

Electronic Supplementary Information (ESI)

**Selective and comprehensive characterization of the quinochalcone
C-glycoside homologs in *Carthamus tinctorius* L. by offline
comprehensive two-dimensional liquid
chromatography/LTQ-Orbitrap MS coupled with versatile data
mining strategies**

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Table S1 Detailed information with respect to the 163 quinochalcone C-glycoside compounds characterized from *C. tinctorius* by the offline comprehensive 2D LC and high-resolution LTQ-Orbitrap MS analysis.

Column selection for the first dimensional (¹D) and the second dimensional (²D) separations

RPLC was primarily selected for the ²D separation. Five columns of the RP separation mechanism were tested, comprising BEH C18 (2.1 × 100 mm, 1.7 μm; Waters, Milford, MA, USA), HSS T3 (2.1 × 100 mm, 1.8 μm; Waters), BEH Shield RP-18 (2.1 × 100 mm, 1.7 μm; Waters), Zorbax SB (2.1 × 100 mm, 1.8 μm; Agilent, Waldbronn, Germany), and Zorbax SB-Aq (2.1 × 100 mm, 1.8 μm; Agilent). Afterwards, the columns of versatile separation mechanisms or with different bonding groups were examined to compare the separation difference (orthogonality) compared with the selected ²D column. The candidate columns tested for the ¹D separation included XBridge Amide (4.6 × 150 mm, 3.5 μm; Waters) and Acchrom XAmide (4.6 × 150 mm, 5 μm; Acchrom, Beijing, China) of the HILIC mode, the RP columns bonded with different hydrophobic groups, BEH Phenyl (2.1 × 100 mm, 1.7 μm; Waters), HSS PFP (2.1 × 100 mm, 1.8 μm; Waters), CSH Phenyl-Hexyl (2.1 × 100 mm, 1.7 μm; Waters), and a cyano column Xselect HSS Cyano (2.1 × 100 mm, 1.8 μm; Waters). The separation differentiation amongst different column combinations was evaluated by comparing the linearity aggression correlation coefficient (R^2) of the distribution of fifteen major *C. tinctorius* components.

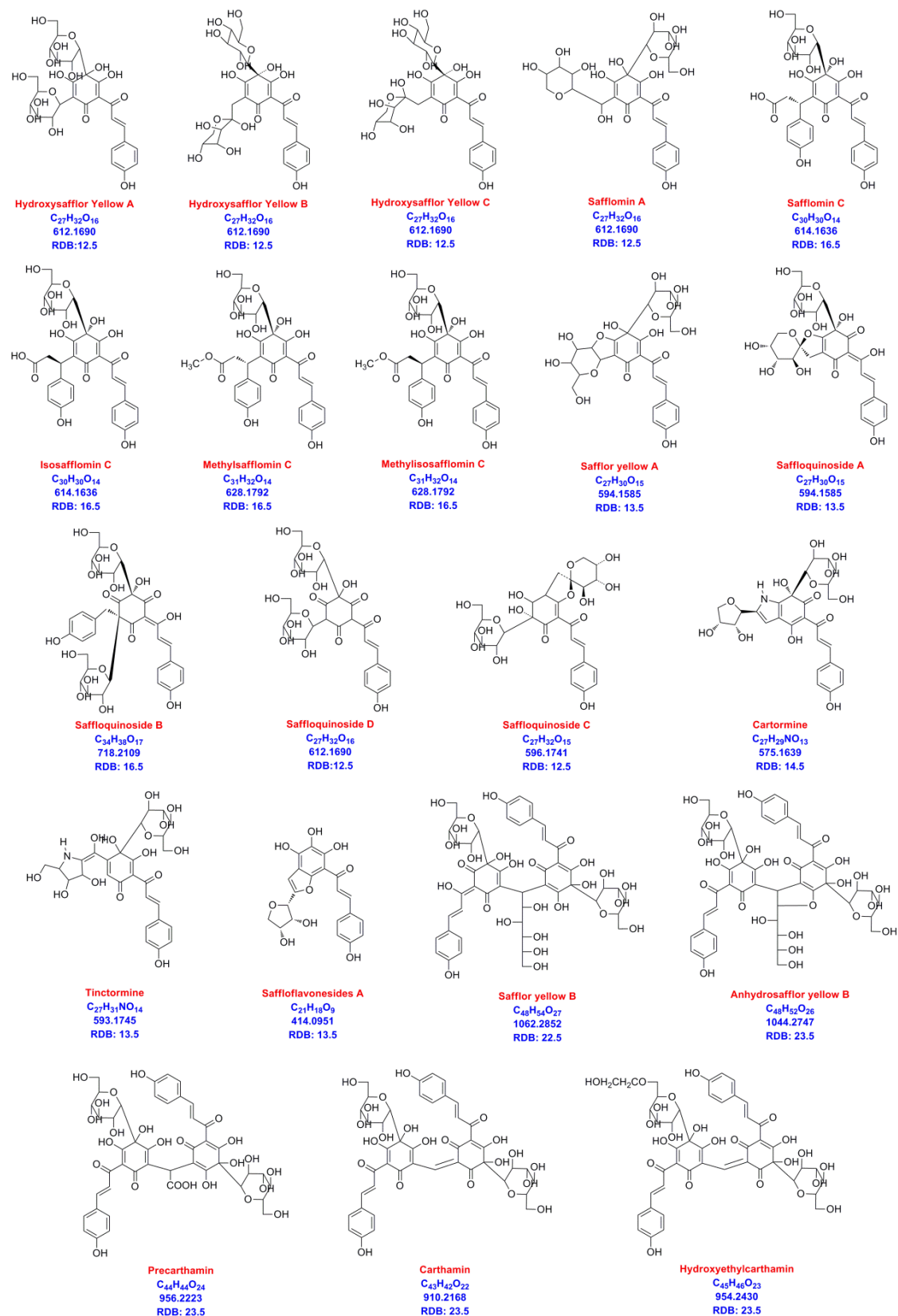


Fig. S1 Structures of 21 known quinochalcone C-glycosides previously isolated from *Carthamus tinctorius* L..

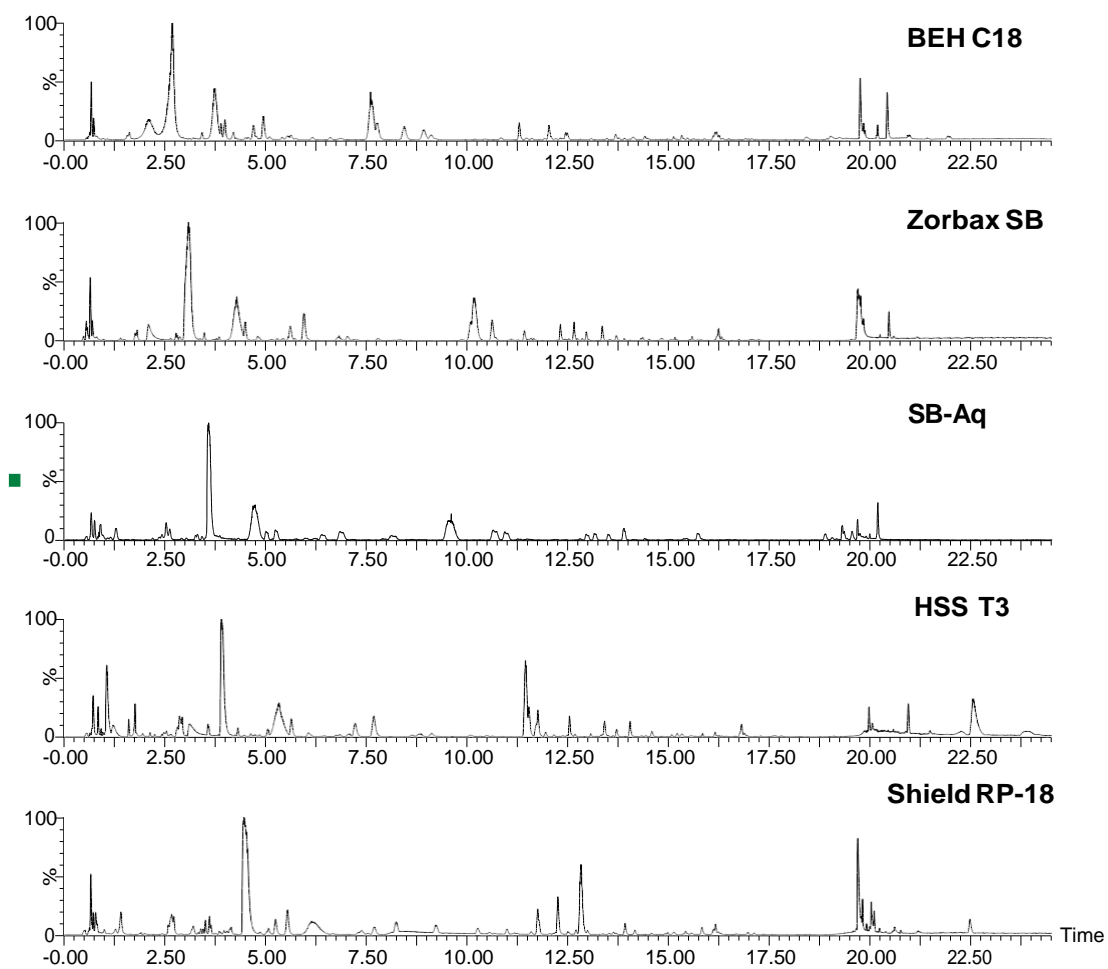


Fig. S2 Comparison of five different RP stationary phases on the selectivity of *C. tinctorius* components. Data were acquired on a Waters UPLC/QTOF instrument.

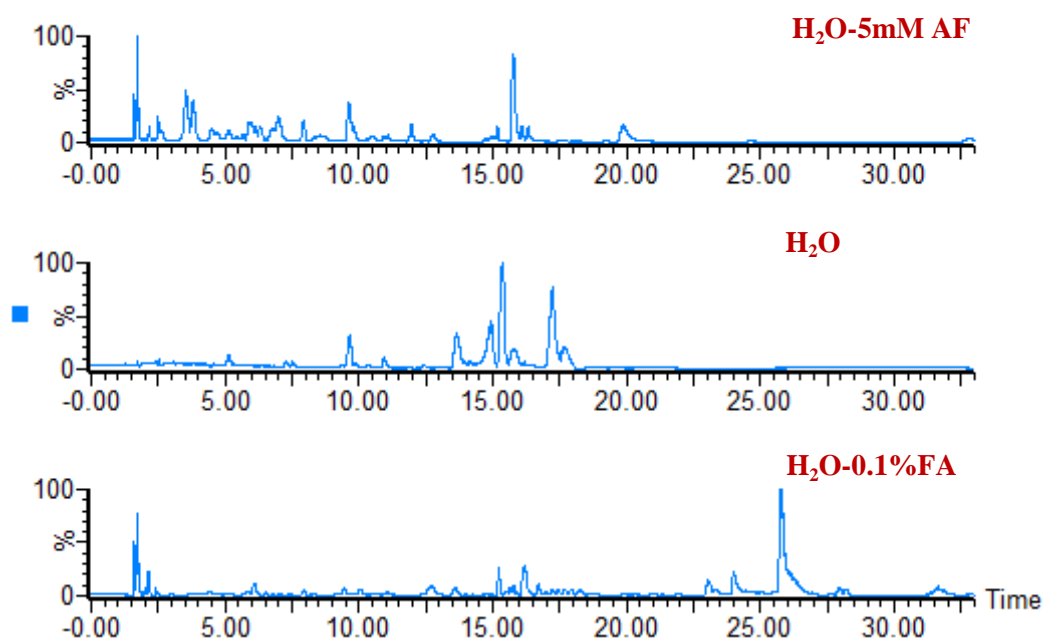


Fig. S3 The ¹D HILIC separation of *C. tinctorius* components using different mobile phases. AF, ammonium formate; FA, formic acid. Data were acquired on a Waters UPLC/QTOF instrument.

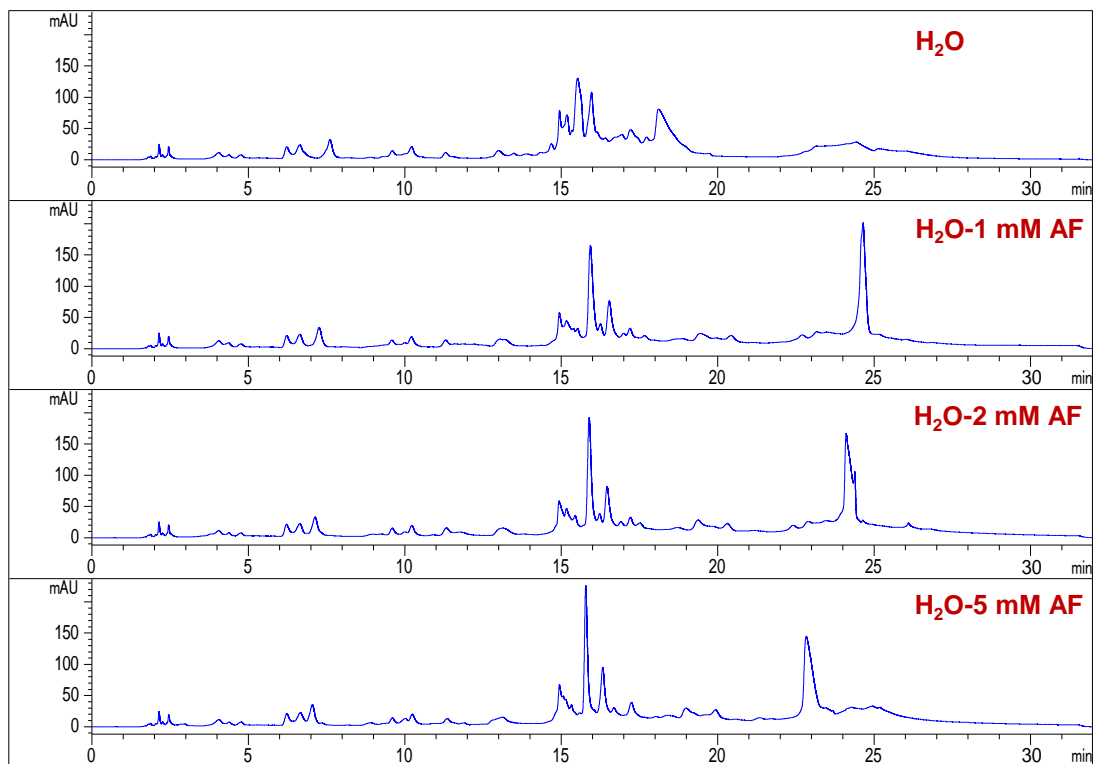


Fig. S4 Comparison of the addition of different concentrations of ammonium formate (AF) in the mobile phase on the separation of *C. tinctorius* components.

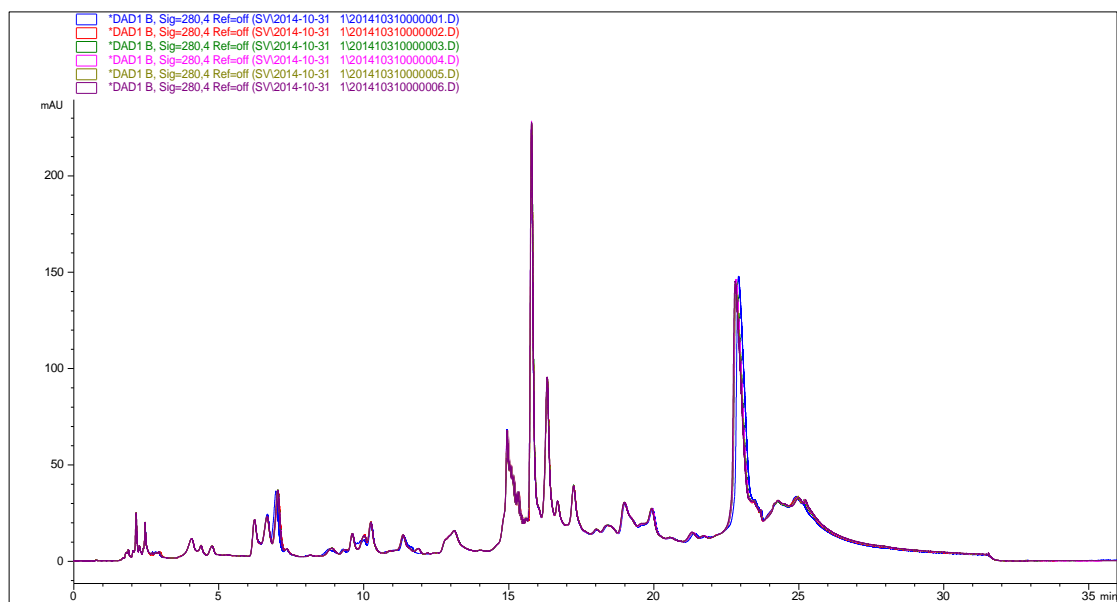


Fig. S5 A precision test of the ¹D HILIC method (n=6).

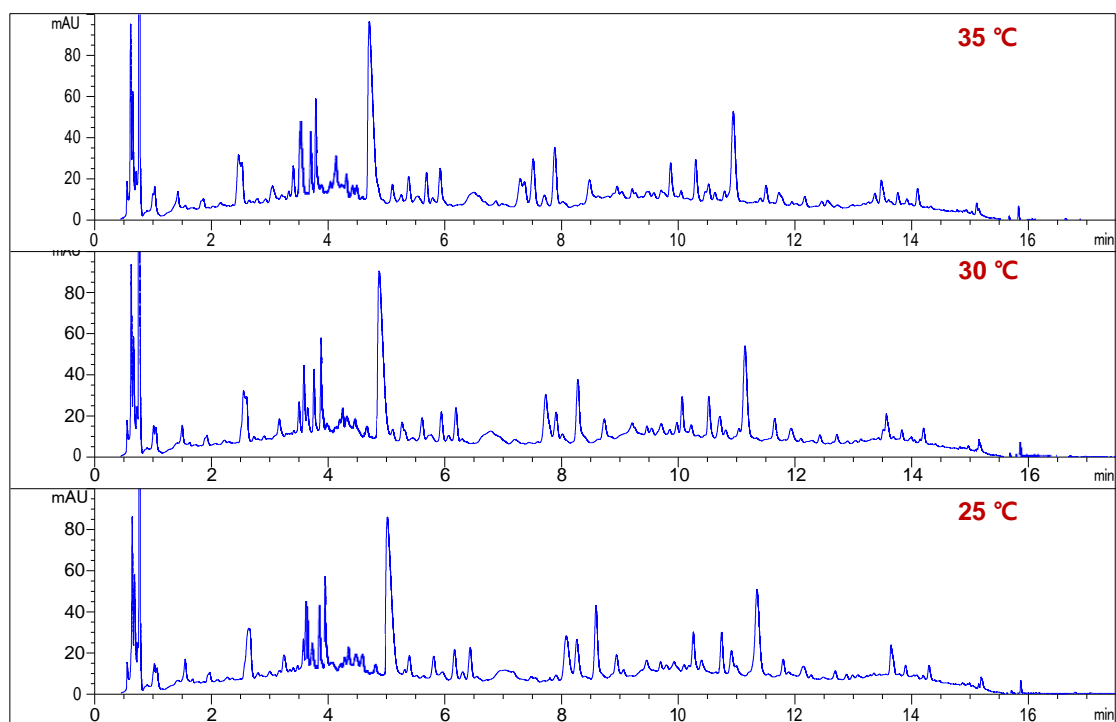


Fig. S6 Comparison of different column temperature on the ^2D separation of *C. tinctorius* components.

HSYA

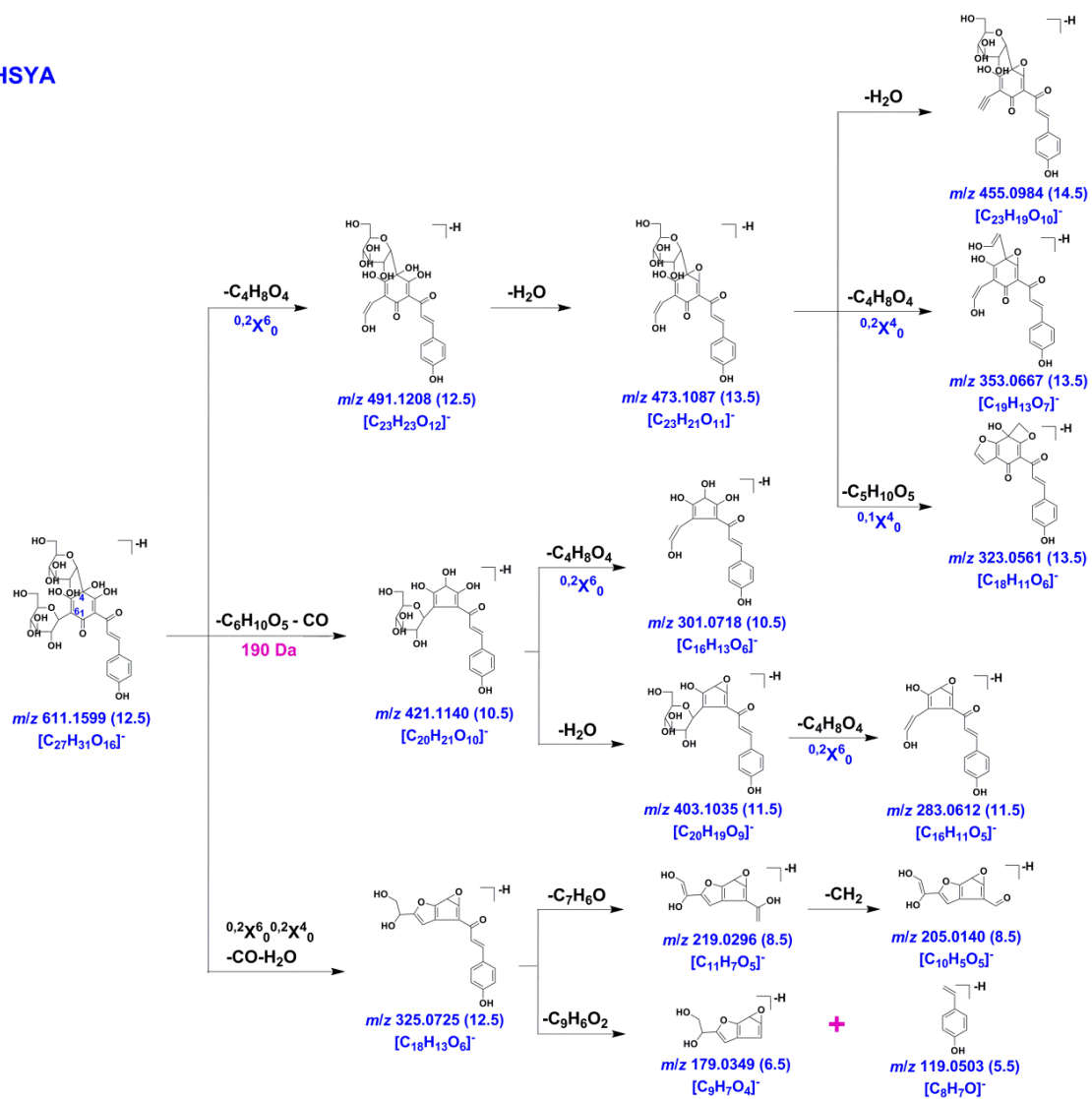


Fig. S7 The proposed fragmentation pathways for HSYA based on the negative mode CID-MS³ data obtained on an LTQ-Orbitrap hybrid mass spectrometer.

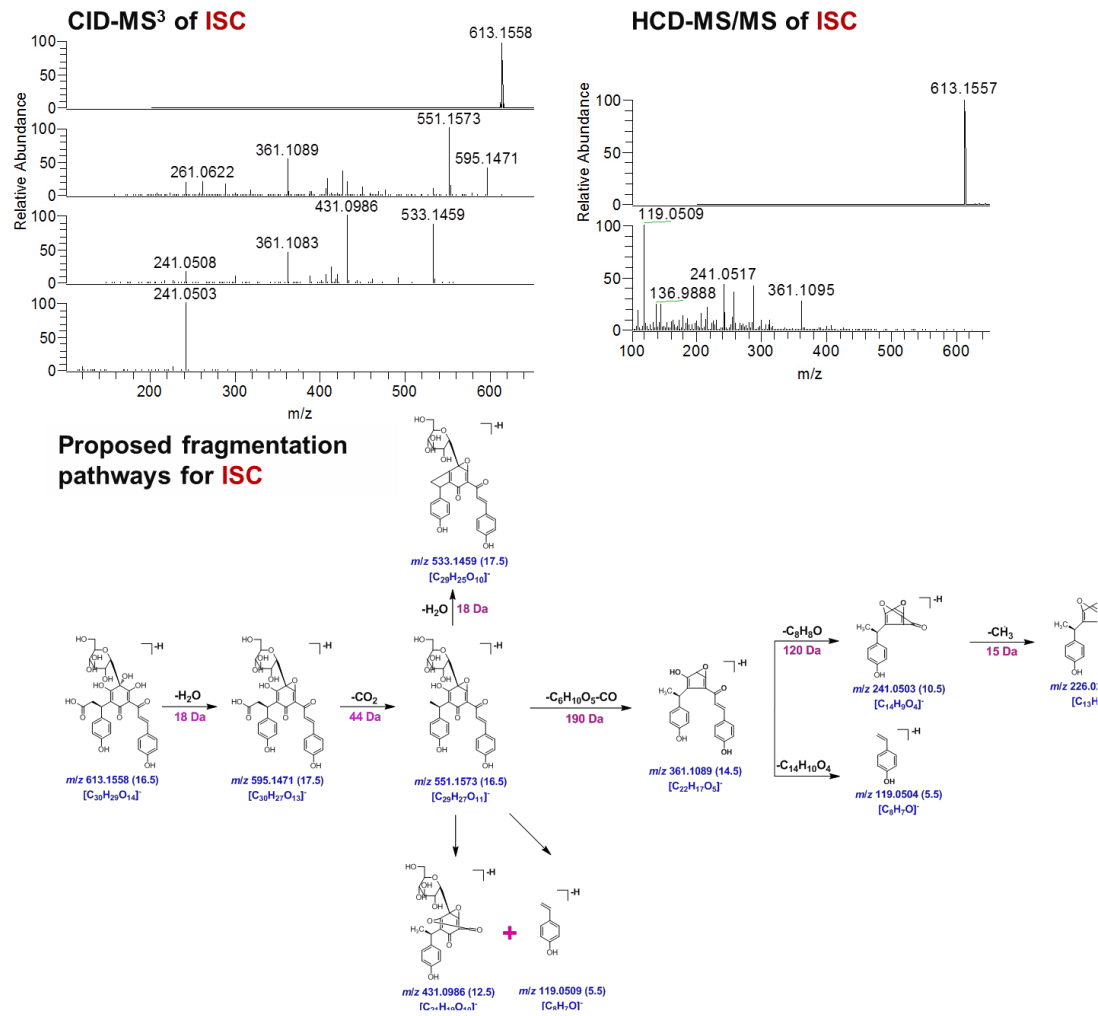


Fig. S8 The CID-MS³ and HCD-MS/MS spectra and proposed fragmentation pathways for ISC.

AnHSYB

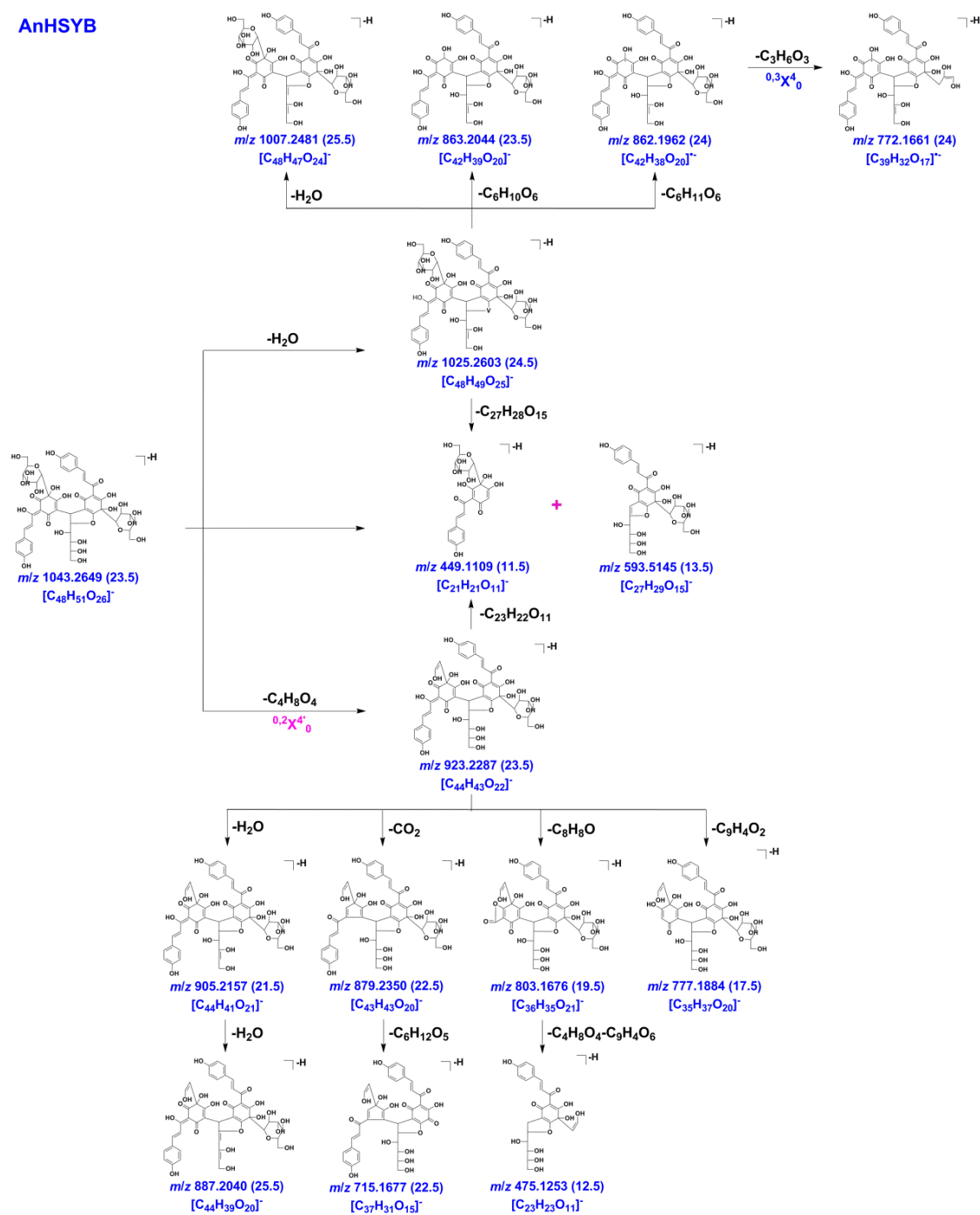


Fig. S9 The proposed fragmentation pathways for AnHSYB based on the negative mode CID-MS³ and HCD-MS/MS data obtained on an LTQ-Orbitrap hybrid mass spectrometer.

Table S1 Detailed information with respect to the 163 quinochalcone C-glycoside compounds characterized from *C. tinctorius* by the offline comprehensive 2D LC and high-resolution LTQ-Orbitrap MS analysis.

No.	t _R (min)	Fr.	[M-H] ⁻	Observed m/z	Mass error	RDB	CID-MS ³	HCD-MS ² (abundance in %)	Identification
1 ^c	2.95	9	[C ₃₂ H ₃₁ O ₁₅] ⁻	655.1170	4.3	17.5	MS ² [655]: 637.1594, 619.1487, 611.1628 MS ³ [655→637]: 619.1473, 517.1156, 491.1196 MS ³ [655→619]: 473.1094, 601.137	MS ² [655]: 325.0714, 283.061, 119.0504	X-Glc-C ₁₁ H ₁₀ O ₄
2 ^c	2.99	10	[C ₃₃ H ₃₄ NO ₁₈] ⁻	732.1817	4.8	17.5	MS ² [732]: 611.1628, 491.1203, 403.1042 MS ³ [732→611]: 491.1197, 403.1036, 325.0718 MS ³ [732→491]: 473.1091, 283.0612, 301.0718	MS ² [732]: 119.0504, 283.0612, 325.0718	X-2Glc-C ₆ H ₃ NO ₂
3 ^c	3.51	10	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1615	-0.4	12.5	MS ² [611]: 491.1201, 473.1101 MS ³ [611→491]: 473.1087, 323.0561, 283.0612 MS ³ [611→473]: 323.0561, 455.0984, 353.0514	MS ² [611]: 328.0593, 119.0506, 208.0017	Isomer of Hydroxysafflor yellow A
4 ^c	3.53	9	[C ₂₁ H ₂₃ O ₁₂] ⁻	467.1198	0.7	10.5	MS ² [467]: 449.1089, 329.0878, 261.0617 MS ³ [467→449]: 317.067, 431.0984, 285.062 MS ³ [467→329]: 311.077, 179.035, 139.0402	MS ² [467]: 153.0195, 215.0714, 207.0511, 119.0504	X-Glc-H ₂ O
5 ^c	3.55	8	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1633	2.5	12.5	MS ² [611]: 491.1205, 473.1101 MS ³ [611→491]: 473.1095, 283.0615, 323.0564 MS ³ [611→473]: 323.0558, 455.0980, 353.0511	MS ² [611]: 328.0591, 208.0016, 119.0505	Isomer of Hydroxysafflor yellow A
6 ^c	3.68	10	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1632	2.4	12.5	MS ² [611]: 491.1195, 473.1092 MS ³ [611→491]: 473.1092, 283.0613, 323.0562 MS ³ [611→473]: 323.0562, 455.0984, 353.0515	MS ² [611]: 328.0591, 119.0505, 208.0015	Isomer of Hydroxysafflor yellow A
7 ^c	3.71	5	[C ₂₆ H ₂₄ NO ₁₅] ⁻	590.1147	-0.67	15.5	MS ² [590]: 572.1049, 257.0457, 465.1041 MS ³ [590→572]: 529.0989 MS ³ [590→257]: 136.9880, 119.0501	MS ² [590]: 273.0405, 119.0504, 245.0456	Z-Glc-C ₅ H ₂ O ₅
8 ^c	3.71	10	[C ₃₉ H ₄₅ O ₂₄] ⁻	897.2325	2.1	17.5	MS ² [897]: 897.2210, 777.1894, 449.1098 MS ³ [897→897]: 716.1602, 861.2101, 626.1285 MS ³ [897→777]: 759.1785, 569.1312, 733.1989	MS ² [897]: 153.0196, 435.0725, 287.0563	Unknown (450+448)

9 °	3.72	8	[C ₂₇ H ₃₄ NO ₁₆] ⁻	628.1895	1.8	11.5	MS ² [628]: 611.1619, 491.1195, 403.1035 MS ³ [628→611]: 491.1192, 521.1298, 403.1031 MS ³ [628→491]: 473.1089, 283.0612, 323.0561	MS ² [628]: 325.0723, 119.0505, 283.0617	X-2Glc-NH ₃
10 °	3.76	5	[C ₂₆ H ₂₆ NO ₁₆] ⁻	608.1252	-0.8	14.5	MS ² [608]: 356.0779, 257.0458, 564.1365, 269.0458	MS ² [608]: 119.0504, 269.0457, 136.9882	Z-Glc-C ₅ H ₄ O ₆
11 °	3.90	10	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1630	2.0	12.5	MS ² [611]: 491.1195, 489.1253, 473.1091 MS ³ [611→491]: 473.1085, 283.0611, 323.0559	MS ² [611]: 328.0589, 119.0505, 489.1253, 208.0017	Isomer of Hydroxysafflor yellow A
12 °	3.93	10	[C ₃₆ H ₃₉ O ₁₇] ⁻	743.2159	-4.5	17.5	MS ² [743]: 491.1206, 611.1631, 628.1894 MS ³ [743→491]: 473.1092, 283.0613, 323.0562 MS ³ [743→611]: 491.1193	MS ² [743]: 119.0504, 328.0584, 283.0610	X-2Glc-C ₉ H ₈ O
13 °	4.03	10	[C ₂₇ H ₃₁ O ₁₇] ⁻	627.1580	2.1	12.5	MS ² [627]: 419.0991, 583.1678, 609.1469 MS ³ [627→419]: 299.0557, 329.0662, 401.0872 MS ³ [627→583]: 493.1355, 565.1565, 475.1248	MS ² [627]: 119.0504, 178.9987, 299.0562	Isomer of Methylsafflorin C or Methylisosafflorin C
14 °	4.14	10	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1623	0.9	12.5	MS ² [611]: 521.1300, 491.1194, 371.0772 MS ³ [611→521]: 503.11, 313.0718, 401.0876 MS ³ [611→491]: 371.0773, 327.0875, 473.109	MS ² [611]: 119.0505, 300.0640, 358.0695	Isomer of Hydroxysafflor yellow B/C or Safflorin A
15 °	4.24	10	[C ₃₃ H ₄₁ O ₂₁] ⁻	773.2141	-0.6	13.5	MS ² [773]: 653.1743, 487.1263, 565.1583 MS ³ [773→653]: 635.1624, 445.1147, 463.1253 MS ³ [773→487]: 325.0714, 459.1292, 443.1343	MS ² [773]: 487.1248, 445.1144, 119.0506	X-3Glc
16 °	4.29	5	[C ₂₆ H ₂₇ O ₁₆] ⁻	595.1310	1.0	13.5	MS ² [595]: 449.1095, 287.0564, 407.0988 MS ³ [595→449]: 431.0977, 299.0557, 287.0557	MS ² [595]: 287.0562, 119.0504, 257.0458	X-Glc-C ₅ H ₆ O ₅
17 °	4.41	5	[C ₂₆ H ₂₇ O ₁₆] ⁻	595.1307	0.5	13.5	MS ² [595]: 449.1093, 287.0563, 407.0987 MS ³ [595→449]: 431.0975, 299.0558, 287.0558	MS ² [595]: 119.0504, 287.0561, 257.0455	X-Glc-C ₅ H ₆ O ₅
18 °	4.44	7	[C ₂₀ H ₁₉ O ₁₁] ⁻	435.0945	2.8	11.5	MS ² [435]: 417.0832, 315.0511, 245.0459 MS ³ [435→417]: 273.0404, 245.0455, 297.0252 MS ³ [435→315]: 245.0453, 287.0558	MS ² [435]: 119.0505, 245.0457, 273.0406	Unknown
19 °	4.48	10	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1623	0.9	12.5	MS ² [611]: 521.1309, 593.1522, 445.1148 MS ³ [611→521]: 503.1200, 313.0722, 358.0698 MS ³ [611→593]: 503.1200, 473.1095, 575.1407	-	Isomer of Hydroxysafflor yellow B/C or Safflorin A
20 °	4.49	8	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1636	3.0	12.5	MS ² [611]: 491.1193, 551.1405, 403.1032	MS ² [611]: 325.0714, 283.061, 491.1190	Isomer of Hydroxysafflor yellow A

							MS ³ [611→491]: 473.1086, 283.0611, 301.0717 MS ³ [611→473]: 491.1192		
21 ^c	4.60	10	[C ₃₉ H ₄₅ O ₂₄] ⁻	897.2316	1.1	17.5	MS ² [897]: 879.2219, 777.1900, 449.1102, 429.1051 MS ³ [897→897]: 716.1596, 861.2094, 449.1091 MS ³ [897→777]: 759.1787, 569.1312, 733.1993	MS ² [897]: 119.0506, 153.0196, 287.0565	Unknown (450+448)
22	4.62	9	[C ₂₇ H ₃₁ O ₁₇] ⁻	627.1570	0.6	12.5	MS ² [627]: 419.0987, 609.1467, 299.0563 MS ³ [627→419]: 299.0561 MS ³ [627→609]: 401.0880, 419.0987, 281.0457	MS ² [627]: 153.0196, 119.0505, 125.0247	Methylsafflomin C/ Methylisosafflomin C
23 ^c	4.80	8	[C ₂₇ H ₃₁ O ₁₇] ⁻	627.1573	1.1	12.5	MS ² [627]: 463.1102, 481.1207, 419.0991 MS ³ [627→463]: 343.0667, 445.0983, 403.0878 MS ³ [627→481]: 361.0779, 463.1097, 343.0673	MS ² [627]: 153.0195, 119.0505, 299.0560	Isomer of Methylsafflomin C or Methylisosafflomin C
24 ^c	4.90	12	[C ₄₈ H ₅₁ O ₂₆] ⁻	1043.2683	0.9	23.5	MS ² [1043]: 593.1525, 449.1100, 473.1100, 1025.2584 MS ³ [1043→593]: 515.1201, 473.1095, 365.0670 MS ³ [1043→449]: 431.0985, 299.0563, 287.0563	MS ² [1043]: 286.0485, 119.0505, 299.0563, 449.1093	Isomer of Anhydrosafflor Yellow B
25 ^d	4.94	12	[C ₅₀ H ₅₁ O ₃₀] ⁻	1131.2487	1.4	25.5	MS ² [1131]: 1113.2374, 505.0998, 637.1421 MS ³ [1131→1131]: 1095.2268, 625.1416, 949.1896 MS ³ [1131→505]: 297.0408, 461.1094, 271.0615	MS ² [1131]: 119.0504, 299.0197, 271.0248, 463.0883	(C ₁₇ H ₁₂ O ₈ -Glc)+(quercetin- Glc-Glc)
26 ^c	4.95	9	[C ₃₃ H ₄₁ O ₂₁] ⁻	773.2185	1.6	13.5	MS ² [773]: 491.1199, 565.1567, 473.1094 MS ³ [773→491]: 473.1058, 283.061, 301.0715 MS ³ [773→565]: 325.0717, 445.0988, 547.146	MS ² [773]: 119.0504, 325.0717, 283.0612	X-3Glc
27	4.98	8	[C ₂₇ H ₃₁ O ₁₇] ⁻	627.1573	1.1	12.5	MS ² [627]: 437.1094, 419.0989, 609.1468 MS ³ [627→437]: 299.0564, 419.0989, 269.0458 MS ³ [627→419]: 2999.0564	MS ² [627]: 207.0513, 419.0988, 119.0506	Methylsafflomin C/ Methylisosafflomin C
28 ^c	5.04	7	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1627	1.6	12.5	MS ² [611]: 491.1201, 521.1307, 593.152 MS ³ [611→491]: 329.0670, 473.1093, 283.0616 MS ³ [611→521]: 359.0774, 503.1199, 313.0718	MS ² [611]: 328.0588, 119.0504, 299.0562	Isomer of Hydroxysafflor yellow A
29 ^c	5.08	7	[C ₂₆ H ₂₇ O ₁₅] ⁻	579.1361	1.0	13.5	MS ² [579]: 371.0776, 561.1257, 287.0564 MS ³ [579→371]: 311.056, 251.0197, 353.0666 MS ³ [579→561]: 501.1044, 373.0932, 543.1151	MS ² [579]: 119.0505, 187.0403, 257.046	X-Glc-C ₅ H ₆ O ₄
30 ^c	5.14	6	[C ₂₀ H ₂₁ O ₁₁] ⁻	437.1095	1.3	10.5	MS ² [437]: 299.0563, 419.0988, 291.0725 MS ³ [437→299]: 178.9985	MS ² [437]: 119.0504, 178.9987, 299.0561	Unknown

31 °C	5.15	7	[C ₂₈ H ₃₁ O ₁₇] ⁻	639.1569	0.3	13.5	MS ² [437→419]: 299.056 MS ² [639]: 549.1259, 419.0990, 519.1152 MS ³ [639→549]: 419.0979, 519.1140, 531.1140 MS ³ [639→419]: 299.0558	MS ² [639]: 119.0504, 299.0561, 145.0296	Y-2Glc-O
32 °C	5.17	9	[C ₃₃ H ₄₁ O ₂₁] ⁻	773.2153	0.9	13.5	MS ² [773]: 491.1204, 565.1573, 683.1839 MS ³ [773→491]: 473.1089, 283.0612, 301.0717 MS ³ [773→565]: 325.0715, 445.0982, 547.1457	MS ² [773]: 119.0504, 325.0718, 205.0143	X-3Glc
33	5.18	8	[C ₂₇ H ₃₁ O ₁₇] ⁻	627.1583	2.5	12.5	MS ² [627]: 609.147, 437.1096, 419.099 MS ³ [627→609]: 401.0882, 281.0458, 419.0988 MS ³ [627→437]: 299.0559, 419.098, 26.0454	MS ² [627]: 187.0401, 207.051, 119.0504	Methylsafflomin C/ Methylisosafflomin C
34 °C	5.19	10	[C ₄₁ H ₄₅ O ₂₆] ⁻	953.2215	1.1	19.5	MS ² [953]: 935.2113, 833.1799, 503.1054 MS ³ [953→935]: 773.158, 917.2003, 744.1552 MS ³ [953→833]: 815.1684, 735.179, 625.1207	MS ² [953]: 287.0561, 119.0504, 197.0092	(X-Glc)+C ₂₀ H ₂₃ O ₁₅
35 °C	5.20	9	[C ₃₃ H ₃₉ O ₂₂] ⁻	787.1942	0.5	14.5	MS ² [787]: 743.2044, 725.1946 MS ³ [787→743]: 653.1731, 725.1945, 623.1628 MS ³ [787→725]: 587.1406, 605.1512, 707.1826	MS ² [787]: 287.0560, 119.0505, 257.0455	X-2Glc-C ₆ H ₈ O ₆
36 °C	5.25	8	[C ₃₃ H ₃₉ O ₂₂] ⁻	787.1955	2.1	14.5	MS ² [787]: 743.2059, 725.1962 MS ³ [787→743]: 653.1733, 725.1946, 623.163 MS ³ [787→725]: 587.1415, 707.1838, 605.1522	MS ² [787]: 287.0563, 119.0505, 257.0458	X-2Glc-C ₆ H ₈ O ₆
37	5.25	7	[C ₂₇ H ₃₁ O ₁₅] ⁻	595.1685	2.3	12.5	MS ² [595]: 355.0832, 385.0937, 4753.1258 MS ³ [595→355]: 313.0713, 325.0713, 265.0351 MS ³ [595→385]: 235.0249, 209.0456, 249.0405	MS ² [595]: 355.0824, 385.0929, 313.0719	Saffloquinoside C or isomer
38 °C	5.37	9	[C ₂₇ H ₃₁ O ₁₇] ⁻	627.1567	1.7	12.5	MS ² [627]: 419.0987, 437.1092, 299.0564 MS ³ [627→419]: 299.0563, 329.0668, 178.9987 MS ³ [627→437]: 299.0564, 419.0987, 269.0457	MS ² [627]: 207.0512, 119.0505, 257.0457	Isomer of Methylsafflomin C or Methylisosafflomin C
39 °C	5.54	9	[C ₂₇ H ₃₁ O ₁₇] ⁻	627.1567	1.4	12.5	MS ² [627]: 609.1461, 437.1088, 401.0878 MS ³ [627→609]: 401.0875, 311.056, 383.0770 MS ³ [627→437]: 299.0558, 419.0978	MS ² [627]: 207.0510, 119.0504, 257.0456	Isomer of Methylsafflomin C or Methylisosafflomin C
40 °C	5.62	7	[C ₂₀ H ₂₁ O ₁₁] ⁻	437.1091	0.4	10.5	MS ² [437]: 299.0562, 291.0724, 419.0988	MS ² [437]: 119.0504, 153.0195, 178.9987	Y-Glc-2C

							MS ³ [437→299]: 178.9986 MS ³ [437→291]: 273.0611, 153.0193, 141.0196		
41 °C	5.69	7	[C ₂₇ H ₂₉ O ₁₆] ⁻	609.1463	0.3	13.5	MS ² [609]: 419.0991, 519.1154, 591.1364 MS ³ [609→419]: 299.0558 MS ³ [609→519]: 419.098, 299.056	MS ² [609]: 119.0505, 299.056, 178.9988	Y-2Glc—CH ₂
42 °C	5.71	8	[C ₃₂ H ₃₉ O ₂₀] ⁻	743.2040	0.0	13.5	MS ² [743]: 491.1199, 535.1462, 325.0721 MS ³ [743→491]: 473.1089, 283.0612, 301.0717 MS ³ [743→535]: 325.0717, 517.1354, 415.0882	MS ² [743]: 119.0505, 325.072, 205.0144	X-2Glc-C ₅ H ₈ O ₄
43 °C	5.72	7	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1632	2.4	12.5	MS ² [611]: 521.1306, 445.1145, 593.1519 MS ³ [611→491]: 503.1199, 313.0719, 358.0695 MS ³ [611→473]: 325.0563, 299.0771, 427.1032	MS ² [611]: 119.0504, 287.0562, 207.0511	Isomer of Hydroxysafflor yellow B/C or Safflomin A
44 °C	5.76	12	[C ₄₈ H ₅₁ O ₂₆] ⁻	1043.2681	0.6	23.5	MS ² [1043]: 593.1524, 449.1099, 473.1099, 1025.2574 MS ³ [1043→593]: 515.1200, 473.1093, 365.0669 MS ³ [1043→449]: 431.0985, 287.0564, 299.0565	MS ² [1043]: 286.0487, 119.0505, 299.0565	Isomer of Anhydrosafflor Yellow B
45 °C	5.79	7	[C ₂₇ H ₃₁ O ₁₇] ⁻	627.1572	0.8	12.5	MS ² [627]: 419.0993, 609.1474, 583.1683 MS ³ [627→419]: 299.0562, 329.0668 MS ³ [627→609]: 447.0937, 519.1148, 419.0985	MS ² [627]: 299.0561, 119.0505, 178.9988	Isomer of Methylsafflomin C or Methylisosafflomin C
46 °C	5.86	9	[C ₃₃ H ₄₁ O ₂₁] ⁻	773.2153	0.9	13.5	MS ² [773]: 653.1733, 403.1042, 635.163 MS ³ [773→653]: 635.1625, 465.1256, 323.0565 MS ³ [773→403]: 325.0716, 385.0928, 283.061	MS ² [773]: 119.0504, 325.0714, 283.061, 205.0142	X-3Glc
47 °C	5.89	7	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1619	0.2	12.5	MS ² [611]: 521.13, 445.114, 593.1511 MS ³ [611→521]: 503.1193, 313.0716 MS ³ [611→445]: 325.0564, 299.0771, 427.1036	MS ² [611]: 119.0505, 287.0562, 207.0512	Isomer of Hydroxysafflor yellow B/C or Safflomin A
48 °C	5.96	8	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1602	-2.5	12.5	MS ² [611]: 491.1209, 325.0725, 403.1046 MS ³ [611→491]: 473.1088, 283.0612, 301.0717 MS ³ [611→325]: 205.0142, 219.0298, 179.035	MS ² [611]: 119.0507, 325.0726, 205.0149	Isomer of Hydroxysafflor yellow A
49 °C	5.97	5	[C ₂₇ H ₂₉ O ₁₄] ⁻	577.1569	1.1	13.5	MS ² [577]: 457.1145 MS ³ [577→457]: 337.0719	MS ² [577]: 217.0143, 337.0717, 119.0504	X-2Glc—2OH
50 °C	5.99	8	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1596	-3.5	12.5	MS ² [611]: 491.1211, 325.0726, 403.1047, 473.1107	MS ² [611]: 325.0721, 119.0507, 205.0147, 283.0616, 163.0041	Isomer of Hydroxysafflor yellow A

							MS ³ [611→491]: 473.1092, 283.0614, 301.0719, 323.0563 MS ³ [611→325]: 205.0143, 219.0300, 179.050		
51 ^c	6.02	10	[C ₃₉ H ₃₅ O ₁₅] ⁻	743.1951	4.1	22.5	MS ² [743]: 419.0991, 437.1096, 299.0566 MS ³ [743→419]: 299.0563, 329.0668 MS ³ [743→437]: 299.0564, 419.0986, 269.0460	MS ² [743]: 178.9986, 299.056, 119.0504	Unknown
52 ^b	6.05	8	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1599	-3.0	12.5	MS ² [611]: 491.1208, 325.0725, 403.1045, 473.1104 MS ³ [611→491]: 473.1087, 283.0612, 301.0717, 323.0560 MS ³ [611→325]: 205.0140, 219.0296, 179.0349	MS ² [611]: 325.0721, 119.0507, 205.0147, 283.0616, 163.0041	Hydroxysafflor yellow A
53 ^c	6.06	10	[C ₂₁ H ₂₁ O ₁₃] ⁻	481.0990	0.5	11.5	MS ² [481]: 419.0981, 463.0879, 299.056 MS ³ [481→419]: 299.0561 MS ³ [481→463]: 419.0982, 245.0457, 445.0775	MS ² [481]: 119.0504, 178.9987, 299.0561	Y-C ₅ H ₁₀ O ₇
54 ^c	6.07	9	[C ₃₃ H ₄₁ O ₂₁] ⁻	773.2145	-0.1	13.5	MS ² [773]: 491.1204, 653.1735, 565.1573 MS ³ [773→491]: 473.12091	MS ² [773]: 325.0717, 119.0504, 205.0143, 283.0612	X-3Glc
55 ^c	6.09	8	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1602	-2.5	12.5	MS ² [611]: 491.1210, 325.0726, 403.1047 MS ³ [611→491]: 473.1092, 283.0614, 301.0719, 323.0563 MS ³ [611→325]: 205.0141, 219.0297, 179.0349	MS ² [611]: 119.0507, 325.0724, 205.0148, 283.0619, 163.0042	Isomer of Hydroxysafflor yellow A
56 ^c	6.20	6	[C ₁₉ H ₁₉ O ₁₀] ⁻	407.0984	0.1	10.5	MS ² [407]: 287.056, 261.0616, 185.0092 MS ³ [407→287]: 257.0452, 227.0195, 185.0091 MS ³ [407→264]: 141.0194, 197.0296, 111.0089	MS ² [407]: 119.0504	X-C ₄ H ₈ O ₄
57 ^c	6.21	8	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1615	-0.4	12.5	MS ² [611]: 491.1208, 403.1045, 325.0725, 473.1103 MS ³ [611→491]: 473.1086, 283.0611, 301.0716, 323.0559 MS ³ [611→403]: 325.0715, 385.0926, 283.0610	MS ² [611]: 119.0505, 325.0721, 205.0145, 283.0615, 163.0040	Isomer of Hydroxysafflor yellow A
58 ^c	6.41	10	[C ₂₃ H ₂₃ O ₁₄] ⁻	523.1102	1.7	12.5	MS ² [523]: 271.0614, 479.12, 315.0512 MS ³ [523→271]: 151.0036, 119.0503, 165.0193	MS ² [523]: 119.0504, 151.0038, 276.0712	Y-Glc-CO ₂ -H ₂ O
59 ^c	6.42	8	[C ₂₈ H ₂₉ O ₁₈] ⁻	653.1371	1.7	14.5	-	MS ² [653]: 287.051, 119.0504, 257.0456	X-Glc-C ₇ H ₈ O ₇
60 ^c	6.45	4	[C ₂₆ H ₂₉ O ₁₅] ⁻	581.1516	0.6	12.5	MS ² [581]: 553.1562, 421.1138, 443.0982, 243.0663, 535.1667	MS ² [581]: 119.0504, 145.0296, 211.0611	X-2Glc-CH ₂ O
61 ^c	6.53	6	[C ₁₉ H ₁₉ O ₁₀] ⁻	407.0989	1.4	10.5	MS ² [407]: 287.0559, 261.0615, 257.0455 MS ³ [407→287]: 257.0453, 243.0660	MS ² [407]: 119.0504, 136.9882, 187.0401	X-C ₄ H ₈ O ₄
62 ^c	6.57	6	[C ₃₀ H ₃₅ O ₁₆] ⁻	651.1947	2.5	13.5	-	MS ² [651]: 119.0504, 163.0402	Unknown

63 °C	6.64	6	[C ₂₇ H ₃₁ O ₁₇] ⁻	627.1545	2.1	12.5	-	MS ² [627]: 299.0558, 178.9986, 119.0504	Isomer of Methylsafflorin C or Methylisosafflorin C (X-Glc—C)+(Y-Glc-Glc)
64 °C	6.69	10	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.262	-0.1	23.5	MS ² [1059]: 939.2216, 1041.2532, 817.1844, 591.1367, 449.1098 MS ³ [1059→939]: 817.1831, 799.1727, 654.1229 MS ³ [1059→1041]: 919.2156, 757.1624, 879.199	MS ² [1059]: 193.0143, 119.0504, 87.056	
65 °C	6.70	6	[C ₁₉ H ₁₉ O ₁₀] ⁻	407.0986	0.6	10.5	MS ² [407]: 287.0558, 261.0613, 257.0453 MS ³ [407→287]: 257.0454, 227.0195, 243.0661	MS ² [407]: 328.0587, 287.0561, 358.0693	X-C ₄ H ₈ O ₄
66 °C	6.77	10	[C ₄₈ H ₅₃ O ₂₈] ⁻	1077.272	-0.8	22.5	MS ² [1077]: 1059.2617, 957.2302, 939.2204	MS ² [1077]: 119.0503, 153.0194, 299.056	2X-3Glc-O
67 °C	6.78	10	[C ₂₇ H ₂₉ O ₁₅] ⁻	593.1522	1.6	13.5	MS ² [593]: 473.1089, 503.1201, 353.0517 MS ³ [593→473]: 323.0565, 403.1039, 413.0729	MS ² [593]: 119.0504, 205.0144, 473.1092	Isomer of Safflor Yellow A or Saffloquinoside A
68 °C	6.80	6	[C ₂₄ H ₂₃ O ₁₃] ⁻	519.1149	0.9	13.5	MS ² [519]: 501.1037, 311.056, 287.0560	MS ² [519]: 119.0504, 187.0401, 257.0455	X-Glc-C ₃ H ₂ O ₂
69 °C	6.88	7	[C ₂₁ H ₂₁ O ₁₁] ⁻	449.1089	-0.1	11.5	MS ² [449]: 431.0977, 207.0509, 259.061 MS ³ [449→431]: 299.0563, 311.0562 MS ³ [449→207]: 189.0402, 129.0192, 75.0087	MS ² [449]: 119.0504, 153.0195, 207.051	Y-C ₃ H ₁₀ O ₅
70 °C	6.92	11	[C ₂₇ H ₂₉ O ₁₅] ⁻	593.1526	2.4	13.5	MS ² [593]: 515.1204, 365.0672, 497.0779 MS ³ [593→515]: 365.0668, 347.0563, 497.1093 MS ³ [593→365]: 245.0089	MS ² [593]: 365.0667, 220.0014, 119.0504	Isomer of Safflor Yellow A or Saffloquinoside A
71 °C	7.06	10	[C ₄₄ H ₄₁ O ₂₆] ⁻	985.1887	-0.4	24.5	MS ² [985]: 505.0988, 449.1089, 479.0831 MS ³ [985→505]: 297.0404, 461.1091, 271.0612	-	Unknown (450+536)
72 °C	7.12	7	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1625	1.2	12.5	MS ² [611]: 521.1309, 593.1522, 445.1148, 491.1203 MS ³ [611→521]: 503.1193, 313.0718, 358.0693 MS ³ [611→593]: 503.1191, 445.1135, 575.1399	MS ² [611]: 119.0505, 287.0559, 207.0510	Isomer of Hydroxysafflor yellow B/C or Safflorin A
73 °C	7.14	6	[C ₂₂ H ₂₃ O ₁₂] ⁻	479.1195	0.1	11.5	-	MS ² [479]: 119.0504, 145.0296	Unknown
74 °C	7.18	10	[C ₅₄ H ₆₁ O ₃₃] ⁻	1237.312	1.6	24.5	MS ² [1237]: 787.1948, 611.163, 491.1205 MS ³ [1237→787]: 667.1521, 697.1623, 505.0991 MS ³ [1237→611]: 491.1199, 521.1305, 403.1038	MS ² [1237]: 299.0198, 286.0483, 301.0350	(X-Glc)+(Y-Glc-Glc-C ₄ H ₈ O ₄ -CO ₂)
75 °C	7.43	5	[C ₂₇ H ₂₉ O ₁₄] ⁻	577.1566	0.5	13.5	MS ² [577]: 457.1139, 379.0822, 499.1246 MS ³ [577→457]: 379.0822 MS ³ [577→379]: 259.0248, 273.0405, 285.0405	MS ² [577]: 259.0248, 379.0823, 119.0504	X-Glc-C ₆ H ₈ O ₃
76 °C	7.84	7	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1630	2.1	12.5	MS ² [611]: 521.1309, 445.1148, 593.1522, 313.0722	-	Isomer of Hydroxysafflor yellow B/C or Safflorin A

							MS ³ [611→521]: 503.1199, 313.0720, 358.0696 MS ³ [611→445]: 325.0562, 427.1029, 299.0770		
77 °C	7.98	10	[C ₄₈ H ₅₁ O ₂₆] ⁻	1043.2683	0.9	23.5	MS ² [1043]: 1025.2582, 923.2264, 593.1523, 449.1099 MS ³ [1043→1025]: 863.2048, 1007.2472, 407.0991 MS ³ [1043→923]: 905.2142, 715.1665, 475.1252	MS ² [1043]: 119.0504, 287.0561, 257.0456	Isomer of Anhydrosafflor Yellow B
78 °C	8.05	7	[C ₃₃ H ₄₁ O ₂₀] ⁻	757.2206	1.2	13.5	-	MS ² [757]: 287.0561, 164.9831, 119.0504	X-3Glc-O
79 °C	8.05	10	[C ₃₀ H ₃₃ O ₁₉] ⁻	697.120	-0.2	14.5	MS ² [697]: 491.1205, 653.1733, 611.1630 MS ³ [697→491]: 473.1089, 283.0611, 301.0717 MS ³ [697→653]: 491.1200, 533.1307, 445.1144	MS ² [697]: 119.0504, 283.0612, 328.0589, 163.0038	X-2Glc-C ₃ H ₂ O ₃
80 °C	8.19	10	[C ₂₈ H ₂₉ O ₁₈] ⁻	653.1371	1.9	14.5	MS ² [653]: 591.1364, 419.0991, 299.0565 MS ³ [653→591]: 501.1039, 471.0931 MS ³ [653→419]: 299.056	MS ² [653]: 299.0562, 178.9988, 119.0505	Y-Glc-C ₈ H ₈ O ₇
81 °C	8.21	7	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1620	0.3	12.5	MS ² [611]: 521.1317, 445.1154, 593.1530 MS ³ [611→521]: 503.1198, 313.0718, 358.0694 MS ³ [611→445]: 325.0566, 299.0774, 427.1036	MS ² [611]: 119.0506, 287.0565, 358.0699	Isomer of Hydroxysafflor yellow B/C or Safflomin A
82 °C	8.78	10	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.262	-0.7	23.5	MS ² [1059]: 731.1626, 593.1521, 1041.2526 MS ³ [1059→731]: 713.1521, 523.1046, 283.0616	MS ² [1059]: 119.0504, 257.0456, 136.9882	(X-Glc-C)+(Y-Glc-Glc)
83 °C	8.81	9	[C ₃₆ H ₄₃ O ₂₃] ⁻	843.2194	-0.7	15.5	MS ² [843]: 799.2314, 491.1205 MS ³ [843→799]: 491.1204, 287.0566, 595.1687	MS ² [843]: 287.0558, 164.983, 119.0504	X-3Glc-C ₃ H ₂ O ₂
84 °C	8.91	10	[C ₃₀ H ₂₉ O ₁₄] ⁻	613.1575	1.9	16.5	MS ² [613]: 551.1567, 361.1085, 595.1466 MS ³ [613→551]: 431.0984, 533.1456, 361.1082 MS ³ [613→361]: 241.0505, 119.0505	MS ² [613]: 119.0505, 241.0508, 287.0563	Isomer of SC/ISC
85 °C	8.96	4	[C ₂₇ H ₂₅ O ₁₄] ⁻	573.1248	-0.4	15.5	MS ² [573]: 365.0668, 463.0885, 273.0406 MS ³ [573→365]: 245.0090, 219.0298, 173.0244	MS ² [573]: 119.0504, 143.0504, 187.0402	X-Glc-C ₈ H ₈ O ₃
86 °C	9.05	10	[C ₃₀ H ₂₉ O ₁₅] ⁻	629.1516	0.7	16.5	MS ² [629]: 419.0984, 437.1088, 299.0562 MS ³ [629→419]: 299.0557, 178.9985, 329.0661 MS ³ [629→437]: 299.056, 419.0984	MS ² [629]: 178.9989, 299.0566, 119.0505	Y-Glc-C ₈ H ₈ O ₄
87 °C	9.12	10	[C ₂₉ H ₂₉ O ₁₉] ⁻	681.1318	1.3	15.5	MS ² [681]: 663.1213, 619.1316, 407.0991 MS ³ [681→663]: 619.131, 407.0988 MS ³ [681→619]: 407.0986, 389.088, 287.0562	MS ² [681]: 287.0561, 119.0504, 257.0456	X-Glc-C ₈ H ₈ O ₈

88 ^c	9.16	7	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1625	1.2	12.5	MS ² [611]: 521.1301, 445.1141, 593.1511 MS ³ [611→521]: 503.1201, 313.0719, 358.0696 MS ³ [611→445]: 325.0568, 299.0777, 427.1036	-	Isomer of Hydroxysafflor yellow B/C or Safflomin A
89 ^c	9.16	10	[C ₃₀ H ₂₉ O ₁₄] ⁻	613.1574	1.8	16.5	MS ² [613]: 551.1568, 361.1086 MS ³ [613→551]: 431.0979, 533.1453, 361.1078 MS ³ [613→361]: 241.0505, 226.0217, 119.0503	MS ² [613]: 119.0505, 241.0508, 287.0562	Isomer of SC/ISC
90 ^c	9.31	7	[C ₂₇ H ₂₇ O ₁₄] ⁻	575.1415	1.6	14.5	MS ² [575]: 515.1196, 407.0772, 365.0667 MS ³ [575→515]: 347.0562, 365.0668, 351.0723 MS ³ [575→407]: 335.0561	-	X-2Glc—2H ₂ O
91 ^c	9.34	7	[C ₂₇ H ₂₉ O ₁₅] ⁻	593.1525	2.3	13.5	MS ² [593]: 503.1196, 575.1407, 473.0939 MS ³ [593→503]: 365.05841, 485.1092, 335.0565 MS ³ [593→575]: 485.1095	MS ² [611]: 119.0504, 145.0297	Isomer of Safflor Yellow A or Saffloquinoside A
92 ^c	9.34	12	[C ₄₈ H ₅₁ O ₂₆] ⁻	1043.2682	0.8	23.5	MS ² [1043]: 449.1091, 593.1515, 1025.2565 MS ³ [1043→449]: 431.0985, 299.0563, 287.0563 MS ³ [1043→593]: 515.1198, 365.0667, 473.1091	MS ² [1043]: 286.0485, 119.0505, 449.1093	Isomer of Anhydrosafflor Yellow B
93 ^c	9.45	10	[C ₄₈ H ₅₁ O ₂₈] ⁻	1075.257	0.2	23.5	MS ² [1075]: 1057.2483, 955.2164, 816.1768	MS ² [1075]: 193.0143, 178.9987, 119.0504	2X-2Glc-2CO-C ₄ H ₈ O ₄
94 ^c	9.53	10	[C ₄₈ H ₅₁ O ₂₆] ⁻	1043.266	2.2	23.5	MS ² [1043]: 1025.2594, 923.2278, 449.1105 MS ³ [1043→1025]: 863.2034, 1007.2465, 772.1646 MS ³ [1043→923]: 905.2159, 715.1678, 475.1255	MS ² [1043]: 119.0506, 287.0563, 257.0457	Isomer of Anhydrosafflor Yellow B
95 ^d	9.58	10	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.2614	-0.1	23.5	-	MS ² [1059]: 119.0503, 193.0141, 2877.0558, 257.0453	(X-Glc—C)+(Y-Glc-Glc)
96 ^c	9.59	7	[C ₂₇ H ₃₁ O ₁₆] ⁻	611.1631	2.3	12.5	MS ² [611]: 521.1302, 593.1512, 445.1142 MS ³ [611→521]: 503.1198, 313.0718, 358.0695 MS ³ [611→593]: 503.1200, 575.1413, 533.1306	-	Isomer of Hydroxysafflor yellow B/C or Safflomin A
97 ^c	9.73	10	[C ₄₈ H ₅₁ O ₂₆] ⁻	1043.2680	0.1	23.5	MS ² [1043]: 1025.2578, 923.2261, 449.1096 MS ³ [1043→1025]: 863.2047, 1007.2477, 772.1656 MS ³ [1043→923]: 905.2163, 475.1258, 715.1678	MS ² [1043]: 119.0504, 287.0562, 257.0455	Isomer of Anhydrosafflor Yellow B
98	9.80	7	[C ₂₇ H ₃₀ NO ₁₄] ⁻	592.1690	3.1	13.5	MS ² [592]: 472.1103, 364.0830, 446.1310 MS ³ [592→472]: 244.0251, 286.0355, 364.0670 MS ³ [592→364]: 244.0249	MS ² [592]: 233.0331, 364.0826, 339.0749	Tinctormine

99 °C	9.87	9	[C ₅₅ H ₆₁ O ₃₃] ⁻	1249.3090	-1.1	25.5	MS ² [1249]: 1231.3007, 419.0991, 437.1097	MS ² [1249]: 299.0566, 178.9985, 119.053	Unknown
100 °C	10.04	8	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.2642	0.0	23.5	MS ² [1059]: 1041.2528, 593.1522, 731.1627 MS ³ [1059→1041]: 1023.2422, 895.2151, 951.2206 MS ³ [1059→593]: 515.1198, 365.0668	MS ² [1059]: 119.0505, 257.0457, 136.9883	(X-Glc—C)+(Y-Glc-Glc)
101 °C	10.04	10	[C ₄₈ H ₅₁ O ₂₆] ⁻	1043.2697	2.2	23.5	MS ² [1043]: 1025.594, 923.2280, 449.1106 MS ³ [1043→1025]: 863.2033, 1007.2465, 772.1649 MS ³ [1043→923]: 905.2159, 715.1678, 475.1255	MS ² [1043]: 119.0505, 287.0562, 257.0457	Isomer of Anhydrosafflor Yellow B
102	10.07	7	[C ₂₇ H ₂₉ O ₁₅] ⁻	593.1526	2.5	13.5	MS ² [593]: 447.1149, 473.0967, 327.0725 MS ³ [593→447]: 327.0722, 177.0194, 297.0616 MS ³ [593→473]: 177.0192	MS ² [593]: 119.0505, 177.0195, 310.0482	Safflor Yellow A/ Saffloquinoside A
103 °C	10.13	8	[C ₃₁ H ₂₉ O ₁₀] ⁻	561.1733	-2.7	17.5	MS ² [561]: 373.1249, 441.1146, 353.114 MS ³ [561→373]: 253.0828, 223.0723 MS ³ [561→441]: 373.1248	MS ² [561]: 119.0505, 265.083, 223.0725	Unknown
104 °C	10.17	6	[C ₃₁ H ₃₂ NO ₁₃] ⁻	626.1884	0.7	16.5	MS ² [626]: 461.1091, 449.1093 MS ³ [626→461]: 341.0513	MS ² [626]: 298.0482, 341.0514, 178.9987	X-Glc-C ₁₀ H ₁₁ NO ₂
105 °C	10.18	10	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.263	-0.12	23.5	MS ² [1059]: 731.1631, 1041.2533, 833.1948 MS ³ [1059→731]: 713.1523, 523.1047, 283.0617 MS ³ [1059→1041]: 1023.2406, 879.1987, 921.2101	MS ² [1059]: 119.0504, 257.0456, 136.9882, 287.0561	(X-Glc—C)+(Y-Glc-Glc)
106 °C	10.23	8	[C ₂₇ H ₃₀ NO ₁₃] ⁻	576.1737	2.52	13.5	MS ² [576]: 449.1098, 388.1256, 430.1364 MS ³ [576→449]: 431.0983, 299.0562, 287.0562 MS ³ [576→388]: 261.0614, 344.1348	MS ² [576]: 119.0505, 240.0879, 287.0562	Y-Glc-C ₅ H ₉ NO ₂
107 °C	10.35	7	[C ₃₀ H ₂₉ O ₁₅] ⁻	629.1524	1.9	16.5	MS ² [629]: 419.0989, 437.193, 299.0564 MS ³ [629→419]: 299.0563 MS ³ [629→437]: 299.0557, 419.0976	MS ² [629]: 119.0504, 178.9987, 299.0561	Y-Glc-C ₈ H ₈ O ₄
108 °C	10.35	10	[C ₃₀ H ₂₉ O ₁₅] ⁻	629.1528	2.5	16.5	MS ² [629]: 419.0991, 437.1096, 299.0565 MS ³ [629→419]: 299.0561, 329.0667, 178.9987 MS ³ [629→437]: 299.0564, 419.0988, 269.0458	MS ² [629]: 119.0505, 178.9988, 299.0562	Y-Glc-C ₈ H ₈ O ₄
109 °C	10.41	8	[C ₂₄ H ₂₆ NO ₁₂] ⁻	520.1465	0.8	12.5	MS ² [520]: 332.0989, 400.0889, 312.088 MS ³ [520→332]: 212.0563, 182.0458, 302.0876 MS ³ [520→400]: 332.0986	MS ² [520]: 119.0504, 182.046, 194.046	Z-Glc-C ₃ H ₄ O ₂
110 °C	10.45	8	[C ₂₅ H ₂₆ NO ₁₄] ⁻	564.1368	1.6	13.5	-	MS ² [564]: 119.0503, 194.0457, 182.0458	Unknown

111 °C	10.57	4	[C ₂₇ H ₃₁ O ₁₄] ⁻	579.1724	0.8	12.5	MS ² [579]: 271.0610 MS ³ [579→271]: 151.0035, 177.0191	MS ² [579]: 271.0613, 151.0038, 119.0504	X-2Glc-2O
112 °C	10.57	12	[C ₂₁ H ₂₁ O ₁₁] ⁻	449.1099	2.1	11.5	MS ² [449]: 431.0985, 299.0562, 287.0562, 207.0510 MS ³ [449→431]: 299.0560, 311.0559, 281.0454, 413.0877 MS ³ [449→299]: 178.9984, 255.0660, 271.0610	MS ² [449]: 119.0505, 286.0484, 153.0195,	Y-C ₃ H ₁₀ O ₅
113 °C	10.58	9	[C ₅₄ H ₆₁ O ₃₁] ⁻	1205.326	0.5	24.5	MS ² [1205]: 449.1092, 491.1198, 611.162 MS ³ [1205→449]: 299.0564, 431.0986, 287.0565 MS ³ [1205→491]: 473.109, 283.0612, 328.0588	MS ² [1205]: 119.0504, 286.0482, 153.0195	(X-Glc-Glc OH)+(X-Glc-Glc) —
114 °C	10.59	10	[C ₃₉ H ₃₅ O ₁₄] ⁻	727.1999	-4.6	22.5	MS ² [727]: 595.1473, 709.1901, 539.1534 MS ³ [727→595]: 427.0828, 475.0887, 449.1094 MS ³ [727→709]: 577.1351, 692.1623, 589.1466	MS ² [727]: 119.0505, 131.0465, 241.0507	Y-Glc-C ₁₇ H ₁₄ O ₃
115 °C	10.67	12	[C ₂₂ H ₂₂ NO ₁₁] ⁻	476.1202	0.7	12.5	MS ² [476]: 356.0624, 458.1097, 268.0617, 288.0726 MS ³ [476→491]: 288.0722, 168.0302, 338.0515 MS ³ [476→473]: 326.0667, 338.0668, 308.0562	MS ² [476]: 119.0505, 180.0304, 168.0304	Z-Glc-CO
116 °C	10.83	10	[C ₄₀ H ₃₇ O ₁₄] ⁻	741.2161	-3.8	22.5	MS ² [741]: 553.1689, 723.2059, 603.1634 MS ³ [741→553]: 287.0778, 407.0989, 459.1263 MS ³ [741→723]: 603.1631, 577.1362, 705.1948	MS ² [741]: 145.0621, 119.0505, 241.0508	X-Glc-C ₁₉ H ₁₆ O ₃
117	10.89	7	[C ₂₇ H ₂₉ O ₁₅] ⁻	593.1523	1.9	13.5	MS ² [593]: 473.0939, 447.1145, 503.1197 MS ³ [593→473]: 405.1039, 285.0616 MS ³ [593→447]: 297.062	MS ² [593]: 119.0503, 405.0979, 241.0506	Safflor Yellow A/ Saffloquinoside A
118 °C	10.90	10	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.264	1.5	23.5	MS ² [1059]: 731.163, 465.1049, 1041.2532 MS ³ [1059→31]: 713.1519, 523.1042, 283.0616 MS ³ [1059→465]: 447.0925, 297.0401, 315.0506	MS ² [1059]: 119.0504, 287.056, 257.0455	(X-Glc—C)+(Y-Glc-Glc)
119 °C	11.01	10	[C ₂₇ H ₂₆ NO ₁₄] ⁻	588.1372	0.7	15.5	-	MS ² [588]: 248.0562, 119.0504, 269.0453	Unknown
120 °C	11.07	5	[C ₂₂ H ₂₁ O ₁₂] ⁻	477.1038	-0.1	12.5	MS ² [477]: 459.0938, 287.0564, 269.0458 MS ³ [477→459]: 339.0508, 327.0508, 271.0612 MS ³ [477→287]: 257.0453	MS ² [477]: 119.0504, 314.0432, 269.0456	X-Glc-CO
121 °C	11.25	8	[C ₂₅ H ₂₈ NO ₁₂] ⁻	534.1628	2.16	12.5	MS ² [534]: 346.1148, 414.1049, 326.1039 MS ³ [534→346]: 266.072, 302.088, 182.0459 MS ³ [534→414]: 346.1141	MS ² [534]: 119.0504, 194.0459, 182.0459	X-Glc-C ₄ H ₇ NO

122 °c	11.51	10	[C ₂₉ H ₂₇ O ₁₈] ⁻	663.1215	1.8	16.5	MS ² [663]: 619.1315, 407.0992 MS ³ [663→619]: 407.0988, 389.0882, 287.0564 MS ³ [663→403]: 287.0561, 257.0455, 261.0615	MS ² [663]: 287.0562, 119.0505, 257.0456	X-Glc-C ₈ H ₆ O ₇
123	11.55	5	[C ₂₇ H ₂₈ NO ₁₃] ⁻	574.1574	1.4	14.5	MS ² [574]: 454.0993, 424.1040, 466.1145 MS ³ [574→454]: 304.0461, 346.0565, 436.0882 MS ³ [574→424]: 364.0821	MS ² [574]: 364.0826, 338.067, 244.0252	Cartormine
124 °c	11.66	5	[C ₂₇ H ₂₈ NO ₁₄] ⁻	590.1521	1.0	14.5	MS ² [590]: 530.1312, 470.0947, 410.0735 MS ³ [590→530]: 410.0726, 380.0772, 512.1194 MS ³ [590→470]: 410.0732	MS ² [590]: 230.0095, 260.02, 367.0697	Z-Glc-C ₆ H ₆ O ₄
125 °c	11.69	5	[C ₂₈ H ₂₉ O ₁₇] ⁻	637.1409	-0.1	14.5	MS ² [637]: 619.1315, 575 MS ³ [637→619]: 575.1406, 601.1197, 287.0562	MS ² [637]: 119.0505, 287.0561, 338.0432	X-Glc-C ₇ H ₈ O ₆
126 °c	11.84	5	[C ₃₀ H ₂₉ O ₁₃] ⁻	597.1619	1.0	16.5	MS ² [597]: 477.1197, 507.1302, 579.1514 MS ³ [597→477]: 313.0722, 339.0878 MS ³ [597→507]: 369.0982, 343.0826	MS ² [597]: 313.0718, 119.0504, 339.0874	X-Glc-C ₉ H ₈ O ₂
127 °c	11.98	10	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.2630	0.2	23.5	MS ² [1059]: 621.1474, 1041.2532, 651.1579 MS ³ [1059→621]: 501.1044, 603.1361, 531.1149 MS ³ [1059→1041]: 595.1674, 407.0987, 287.0564	MS ² [1059]: 119.0505, 299.056, 178.9987	(X-Glc—C)+(Y-Glc-Glc)
128 °d	12.13	11	[C ₅₀ H ₅₁ O ₃₀] ⁻	1131.2480	2.0	25.5	MS ² [1131]: 1113.2384, 505.1003, 637.1428 MS ³ [1131→1113]: 1095.228, 625.1424, 949.1906 MS ³ [1131→505]: 297.0406, 461.1093, 271.0614	MS ² [1131]: 625.1414, 463.0886, 299.0199, 271.0250, 187.0402, 151.0039, 119.0505	(C ₁₇ H ₁₂ O ₈ -Glc)+(quercetin-Glc-Glc)
129 °d	12.25	10	[C ₅₆ H ₆₁ O ₃₄] ⁻	1277.3070	1.4	26.5	MS ² [1277]: 1259.2957, 505.0999, 783.2001 MS ³ [1277→1259]: 1241.2847, 1095.2477, 771.1996 MS ³ [1277→505]: 297.0401, 461.1084, 271.0609	MS ² [1277]: 119.0504, 301.0358, 151.0039, 771.1971	(C ₁₇ H ₁₂ O ₈ -Glc)+(quercetin-Glc-Rha-Glc)
130 °c	12.44	4	[C ₃₀ H ₂₇ O ₁₄] ⁻	611.1414	1.3	17.5	MS ² [611]: 403.0826, 421.0930, 593.1304 MS ³ [611→403]: 283.0243, 361.0710, 241.0139 MS ³ [611→421]: 275.0560, 257.0455, 377.1029	MS ² [611]: 119.0505, 187.0402	Isomer of Hydroxysafflor yellow A
131 °c	12.46	8	[C ₂₄ H ₂₆ NO ₁₁] ⁻	504.1514	0.6	12.5	MS ² [504]: 316.1041, 384.0941, 486.1412 MS ³ [504→316]: 196.0614 MS ³ [504→384]: 316.1036, 196.0615	MS ² [504]: 119.0504, 208.0615, 196.0615	Z-Glc-C ₃ H ₄ O
132 °c	12.46	9	[C ₄₁ H ₄₁ O ₂₁] ⁻	869.2139	-0.7	21.5	MS ² [869]: 851.2053, 593.1525, 473.1099	MS ² [869]: 119.0504, 136.9882, 257.0455	2X-Glc-C ₃ H ₆ O ₄

							MS ³ [869→851]: 705.167, 833.193, 689.1509 MS ³ [869→593]: 515.1201, 365.0669		
133 ^c	12.53	9	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.263	0.7	23.5	MS ² [1059]: 731.162, 1041.2517, 851.2042 MS ³ [1059→731]: 713.1514, 523.1038, 283.0614 MS ³ [1059→1041]: 909.2147, 1023.2403	MS ² [1059]: 119.0504, 287.0561, 257.0455	(X-Glc—C)+(Y-Glc-Glc)
134 ^c	12.58	6	[C ₂₃ H ₂₃ O ₁₂] ⁻	491.1203	1.6	12.5	MS ² [491]: 287.0558, 431.0987 MS ³ [491→287]: 181.0142, 166.9986, 153.0194 MS ³ [491→431]: 287.056, 311.0409, 329.0665	MS ² [491]: 286.0491, 166.9989, 153.0197	X-Glc-C ₂ H ₂ O
135 ^b	12.59	8	[C ₄₈ H ₅₁ O ₂₆] ⁻	1043.265	-2.4	23.5	MS ² [1043]: 1025.2603, 923.2287, 449.1109 MS ³ [1043→1025]: 963.2044, 1007.2481, 772.1661 MS ³ [1043→923]: 905.2157, 715.1677	MS ² [1043]: 119.0506, 287.0565, 257.0459	Anhydrosafflor Yellow B
136 ^c	12.65	9	[C ₄₈ H ₅₁ O ₂₆] ⁻	1043.269	1.5	23.5	MS ² [1043]: 1025.2594, 923.228, 449.1105 MS ³ [1043→1025]: 863.2045, 1007.2478, 772.1658 MS ³ [1043→923]: 905.2157	MS ² [1043]: 119.0505, 287.0566, 257.0457	Isomer of Anhydrosafflor Yellow B
137	13.22	10	[C ₄₈ H ₅₃ O ₂₇] ⁻	1061.22	2.2	22.5	MS ² [1061]: 611.1632, 449.1101, 507.1368 MS ³ [1061→611]: 491.1198, 521.1304, 403.1037 MS ³ [1061→449]: 431.0978, 299.0561, 287.0562	MS ² [1061]: 153.0196, 179.0352, 221.0457	Safflor yellow B
138 ^c	13.38	4	[C ₄₂ H ₄₈ O ₁₂] ⁻	744.3135	-1.3	19	MS ² [744]: 582.2615, 462.2039 MS ³ [744→582]: 462.2039, 342.1461, 436.2245 MS ³ [744→462]: 342.1462	MS ² [744]: 119.0504, 145.0296, 342.1456	Unknown
139 ^d	13.48	10	[C ₄₄ H ₄₁ O ₂₅] ⁻	969.1965	2.4	24.5	MS ² [969]: 505.0999, 951.1848, 297.0409 MS ³ [969→505]: 297.04063, 461.1087, 271.0612 MS ³ [969→951]: 933.1741, 787.137, 463.089	MS ² [969]: 119.0505, 300.0277, 151.0039	(C ₁₇ H ₁₂ O ₈ -Glc)+(quercetin-Glc)
140 ^c	13.53	4	[C ₄₂ H ₄₈ O ₁₂] ⁻	744.3135	-2.2	19	MS ² [744]: 582.2621, 462.2044 MS ³ [744→582]: 462.2033, 342.1458, 436.2240	MS ² [744]: 119.0503, 342.1458, 145.0296	Unknown
141 ^d	13.54	10	[C ₅₀ H ₅₁ O ₂₉] ⁻	1115.2544	2.0	25.5	MS ² [1115]: 505.0991, 1097.2417, 461.1093 MS ³ [1115→505]: 297.0407, 461.109, 271.0615 MS ³ [1115→1097]: 1079.2301, 933.1942, 609.1464	MS ² [1115]: 119.0504, 301.0355, 151.0039	(C ₁₇ H ₁₂ O ₈ -Glc)+(quercetin-Glc-Rha)
142 ^c	13.59	9	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.2630	0.6	23.5	MS ² [1059]: 621.1473, 1041.2531, 827.2263 MS ³ [1059→621]: 501.1046, 603.1362, 513.1047	MS ² [1059]: 119.0503, 299.0558, 178.9986	(X-Glc—C)+(Y-Glc-Glc)

143 ^d	13.72	9	[C ₅₅ H ₆₁ O ₃₂] ⁻	1233.315	-0.6	25.5	MS ² [1059→1041]: 621.1473, 419.0992, 921.215 MS ² [1233]: 771.1989, 461.1092, 609.1463 MS ³ [1233→771]: 609.1472, 301.0358, 463.0889 MS ³ [1233→461]: 271.0612, 151.0038, 253.0506	MS ² [1233]: 301.0356, 119.0504, 271.0251	(Y-Glc)+(quercetin-Glc-Glc-Rha)
144 ^c	13.78	10	[C ₅₀ H ₅₁ O ₂₈] ⁻	1099.257	-0.5	25.5	MS ² [1099]: 1081.2458, 505.0989, 1037.2566 MS ³ [1099→1081]: 1063.2368, 917.1993, 1037.2583 MS ³ [1099→505]: 297.0403, 461.1086, 271.0612	MS ² [1099]: 119.0505, 284.0327, 151.0039	(C ₁₇ H ₁₂ O ₈ -Glc)+(X-Glc-Glc-H ₂ O)
145 ^b	13.90	7	[C ₃₀ H ₂₉ O ₁₄] ⁻	613.1558	-0.8	16.5	MS ² [613]: 551.1573, 361.1089, 595.1471 MS ³ [613→551]: 431.0986, 533.1459, 361.1083 MS ³ [613→361]: 241.0503	MS ² [613]: 119.0509, 241.0507, 287.0570	Isosafflomin C
146 ^d	14.01	10	[C ₅₀ H ₅₁ O ₂₉] ⁻	1115.254	1.8	25.5	MS ² [1115]: 1097.2429, 1053.2533, 505.0999 MS ³ [1115→1097]: 909.1941, 649.1412, 959.1889 MS ³ [1115→1053]: 717.167, 1035.2413, 743.1462	MS ² [1115]: 300.0279, 119.0504, 151.0038	(C ₁₇ H ₁₂ O ₈ -Glc)+(quercetin-Glc-Rha)
147 ^b	14.07	7	[C ₃₀ H ₂₉ O ₁₄] ⁻	613.1572	1.6	16.5	MS ² [613]: 361.109, 551.1574, 425.11 MS ³ [613→361]: 241.0505, 119.0503 MS ³ [613→551]: 431.098, 533.1451, 361.1078	-	Safflomin C
148 ^d	14.12	8	[C ₄₉ H ₅₁ O ₂₈] ⁻	1087.259	1.8	24.5	MS ² [1087]: 625.1422, 461.1100 MS ³ [1087→625]: 463.0886, 301.0355 MS ³ [1087→461]: 271.0616, 151.0039	MS ² [1087]: 299.096, 271.0247, 463.0877	(Y-Glc)+(quercetin-Glc-Glc)
149 ^c	14.14	10	[C ₃₅ H ₃₆ NO ₁₅] ⁻	710.2095	0.6	18.5	MS ² [710]: 595.1471, 522.1629, 387.0883 MS ³ [710→595]: 427.0828, 475.0887, 449.1094 MS ³ [710→522]: 407.0987, 287.0563, 428.1201	MS ² [710]: 119.0504, 241.0506, 287.056	Y-Glc-C ₁₃ H ₁₅ NO ₄
150 ^c	14.17	7	[C ₄₁ H ₃₉ O ₂₁] ⁻	867.1986	-0.4	22.5	MS ² [867]: 459.0933, 287.0563, 849.1882, 407.0984	MS ² [867]: 119.0504, 287.0561, 257.0455	(X-Glc-C ₂ H ₂ O)+C ₂₂ H ₁₉ O ₁₁
151 ^c	14.19	8	[C ₄₈ H ₅₁ O ₂₇] ⁻	1059.265	2.2	23.5	MS ² [1059]: 621.1475, 1041.2535, 827.2267 MS ³ [1059→621]: 603.136, 501.1044, 513.1044 MS ³ [1059→1041]: 621.1474	MS ² [1059]: 119.0505, 287.0564, 299.0564	(X-Glc-C)+(Y-Glc-Glc)
152 ^c	14.23	7	[C ₃₀ H ₃₀ NO ₁₂] ⁻	596.1776	0.3	16.5	MS ² [596]: 450.1413, 476.1205, 408.1306 MS ³ [596→450]: 300.0879, 286.0722, 342.0985 MS ³ [596→476]: 408.1302, 432.1303, 288.0879	MS ² [596]: 119.0504, 244.098, 300.0877	Z-Glc-C ₉ H ₈ O ₂
153 ^c	14.27	10	[C ₅₁ H ₅₃ O ₂₉] ⁻	1129.2700	1.8	25.5	MS ² [1129]: 1111.2585, 505.0999 MS ³ [1129→1111]: 1093.2462, 947.2098	MS ² [1129]: 119.0503, 151.0037, 314.0427	2X-3Glc-C ₃ H ₂ O ₂ -2H

154 °C	14.32	7	[C ₂₆ H ₃₀ NO ₁₁] ⁻	532.1839	2.8	12.5	MS ² [532]: 344.1352, 324.1242, 412.1251 MS ³ [532→344]: 224.0926, 194.0821 MS ³ [532→324]: 204.0665, 119.0503, 132.082	-	X-Glc-C ₅ H ₉ N
155 °C	14.61	10	[C ₄₁ H ₃₂ NO ₁₃] ⁻	746.1895	2.1	26.5	MS ² [746]: 553.1357, 449.1092, 921.2307 MS ³ [746→553]: 363.0873, 535.1249, 345.0769 MS ³ [746→449]: 299.0562, 431.0984, 287.0562	MS ² [746]: 119.0505, 287.0562, 257.0457	X-Y-C ₁₁ H ₁₀ NO
156 °C	14.70	8	[C ₄₄ H ₄₃ O ₂₄] ⁻	955.2169	2.0	23.5	-	MS ² [955]: 119.0504, 286.0484, 151.0039	Isomer of Precarthamin
157 °C	14.76	7	[C ₂₇ H ₃₂ NO ₁₁] ⁻	546.1992	2.1	12.5	MS ² [546]: 426.1408, 358.1509, 338.14 MS ³ [546→426]: 358.1503, 238.1084 MS ³ [546→358]: 238.1083	MS ² [546]: 119.0504, 250.1086, 208.0981	X-Glc-C ₆ H ₁₁ N
158 °C	14.79	7	[C ₄₃ H ₄₃ O ₂₂] ⁻	911.2270	2.0	22.5	MS ² [911]: 461.1098, 449.1099 MS ³ [911→461]: 443.0974 MS ³ [911→449]: 431.0984	MS ² [911]: 286.0481, 119.0503, 151.0037	(X-Glc)+(Y-Glc)
159 °C	14.91	7	[C ₃₀ H ₃₀ NO ₁₁] ⁻	580.1831	1.2	16.5	MS ² [580]: 460.1255, 392.1355, 372.1246 MS ³ [580→460]: 392.1353, 272.0932 MS ³ [580→392]: 272.0926, 242.082	MS ² [580]: 119.0504, 284.0925, 242.0821	Z-Glc-C ₉ H ₈ O
160 °C	15.07	7	[C ₅₀ H ₅₃ O ₂₇] ⁻	1085.2790	0.7	24.5	MS ² [1085]: 461.1091, 449.1091, 1067.2671 MS ³ [1085→461]: 271.0612 MS ³ [1085→449]: 431.0984, 299.0561, 287.0562	MS ² [1085]: 119.0505, 299.0202, 151.0039	(Y-Glc)+(Y-Glc-Glc)
161 °C	15.16	9	[C ₄₄ H ₄₃ O ₂₄] ⁻	955.2167	1.8	23.5	MS ² [955]: 505.0993, 297.0408, 937.2048 MS ³ [955→505]: 461.1094, 297.0407, 271.0615 MS ³ [955→297]: 176.9829, 269.0453, 253.0504	MS ² [955]: 119.0505, 286.0484, 151.0039	Precarthamin
162 °C	15.37	10	[C ₄₄ H ₄₁ O ₂₃] ⁻	937.2055	1.2	24.5	MS ² [937]: 367.0466, 407.0992, 511.0892	MS ² [937]: 119.0504, 287.0558, 136.9881	(X-Glc-C ₂ H ₂ O)+(C ₁₈ H ₁₁ O ₆ -Glc-CO ₂)
163 °C	15.69	7	[C ₂₃ H ₁₇ O ₈] ⁻	421.0938	2.3	15.5	MS ² [421]: 275.0562, 257.0456, 377.1031 MS ³ [421→275]: 187.0764, 231.0662, 213.0556 MS ³ [421→257]: 136.9881, 119.0503	MS ² [421]: 119.0503, 136.9881, 271.0611	X-C ₈ H ₆ O ₂

^a The basic frameworks X, Y, and Z, represent the QCG skeletons with the elemental compositions of C₁₅H₁₂O₆, C₁₆H₁₂O₆, and C₁₅H₁₃NO₅, respectively;

^b identified by comparison with the reference standards;

^c potential new QCG molecules;

^d novel dimers containing QCG and FOG.