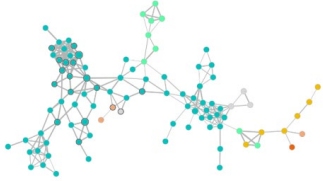
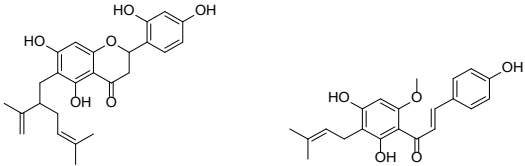
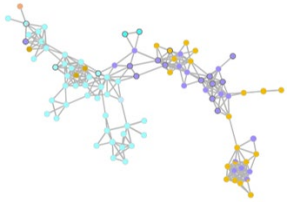
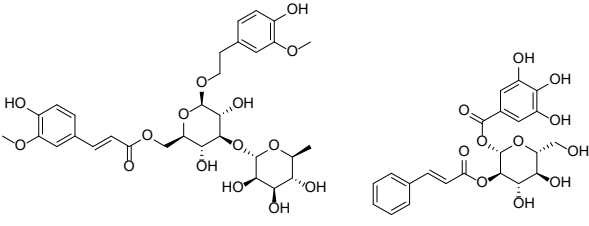

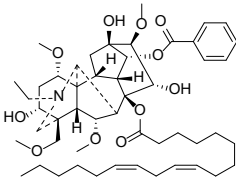
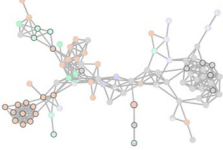


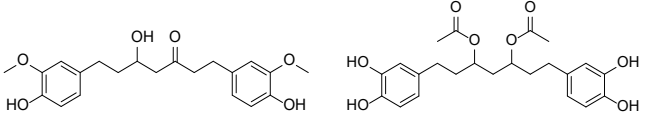
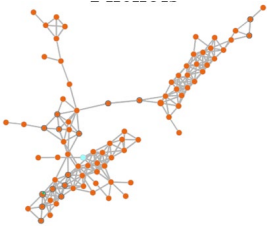
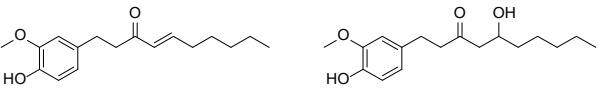
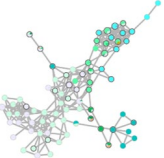
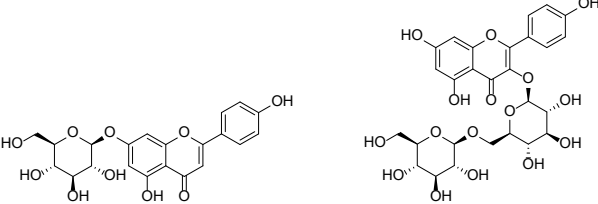
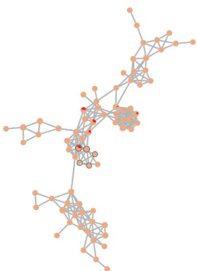
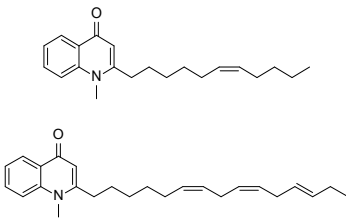

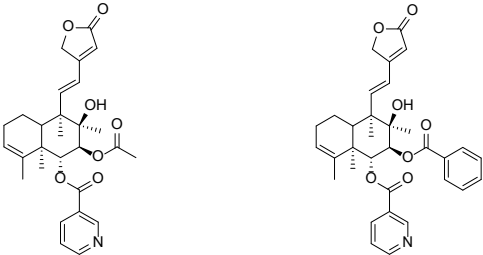
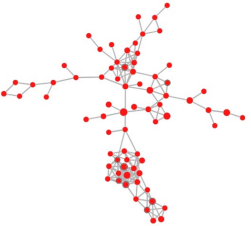
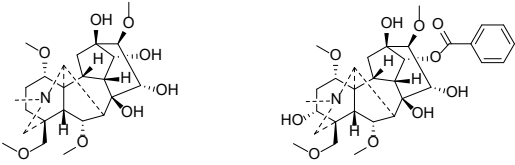

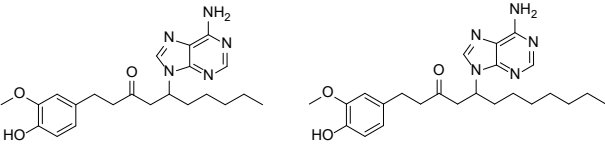
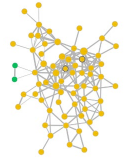
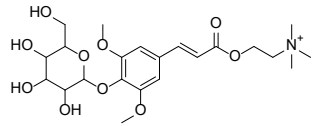
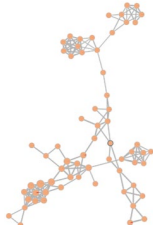
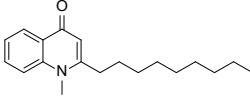
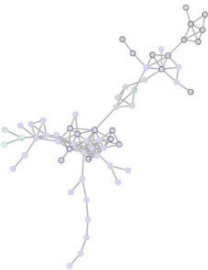
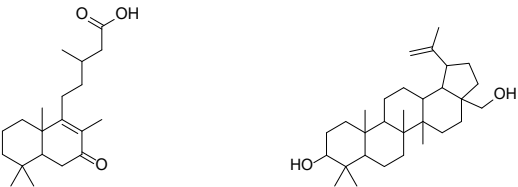

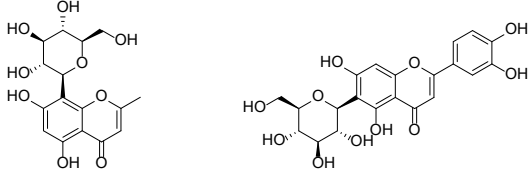

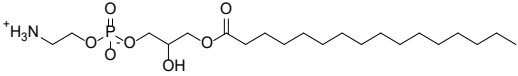



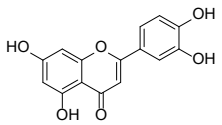
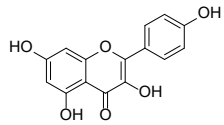
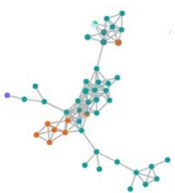
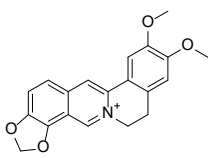
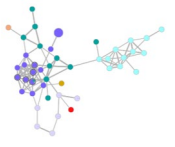
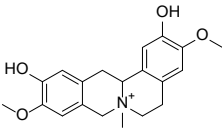
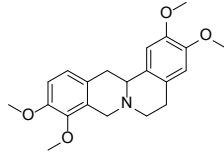
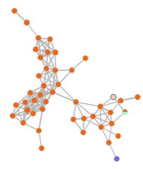
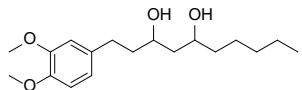
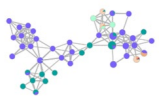
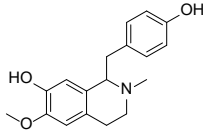
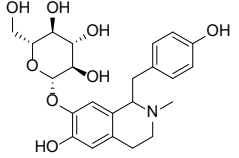
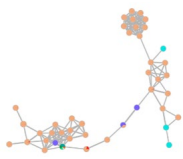
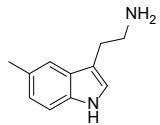
Supporting information

(A) Positive ion data

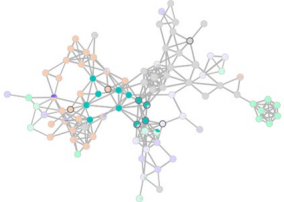
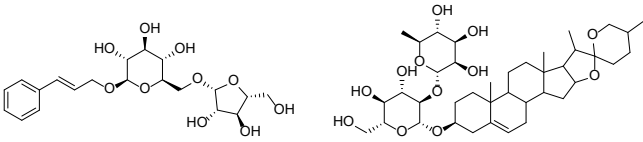
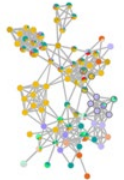
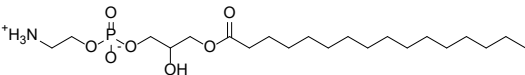

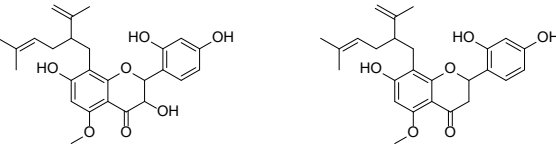
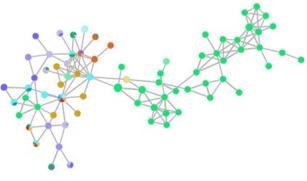
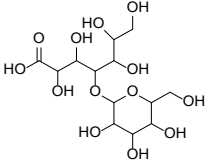
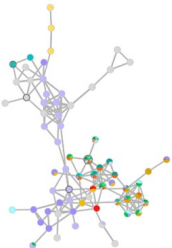
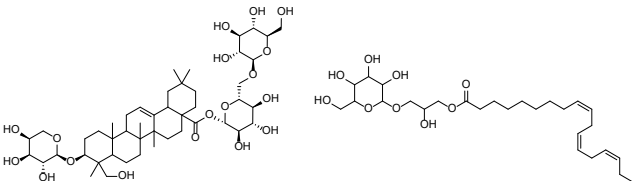
Molecular family	Representative metabolite	Ref. ^a
<p>Flavonoids and chalconoids (1)</p> 	 <p>Kushenol F Xanthohumol</p>	G; T
<p>Phenolic acids derivatives (2)</p> 	 <p>Epimeredinoside A 1-<i>O</i>-Galloyl-2-<i>O</i>-cinnamoylglucose</p>	T
<p>Diterpenoid alkaloids (3)</p> 	 <p>8-<i>O</i>-Linoleoyl-14-<i>O</i>-benzoylaconine</p>	S; Lei et al. (2021) [1]
<p>Benzenoids (4)</p> 	 <p>2-Hydroxycinnamaldehyde 2-Methoxycinnamaldehyde</p>	T
<p>Diarylheptanoids (5)</p> 	 <p>Hexahydrocurcumin 4,4'-(3,5-Diacetoxyheptane-1,7-diyl)bispyrocatechol</p>	G; T

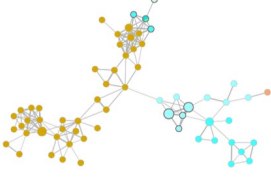
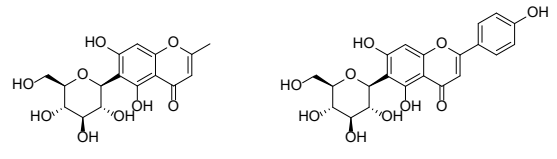
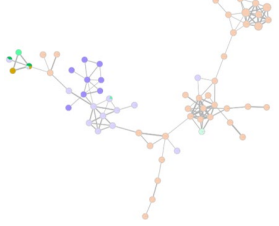
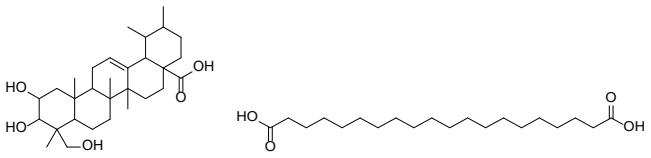
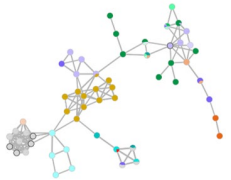
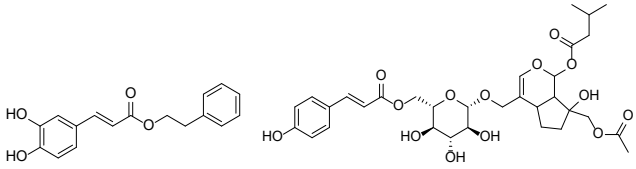
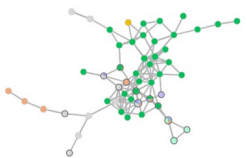
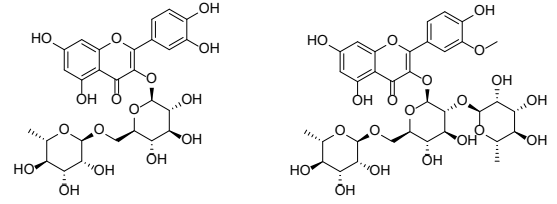
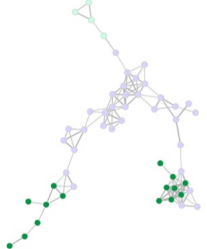
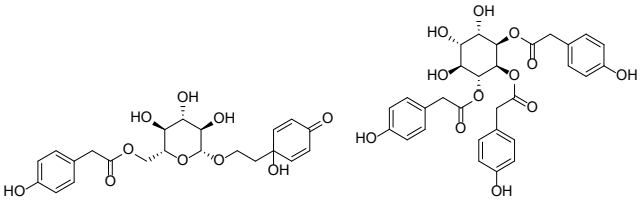
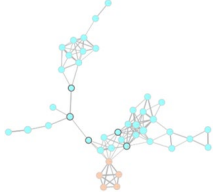
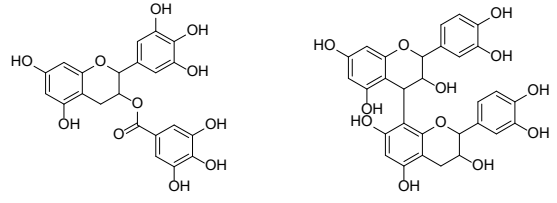
<p>Phenols (6)</p> 	 <p>6-Shogaol 6-Gingerol</p>	<p>T</p>
<p>Flavonoid glycosides (7)</p> 	 <p>Apigetrin Kaempferol-3-gentiobioside</p>	<p>G; T</p>
<p>Quinolones (8)</p> 	 <p>1-Methyl-2-[(Z)-6-undecenyl]-4(1H)-quinolinone 1-Methyl-2-[(6Z,9Z,12E)-6,9,12-pentadecatriene]-4(1H)-quinolinone</p>	<p>G; Ling et al. (2016) [2]</p>
<p>Neo-clerodane diterpenoids (9)</p> 	 <p>Scutebarbatine K Scutebarbatine B</p>	<p>S; Wang et al. (2020) [3]</p>
<p>Diterpenoid alkaloids (10)</p> 	 <p>Hypaconine Benzoylmesaconine</p>	<p>T</p>

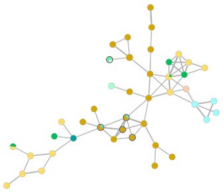
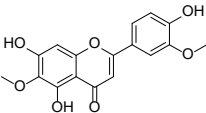
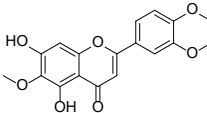
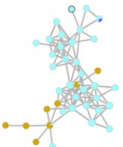
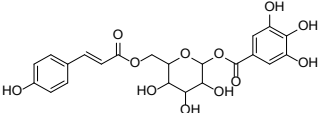
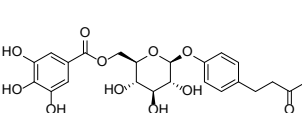
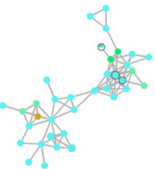
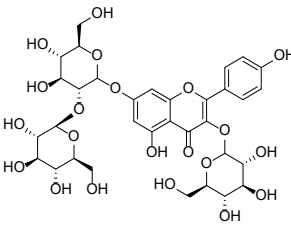
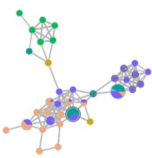
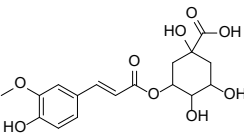
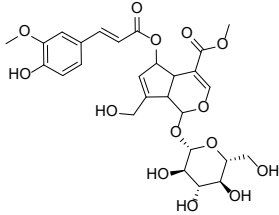
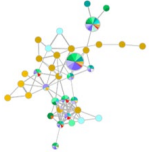
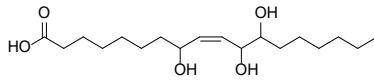
<p>Nucleotide derivatives (11)</p> 	 <p>6-Zingerine 8-Zingerine</p>	<p>S; Araya et al. (2011) [4]</p>
<p>Sinapine derivatives (12)</p> 	 <p>Sinapoylcholine 4-<i>O</i>-hexoside</p>	<p>G</p>
<p>Quinolones (13)</p> 	 <p>1-Methyl-2-nonyl-4(1<i>H</i>)-quinolone</p>	<p>S; Ling et al. (2016) [2]</p>
<p>Terpenoids (14)</p> 	 <p>Agatholic acid isomer Betulinol</p>	<p>G; T</p>
<p>Chromones (15)</p> 	 <p>Biflorin isomer Isoorientin</p>	<p>G; T</p>
<p>Glycerophospholipids (16)</p> 	 <p>1-Palmitoyl-<i>sn</i>-glycero-3-phosphoethanolamine</p>	<p>S</p>

<p>Flavonoids (17)</p> 	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>Luteolin</p> </div> <div style="text-align: center;">  <p>Kaempferol</p> </div> </div>	<p>G; T</p>
<p>Protoberberine alkaloids (18)</p> 	<div style="text-align: center;">  <p>Epiberberine</p> </div>	<p>T</p>
<p>Protoberberine alkaloids (19)</p> 	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>Phellodendrine</p> </div> <div style="text-align: center;">  <p>Tetrahydropalmatine</p> </div> </div>	<p>T</p>
<p>Phenols (20)</p> 	<div style="text-align: center;">  <p>Methyl-6-gingerdiol</p> </div>	<p>S; Asamenew et al. (2019) [5]</p>
<p>Isoquinoline alkaloids (21)</p> 	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p><i>N</i>-Methylcoclaurine</p> </div> <div style="text-align: center;">  <p><i>N</i>-Methylhigenamine-7-glucoopyranoside</p> </div> </div>	<p>S; He et al. (2018) [6]; Sun et al. (2019) [7]</p>
<p>Indole alkaloids (22)</p> 	<div style="text-align: center;">  <p>5-Methyltryptamine</p> </div>	<p>S; Li & Wang (2020) [8]</p>

(B) Negative ion data

Molecular family	Representative metabolite	Ref. ^a
<p data-bbox="292 360 464 389">Glycosides (23)</p> 	 <p data-bbox="584 551 884 580">Cinnamyl alcohol glycoside</p> <p data-bbox="991 551 1163 580">Prosapogenin A</p>	<p data-bbox="1305 479 1358 508">G; T</p>
<p data-bbox="236 678 520 707">Glycerophospholipids (24)</p> 	 <p data-bbox="655 819 1166 848">1-Palmitoyl-<i>sn</i>-glycero-3-phosphoethanolamine</p>	<p data-bbox="1321 775 1342 804">G</p>
<p data-bbox="292 954 464 983">Flavonoids (25)</p> 	 <p data-bbox="687 1167 807 1196">Kushenol I</p> <p data-bbox="1007 1167 1126 1196">Kurarinone</p>	<p data-bbox="1321 1072 1342 1102">T</p>
<p data-bbox="292 1267 464 1296">Glycosides (26)</p> 	 <p data-bbox="719 1469 1102 1498">Hexahydroxyheptanoic acid hexose</p>	<p data-bbox="1321 1373 1342 1402">S</p>
<p data-bbox="292 1559 464 1588">Glycosides (27)</p> 	 <p data-bbox="639 1783 831 1812">Akebia saponin D</p> <p data-bbox="895 1783 1222 1872">9,12,15-Octadecatrienoic acid, 3-(hexopyranosyloxy)-2-hydroxypropyl ester</p>	<p data-bbox="1305 1704 1358 1733">G; T</p>

<p>Chromones (28)</p> 	 <p>Biflorin Isovitexin</p>	<p>G; T; S; El-Saber Batiha et al. (2020) [9]</p>
<p>Lipids and terpenoids (29)</p> 	 <p>Asiatic acid Eicosanedioic acid</p>	<p>S</p>
<p>Phenolic acids derivatives (30)</p> 	 <p>Phenylethyl caffeate Furcatoside A isomer</p>	<p>G; T</p>
<p>Flavonoid glycosides (31)</p> 	 <p>Rutin Typhaneoside</p>	<p>G; T</p>
<p>Phenolic acids derivatives (32)</p> 	 <p>Forsythenside A <i>chiro</i>-Inositol-1,2,3-tris (4-hydroxybenzeneacetate)</p>	<p>S; Wang et al. (2018) [10]; Mo et al. (2017) [11]</p>
<p>Flavonoids (33)</p> 	 <p>Gallocatechin gallate Procyanidin B1</p>	<p>G; T</p>

<p>Flavonoids (34)</p> 	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>Jaccosidin</p> </div> <div style="text-align: center;">  <p>Eupatilin</p> </div> </div>	T
<p>Phenolic acids derivatives (35)</p> 	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>Coumaroyl(-6)Hex-O-galloyl</p> </div> <div style="text-align: center;">  <p>Lindleyin</p> </div> </div>	G; S; Cao et al. (2017) [12]
<p>Flavonoid glycosides (36)</p> 	 <p>Kaempferol-3-glucoside-7-sophoroside</p>	S
<p>Phenolic acids derivatives (37)</p> 	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>3-O-Feruloylquinic acid</p> </div> <div style="text-align: center;">  <p>6-O-Feruloylscandoside methyl ester</p> </div> </div>	G; S; Chen et al. (2016) [13]
<p>Fatty acids (38)</p> 	 <p>8,11,12-Trihydroxy-9Z-octadecenoic acid</p>	S; Sun et al. (2011) [14]

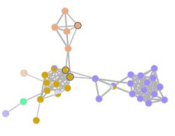
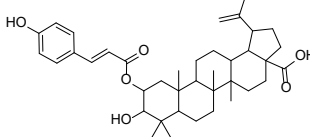
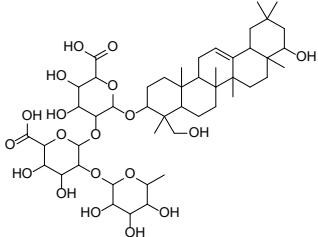

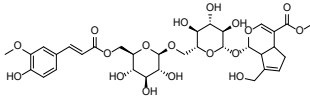
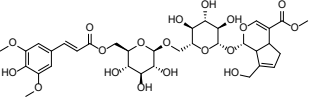
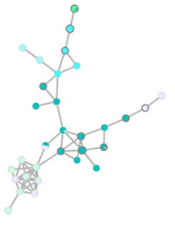
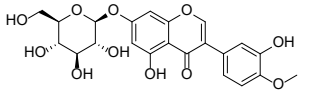
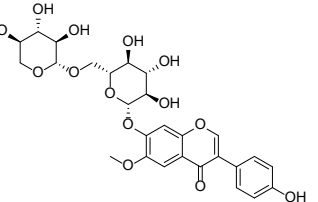
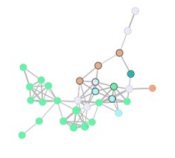
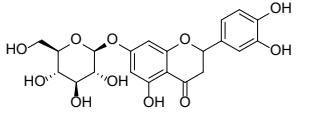
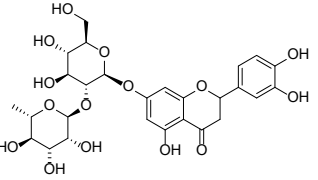
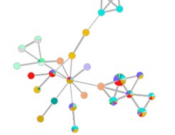
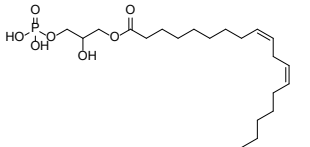
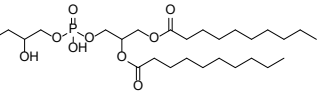
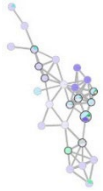
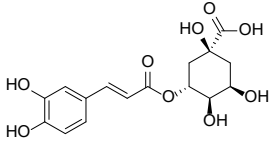

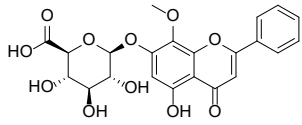
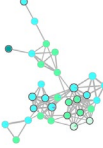
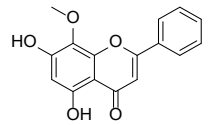

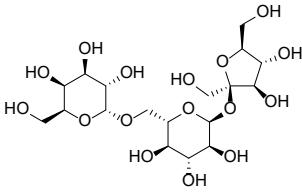

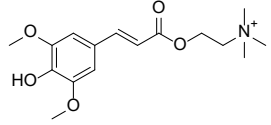

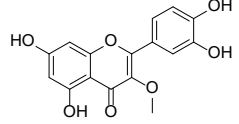

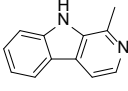
<p>Triterpenoids (39)</p> 	 <p>2-<i>O-E-p</i>-Coumaroyl alphitolic acid</p>	 <p>Soyasapogenol B base + <i>O</i>-HexA-HexA-dHex</p>	<p>G; T; S</p>
<p>Iridoid glycosides (40)</p> 	 <p>6''-<i>O</i>-trans-Feruloylgenipin gentiobioside</p>	 <p>6''-<i>O</i>-trans-Sinapoylgenipin gentiobioside</p>	<p>G; S; Chen et al. (2020) [15]</p>
<p>Flavonoid glycosides (41)</p> 	 <p>Pratenstein 7-<i>O</i>-glucopyranoside</p>	 <p>6'-<i>O</i>-Xylosyl-glycitin</p>	<p>T</p>
<p>Flavonoid glycosides (42)</p> 	 <p>Eriodictyol-7-<i>O</i>-glucoside</p>	 <p>Neoeriocitrin</p>	<p>G; T</p>
<p>Glycerophospholipids (43)</p> 	 <p>1-Linoleylglycerol 3-phosphate</p>	 <p>1,2-Didecanoyl-<i>sn</i>-glycerol- 3-phospho-(1'-<i>sn</i>-glycerol)</p>	<p>S</p>

Fig. S1. Representative metabolites of the major molecular families in the molecular networks of 50% EtOH extracts of the 24 selected TCMs. (A) Positive ion data and (B) negative ion data. ^a G: Public spectral libraries on the GNPS website; T: TCM PCDL; S: Predicted by SIRIUS software.

(A) Positive ion data

Molecular family	Representative metabolite	Ref. ^a
Phenolic acids derivatives (44) 	 Chlorogenic acid	G; T
Flavonoid glycosides (45) 	 Oroxindin	G
Flavonoids (46) 	 Wogonin	G; T
Carbohydrates (47) 	 Raffinose	T
Sinapine derivatives (48) 	 Sinapine	G; T
Flavonoids (49) 	 3-O-Methylquercetin	G
Beta-carboline alkaloids (50) 	 Harman	G

(B) Negative ion data

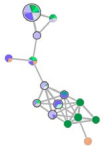
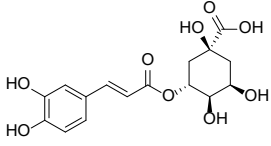
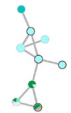
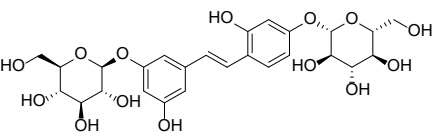
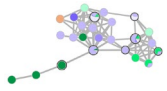
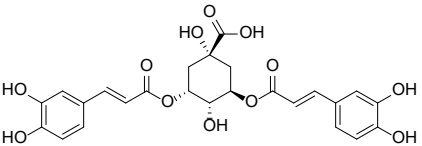

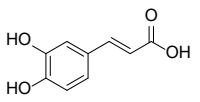
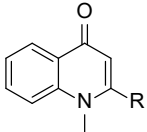
Molecular family	Representative metabolite	Ref. ^a
Phenolic acids derivatives (51) 	 Chlorogenic acid	G; T
Stilbenes (52) 	 Mulberroside A	T
Phenolic acids derivatives (53) 	 Isochlorogenic acid A	T
Phenolic acids (54) 	 Caffeic acid	G; T

Fig. S2. Other smaller representative cold-property and hot-property TCM molecular families in the molecular networks of 50% EtOH extracts of the 24 selected TCMs. (A) Positive ion data and (B) negative ion data. ^a G: Public spectral libraries on the GNPS website; T: TCM PCDL.

Table S1. The accession numbers of the LC-MS/MS data of 50% EtOH extracts of the 24 selected TCMs on the MassIVE website (<https://massive.ucsd.edu>).

TCM	Accession number on the MassIVE website	
	Positive ion data	Negative ion data
BHSSC	MSV000089363	MSV000089364
BLG	MSV000089367	MSV000089368
BZL	MSV000089365	MSV000089366
CXL	MSV000089369	MSV000089370
DH	MSV000089373	MSV000089374
HB	MSV000089371	MSV000089372
HQ	MSV000089375	MSV000089376
HL	MSV000089377	MSV000089378
JYH	MSV000089379	MSV000089380
KS	MSV000089381	MSV000089382
PGY	MSV000089383	MSV000089384
ZZ	MSV000089386	MSV000089387
BYC	MSV000089388	MSV000089389
JH	MSV000089390	MSV000089391
LQ	MSV000089392	MSV000089393
YXC	MSV000089394	MSV000089395
GJ	MSV000089396	MSV000089397
PFZ	MSV000089398	MSV000089399
RG	MSV000089400	MSV000089401
ZWZY	MSV000089402	MSV000089403
BJZ	MSV000089404	MSV000089405
DX	MSV000089406	MSV000089407
BJT	MSV000089408	MSV000089409
BJC	MSV000089410	MSV000089411

Table S2. Summary of the identified metabolites in the major representative hot-property TCM molecular families.

No.	RT (min)	Name	Formula	Calculated <i>m/z</i>	Observed <i>m/z</i>	Error (ppm)	Adduct	Fragment ions (relative abundance in %) ^a	TCM source	Ref. ^b
Positive ion data										
Quinolones										
										
1	8.95 9.07 9.18 11.62 11.77 11.86	R = 13 C + 2 double bonds	C ₂₃ H ₃₁ NO	338.2478	338.2478 338.2476 338.2477 338.2478 338.2489 338.2483	0.00 -0.59 -0.30 0.00 3.25 1.48	[M+H] ⁺	338.2479 (11), 200.1068 (12), 187.0990 (7), 186.0913 (100), 173.0833 (58), 159.0673 (6)	PFZ, ZWZY	Ling et al. (2016) [2]
2	9.73 10.19 12.15 12.28 12.35	R = 15 C + 3 double bonds	C ₂₅ H ₃₃ NO	364.2635	364.2625 364.2631 364.2641 364.2639 364.2626	-2.75 -1.10 1.65 1.10 -2.47	[M+H] ⁺	364.2632 (5), 200.1066 (9), 187.0989 (11), 186.0913 (100), 173.0833 (55), 159.0676 (6)	DX, HB, PFZ, ZWZY	G; Ling et al. (2016) [2]
3	9.82 11.07 11.23 11.54 14.24	R = 11 C + 1 double bond	C ₂₁ H ₂₉ NO	312.2322	312.2309 312.2323 312.2325 312.2316 312.2312	-4.16 0.32 0.96 -1.92 -3.20	[M+H] ⁺	312.2317 (10), 200.1063 (6), 187.0985 (9), 186.0911 (100), 173.0832 (52), 159.0672 (9)	BLG, DX, PFZ, RG, ZWZY	G; Ling et al. (2016) [2]
4	11.77 11.97	R = 12 C + 1 double bond	C ₂₂ H ₃₁ NO	326.2478	326.2474 326.2474	-1.23 -1.23	[M+H] ⁺	326.2465 (16), 200.1059 (10), 187.0983 (6), 186.0908 (100), 173.0830 (53), 159.0670 (5)	ZWZY	Wang et al. (2013) [16]

Other alkaloids

5	3.34 3.65 4.13 5.38	Sinapine and isomers	C ₁₆ H ₂₄ NO ₅	310.1649	310.1649 310.1662 310.1660 310.1655	0.00 4.19 3.55 1.93	[M] ⁺	251.0908 (13), 207.0649 (22), 179.0696 (9), 175.0391 (83), 164.0463 (11), 163.0383 (7), 147.0442 (83), 129.0329 (18), 119.0491 (100), 118.0409 (6)	BJZ, GJ, ZWZY	G; T
6	3.51	Norharman	C ₁₁ H ₈ N ₂	169.0760	169.0760	0.00	[M+H] ⁺	169.0753 (12), 168.0672 (13), 141.0565 (5), 140.0487 (5), 115.0542 (100)	BJT, CXL, HL, ZWZY	G
7	3.89	Harman	C ₁₂ H ₁₀ N ₂	183.0917	183.0917	0.00	[M+H] ⁺	183.0910 (9), 182.0834 (6), 181.0744 (6), 168.0676 (10), 142.0655 (5), 141.0560 (6), 116.0491 (6), 115.0537 (100)	GJ	G

^a The mass spectrum with the highest library match score or signal intensity was selected to represent the fragment ions if more than one molecule was identified as the same metabolite (potential structural isomer).

^b G: Public spectral libraries on the GNPS website; T: TCM PCDL.

RT: Retention time.

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