

Supporting Information for:

**Deciphering the differentiations of Traditional Chinese Medicine
analogous formulae by parallel liquid chromatography-mass
spectrometry coupled with microplate-based assays**

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Table.S1 Detailed MS data of WLS.

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
10.99	MS[Full ms]1440.93(203), 1367.25(212), 1126.54(216), 962.48(223), 726.07(214), 326.31(513), 287.26(1000)		MS2[287.30@35]: 241.17(1000)		MS3[287.30@35-->241.20@35]: 198.00(207), 196.98(93), 179.87(59), 167.84(98), 151.02(546), 126.32(95), 125.22(1000)		242.0830	C ₁₀ H ₁₄ O ₅ N ₂	2.1
11.10	MS[Full ms]1308.25(214), 1185.58(295), 914.98(261), 650.23(249), 326.30(1000)	MS[Full ms]491.96(107), 329.40(148), 328.35(1000), 317.12(104), 310.48(194), 302.43(124), 297.04(107), 212.92(106), 194.41(130), 167.17(146), 158.21(498), 122.56(237), 110.94(231)	MS2[326.30@35]: 278.15(438), 236.07(1000), 164.27(250)		MS3[326.30@35-->236.10@40]: 164.25(1000), 163.35(19)		327.1245	C ₁₅ H ₂₁ O ₇ N	0.5
18.47	MS[Full ms]787.12(102), 494.42(264), 493.42(1000)	MS[Full ms]981.16(174), 919.18(263), 692.60(156), 534.29(124), 533.35(369), 471.39(140), 468.51(330), 467.43(192), 466.32(1000), 285.43(110), 264.92(144), 251.30(162), 122.43(104)	MS2[493.40@35]: 447.30(1000)		MS3[493.40@35-->447.30@40]: 411.23(38), 285.24(1000), 267.31(24), 249.33(131), 179.06(54), 173.29(68), 160.82(37)		448.2291	C ₂₁ H ₃₆ O ₁₀	0.3

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
20.23	MS[Full ms]1261.04(118), 1165.86(105), 1078.82(117), 1013.82(101), 797.16(107), 762.52(117), 756.85(111), 740.22(129), 699.11(126), 563.09(107), 478.99(236), 350.42(173), 349.42(1000)		MS2[349.45@35]: 350.32(111), 349.33(1000), 320.87(32), 241.32(214)				350.0599	C ₁₃ H ₁₈ O ₆ S	1.5
20.74		MS[Full ms]427.42(194), 293.32(184), 266.33(181), 265.30(1000), 177.24(192), 167.04(137), 122.61(224), 111.07(111)		MS2[265.30@35]: 265.25(105), 248.20(1000), 206.32(119), 177.17(939), 120.22(51), 115.15(59), 114.14(57)		MS3[265.30@35-->206.30@40]: 206.99(122), 206.22(1000), 192.19(92), 191.14(449), 162.89(14), 160.53(22), 159.29(11), 147.08(11), 134.18(20), 107.47(52), 105.09(17)	247.1547	C ₁₄ H ₁₇ O ₃ N	3.5
21.54	MS[Full ms]1479.08(297), 1430.46(257), 1395.16(371), 1291.07(335), 1271.18(273), 1205.13(268), 1172.00(261), 974.85(264), 846.56(266), 845.72(251), 844.94(621), 799.48(263), 137.43(1000)	MS[Full ms]823.10(340), 802.33(318), 801.29(750), 495.52(286), 441.71(263), 427.26(405), 411.41(279), 323.11(281), 297.01(417), 273.85(255), 251.17(329), 166.95(291), 122.48(1000),					800.2455	C ₃₉ H ₄₄ O ₁₈	0.5

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
		110.91(531)							
23.47		MS[Full ms]441.45(335), 424.36(212), 315.56(293), 314.50(1000), 296.98(205), 217.29(311), 208.11(206), 167.02(265), 122.51(508)		MS2[314.50@35]: 315.30(72), 314.29(222), 299.31(125), 272.08(81), 271.13(497), 270.21(161), 269.18(1000), 237.28(97), 175.21(148), 145.20(90), 137.23(59), 107.17(114)		MS3[314.50@35-->269.20@40]: 238.18(82), 237.12(564), 209.13(236), 176.12(66), 175.13(1000), 163.11(58), 145.13(500), 143.02(154), 137.11(361), 107.13(804)	313.1751	C ₁₉ H ₂₃ O ₃ N	4.9
26.21	MS[Full ms]1268.73(478), 1159.81(575), 1112.62(418), 1098.51(570), 1090.34(510), 1049.35(518), 826.92(439), 447.15(1000)		MS2[447.20@35]: 401.20(1000)		MS3[447.20@35-->401.20@40]: 269.13(1000), 161.08(277)		402.1508	C ₁₈ H ₂₆ O ₁₀	-0.4
27.99	MS[Full ms]1230.80(308), 1193.85(349), 1110.71(422), 1036.94(390), 1021.29(347), 1004.02(304), 966.89(326), 545.03(509), 415.39(1000)		MS2[415.40@35]: 415.32(245), 387.32(54), 369.18(72), 270.14(53), 269.17(1000), 268.47(70), 161.10(357)		MS3[415.40@35-->269.20@40]: 161.05(1000), 101.37(55), 89.25(77)		416.1246	C ₁₈ H ₂₄ O ₁₁	0.3

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
28.03		MS[Full ms]903.46(102), 403.43(101), 329.59(186), 328.50(1000), 298.36(107), 297.57(183), 296.87(199), 166.92(128), 122.53(409), 110.94(103)		MS2[328.50@35]: 298.17(185), 297.15(1000), 265.25(202)		MS3[328.50@35-->297.20@40]: 283.17(28), 282.14(194), 266.15(165), 265.16(1000), 255.02(24), 237.22(50)	327.1543	C ₁₉ H ₂₁ O ₄ N	4.2
29.06		MS[Full ms]343.53(246), 342.43(1000), 297.29(171), 167.03(141), 122.54(232)		MS2[342.50@35]: 311.16(155), 299.21(156), 298.21(165), 297.17(1000), 279.25(76), 265.27(237)		MS3[342.50@35-->297.20@40]: 283.09(27), 282.14(192), 266.17(145), 265.14(1000), 255.09(24), 237.21(57)	341.1700	C ₂₀ H ₂₃ O ₄ N	4.4
30.99		MS[Full ms]331.50(268), 330.48(1000), 167.08(214), 122.54(572)		MS2[330.50@35]: 299.12(67), 193.29(96), 192.26(1000)		MS3[330.50@35-->299.10@40]: 270.03(82), 267.11(551), 253.33(65), 249.28(103), 239.19(192), 235.19(274), 207.18(61), 176.17(137), 175.08(1000), 144.27(117), 143.19(544), 137.20(535)	329.1700	C ₁₉ H ₂₃ O ₄ N	4.0

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
31.56	MS[Full ms]1426.73(272), 1301.88(315), 1276.91(257), 1268.42(261), 1253.96(329), 1205.29(345), 1110.59(319), 809.22(255), 803.24(258), 754.38(251), 563.47(1000)	MS[Full ms]566.50(477), 565.44(728), 359.06(446), 297.04(593), 237.39(430), 207.99(545), 167.04(602), 122.49(1000), 110.99(521)	MS2[563.50@35]: 545.29(87), 503.34(64), 485.31(64), 474.30(172), 473.30(648), 444.34(220), 443.36(1000), 383.37(221), 354.43(57), 353.37(336)		MS3[563.50@35-->443.40@40]: 383.29(213), 354.30(185), 353.27(1000)		564.1406	C ₂₆ H ₂₈ O ₁₄	-0.1
34.29	MS[Full ms]1431.93(538), 1344.38(320), 1216.21(432), 1147.30(351), 1060.90(359), 989.61(348), 702.84(349), 627.22(1000), 581.37(327), 475.35(408)	MS[Full ms]667.14(390), 601.27(496), 600.19(1000), 453.70(810), 352.28(521), 167.05(334), 122.52(684), 110.92(361)	MS2[581.40@35]: 566.20(93), 419.30(1000), 405.42(65), 404.31(114), 401.31(109), 233.20(92)		MS3[581.40@35-->419.30@40]: 404.21(1000), 389.30(91), 373.33(237)		582.2240	C ₂₈ H ₃₈ O ₁₃	0.9
35.08	MS[Full ms]1391.58(384), 1326.45(415), 1313.66(428), 1284.16(432), 1177.21(421), 1036.39(358), 912.85(357), 787.65(364), 473.15(509), 431.31(470), 301.45(1000)		MS2[301.50@40]: 302.44(67), 301.39(1000), 283.19(132), 273.00(220), 257.18(116), 255.47(60), 243.59(64), 219.14(53), 181.33(51)		MS3[301.50@40-->273.00@45]: 272.95(1000)		302.1479	C ₁₅ H ₂₆ O ₄ S	2.3

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
38.40		MS[Full ms]505.41(234), 440.49(208), 438.13(366), 292.06(323), 267.21(469), 249.35(1000), 122.43(266)		MS2[249.40@35]: 249.15(71), 232.20(57), 231.19(403), 221.17(436), 219.21(80), 217.07(53), 216.11(62), 204.23(287), 199.20(99), 190.09(84), 189.13(574), 188.11(138), 187.11(1000), 173.09(56), 171.26(74), 161.27(164), 159.19(515), 157.22(84), 131.26(103)		MS3[249.40@35-->187.10@40]: 228.18(19), 173.12(12), 172.10(64), 169.21(13), 159.13(1000), 157.17(11), 141.15(41), 132.12(14), 131.13(195), 128.83(14)	248.1121	C ₁₄ H ₁₆ O ₄	3.1
42.46	MS[Full ms]1126.39(374), 1123.25(354), 1056.56(350), 722.46(355), 644.92(303), 516.26(434), 515.22(1000)		MS2[515.20@35]: 353.10(1000), 335.29(60), 191.33(136)		MS3[515.20@35-->353.10@40]: 191.27(1000), 190.53(12), 179.21(245), 173.16(11), 135.35(40)		516.1195	C ₂₅ H ₂₄ O ₁₂	0.6
47.10	MS[Full ms]1453.63(325), 1344.75(357), 1225.02(314), 1129.34(405), 1118.10(329), 1029.21(341), 936.42(310), 821.28(350), 728.44(335), 446.89(301), 317.48(1000)						318.1428	C ₁₅ H ₂₆ O ₅ S	1.5

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)	
48.04	MS[Full ms]1484.59(514), 1461.09(391), 1060.23(415), 821.39(362), 683.28(440), 553.46(366), 515.08(528), 469.48(1000)	MS[Full ms]963.30(159), 555.44(266), 493.55(153), 472.40(190), 471.41(1000), 296.78(261), 122.57(366)	MS2[469.50@35]: 319.28(1000), 275.36(109)		MS3[469.50@35-->319.30@40]: 304.40(32), 276.36(54), 275.25(1000), 274.14(46), 260.40(20), 192.18(233), 177.36(14), 149.19(828), 148.53(14), 134.25(115)		470.1980	C ₂₅ H ₃₀ O ₇ N ₂	0.6	
53.78	MS[Full ms]1455.58(458), 1445.64(486), 1264.00(456), 1131.70(392), 993.52(365), 920.25(381), 722.90(398), 378.97(1000), 333.35(429)		MS2[333.40@35]: 305.26(371), 262.18(103), 261.16(1000), 203.28(229), 189.32(127)		MS3[333.40@35-->261.20@40]: 244.35(57), 243.26(467), 215.25(19), 203.20(928), 202.45(22), 189.24(1000), 175.23(22)		334.1344	C ₁₈ H ₂₂ O ₆	2.8	
58.48	MS[Full ms]1380.40(261), 1310.76(272), 1301.28(445), 1274.11(268), 1191.97(274), 1189.66(362), 311.44(1000)		MS2[311.40@35]: 312.36(168), 311.37(1000), 293.39(94)		MS3[311.40@35-->293.40@40]: 294.35(77), 293.34(1000), 249.32(30), 230.38(11), 143.16(11)		312.0959	C ₁₅ H ₂₀ O ₅ S	2.0	
66.10	MS[Full ms]1481.33(276), 1409.25(281), 1319.19(266), 1243.45(275), 1078.37(291), 860.51(291), 793.47(318), 663.56(358), 580.15(376), 579.12(1000), 534.60(355),	MS[Full ms]619.42(138), 536.57(235), 535.55(1000), 328.47(319), 296.99(101), 187.38(103), 122.53(260)		MS2[535.60@35]: 517.22(935), 499.34(358), 445.34(1000)		MS3[535.60@35-->445.30@40]: 427.22(695), 409.22(314), 401.20(462), 399.22(876), 385.23(457), 383.14(639), 381.23(281), 355.22(1000), 339.26(387), 337.16(273),		534.3265	C ₃₀ H ₄₆ O ₈	3.1

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
	533.55(816), 375.47(468), 329.52(520)					329.10(416), 321.17(273), 298.23(501), 295.10(270), 285.19(276)			
66.40	MS[Full ms]1423.43(193), 1157.18(154), 847.29(157), 742.94(155), 568.31(188), 567.45(719), 521.51(184), 329.55(1000), 281.37(271)	MS[Full ms]1067.42(326), 700.74(281), 699.61(1000), 429.32(267), 415.35(519), 410.25(549), 246.78(264), 226.21(484), 122.56(500)	MS2[329.60@35]: 330.38(348), 329.40(1000), 311.48(116), 293.49(51), 229.42(307), 211.43(138), 171.41(108)		MS3[329.60@35-->229.40@40]: 229.36(1000), 211.33(524), 210.55(61), 209.35(260), 183.13(75), 167.46(73), 127.24(111), 125.33(195)		330.2333	C ₁₈ H ₃₄ O ₅	2.6
68.01	MS[Full ms]1473.20(328), 1417.78(272), 1382.11(304), 1196.95(276), 1119.76(305), 1064.11(258), 1035.35(260), 905.30(324), 822.66(694), 821.57(1000), 622.14(253), 621.36(602)		MS2[821.60@35]: 803.50(107), 759.61(78), 645.53(98), 627.55(67), 351.22(1000)		MS3[821.60@35-->351.20@40]: 333.15(197), 306.85(66), 289.15(482), 193.14(1000), 175.11(171), 174.24(256), 113.18(358)		822.3965	C ₄₂ H ₆₂ O ₁₆	4.4

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
69.38	MS[Full ms]550.43(339), 549.47(1000), 485.66(220)	MS[Full ms]1094.56(116), 1093.52(208), 776.54(101), 589.41(106), 524.79(120), 506.44(256), 505.41(1000), 313.35(334)		MS2[505.40@35]: 487.26(912), 469.36(384), 451.41(76), 415.38(1000)		MS3[505.40@35-->415.40@40]: 397.19(1000), 379.29(237), 353.22(456), 335.27(122), 247.08(139), 205.08(109), 199.18(101)	504.3524	C ₃₀ H ₄₈ O ₆	4.6
70.03		MS[Full ms]505.35(158), 477.46(155), 311.40(197), 310.41(1000), 208.01(201), 166.97(152), 122.44(491)		MS2[310.40@35]: 212.08(70), 211.09(1000), 133.09(93), 100.21(57)		MS3[310.40@35-->211.10@40]: 183.16(20), 150.97(32), 134.09(11), 133.08(1000), 105.12(21)	309.2165	C ₂₁ H ₂₇ ON	5.3
70.33	MS[Full ms]1432.78(285), 1415.47(203), 1260.32(232), 1211.35(216), 1152.16(214), 976.57(212), 932.90(224), 925.49(229), 821.65(204), 568.54(290), 567.51(1000), 551.54(473), 519.57(244)		MS2[567.50@35]: 521.42(1000), 520.60(59), 463.49(393)		MS3[567.50@35-->521.40@40]: 503.42(75), 463.38(1000), 445.43(170), 419.44(64)		522.3539	C ₃₀ H ₅₀ O ₇	1.5
71.48	MS[Full ms]976.51(116), 975.61(142), 592.52(402), 591.47(1000)	MS[Full ms]1177.46(127), 631.64(195), 556.36(101), 548.78(212), 547.62(464), 530.76(335), 529.65(1000),		MS2[547.50@35]: 529.20(1000), 511.36(184), 487.36(52), 469.31(301), 451.40(77)		MS3[547.50@35-->469.30@40]: 451.28(1000), 433.28(90), 259.32(40), 214.92(22), 212.95(21), 184.82(32),	546.3629	C ₃₂ H ₅₀ O ₇	3.8

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
		431.68(202), 334.54(131), 163.26(205), 122.55(133)				135.10(21)			
72.41	MS[Full ms]1134.56(167), 564.99(311), 549.45(347), 548.50(325), 547.45(1000), 295.38(196)	MS[Full ms]547.40(196), 505.63(203), 504.54(326), 503.50(1000), 487.42(298), 333.64(164), 332.76(365), 313.57(202), 296.83(169), 122.44(435)		MS2[503.50@35]: 485.26(1000), 467.40(145), 445.34(293), 413.34(437)		MS3[503.50@35-->485.30@40]: 467.25(1000), 466.39(30), 449.33(299), 431.38(27), 427.17(24), 413.25(734), 411.26(31), 395.28(96), 353.16(148), 317.17(29), 267.13(21), 199.21(29)	502.3367	C ₃₀ H ₄₆ O ₆	3.7
74.75	MS[Full ms]592.42(372), 591.41(1000), 545.37(142)	MS[Full ms]548.48(127), 547.41(400), 530.63(385), 529.56(1000), 487.47(287), 354.86(123), 334.50(128), 122.51(104)					546.3539	C ₃₂ H ₅₀ O ₇	2.6
77.19	MS[Full ms]1191.33(260), 596.58(350), 595.47(1000)		MS2[595.50@35]: 595.38(84), 415.28(1000), 315.25(340), 279.51(102), 241.34(202)		MS3[595.50@35-->415.30@40]: 352.72(42), 279.46(1000), 153.22(488)		596.2913	C ₃₄ H ₄₄ O ₉	-0.1
77.57		MS[Full ms]488.70(321), 487.62(1000)		MS2[487.60@35]: 469.25(889), 451.35(393), 397.33(1000)		MS3[487.60@35-->397.30@40]: 379.22(79), 353.17(1000), 335.21(147), 227.16(64),	486.3418	C ₃₀ H ₄₆ O ₅	4.5

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
						215.07(55), 203.07(109), 201.02(157), 187.07(67), 174.95(87), 161.10(61), 147.10(71)			
77.74	MS[Full ms]1144.31(189), 1143.26(284), 572.58(231), 571.58(1000)		MS2[571.60@35]: 571.41(131), 392.29(65), 391.29(1000), 315.28(390), 255.55(104), 241.38(211)		MS3[571.60@35-->391.30@40]: 256.64(204), 255.47(1000), 153.24(799)		572.2913	C ₃₂ H ₄₄ O ₉	-1.3
78.48	MS[Full ms]1029.46(254), 981.55(260), 769.53(312), 576.69(582), 575.60(1000), 561.54(286), 551.54(444), 265.40(478)	MS[Full ms]532.69(306), 531.61(1000), 529.63(387), 371.73(306), 315.51(280)		MS2[531.60@35]: 531.39(81), 513.28(71), 512.28(195), 471.26(63), 470.29(510), 469.42(65), 453.38(103), 452.33(1000), 451.38(141), 434.37(106), 416.41(241), 415.42(54), 414.26(81)		MS3[531.60@35-->452.30@40]: 434.31(1000), 433.63(194), 382.31(280)	530.3680	C ₃₂ H ₅₀ O ₆	2.2
79.51	MS[Full ms]961.27(278), 926.35(318), 575.55(490), 573.55(1000), 559.72(274)	MS[Full ms]529.69(465), 469.82(319), 415.72(300), 414.62(1000), 315.63(262)		MS2[529.70@35]: 511.28(311), 469.29(730), 452.34(72), 451.37(1000), 433.41(116), 415.39(242), 413.40(66)		MS3[529.70@35-->451.40@40]: 433.26(1000), 381.29(429), 353.20(161), 227.09(215), 199.15(247)	528.3524	C ₃₂ H ₄₈ O ₆	4.4

RT (min)	MS Neg	MS Pos	MS ² Neg	MS ² Pos	MS ³ Neg	MS ³ Pos	MW (HR-MS)	Formula	Error (ppm)
80.93	MS[Full ms]1033.41(230), 991.59(163), 977.65(185), 976.65(499), 975.69(1000), 923.67(216), 535.63(465)	MS[Full ms]474.63(318), 473.58(1000), 455.57(152)	MS2[535.60@35]: 490.41(176), 489.38(703), 472.46(198), 471.43(1000)		MS3[535.60@35-->471.40@40]: 453.45(18), 435.54(66), 417.45(17), 413.45(70), 411.38(11), 395.40(273), 377.45(69), 353.30(22), 339.43(1000), 338.78(22), 311.64(18)		490.3640	C ₃₀ H ₅₀ O ₅	4.1
81.84		MS[Full ms]516.79(291), 515.73(1000), 452.67(171)		MS2[515.70@35]: 497.21(137), 437.29(340), 419.38(223), 383.23(419), 381.36(73), 365.29(1000), 357.27(144), 339.27(532), 219.19(83), 205.18(74), 201.28(55)		MS3[515.70@35-->365.30@40]: 347.34(310), 337.02(210), 271.29(172), 251.30(184), 225.24(153), 215.24(165), 213.02(203), 159.23(269), 147.20(164), 145.15(1000)	514.3731	C ₃₂ H ₅₀ O ₅	2.9