyltyramine	+	3.97E+05	5.83	C17H17NO3	284.1281	284.1278	-1.1	Allii macrostemonis bulbus
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Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
58	3, 4, 5-trimethoxyphenyl β-D-glucopy ranoside	+	4.91E+04	5.94	C18H26O9	387.165	387.1637	-3.26	Magnoliae officinalis cortex
59	2, 3, 4, 9-tetrahydro-1H pyrido[3, 4-b]indole-3-carboxylic acid	+	8.85E+06	6.04	C12H12N2O2	217.0972	217.097	-0.76	Trichosanthis fructus
60	4'-methoxymagnaldehyde E	+	6.42E+05	6.06	C17H16O3	269.1172	269.1169	-1.14	Magnoliae officinalis cortex
61	(2R,3S,4S,5R)-2-butoxy-2,5-bis(hydroxymethyl)oxolane-3,4-diol	+	1.03E+05	6.37	C10H20O6	237.1333	237.1343	4.29	Trichosanthis fructus
62	N-trans-feruloyltyramine	+	4.56E+06	6.45	C18H19NO4	314.1387	314.1385	-0.51	Allii macrostemonis bulbus
63	trans-N-feruloylputrescine	+	6.90E+07	6.55	C14H20N2O3	265.1547	265.1543	-1.29	Magnoliae officinalis cortex
64	Trihydroxy-tetramethoxy-flavone	-	2.47E+05	6.61	C19H18O9	389.0878	389.086	-4.73	Aurantii fructus immaturus
65	ethyl benzoate	+	8.84E+06	6.65	C9H10O2	151.0754	151.0753	-0.38	Cinnamomi ramulus

66	chlorogenic Acid	-	3.74E+07	6.94	C16H18O9	353.0878	353.0881	0.83	Magnoliae officinalis cortex
67	4-(2-formyl-5-hydroxy methylpyrrol-1-yl)-butyric acid	-	3.07E+06	7.07	C10H13NO4	210.0772	210.077	-0.95	Trichosanthis fructus
68	cucurbitacin B	+	5.24E+05	7.21	C32H46O8	559.3265	559.3265	0	Trichosanthis fructus
69	caffeicacid	-	3.18E+07	7.24	C9H8O4	179.035	179.0344	-3.19	Magnoliae officinalis cortex
70	pinoresionol-4-O-β-D-glucopyranoside	+	1.02E+06	7.87	C26H32O11	521.2017	521.2016	-0.27	Magnoliae officinalis cortex
71	reticuline	+	3.20E+07	7.92	C19H23NO4	330.17	330.1696	-1.1	Magnoliae officinalis cortex
72	syringaldehyde	+	6.98E+06	8.35	C9H10O4	183.0652	183.0653	0.48	Cinnamomi ramulus/Magnoliae officinalis cortex
73	5, 7-Dihydroxycoumarin	-	1.83E+07	8.44	C9H6O4	177.0193	177.0187	-3.43	Aurantii fructus immaturus
74	sinapic Acid	-	2.79E+05	8.57	C11H12O5	223.0612	223.061	-0.81	Magnoliae officinalis cortex
75	acteoside	-	3.99E+08	8.62	C29H36O15	623.1981	623.1985	0.56	Magnoliae officinalis cortex

Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
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76	coniferol alcohol	+	1.79E+06	8.63	C10H12O3	181.0859	181.0861	0.94	Magnoliae officinalis cortex
77	umbelliferone	+	7.34E+07	8.63	C9H6O3	163.039	163.0388	-1.3	Aurantii fructus immaturus
78	kaempferol-3-O- β -rutinoside	-	4.55E+07	8.67	C27H30O15	593.1512	593.1514	0.4	Trichosanthis fructus
79	lonicerin	-	4.55E+07	8.67	C27H30O15	593.1512	593.1514	0.4	Aurantii fructus immaturus
80	S-(+)-dehydrovomifoliol	+	1.15E+06	8.71	C13H18O3	223.1329	223.1329	0.15	Magnoliae officinalis cortex
81	coniferin	-	5.63E+05	8.82	C16H22O8	341.1242	341.1246	1.12	Magnoliae officinalis cortex
82	p-Hydroxy-cinnamic acid	-	2.60E+07	8.97	C9H8O3	163.0401	163.0393	-4.59	Allii macrostemonis bulbus
83	(+) -lyoniresinol	-	3.77E+05	9.02	C22H28O8	419.1711	419.1713	0.44	Cinnamomi ramulus
84	acanthoside D	-	6.41E+05	9.13	C34H46O18	741.2611	741.2614	0.29	Allii macrostemonis bulbus
85	lariciresinol	-	3.81E+06	9.28	C20H24O6	359.15	359.1503	0.72	Magnoliae officinalis cortex
86	limonexin	+	1.35E+06	9.34	C26H30O10	503.1912	503.1887	-4.87	Aurantii fructus immaturus
87	(-)-Loliolide	+	1.18E+07	9.37	C11H16O3	197.1172	197.1172	0.14	Trichosanthis fructus
88	loliolide	+	1.18E+07	9.37	C11H16O3	197.1172	197.1172	0.14	Magnoliae officinalis cortex
89	cinnamic acid	+	1.52E+06	9.39	C9H8O2	149.0597	149.0597	0.19	Magnoliae officinalis cortex

90	asimilobine	+	1.39E+08	9.44	C17H17NO2	268.1332	268.1328	-1.48	Magnoliae officinalis cortex
91	cinnamyl Acetate	+	3.39E+06	9.54	C11H12O2	177.091	177.091	-0.12	Magnoliae officinalis cortex
92	(-) -secoisolariciresinol	-	1.21E+06	9.55	C20H26O6	361.1657	361.1653	-0.96	Cinnamomi ramulus
93	methylcaffeate	-	1.08E+07	9.55	C10H10O4	193.0506	193.0502	-2.22	Magnoliae officinalis cortex
94	sinapaldehyde	+	5.59E+06	9.57	C11H12O4	209.0808	209.0808	0.01	Cinnamomi ramulus
95	(E) -3-(4-Hydroxy-3, 5-Di methoxyphenyl)acrylaldehyde	+	5.59E+06	9.57	C11H12O4	209.0808	209.0808	0.01	Magnoliae officinalis cortex
96	tricin	+	1.11E+06	9.79	C17H14O7	331.0812	331.0807	-1.45	Trichosanthis fructus

Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
97	afzelin	+	9.99E+05	9.79	C21H20O10	433.1129	433.1124	-1.21	Magnoliae officinalis cortex
98	eriodictyol	+	8.50E+07	9.79	C15H12O6	289.0707	289.0703	-1.1	Aurantii fructus immaturus
99	isovitexin	+	9.99E+05	9.79	C21H20O10	433.1129	433.1124	-1.21	Aurantii fructus immaturus

100	eriocitrin	-	4.04E+08	9.81	C27H32O15	595.1668	595.1672	0.56	Aurantii fructus immaturus
101	manglieside D	-	3.17E+06	9.93	C26H34O11	521.2028	521.2032	0.8	Magnoliae officinalis cortex
102	icaraside E5	-	3.17E+06	9.93	C26H34O11	521.2028	521.2032	0.8	Magnoliae officinalis cortex
103	coniferaldehyde	+	1.11E+07	9.94	C10H10O3	179.0703	179.0702	-0.19	Magnoliae officinalis cortex
104	kaempferol-3-O- β -D-glucoside-7-O- α -rhamnoside	-	4.38E+05	10.24	C33H40O20	755.204	755.2007	-4.34	Trichosanthis fructus
105	seselin	+	3.58E+05	10.35	C14H12O3	229.0859	229.0861	0.74	Aurantii fructus immaturus
106	coumarin	+	2.14E+08	10.43	C9H6O2	147.0441	147.044	-0.16	Cinnamomi ramulus
107	quercetin-3-O- α -D-nucleoside	-	3.19E+05	10.45	C20H18O11	433.0776	433.0786	2.2	Trichosanthis fructus
108	syringaresinol-4'-O- β -D-glucopyranoside	-	1.36E+07	10.5	C28H36O13	579.2083	579.2061	-3.79	Magnoliae officinalis cortex
109	lirioresinol A	+	2.21E+06	10.51	C22H26O8	419.17	419.1696	-1.01	Magnoliae officinalis cortex
110	D-apiose	-	2.26E+06	10.52	C5H10O5	149.0456	149.046	3.26	Magnoliae officinalis cortex
111	L-Arabinose	-	2.26E+06	10.52	C5H10O5	149.0456	149.046	3.26	Allii macrostemonis bulbus
112	apigenin-6,8-C- β -glucoside	-	4.88E+05	10.59	C26H28O14	563.1406	563.1421	2.59	Trichosanthis fructus
113	2,7-dimethyl-2,4-diene deca- α , ω -diacid-8-O- β -D-glu	-	1.30E+07	10.59	C18H28O10	403.161	403.1611	0.4	Trichosanthis fructus

114	2-isopropylphenol	+	3.48E+05	10.61	C9H12O	137.0961	137.096	-0.71	Magnoliae officinalis cortex
115	choerospondin	+	8.35E+07	10.81	C21H22O10	435.1286	435.1279	-1.61	Magnoliae officinalis cortex
116	puerarin	+	9.78E+06	10.81	C21H20O9	417.118	417.1172	-1.9	Aurantii fructus immaturus
117	prunin	+	8.35E+07	10.81	C21H22O10	435.1286	435.1279	-1.61	Aurantii fructus immaturus
118	natsudaïdai, natsu-daïdai	+	7.99E+07	10.81	C21H22O9	419.1337	419.1329	-1.88	Aurantii fructus immaturus

Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
119	naringenin-7-O- β -D-glucopyranoside	+	1.16E+07	10.81	C33H42O18	727.2444	727.2427	-2.27	Aurantii fructus immaturus
120	naringin	-	2.46E+09	10.82	C27H32O14	579.1719	579.1721	0.22	Aurantii fructus immaturus
121	michealbine	+	4.39E+05	11.01	C17H15NO3	282.1125	282.1124	-0.26	Magnoliae officinalis cortex
122	phellopterin	-	1.10E+06	11.05	C17H16O5	299.0925	299.0929	1.32	Aurantii fructus immaturus
123	honokitriol	-	6.41E+06	11.27	C18H20O5	315.1238	315.1241	1	Magnoliae officinalis cortex
124	quercetin-3-O- β -D-glucofuranoside	-	5.13E+05	11.29	C21H20O12	463.0882	463.0883	0.25	Trichosanthis fructus

125	luteolin	+	3.45E+05	11.31	C15H10O6	287.055	287.0552	0.58	Trichosanthis fructus
126	eugenol	+	8.02E+06	11.31	C10H12O2	165.091	165.0906	-2.35	Cinnamomi ramulus/Magnoliae officinalis cortex
127	hesperidin	-	4.39E+09	11.32	C28H34O15	609.1825	609.1827	0.31	Aurantii fructus immaturus
128	diosmetin-7-O- β -D-glucoside	+	3.84E+06	11.33	C22H22O11	463.1235	463.1227	-1.62	Trichosanthis fructus
129	hesperitin-7-O- β -D-glucoside	+	2.12E+08	11.33	C22H24O11	465.1391	465.1386	-1.14	Aurantii fructus immaturus
130	dihydroxy-trimethoxy-flavone	+	3.37E+07	11.33	C18H16O7	345.0969	345.0964	-1.46	Aurantii fructus immaturus
131	homoeriodictyol	+	1.60E+09	11.33	C16H14O6	303.0863	303.0858	-1.63	Aurantii fructus immaturus
132	isosakuranin	+	2.81E+08	11.33	C22H24O10	449.1442	449.1437	-1.21	Aurantii fructus immaturus
133	4',6-dihydroxy-4-methoxyisoaurone	+	1.03E+06	11.35	C16H12O5	285.0758	285.0747	-3.77	Trichosanthis fructus
134	ehletianol C	-	3.65E+05	11.57	C30H36O10	555.2236	555.2241	0.99	Trichosanthis fructus
135	4-allyl-2-(2'-methylbenzofuran-5'-yl) phenol	+	1.65E+06	11.77	C18H16O2	265.1223	265.1223	-0.1	Magnoliae officinalis cortex
136	lirinidine	+	6.15E+06	11.77	C18H19NO2	282.1489	282.1488	-0.31	Magnoliae officinalis cortex
137	roemerine	+	4.12E+06	11.77	C18H17NO2	280.1332	280.1332	-0.11	Magnoliae officinalis cortex

138	(7aS)-7-Methyl-6, 7, 7a, 8-tetrahydro-5H- [1, 3] benzo dioxolo [6, 5, 4-de] benzo [g] quinoline	+	4.12E+06	11.77	C18H17NO2	280.1332	280.1332	-0.11	Magnoliae officinalis cortex
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Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
139	chinenoside V	+	6.16E+05	11.87	C45H72O19	917.4741	917.4709	-3.46	Allii macrostemonis bulbus
140	apigenin	+	4.30E+05	12.05	C15H10O5	271.0601	271.0589	-4.54	Trichosanthis fructus/Aurantii fructus immaturus
141	rhoifolin	-	1.88E+07	12.07	C27H30O14	577.1563	577.1568	0.9	Aurantii fructus immaturus
142	quercetin	+	1.15E+05	12.18	C15H10O7	303.0499	303.0501	0.49	Trichosanthis fructus
143	anonaine	+	2.94E+07	12.21	C17H15NO2	266.1176	266.1174	-0.6	Magnoliae officinalis cortex
144	sinapaldehyde-4-O- β -D-glucopyranoside	-	1.99E+06	12.25	C17H22O9	369.1191	369.1194	0.74	Magnoliae officinalis cortex
145	cadinol	+	7.02E+05	12.31	C20H20O6	357.1333	357.1332	-0.14	Magnoliae officinalis cortex
146	isorhamnetin-3-O- β -D-glucoside	-	4.49E+06	12.4	C22H22O12	477.1038	477.104	0.32	Magnoliae officinalis cortex
147	meranzin	+	3.85E+07	12.47	C15H16O4	261.1121	261.1118	-1.36	Aurantii fructus immaturus

148	cinnamaldehyde	+	8.40E+07	12.59	C9H8O	133.0648	133.0648	0.34	Cinnamomi ramulus
149	bergaptol	-	1.81E+07	12.76	C11H6O4	201.0193	201.0191	-1.2	Aurantii fructus immaturus
150	xanthotoxol	-	1.81E+07	12.76	C11H6O4	201.0193	201.0191	-1.2	Aurantii fructus immaturus
151	poriferast-5-ene-3 β ,4 β -diol	+	9.24E+04	12.9	C35H54O10	635.379	635.3761	-4.52	Trichosanthis fructus
152	7-O-6'' -Malonylnaringin	+	4.91E+05	12.9	C30H33O17	666.179	666.1781	-1.43	Aurantii fructus immaturus
153	poncirin	+	7.46E+07	12.93	C28H34O14	595.2021	595.2017	-0.79	Aurantii fructus immaturus
154	sakuranetin	+	3.34E+07	12.93	C16H14O5	287.0914	287.0909	-1.7	Aurantii fructus immaturus
155	isosakuranetin	+	3.34E+07	12.93	C16H14O5	287.0914	287.0909	-1.7	Aurantii fructus immaturus
156	magnaldehyde C	-	6.81E+05	12.97	C18H18O5	313.1082	313.1087	1.67	Magnoliae officinalis cortex
157	cucurbitacin D	+	1.07E+05	13.06	C30H44O7	517.316	517.3157	-0.47	Trichosanthis fructus
158	limonin	+	2.37E+08	13.31	C26H30O8	471.2013	471.2007	-1.26	Aurantii fructus immaturus
159	magnatriol B	-	3.70E+07	13.34	C15H14O3	241.087	241.087	-0.25	Magnoliae officinalis cortex

Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT	Formula	Expected	Measured	Delta	Source
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				(time)		(m/z)	(m/z)	(m/z)	
160	randaiol	-	3.70E+07	13.34	C15H14O3	241.087	241.087	-0.25	Magnoliae officinalis cortex
161	α -spinasterol-3-O- β -D-glucoside	+	3.38E+07	13.49	C35H58O6	575.4306	575.4329	3.9	Trichosanthis fructus
162	alpha-Spinasterol glucoside	+	3.38E+07	13.49	C35H58O6	575.4306	575.4329	3.9	Trichosanthis fructus
163	magnolignan E	-	5.81E+06	13.63	C18H18O4	297.1132	297.1137	1.51	Magnoliae officinalis cortex
164	magnolignan A	-	4.29E+06	13.76	C18H20O4	299.1289	299.1294	1.72	Magnoliae officinalis cortex
165	3-(2-Methoxyphenyl)acrylaldehyde	+	1.66E+08	13.95	C10H10O2	163.0754	163.0752	-1.1	Cinnamomi ramulus
166	benzenepropanal	+	1.58E+07	13.95	C9H10O	135.0804	135.0804	-0.31	Cinnamomi ramulus
167	methoxycinnamaldehyde	+	1.66E+08	13.95	C10H10O2	163.0754	163.0752	-1.1	Cinnamomi ramulus
168	cucurbitacin E	+	6.26E+05	14.18	C32H44O8	557.3109	557.3087	-4.01	Trichosanthis fructus
169	yellow powder	+	3.09E+06	14.21	C17H12N2O4	309.087	309.0869	-0.41	Trichosanthis fructus
170	clovanemagnolol	+	1.24E+06	14.24	C33H42O3	487.3207	487.3222	3.21	Magnoliae officinalis cortex
171	caryolanemagnolol	+	1.24E+06	14.24	C33H42O3	487.3207	487.3222	3.21	Magnoliae officinalis cortex
172	piperitenone	+	5.34E+05	14.31	C10H14O	151.1117	151.1117	0	Magnoliae officinalis cortex

173	opercurins A	-	4.81E+05	14.61	C38H56O13	719.3648	719.3661	1.78	Trichosanthis fructus
174	liriodenine	+	5.41E+06	14.73	C17H9NO3	276.0655	276.0654	-0.55	Magnoliae officinalis cortex
175	oxoushinsunine	+	5.41E+06	14.73	C17H9NO3	276.0655	276.0654	-0.55	Magnoliae officinalis cortex
176	bergapten	+	1.58E+06	14.73	C12H8O4	217.0495	217.0497	0.52	Aurantii fructus immaturus
177	1-acetyl-3-carboxy- β -carboline	+	3.00E+05	14.99	C14H10N2O3	255.0764	255.0763	-0.43	Trichosanthis fructus
178	23, 24-dihydrocucurbitacin D	-	4.15E+05	15	C30H46O7	517.3171	517.3174	0.59	Trichosanthis fructus
179	lunularic acid	-	6.67E+05	15.08	C15H14O4	257.0819	257.0821	0.63	Allii macrostemonis bulbus
180	marmin	+	1.34E+06	15.3	C19H24O5	333.1696	333.1693	-0.92	Aurantii fructus immaturus
181	trimehydroxy-trimethoxy-flavone	+	2.93E+05	15.35	C18H16O8	361.0918	361.0915	-0.83	Aurantii fructus immaturus

Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
182	magnaldehyde D	-	6.71E+06	15.46	C16H14O3	253.087	253.0872	0.73	Magnoliae officinalis cortex
183	magnaldehyde E	-	6.71E+06	15.46	C16H14O3	253.087	253.0872	0.73	Magnoliae officinalis cortex

184	chrysoeriol	-	2.92E+06	15.62	C16H12O6	299.0561	299.0565	1.37	Trichosanthis fructus
185	diosmetin	-	2.92E+06	15.62	C16H12O6	299.0561	299.0565	1.37	Trichosanthis fructus/Aurantii fructus immaturus
186	blumenol A	+	8.81E+06	15.86	C13H20O3	225.1485	225.1484	-0.43	Magnoliae officinalis cortex
187	O-methyleugenol	+	2.91E+06	16.12	C11H14O2	179.1067	179.1067	0.42	Magnoliae officinalis cortex
188	imperatorin	+	1.34E+06	16.22	C16H14O4	271.0965	271.0963	-0.88	Aurantii fructus immaturus
189	blumenol B	+	4.97E+06	16.29	C13H22O3	227.1642	227.1641	-0.47	Magnoliae officinalis cortex
190	magnaldehyde B	-	9.68E+06	16.43	C18H16O3	279.1027	279.1031	1.39	Magnoliae officinalis cortex
191	randainal	-	9.68E+06	16.43	C18H16O3	279.1027	279.1031	1.39	Magnoliae officinalis cortex
192	chinenoside IV	-	2.26E+06	16.58	C50H80O23	1047.5018	1047.4993	-2.38	Allii macrostemonis bulbus
193	linalyl acetate	-	1.01E+07	16.76	C12H20O2	195.139	195.1387	-2.02	Magnoliae officinalis cortex
194	bornyl acetate	-	1.01E+07	16.76	C12H20O2	195.139	195.1387	-2.02	Magnoliae officinalis cortex
195	4'-methoxymagnaldehyde B	-	3.26E+05	17.09	C19H18O3	293.1183	293.1187	1.34	Magnoliae officinalis cortex
196	agarofuran	+	2.13E+06	17.15	C15H24O	221.19	221.19	0.26	Magnoliae officinalis cortex

197	laxogenin	+	1.41E+05	17.15	C27H42O4	431.3156	431.3161	1.11	Allii macrostemonis bulbus
198	nobiletin	+	5.76E+08	17.41	C21H22O8	403.1387	403.1383	-1.08	Aurantii fructus immaturus
199	3', 4', 3, 5, 6, 7, 8-Heptamethoxy-flavone	+	3.77E+08	17.61	C22H24O9	433.1493	433.1488	-1.17	Aurantii fructus immaturus
200	trichosanatin	+	1.14E+05	17.86	C27H28N2O4	445.2122	445.2119	-0.6	Trichosanthis fructus
201	5, 6, 7, 4'-Tetramethoxyflavone	+	8.17E+07	17.89	C19H18O6	343.1176	343.1174	-0.7	Aurantii fructus immaturus
202	isoimperatorin	-	4.49E+06	17.93	C16H14O4	269.0819	269.0824	1.62	Aurantii fructus immaturus

Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
203	paeonol	+	9.97E+06	18.02	C9H10O3	167.0703	167.0703	0.25	Trichosanthis fructus
204	7(Z),10(Z),13(Z)-hexadecatrienoic acid	+	2.89E+05	18.09	C16H26O2	251.2006	251.1995	-4.25	Trichosanthis fructus
205	caryophyllene	+	2.31E+07	18.09	C15H24	205.1951	205.195	-0.21	Magnoliae officinalis cortex
206	tangeretin	+	4.27E+08	18.82	C20H20O7	373.1282	373.1277	-1.16	Aurantii fructus immaturus
207	gitogenin	+	3.56E+05	18.9	C27H44O4	433.3312	433.3305	-1.62	Allii macrostemonis bulbus

208	magnolignan G	-	6.90E+04	19.79	C36H36O8	595.2337	595.2346	1.48	Magnoliae officinalis cortex
209	obovatoI	-	3.34E+07	20.12	C18H18O3	281.1183	281.1186	1.07	Magnoliae officinalis cortex
210	magnolol	-	3.84E+08	20.45	C18H18O2	265.1234	265.1236	0.62	Magnoliae officinalis cortex
211	4'-methoxymagnodialdehyde	+	3.68E+05	20.81	C19H16O4	309.1121	309.1119	-0.65	Magnoliae officinalis cortex
212	geranylacetone	+	7.16E+05	21.29	C13H22O	195.1743	195.1744	0.19	Trichosanthis fructus
213	punicic acid	+	5.30E+06	22.72	C18H30O2	279.2319	279.2317	-0.72	Trichosanthis fructus
214	linolenic acid	+	5.30E+06	22.72	C18H30O2	279.2319	279.2317	-0.72	Allii macrostemonis bulbus
215	auraptene	+	3.31E+05	23.57	C19H22O3	299.1642	299.1637	-1.58	Aurantii fructus immaturus
216	tigogenin	+	2.23E+05	23.65	C27H44O3	417.3363	417.3358	-1.14	Allii macrostemonis bulbus
217	magnoflorine	+	7.05E+04	25.13	C19H24NO3	315.1829	315.1842	4.23	Magnoliae officinalis cortex
218	magnocurarine	+	7.05E+04	25.13	C19H24NO3	315.1829	315.1842	4.23	Magnoliae officinalis cortex
219	tianshic acid	+	3.20E+08	25.75	C18H34O5	331.2479	331.2477	-0.66	Trichosanthis fructus
220	palmitoleic acid	-	7.33E+04	26.65	C16H30O2	253.2173	253.2172	-0.48	Trichosanthis fructus
221	isosalsoline	+	2.09E+07	26.86	C18H32O	265.2526	265.2522	-1.48	Magnoliae officinalis cortex

222	7-Hexadecyn-1-ol	+	8.30E+05	26.93	C16H30O	239.2369	239.2367	-1.15	Trichosanthis fructus
223	linoleic acid	-	9.30E+05	27.05	C18H32O2	279.233	279.2333	1.39	Trichosanthis fructus/Allii macrostemonis bulbus

Continued Table S1: Identification of chemical constituents of TTN by UPLC-UESI-Q Exactive Focus

No.	Compound Name	+/-	Area	RT (time)	Formula	Expected (m/z)	Measured (m/z)	Delta (m/z)	Source
224	piperitylmagnolol	-	1.97E+06	27.43	C28H34O2	401.2486	401.2489	0.83	Magnoliae officinalis cortex
225	bornylmagnolol	-	1.97E+06	27.43	C28H34O2	401.2486	401.2489	0.83	Magnoliae officinalis cortex
226	tembetarine	+	1.29E+06	28.04	C20H26NO4	345.1935	345.1928	-1.88	Magnoliae officinalis cortex
227	palmitic acid	-	8.04E+06	28.05	C16H32O2	255.233	255.2329	-0.04	Trichosanthis fructus/Magnoliae officinalis cortex/Allii macrostemonis bulbus
228	oleic acid	-	1.94E+07	28.05	C18H34O2	281.2486	281.2487	0.53	Trichosanthis fructus/Allii macrostemonis bulbus/Magnoliae officinalis cortex
229	eudesobovatoI A	+	6.33E+04	28.94	C33H44O4	505.3312	505.3311	-0.37	Magnoliae officinalis cortex
230	cis-11-eicosenoic acid	-	3.12E+05	29.33	C20H38O2	309.2799	309.2805	1.8	Trichosanthis fructus