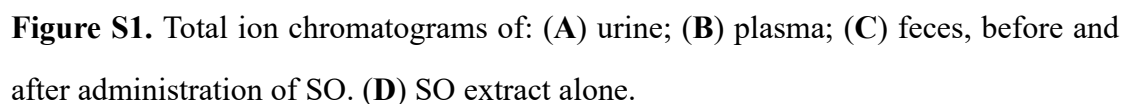
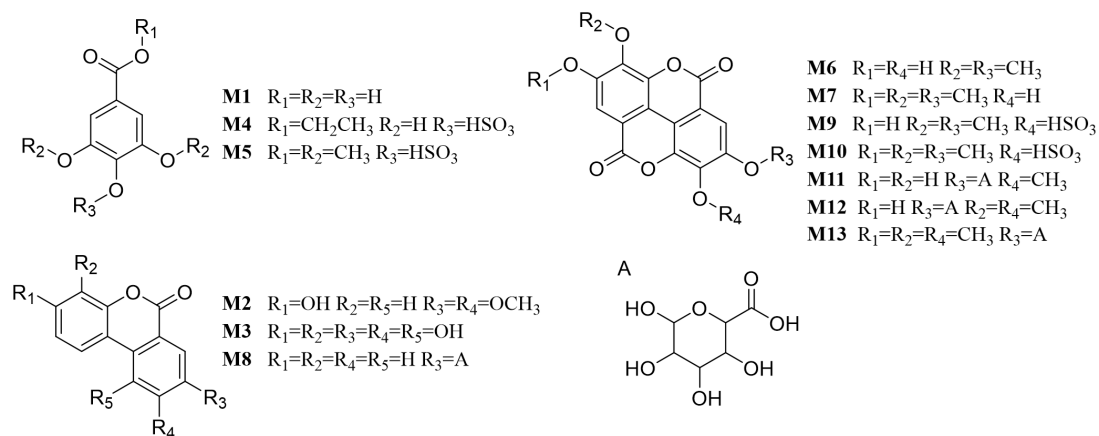
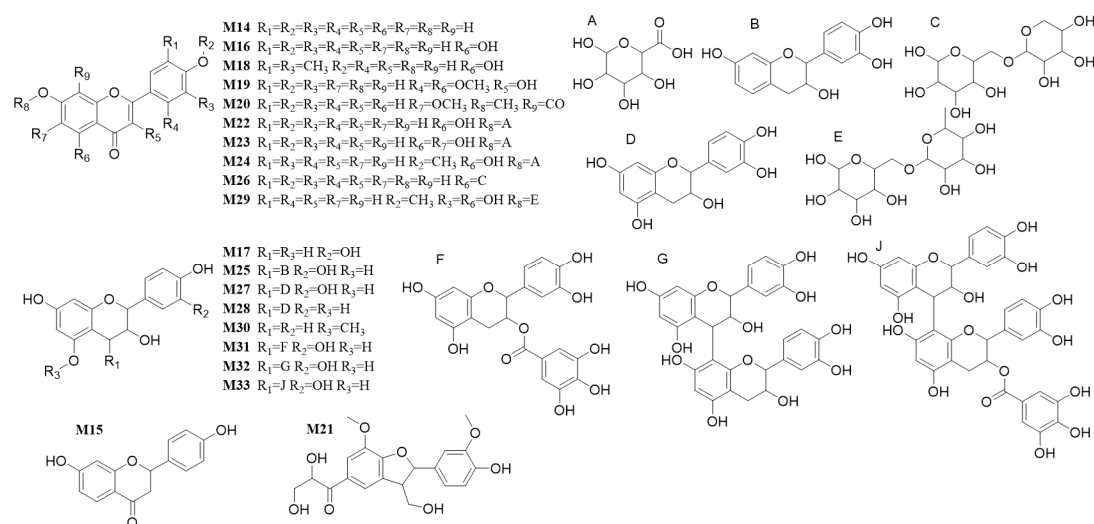


# Rapid Profiling of Metabolites Combined with Network Pharmacology to Explore the Potential Mechanism of *Sanguisorba officinalis* L. against Thrombocytopenia

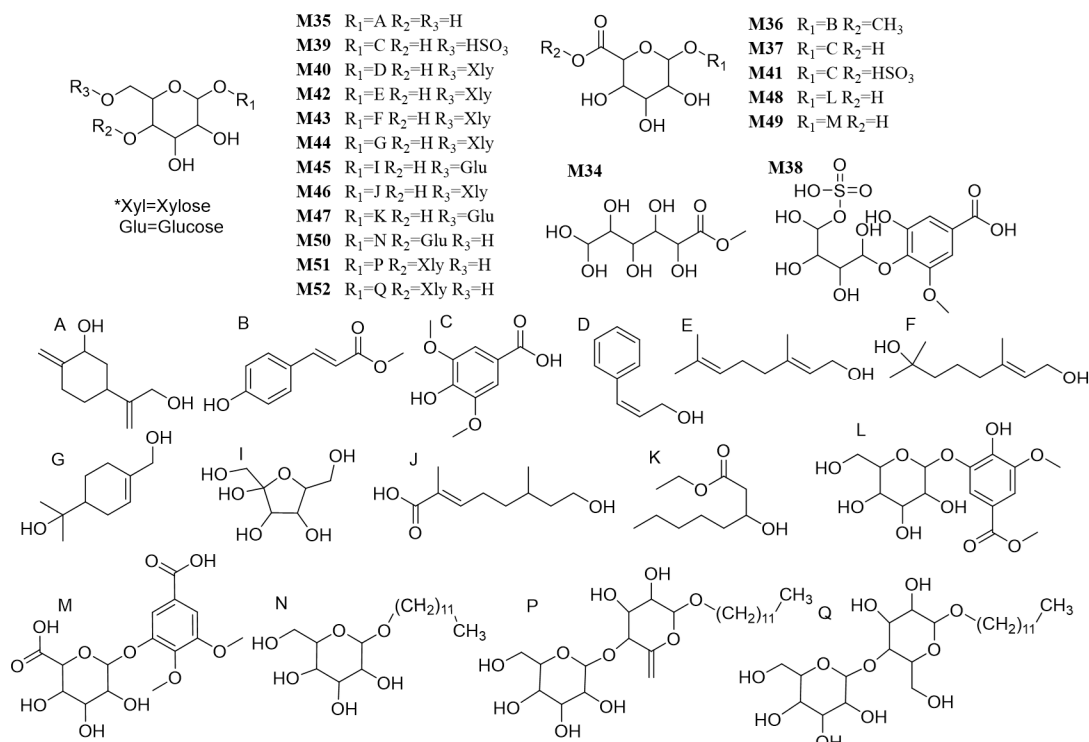




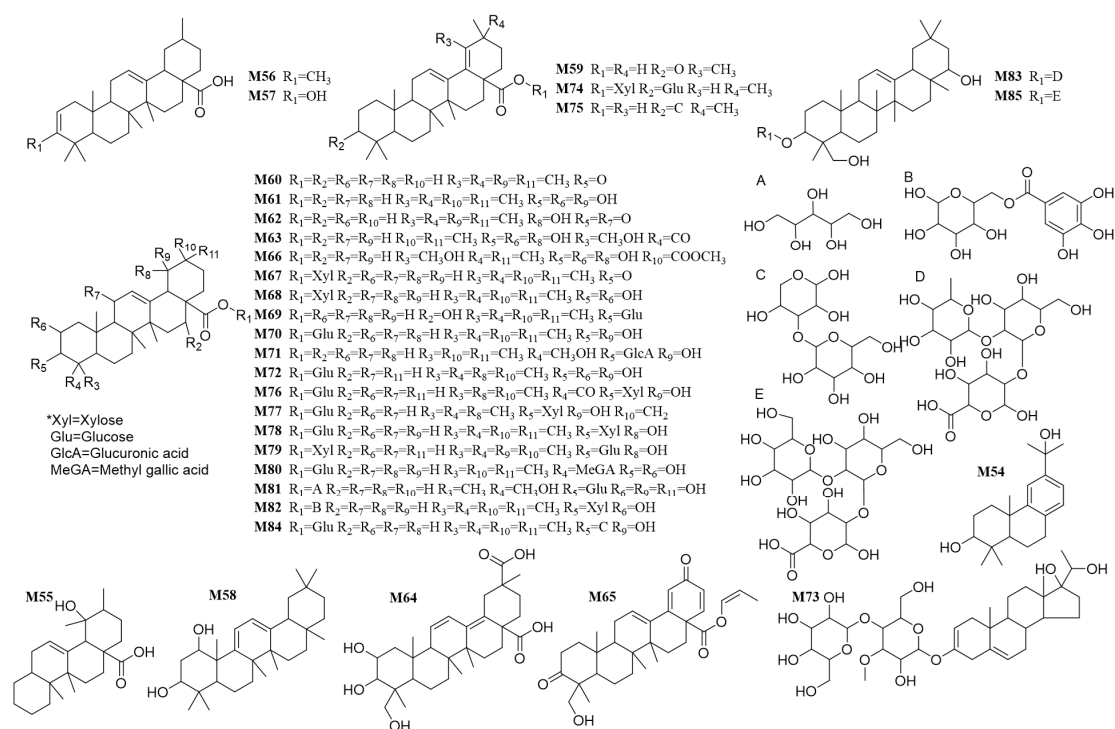
**Figure S2.** Metabolites of ellagic acids (EAs) in vivo.



**Figure S3.** Metabolites of flavonoids in vivo.



**Figure S4.** Metabolites of glycosides in vivo.



**Figure S5.** Metabolites of saponins in vivo.

**Table S1.** Structures of the tentatively characterized compounds in *Sanguisorba officinalis* L.

Metabolites	Class	Ion type	Molecular Formula	Molecular ion	Retention Time (min)	ppm	Fragments	References
<b>M1</b>	EA	[M–H] <sup>–</sup>	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub>	169.0143	2.555	3.5	125.0245, 107.0136, 97.0295, 79.0188	[1]
<b>M2</b>	EA	[M–H] <sup>–</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>	271.0618	9.940	4.2	243.0564, 227.0609, 109.0653	[2]
<b>M3</b>	EA	[M–H] <sup>–</sup>	C <sub>13</sub> H <sub>8</sub> O <sub>7</sub>	275.0201	1.532	3.3	195.0663, 165.0559, 151.0769	[3]
<b>M4*</b>	EA	[M–H] <sup>–</sup>	C <sub>9</sub> H <sub>10</sub> O <sub>8</sub> S	277.0022	7.146	1.4	197.0457, 182.0226, 166.9989	–
<b>M5</b>	EA	[M–H] <sup>–</sup>	C <sub>10</sub> H <sub>12</sub> O <sub>8</sub> S	291.0185	9.400	3.5	211.0606, 181.0137, 153.0191	[4]
<b>M6</b>	EA	[M–H] <sup>–</sup>	C <sub>16</sub> H <sub>10</sub> O <sub>8</sub>	329.0307, 331.0450	11.422	2.9	315.0104, 298.9837, 285.0048	[5]
<b>M7</b>	EA	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>12</sub> O <sub>8</sub>	345.0602	16.093	–2.4	330.0369, 313.0346, 285.0395	[6]

<b>M8</b>	EA	[M–H] <sup>–</sup>	C <sub>19</sub> H <sub>16</sub> O <sub>9</sub>	387.0711	11.851	–1.3	211.0614, 181.0145, 175.0252, 153.0194	[2]
<b>M9*</b>	EA	[M–H] <sup>–</sup>	C <sub>16</sub> H <sub>10</sub> O <sub>11</sub> S	408.9878	16.918	3.0	329.0305, 314.0069, 298.9836, 270.9888	–
<b>M10*</b>	EA	[M–H] <sup>–</sup>	C <sub>17</sub> H <sub>12</sub> O <sub>11</sub> S	423.0024	12.678	0.5	343.0461, 328.0225, 312.9991, 297.9760	–
<b>M11*</b>	EA	[M–H] <sup>–</sup>	C <sub>21</sub> H <sub>16</sub> O <sub>14</sub>	491.0471	9.384	1.8	315.0143, 299.9911, 96.9597	–
<b>M12</b>	EA	[M–H] <sup>–</sup>	C <sub>22</sub> H <sub>18</sub> O <sub>14</sub>	505.0617	9.805	–0.3	329.0294, 314.0056	[7]
<b>M13</b>	EA	[M–H] <sup>–</sup>	C <sub>23</sub> H <sub>20</sub> O <sub>14</sub>	519.0763	11.761	–2.3	343.0454, 328.0218, 312.9984, 297.9747	[8]
<b>M14</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>10</sub> O <sub>4</sub>	255.0651	12.614	–2.5	237.0548, 227.0702, 199.0752, 153.0692, 137.0236	[9]
<b>M15</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	257.0802	12.748	–4.6	239.0686, 163.0376, 137.0223, 95.0481	[10]

<b>M16</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	271.0593	14.919	−4.9	253.0492, 215.0692, 197.0589, 169.0639, 153.0173	[11]
<b>M17</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>	291.0869	6.915	0.1	147.0439, 139.0387, 123.0438, 119.0493	[12]
<b>M18*</b>	Flavonoid s	[M−H] <sup>−</sup>	C <sub>17</sub> H <sub>14</sub> O <sub>7</sub>	329.0664	15.031	0.8	299.0192, 271.0244, 259.1539, 227.0344, 161.0240	–
<b>M19</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>17</sub> H <sub>14</sub> O <sub>7</sub>	331.0814	15.209	−1.1	253.0847, 211.0745	[13]
<b>M20</b>	Flavonoid s	[M+CH <sub>3</sub> OH+H] <sup>+</sup>	C <sub>19</sub> H <sub>16</sub> O <sub>6</sub>	373.1279	11.856	−2.2	313.1087, 271.0968	[14]
<b>M21</b>	Flavonoid s	[M+NH <sub>4</sub> ] <sup>+</sup>	C <sub>20</sub> H <sub>22</sub> O <sub>8</sub>	408.1645	12.136	−3.2	373.1283, 313.1057, 281.0795	[15]
<b>M22</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>21</sub> H <sub>18</sub> O <sub>10</sub>	431.0968	8.772	−2.4	255.0648, 199.0752, 181.0650	[16]
<b>M23</b>	Flavonoid s	[M−H] <sup>−</sup>	C <sub>21</sub> H <sub>18</sub> O <sub>11</sub>	445.0768	10.284	−0.6	269.0455, 175.0249	[17]

<b>M24</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>22</sub> H <sub>20</sub> O <sub>11</sub>	461.1069	8.993	−3.2	285.0756	[18]
<b>M25*</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>26</sub> O <sub>11</sub>	563.1549	8.852	−0.8	435.1078, 423.1078, 411.1065, 393.0963, 283.0597, 165.0547	–
<b>M26</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>26</sub> H <sub>28</sub> O <sub>14</sub>	565.1540	8.706	−3.0	547.1404, 529.1314, 511.1216, 184.1116, 379.0805, 325.0692	[19]
<b>M27</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>30</sub> H <sub>26</sub> O <sub>12</sub>	579.1491	6.792	−1.9	427.1038, 409.0925, 301.0712, 287.0555, 275.0556	[20]
<b>M28</b>	Flavonoid s	[M+Na] <sup>+</sup>	C <sub>30</sub> H <sub>26</sub> O <sub>11</sub>	585.1375	8.423	0.4	433.0889, 415.0787, 303.0729, 277.0304, 153.0186	[21]
<b>M29</b>	Flavonoid s	[M+Na] <sup>+</sup>	C <sub>30</sub> H <sub>26</sub> O <sub>12</sub>	601.1325	6.770	0.5	449.0847, 431.0736, 311.0523, 279.0266	[22]
<b>M30</b>	Flavonoid s	[2M+K] <sup>+</sup>	C <sub>16</sub> H <sub>16</sub> O <sub>5</sub>	615.1634	8.309	0.2	–	[23]
<b>M31</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>37</sub> H <sub>30</sub> O <sub>16</sub>	731.1602	8.423	−1.4	579.1129, 411.1066, 331.0443, 303.0498, 291.0859, 287.0547, 163.0389, 153.0179	[20]

<b>M32</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>45</sub> H <sub>38</sub> O <sub>18</sub>	867.2136	7.049	– 0.05	715.1645, 577.1329, 427.1014, 407.0754, 289.0702, 247.0597, 163.0388	[24]
<b>M33</b>	Flavonoid s	[M+H] <sup>+</sup>	C <sub>52</sub> H <sub>42</sub> O <sub>22</sub>	1019.2249	7.901	0.3	867.1784, 729.1450, 697.1542, 579.1144, 559.1233, 411.1073	[25]
<b>M34</b>	Glycosides	[M–H] <sup>–</sup>	C <sub>7</sub> H <sub>14</sub> O <sub>8</sub>	225.0618	1.058	3.4	113.0239, 101.0245, 89.0243, 71.0139	[26]
<b>M35</b>	Glycosides	[M+NH <sub>4</sub> ] <sup>+</sup>	C <sub>16</sub> H <sub>26</sub> O <sub>7</sub>	348.2020	13.257	–0.7	147.0811, 137.1327, 123.1158, 95.0850	[27]
<b>M36</b>	Glycosides	[M–H] <sup>–</sup>	C <sub>17</sub> H <sub>20</sub> O <sub>9</sub>	367.1047	0.953	4.8	307.0840, 277.0735	[28]
<b>M37</b>	Glycosides	[M–H] <sup>–</sup>	C <sub>15</sub> H <sub>18</sub> O <sub>11</sub>	373.0769	1.312	–0.5	197.0451, 182.0215	[29]
<b>M38*</b>	Glycosides	[M–H] <sup>–</sup>	C <sub>12</sub> H <sub>16</sub> O <sub>13</sub> S	399.0244	3.017	2.7	301.0579, 241.0363, 211.0258, 169.0145	–
<b>M39</b>	Glycosides	[M–H] <sup>–</sup>	C <sub>15</sub> H <sub>20</sub> O <sub>13</sub> S	439.0564	6.784	4.0	359.0992, 241.0028, 197.0453, 182.0219	[30]



<b>M40</b>	Glycosides	$[M+NH_4]^+$	$C_{20}H_{28}O_{10}$	446.2024	9.243	−0.5	241.0705, 117.0698, 115.0541, 91.0543	[31]
<b>M41</b>	Glycosides	$[M-H]^-$	$C_{15}H_{18}O_{14}S$	453.0340	1.201	0.2	373.0778, 277.0022, 197.0453	–
<b>M42</b>	Glycosides	$[M+Na]^+$	$C_{21}H_{36}O_{10}$	466.2642 471.2202	12.269	−0.8	259.0816, 241.0709, 223.0602, 163.0601	[32]
<b>M43</b>	Glycosides	$[M+NH_4]^+$	$C_{21}H_{38}O_{11}$	484.2752 489.2301	8.682	−1.2	295.1027, 259.0818, 241.0711, 163.0601	[33]
<b>M44</b>	Glycosides	$[M+Na]^+$	$C_{21}H_{36}O_{11}$	487.2150	9.460	−1.1	355.1725, 335.0947	[34]
<b>M45</b>	Glycosides	$[M-H]^-$	$C_{18}H_{32}O_{16}$	503.1610	1.047	−1.5	353.1069, 263.0763, 131.0351	[22]
<b>M46*</b>	Glycosides	$[M+Na]^+$	$C_{21}H_{36}O_{12}$	503.2100	8.509	−0.9	335.0957, 317.0845, 229.0684, 209.1153, 185.0425	–
<b>M47</b>	Glycosides	$[M-H]^-$	$C_{22}H_{40}O_{13}$	511.2409	8.547	3.6	333.1929, 311.0991, 293.0882, 211.0672, 179.0565	[35]

<b>M48*</b>	Glycosides	$[M+Na]^+$	$C_{21}H_{28}O_{16}$	559.1268	6.767	−1.3	383.0945, 221.0418, 185.0418	–
<b>M49*</b>	Glycosides	$[M+K]^+$	$C_{21}H_{26}O_{17}$	589.0802	1.275	−0.8	413.0477, 237.0162, 214.9946	–
<b>M50</b>	Glycosides	$[M+H]^+$	$C_{30}H_{56}O_{16}$	673.3621	17.982	−3.8	511.3095, 493.2995	[36]
<b>M51*</b>	Glycosides	$[M+H]^+$	$C_{35}H_{62}O_{19}$	787.3938	17.333	−2.5	671.3464, 625.3409	–
<b>M52*</b>	Glycosides	$[2M+Na]^+$	$C_{15}H_{18}O_{11}$	771.1559	7.957	−4.8	397.0731, 221.0415, 199.0212	–
<b>M53*</b>	Glycosides	$[M+H]^+$	$C_{35}H_{64}O_{20}$	805.4052	14.549	−2.1	689.3567, 643.3521, 493.3004	–
<b>M54</b>	Saponins	$[M+H]^+$	$C_{20}H_{30}O_2$	303.2319	21.010	−1.7	145.1018, 131.0862, 105.0704	[37]
<b>M55*</b>	Saponins	$[M+H]^+$	$C_{23}H_{36}O_3$	361.2731	17.917	−3.2	343.2634, 201.1636, 137.0961	–

<b>M56*</b>	Saponins	$[M+H]^+$	$C_{30}H_{44}O_2$	437.3410	14.784	−2.2	391.3353, 201.1635	–
<b>M57*</b>	Saponins	$[M+H]^+$	$C_{29}H_{44}O_3$	441.3364	16.395	−1.1	423.3244, 351.2704	[38]
<b>M58</b>	Saponins	$[M+H]^+$	$C_{30}H_{48}O_2$	441.3711	21.028	−4.8	423.3610, 405.3508, 369.3138, 247.2049, 203.1785	[39]
<b>M59</b>	Saponins	$[M+H]^+$	$C_{30}H_{44}O_3$	453.3373	14.119	0.9	435.3261, 407.3320, 335.2726, 201.1645	[40]
<b>M60</b>	Saponins	$[M+H]^+$	$C_{30}H_{46}O_3$	455.3528	14.763	−0.6	437.3411, 409.3463, 391.3357, 201.1636	[41]
<b>M61*</b>	Saponins	$[M-H]^-$	$C_{30}H_{48}O_5$	487.3423	19.449	−0.1	373.1829	–
<b>M62</b>	Saponins	$[M+NH_4]^+$	$C_{30}H_{44}O_5$	502.3530	20.878	−0.5	467.3152, 449.3069, 421.3106, 403.2994	[42]
<b>M63</b>	Saponins	$[M-H]^-$	$C_{30}H_{46}O_7$	517.3181	13.307	3.0	473.3279, 455.3195, 407.2962, 365.0313	[43]
<b>M64</b>	Saponins	$[M+NH_4]^+$	$C_{30}H_{44}O_7$	534.3428	18.326	−0.5	487.3044, 471.3112, 435.2853, 409.3093, 365.2845	[44]

<b>M65*</b>	Saponins	$[M+FA-H]^-$	$C_{31}H_{40}O_5$	537.2879	18.305	4.9	501.3200, 491.2321	–
<b>M66*</b>	Saponins	$[M-H]^-$	$C_{31}H_{48}O_8$	547.3293	16.661	4.0	501.3237, 483.3118, 439.3231	–
<b>M67</b>	Saponins	$[M+H]^+$	$C_{35}H_{54}O_7$	587.3943	14.741	–0.8	455.3508, 437.3415, 409.3427	[45]
<b>M68</b>	Saponins	$[M+H]^+$	$C_{35}H_{56}O_8$	605.4055	14.784	0.3	455.3513, 437.3418	[46]
<b>M69</b>	Saponins	$[M+NH_4]^+$	$C_{36}H_{58}O_9$	652.4413	17.982	–1.7	473.3624, 455.3507, 437.3411, 391.3358, 163.1481	[47]
<b>M70</b>	Saponins	$[M+Na]^+$	$C_{36}H_{58}O_9$	657.3965	17.982	–2.1	495.3445, 185.0420	[48]
<b>M71</b>	Saponins	$[M-H]^-$	$C_{36}H_{56}O_{11}$	663.3758	13.392	2.0	617.3656, 487.3443, 175.0243	[49]
<b>M72</b>	Saponins	$[M+NH_4]^+$	$C_{36}H_{58}O_{10}$	668.4364	14.271	–1.4	489.4364, 471.3467, 407.3304	[50]
<b>M73</b>	Saponins	$[M+CH_3OH+H]^+$	$C_{34}H_{54}O_{13}$	703.3901	17.982	–0.5	657.3850, 477.3221, 185.0303	[51]

<b>M74*</b>	Saponins	$[M+NH_4]^+$	$C_{41}H_{64}O_{12}$	766.4732	17.312	−1.2	455.3526, 437.3405, 409.3471	–
<b>M75</b>	Saponins	$[M+Na]^+$	$C_{41}H_{64}O_{12}$	771.4285	17.312	−1.4	609.3758, 565.3870, 185.0424	[52]
<b>M76</b>	Saponins	$[M+H]^+$	$C_{41}H_{64}O_{14}$	781.4371	12.549	0.4	649.3947, 487.3421, 469.3316, 423.3255	[53]
<b>M77</b>	Saponins	$[M+NH_4]^+$	$C_{41}H_{64}O_{13}$	782.4690	15.236	− 0.08	603.3898, 557.3835, 471.3477, 453.3365, 425.3426, 407.3312, 180.0869	[54]
<b>M78</b>	Saponins	$[M+NH_4]^+$	$C_{41}H_{66}O_{13}$	784.4832	14.699	−1.9	455.3509, 437.3410, 409.3459	[55]
<b>M79</b>	Saponins	$[M+Na]^+$	$C_{41}H_{66}O_{13}$	789.4384	14.741	−2.1	627.3859, 185.0422	[56]
<b>M80</b>	Saponins	$[M+Na]^+$	$C_{43}H_{62}O_{14}$	825.4022	14.592	−1.8	641.3898	[57]
<b>M81*</b>	Saponins	$[M+H]^+$	$C_{40}H_{66}O_{18}$	835.4316	14.522	−1.3	789.4263, 627.3727, 537.3434, 477.3229	–

<b>M82</b>	Saponins	$[M+NH_4]^+$	$C_{48}H_{70}O_{17}$	936.4963	15.039	0.7	455.3523, 437.3416, 391.3366, 153.0182	[58]
<b>M83</b>	Saponins	$[M+H]^+$	$C_{48}H_{78}O_{18}$	943.5229	17.539	−3.9	797.4654, 599.3913, 441.3704, 423.3600	[59]
<b>M84</b>	Saponins	$[M+NH_4]^+$	$C_{47}H_{76}O_{18}$	946.5385	14.763	1.0	605.4053, 455.3520, 437.3423, 409.3477, 163.0606	[60]
<b>M85</b>	Saponins	$[M+H]^+$	$C_{48}H_{78}O_{19}$	959.5192	17.208	−2.5	797.4646, 617.4027, 599.3929, 441.3709, 423.3609, 163.0591	[61]
<b>M86</b>	Others	$[M-H]^-$	$C_7H_6O_2$	121.0292	7.980	2.0	93.0335	[62]
<b>M87*</b>	Others	$[M-H]^-$	$C_5H_6O_4$	129.0193	1.123	4.0	111.0088, 87.0089, 85.0296, 67.0191	–
<b>M88*</b>	Others	$[M+H]^+$	$C_{10}H_{16}O$	153.1278	10.001	−0.9	105.0697, 91.0542, 79.0537	–
<b>M89</b>	Others	$[M+NH_4]^+$	$C_6H_8N_2O_2$	158.0923	0.924	−4.1	70.0651	[63]

<b>M90</b>	Others	$[M+H]^+$	$C_{11}H_{14}O$	163.1119	8.750	−2.4	–	[64]
<b>M91</b>	Others	$[M+H]^+$	$C_{10}H_{10}O_3$	179.0704	7.208	−2.3	164.0470, 91.0538, 77.0387	[65]
<b>M92*</b>	Others	$[M+H]^+$	$C_{11}H_{16}O_2$	181.1220	8.750	−4.7	152.0598, 121.1001, 93.0694, 79.0542	–
<b>M93</b>	Others	$[M-H]^-$	$C_{10}H_{10}O_4$	193.0504	9.959	1.6	133.0296	[66]
<b>M94</b>	Others	$[M-H]^-$	$C_{12}H_{18}O_4$	225.1127	8.621	0.07	97.0658, 59.0137	[67]
<b>M95</b>	Others	$[M+H]^+$	$C_{14}H_{12}O_3$	229.0856	20.394	−3.7	151.0387, 105.0337	[68]
<b>M96</b>	Others	$[M+H]^+$	$C_{14}H_{24}O_3$	241.1802	20.851	−0.7	93.0706, 83.0497	[69]
<b>M97</b>	Others	$[M+H]^+$	$C_{15}H_{18}O_6$	295.1172	19.856	−3.3	133.0645, 107.0840, 105.0685	[70]

<b>M98*</b>	Others	$[M+H]^+$	$C_{14}H_{30}O_4S$	295.1930	20.167	−2.6	193.1251, 189.1633, 133.0642, 67.0542	–
<b>M99</b>	Others	$[M+H]^+$	$C_{19}H_{30}O_3$	307.2263	20.649	−3.3	165.1270, 109.0648, 81.0697	[71]
<b>M100*</b>	Others	$[M+H]^+$	$C_{18}H_{34}O_4$	315.2533	20.872	−0.7	185.1178, 139.1121, 121.1017	–
<b>M101*</b>	Others	$[M-H]^-$	$C_{22}H_{36}O_2$	331.2631	20.871	−1.8	287.2723	–
<b>M102</b>	Others	$[M+H]^+$	$C_{20}H_{22}O_8$	391.1389	11.769	−1.0	195.0656, 151.0397, 137.0601	[16]
<b>M103*</b>	Others	$[M+Na]^+$	$C_{28}H_{41}NO_4$	478.2914	20.177	−4.0	337.2717, 306.2776	–
<b>M104</b>	Others	$[M+Na]^+$	$C_{30}H_{45}NO_4$	506.3228	20.918	−3.6	365.3030, 240.0987	[72]

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\*: structures were reported for the first time.



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