# Supplementary Material

# Unraveling the Mechanism of Xiaochaihu Granules in Alleviating Yeast-Induced Fever Based on Network Analysis and Experimental Validation

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**Table S1** The general information of reference standards

| No. | Compounds | Batch number | Source |
|---|---|---|---|
| 1 | Baicalin | 715-200010 | a |
| 2 | Citric acid | 100396-201302 | a |
| 3 | Baicalein | 111595-201808 | a |
| 4 | Wogonoside | DST190709-026 | b |
| 5 | Wogonin | 111514-201706 | a |
| 6 | Scutellarin | 110842-200403 | a |
| 7 | Succinic acid | 110896-200001 | a |
| 8 | Calycosin-7-*O*-β-D-glucoside | 111920-201606 | a |
| 9 | Formononetin | C-018-181216 | b |
| 10 | Chlorogenic acid | 110753-201415 | a |
| 11 | Neochlorogenic acid | P20A11L121936 | c |
| 12 | Chrysin | 111701-200501 | a |
| 13 | Rutin | 110080-9705 | a |
| 14 | Liquiritigenin | F1912131 | f |
| 15 | Isoliquiritigenin | F2001050 | f |
| 16 | Isoliquiritin | Y15A10H95344 | c |
| 17 | Schaftoside | Z25O10B101118 | c |
| 18 | Isoschaftoside | P13D11S134210 | c |
| 19 | Liquiritin apioside | 5569 | i |
| 20 | Saikosaponin c | M12O11S126866 | c |
| 21 | Caffeic acid | 110885-200102 | a |

| No. | Compounds | Batch number | Source |
|---|---|---|---|
| 22 | Saikosaponin A | 150102 | e |
| 23 | Saikosaponin B1 | P09M10F82675 | c |
| 24 | Saikosaponin B2 | Z04S9L69482 | c |
| 25 | L-Malic acid | 191123-038 | b |
| 26 | Phenprobamate | B21910 | h |
| 27 | Proline | BCBZ5040 | g |
| 28 | Glutamic acid | 111576-200201 | a |
| 29 | Aspartic acid | 140691-201602 | a |
| 30 | Arginine | 140685-201305 | a |
| 31 | Liquiritin | 111610-201106 | a |
| 32 | Glycyrrhizic Acid | P24J10F91300 | c |
| 33 | Glycyrrhetinic Acid | 471-53-4 | d |
| 34 | Lobetyolin | 220321 | e |

a: National Institutes for Food and Drug Control. b: Zhongshan CN-Biotechnology Co., Ltd. c：Shanghai yuanye Bio-Technology Co., Ltd. d：Beijing Qisong Biotechnology Co., Ltd. e：Zhongshan UNO Biotechnology Development Co., Ltd. f：Shanghai Aladdin Biochemical Technology Co., Ltd. g：Sigma-Aldrich. h：Guangzhou Meilun Biotechnology Co., Ltd. I: Nature standard

**Table S2** Identification of chemical components in XCHG by UFLC-Triple TOF-MSMS

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $C_6H_{14}N_4O_2$ | 2.15 | 175.1188 （-0.6） | 173.1038 （-3.4） | 175.1183$[M+H]^+$, 158.0917$[M+H-NH_3]^+$, 130.0962$[M+H-CH_3N_2]^+$, 116.0699$[M+H-CH_3N_2-NH3]^+$, 70.0645$[M+H-CH_3N_2-NH_3-HCOOH]^+$ | 173.1030$[M-H]^-$, 131.0819$[M-H-CH_3N_2]^-$, | L(+)-Arginine [a, c] | Organic acid | CH, HQ, JBX, DS, DZ, GC | |
| 2 | $C_{24}H_{42}O_{21}$ | 2.3 | ND | 665.2107 （-5.8） | ND | 665.2090$[M-H]^-$, 485.1492$[M-H-Glc-H_2O]^-$, 443.1412$[M-H-Glc-C_2H_4O_2]^-$, 383.1145$[M-H-Glc-C_4H_8O_4]^-$, 341.1058$[M-H-2Glc]^-$, 179.0542 | Stachyose [c] | Saccharides | HQ, DZ | |
| 3 | $C_4H_7NO_4$ | 2.3 | 134.0443 （-3.5） | 132.0299 （-2.7） | ND | ND | Aspartic acid [a] | Organic acid | CH, JBX, DZ, GC | |
| 4 | $C_5H_9NO_4$ | 2.33 | 148.0599 （-2.5） | 146.0456 （-1.8） | ND | ND | Glutamic acid [a] | Organic acid | CH, SJ, DZ, GC | |
| 5 | $C_5H_{12}O_5$ | 2.33 | 153.0755 （-1.5） | 151.0607 （-3.3） | 99.0434$[M+H-3H_2O]^+$, 69.0331$[M+H-3H_2O-CH_2O]^+$, 57.0329 | 151.0592$[M-H]^-$, 101.0237$[M-H-H_2O-CH_4O]^-$, 89.0227$[M-H-H_2O-CH_2O_2]^-$, 71.0128$[M-H-2H_2O-CH_2O_2]^-$, 59.0130 | D-Arabitol or Ribitol [c] | Saccharides | CH | |
| 6 | $C_6H_{12}O_6$ | 2.34 | ND | 179.0556 （-2.4） | ND | 179.0531$[M-H]^-$, 89.0226$[M-H-C_3H_7O_3]^-$, 71.0127$[M-H-C_3H_7O_3-H_2O]^-$, 59.0129$[M-H-C_4H_9O_4]^-$, | D-Tagatose or D-Glucose | Saccharides | CH, HQ, DS, SJ, DZ, GC | [1] |
| 7 | $C_6H_{12}O_7$ | 2.34 | ND | 195.0505 （-2.6） | ND | 195.0499$[M-H]^-$, 129.0191$[M-H-HCOOH-CH_2O]^-$, | Galactonic acid [c] | Glycosides | CH, HQ, DS, DZ, GC | |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | 75.0086[M-H-HCOOH-$CH_2O$-$3H_2O$]$^-$, | | | | |
| 8 | $C_5H_{11}NO_2$ | 2.36 | 118.0857 （-4.7） | ND | ND | ND | Valine | Organic acid | CH, HQ, DS, DZ, GC | [2] |
| 9 | $C_6H_{13}NO_5$ | 2.36 | 180.8650 （-1.0） | ND | 180.0872[M+H]$^+$, 162.0747[M+H-$H_2O$]$^+$, 144.0642[M+H-$2H_2O$]$^+$, 84.0434[M+H-$2H_2O$-$C_2H_4O_2$]$^+$, 72.0436[M+H-$2H_2O$-$C_3H_5O_2$]$^+$, | ND | Glucosamine Hydrochloride [c] | Saccharides | HQ, DS, DZ, GC | |
| 10 | $C_5H_9NO_2$ | 2.40 | 116.0700 （-4.9） | ND | 116.0700[M+H]$^+$, 70.0646[M+H-HCOOH]$^+$, | ND | Proline [a, c] | Organic acid | HQ, JBX, DS, SJ, DZ, GC | |
| 11 | $C_{12}H_{22}O_{11}$ | 2.40 | 343.1234 （-0.2） | 341.1071 （-5.3） | ND | 341.1058[M-H]$^-$, 179.0555[M-H-$C_6H_{11}O_5$]$^-$, 161.0462[M-H-$C_6H_{11}O_5$-$H_2O$]$^-$, 89.0243[M-H-$C_2H_6O_2$]$^-$, | Sucrose [c] | Saccharides | HQ, DS, SJ, DZ, GC | |
| 12 | $C_6H_6O_3$ | 2.40 | 127.0382 （-2.9） | ND | 127.0388[M+H]$^+$, 109.0282[M+H-$H_2O$]$^+$, 81.0329[M+H-$H_2O$-CO]$^+$, 69.0331[M+H-$C_2HO_2$]$^+$, | ND | 5-Hydroxymethylfurfural [c] | Others | CH, JBX, DS, SJ, DZ, GC | |
| 13 | $C_7H_{12}O_6$ | 2.44 | ND | 191.0194 （-3.5） | ND | 191.0546[M-H]$^-$, 127.0383[M-H-$H_2O$-HCOOH]$^-$, 85.0285 | Quinic acid [c] | Phenolic acids | CH, DS | |
| 14 | $C_5H_5N_5$ | 2.47 | 136.0612 （-3.9） | ND | 136.0613[M+H]$^+$, 119.0349[M+H-$NH_3$]$^+$, | ND | Adenine [c] | Others | CH, HQ, JBX, GC | |
| 15 | $C_4H_6O_5$ | 2.59 | ND | 133.0141 （-1.4） | ND | 133.0136[M-H]$^-$, 115.0030[M-H-$H_2O$]$^-$, 71.0132[M-H-$H_2O$-$CO_2$]$^-$, | Malic acid [a, c] | Organic acid | CH, HQ, JBX, DS, SJ, DZ | |
| 16 | $C_4H_4O_4$ | 2.6 | ND | 115.0032 （-4） | ND | 114.9981[M-H]$^-$, 71.0136[M-H-$CO_2$]$^-$, | Fumaric acid [c] | Organic acid | HQ, DS, DZ | |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | $C_6H_8O_7$ | 3.23 | 193.0336 （-3.3） | 191.0193 （-0.8） | 139.0020$[M+H-3H_2O]^+$, 129.0173$[M+H-H_2O-HCOOH]^+$, 111.0073$[M+H-2H_2O-HCOOH]^+$, 68.9967 | 191.0195$[M-H]^-$, 111.0087$[M-H-2H_2O-CO_2]^-$, 87.0090$[M-H-2H_2O-2CO_2]^-$, | Citric acid [a,c] | Organic acid | CH, HQ, DS, SJ, DZ, GC | |
| 18 | $C_9H_{12}N_2O_6$ | 3.34 | ND | 243.0611 （-1.7） | ND | 243.0613$[M-H]^-$, 200.0529$[M-H-CO_2]^-$, | Uridine [c] | Glycosides | CH, HQ, JBX, DS, GC | |
| 19 | $C_{10}H_{13}N_5O_4$ | 3.52 | 268.1038 （-0.7） | ND | 268.1043$[M+H]^+$, 136.0614$[M+H-C_5H_9O_4]^+$, | ND | Adenosine [c] | Glycosides | CH, HQ, DS, GC | [3] |
| 20 | $C_6H_{13}NO_2$ | 3.66 | 132.1014 （-2.3） | 130.0863 （-4.6） | 132.1017$[M+H]^+$, 86.0960$[M+H-HCOOH]^+$, 69.0695$[M+H-HCOOH-NH_3]^+$ | 130.0860$[M-H]^-$, 113.0243$[M-H-NH_3]^-$, 88.0401$[M-HCOOH-NH_3]^-$, | Isoleucine | Organic acid | JBX,DS | [3] |
| 21 | $C_4H_6O_4$ | 3.75 | ND | 117.0189 （-3.6） | ND | 117.0177$[M-H]^-$, 99.0089$[M-H-H_2O]^-$, 73.0287$[M-H-CO_2]^-$, | Succinic acid [a, c] | Organic acid | CH, DS | |
| 22 | $C_{10}H_{13}N_5O_5$ | 3.81 | 284.0990 （0.1） | 282.0836 （-2.7） | 284.1239$[M+H]^+$, 152.0564$[M+H-C_5H_9O_4]^+$, 135.0292$[M+H-C_5H_9O_4$-NH3$]^+$, 88.0749$[M+H-C_5H_9O_4$-$NH_3$-$CH_2NO]^+$, | 282.0829$[M-H]^-$, 150.0413$[M-H-C_5H_9O_4]^-$, 133.0143$[M-H-C_5H_9O_4$-$NH_3]^-$, | Guanosine [c] | Glycosides | CH, HQ, JBX, DS | |
| 23 | $C_9H_{11}NO_2$ | 5.37 | 166.0860 （-1.7） | 164.0709 （-3.2） | 166.0861$[M+H]^+$, 120.0799$[M+H-HCOOH]^+$, 103.0533$[M+H-HCOOH-NH_3]^+$, | 164.8333$[M-H]^-$, 147.0429$[M-H-NH_3]^-$, 120.9367$[M-H-CO_2]^-$, 103.0563$[M-H-NH_3-CO_2]^-$, | Phenylalanine [a, c] | Organic acid | HQ, JBX | |
| 24 | $C_{14}H_{21}NO_4$ | 6.02 | 268.1540 （-0.3） | ND | 268.1530$[M+H]^+$, 161.0589$[M+H-C_4H_{11}NO-H_2O]^+$, 88.0750 | ND | Codonopsine | Alkaloids | DS | [4] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | $C_{16}H_{18}O_9$ | 7.78 | 355.1012 （-3.1） | 353.0851 （-6.4） | 163.0385[M+H-$C_7H_{11}O_6$]$^+$, 145.0265[M+H-$C_9H_7O_3$-HCOOH] 135.0401[M+H-$C_8H_{11}O_7$]$^+$, | 353.0857[M-H]$^-$, 191.0550[M-H-$C_9H_7O_3$]$^-$, 179.0345[M-H-$C_7H_{11}O_5$]$^-$, 173.0461[M-H-$C_9H_7O_3$-$H_2O$]$^-$, 135.0439[M-H--$C_7H_{11}O_5$-$CHO_2$]$^-$, | Neochlorogenic acid [a] | Phenylpropanoids | CH | |
| 26 | $C_7H_6O_3$ | 9.44 | ND | 137.0238 （-3.8） | ND | 137.0228[M-H]$^-$, 119.0157[M-H-$H_2O$]$^-$, | Protocatechuic aldehyde [c] | Phenolic acids | GC | |
| 27 | $C_9H_{10}O_3$ | 9.55 | ND | 165.0553 （-1.3） | ND | 165.0560[M-H]$^-$, 121.0653[M+COOH]$^-$, 93.0352[M+COOH-$C_2H_4$]$^-$, 59.0130 | Desaminotyrosine [c] | Phenylpropanoids | GC | |
| 28 | $C_{16}H_{18}O_9$ | 9.97 | 355.1022 （-0.3） | 353.0855 （-6.6） | 163.0376[M+H-$C_7H_{11}O_6$]$^+$, 145.0280[M+H-$C_9H_7O_3$-HCOOH] 135.0429[M+H-$C_8H_{11}O_7$]$^+$, | 353.0860[M-H]$^-$, 191.0549[M-H-$C_9H_7O_3$]$^-$, | Chlorogenic acid[a, c] | Phenylpropanoids | CH，HQ | |
| 29 | $C_{21}H_{22}O_9$ | 10.34 | 419.1338 （0.2） | ND | 257.0794[M+H-Glc]$^+$, | ND | Isomer of liquiritin | Flavonoids | GC | [1] |
| 30 | $C_{27}H_{30}O_{15}$ | 11.4 | 595.1634 （-1.3） | 593.1482 （-4.8） | 595.1641, 577.1126[M+H-$H_2O$]$^+$, 559.1375[M+H-2$H_2O$]$^+$, 457.1091[M+H-$H_2O$-$C_4H_8O_4$]$^+$, 427.1029[M+H-$H_2O$-$C_5H_{10}O_5$]$^+$, 325.0767[M+H-$C_5H_{10}O_5$-$C_4H_8O_4$]$^+$ | 593.1483, 473.1060[M-H-$C_4H_8O_4$]$^-$, 353.0645[M-H-2$C_4H_8O_4$]$^-$ | Vicenin-2 (Apigenin-6,8-di-*C*-glucoside) [b] | Flavonoids | HQ, | [5] |
| 31 | $C_9H_8O_4$ | 11.45 | ND | 179.0344 （-3.2） | ND | 179.0342[M-H]$^-$, 135.0449[M-H-$CO_2$]$^-$, | Caffeic acid [a] | Phenolic acids | CH, GC，HQ | |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | $C_{26}H_{28}O_{14}$ | 12.67 | 565.155 （-0.4） | 563.1374 （-5.6） | 565.1524$[M+H]^+$, 547.1394$[M+H-H_2O]^+$, 529.1295$[M+H-2H_2O]^+$ 511.1207$[M+H-3H_2O]^+$, 481.1100$[M+H-3H_2O-2CH_2O]^+$, 427.1004$[M+H-H_2O-C_4H_8O_4]^+$, 409.0909$[M+H-2H_2O-C_4H_8O_4]^+$, 379.0801$[M+H-2H_2O-C_4H_8O_4-2CH_2O]^+$, | 563.1354$[M-H]^-$, 473.1079$[M-H-C_3H_6O_3]^-$ 443.0963$[M-H-C_4H_8O_4]^-$, 383.0732$[M-H-C_4H_8O_4-C_2H_4O_2]^-$, 353.0662$[M-H-C_3H_6O_3-C_4H_8O_4]^-$, | Schaftoside [a, c] | Flavonoids | HQ, GC | [6] |
| 33 | $C_{21}H_{20}O_9$ | 12.97 | 417.1167 (-3.1) | ND | 417.1190 255.0655$[M+H-Glc]^+$ | ND | Sophoraflavone B | Flavonoids | GC | [6] |
| 34 | $C_{26}H_{28}O_{14}$ | 13.17 | 565.1542 （-1.7） | 563.1366 （-5.8） | 565.1578$[M+H]^+$, 547.1413$[M+H-H_2O]^+$, 529.1316$[M+H-2H_2O]^+$, 481.1199$[M+H-3H_2O-CH_2O]^+$, 457.1180$[M+H-H_2O-C_3H_6O_3]^+$, 427.1149$[M+H-H_2O-C_4H_8O_4]^+$, 397.0939$[M+H-H_2O-C_4H_8O_4-CH_2O]^+$, 325.0721$[M+H-2C_4H_8O_4]^+$, | 563.1358$[M-H]^-$, 473.1205$[M-H-C_3H_6O_3]^-$, 443.0925$[M-H-C_4H_8O_4]^-$, 383.0741$[M-H-C_4H_8O4-C_2H_4O_2]^-$, 353.0647$[M-H-C_3H_6O_3-C_4H_8O_4]^-$, | Isoschaftoside [a, c] | Flavonoids | HQ, GC | |
| 35 | $C_{27}H_{30}O_{14}$ | 13.35 | ND | 577.1527 （-6.1） | ND | 577.1513$[M-H]^-$, 457.1140$[M-H- C_4H_8O_4]^-$, 337.0685$[M-H- 2C_4H_8O_4]^-$ | Chrysin-6,8-di-C-glucoside | Flavonoids | HQ | [7] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | $C_{27}H_{32}O_{14}$ | 13.75 | 581.1846 （-0.1） | ND | 581.1871$[M+H]^+$, 419.1337$[M+H-Glc]^+$, 257.0808$[M+H-2Glc]^+$, | ND | Glucoliquiritin | Flavonoids | GC | [6,8] |
| 37 | $C_{27}H_{30}O_{14}$ | 14.08 | 579.1700 （-1.5） | 577.1530 （-5.7） | 579.1665$[M+H]^+$, 561.1592$[M+H-H_2O]^+$, 543.1511$[M+H-2H_2O]^+$, 423.1077$[M+H-2H_2O-C_7H_5O_2]^+$, | 577.1510$[M-H]^-$, 457.1161$[M-H- C_4H_8O_4]^-$, 383.0722$[M-H- C_4H_8O_4-C_3H_6O_2]^-$ | Isoviolanthin | Flavonoids | GC | [6,9] |
| 38 | $C_{22}H_{22}O_{10}$ | 14.36 | 447.1287 （0.4） | ND | 447.1288$[M+H]^+$ 285.0752$[M+H-Glc]^+$, 270.0612$[M+H-Glc-CH_3]^+$, | ND | Calycosin-7-o-glucoside [a, c] | Flavonoids | GC | |
| 39 | $C_{27}H_{30}O_{16}$ | 14.6 | 611.1593 （-0.7） | 609.1026 （-5.8） | 611.1654$[M+H]^+$, 465.1046$[M+H-C_6H_{11}O_4]^+$, 303.0499$[M+H-C_{12}H_{21}O_9]^+$, | 609.1435$[M-H]^-$, 300.0262$[M-H-C_{12}H_{21}O_9]^-$, | Rutin[a, c] | Flavonoids | CH, DZ, GC | |
| 40 | $C_{21}H_{22}O_9$ | 14.62 | 419.1329 （-1.9） | 417.1158 （-7.4） | 257.0809$[M+H-Glc]^+$, 137.0229$[M+H-Glc-C_7H_5O_2]^+$, | 417.1188$[M-H]^-$, 255.0649$[M-H-Glc]^-$, 135.0069$[M-H-Glc-C_7H_5O_2]^-$, 119.0497 | Neoliquiritin | Flavonoids | GC | [10-12] |
| 41 | $C_{15}H_{12}O_4$ | 14.72 | 257.0806 （-0.7） | ND | 257.0815$[M+H]^+$, 147.0429$[M+H-C_6H_5O_2]^+$, 137.0224$[M+H-C_8H_7O]^+$, | ND | Isomer of isoliquiritigenin [c] | Flavonoids | GC | |
| 42 | $C_{26}H_{30}O_{13}$ | 14.74 | 551.1744 （-2.8） | 549.1571 （-7） | 257.0807$[M+H-Api-Glc]^+$, | 549.1563$[M-H]^-$, 255.0659$[M-H-Api-Glc]^-$, | Liquiritin apioside [a] | Flavonoids | GC | |
| 43 | $C_{15}H_{12}O_4$ | 15.00 | 257.0805 （-0.8） | ND | 257.0807$[M+H]^+$ 147.0432$[M+H-C_6H_5O_2]^+$, 137.0228$[M+H-C_8H_7O]^+$, | ND | Isomer of liquiritigenin [c] | Flavonoids | GC | |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | $C_{21}H_{22}O_9$ | 15.01 | 419.1321 （-3.0） | 417.1160 （-6.7） | 257.0801[M+H-Glc]$^+$, 137.0218[M+H-Glc-$C_8H_7O$]$^+$, | 417.1164[M-H]$^-$, 255.0657[M-H-Glc]$^-$, 135.0086[M-H-Glc-$C_8H_7O$]$^-$, | Liquiritin [a, c] | Flavonoids | GC | |
| 45 | $C_{29}H_{36}O_{15}$ | 15.02 | ND | 623.1947 （-5.6） | ND | 623.1940[M-H]$^-$, 461.1611[M-H-Glc]$^-$, 161.0234 | Acteoside [c] | Phenylpropanoids | HQ, GC | |
| 46 | $C_{21}H_{20}O_{12}$ | 15.14 | 465.1018 （-2.0） | 463.0852 （-6.5） | 465.0951[M+H]$^+$, 289.0698[M+H-$C_6H_8O_6$]$^+$, 169.0116[M+H-$C_6H_8O_6$-$C_8H_8O$]$^+$, | 417.1171[M+COOH]$^-$, 255.0655[M-H-HCOOH-Glc]$^-$, 135.0081[M-H-HCOOH-Glc-$C_8H_7O$]$^-$, | Viscidulin I, 2′-O-glucoside | Flavonoids | HQ | [13] |
| 47 | $C_{21}H_{18}O_{12}$ | 15.6 | 463.0864 （-1.5） | 461.0696 （-6.4） | 463.0865[M+H]$^+$, 287.0548[M+H-$C_6H_8O_6$]$^+$, | 461.0672[M-H]$^-$, 285.0396[M-H-$C_6H_8O_6$]$^-$, | Scutellarin [a] | Flavonoids | HQ | |
| 48 | $C_{21}H_{20}O_{12}$ | 15.88 | 465.1024 （-0.8） | 463.0848 （-7.2） | 465.1087[M+H]$^+$, 289.0699[M+H-$C_6H_8O_6$]$^+$, 169.0136[M+H-$C_6H_8O_6$-$C_8H_8O$]$^+$, | 463.0817[M-H]$^-$, 287.0537[M-H-$C_6H_8O_6$]$^-$, 269.0432[M-H-$C_6H_8O_6$-$H_2O$]$^-$, 166.9969[M-H-$C_6H_8O_6$-$C_8H_8O$]$^-$, | Carthamidin-7-O-glucuronide | Flavonoids | HQ | [14] |
| 49 | $C_{27}H_{30}O_{15}$ | 16.43 | 595.1634 （-0.6） | ND | 595.1688[M+H]$^+$, 433.1116[M+H-Glc]$^+$, 271.0596[M+H-2Glc]$^+$, | ND | Oroxin B [c] | Flavonoids | HQ | |
| 50 | $C_{23}H_{24}O_{12}$ | 16.56 | 493.1325 （-2.2） | ND | 493.1290[M+H]$^+$ 331.0795[M+H-Glc]$^+$, | ND | 5,2',6'-Trihydroxy-7,8-dimethoxyflavone 2′-O-glucoside | Flavonoids | HQ | [15] |
| 51 | $C_{21}H_{20}O_9$ | 16.8 | 417.1173 （-1.6） | 415.1011 (-5.6) | 417.1176, 399.1053[M+H-$H_2O$]$^+$, 381.0955[M+H-2$H_2O$]$^+$, 297.0748[M+H-$C_4H_8O_4$]$^+$, 279.0661[M+H-$H_2O$-$C_4H_8O_4$]$^+$ | 415.1016, 295.0607[M-H-$C_4H_8O_4$]$^-$, 267.0662[M-H-$C_4H_8O_4$-CO]$^-$ | Chrysin 8-C-glucoside [c] | Flavonoids | HQ | [5,16] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 52 | $C_{21}H_{22}O_{10}$ | 17.43 | ND | 433.1108 (-4.7) | ND | 433.1113<br>271.0600[M-H-Glc]- ,<br>151.0020[M-H-Glc-$C_7H_4O_2$]- | 5-Hydroxylliquiritin | Flavonoids | GC | [17] |
| 53 | $C_{20}H_{28}O_8$ | 18.01 | ND | 441.1740 （-3.5） | ND | 441.1735[M+COOH]$^-$,<br>215.1064[M-H-$C_6H_{12}O_6$]$^-$,<br>179.0549[M-H-$C_{14}H_{16}O_2$]$^-$,<br>143.0719[$C_7H_{11}O_3$]$^-$<br>89.0217[M-H- $C_6H_{11}O_5$-$C_7H_{12}O_3$]$^-$, | Lobetyolin [a] | Glycosides | DS | [4] |
| 54 | $C_{22}H_{20}O_{12}$ | 18.18 | 477.1007 （-2.5） | 475.0847 （-7.3） | 477.0995[M+H]$^+$,<br>301.0694[M+H- $C_6H_8O_6$]$^+$,<br>286.0463[M+H-$C_6H_8O_6$-$CH_3$]$^+$ | 475.0829[M-H]$^-$,<br>299.0550[M-H- $C_6H_8O_6$]$^-$,<br>284.0326[M-H- $C_6H_8O_6$-$CH_3$]$^-$,<br>175.0257[M-H-$C_{16}H_{12}O_6$]$^-$ | 5,7,2'-Trihydroxy-6-methoxyflavone-7-*O*-glucuronide | Flavonoids | HQ | [5] |
| 55 | $C_{21}H_{22}O_9$ | 18.48 | 419.1329 （-1.7） | ND | 419.1469[M+H]$^+$,<br>257.0811[M+H-Glc]$^+$,<br>239.0649[M+H-Glc-$H_2O$]$^+$,<br>149.0234, 137.0219 | ND | Isomer of liquiritin | Flavonoids | GC | [18] |
| 56 | $C_{26}H_{30}O_{13}$ | 18.49 | 551.1738 （-3.9） | 549.1575 （-6.4） | 419.1327[M+H-Api]$^+$,<br>257.0807[M+H-Api-Glc]$^+$,<br>137.0227[M+H-Api-Glc-$C_7H_5O_2$]$^+$, | 549.1570[M-H]$^-$,<br>255.0642[M-H-Api-Glc]$^-$,<br>135.0081[M-H-Api-Glc-$C_7H_5O_2$]$^-$, | Isoliquiritin apioside | Flavonoids | GC | [10] |
| 57 | $C_{26}H_{30}O_{13}$ | 18.84 | 551.1732 （-3.2） | 549.1577 （-6.7） | 551.1738[M+H]$^+$,<br>419.1325[M+H-Api]$^+$,<br>257.0796[M+H-Api-Glc]$^+$,<br>137.0210[M+H-Api-Glc-$C_7H_5O_2$]$^+$, | 549.1563[M-H]$^-$,<br>429.1024[M-H-$C_7H_5O_2$]$^-$,<br>255.0637[M-H-Api-Glc]$^-$, | Liguiritigenin-7-O-D-apiosyl-4′-O-D-glucoside | Flavonoids | GC | [10] |
| 58 | $C_{22}H_{22}O_9$ | 19.06 | 431.1324 （-3.0） | | 269.0803[M+H-Glc]$^+$, | ND | Ononin [c] | Flavonoids | GC | [18] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 59 | $C_{15}H_{10}O_6$ | 19.13 | 287.0542 （-1.2） | 285.0384 （-5.3） | 287.0540$[M+H]^+$, 269.0432$[M+H-H_2O]^+$, 241.0489$[M+H-H_2O-CO]^+$, 153.0162$[M+H-C_8H_6O_2]^+$, 139.0014$[M+H-C_9H_6O_2]^+$, | 285.0391$[M-H]^-$, 151.0024$[M-H-C_8H_6O_2]^-$, 107.0142$[M-H-C_8H_6O_2-CO_2]^-$, | Scutellarein | Flavonoids | HQ | [5] |
| 60 | $C_{21}H_{20}O_9$ | 19.17 | 417.1160 (-0.5) | 415.1030 (-1.2) | 417.1166, 381.0976$[M+H-2H_2O]^+$, 351.0848$[M+H-2H_2O-CH_2O]^+$, 321.0786$[M+H-2H_2O-C_2H_4O_2]^+$, 297.0746$[M+H-C_4H_8O_4]^+$, 267.0635$[M+H-C_5H_{10}O_5]^+$ | 415.1003, 325.0710$[M-H-C_3H_6O_3]^-$, 295.0572$[M-H-C_4H_8O_4]^-$, 267.0645$[M-H-C_4H_8O_4-CO]^-$, | Chrysin 6-C-glucoside | Flavonoids | HQ | [5,16] |
| 61 | $C_{21}H_{18}O_{12}$ | 19.24 | 463.0854 （0.6） | ND | 287.0532$[M+H- C_6H_8O_6]^+$, 269.0432$[M+H- C_6H_8O_6 -H_2O]^+$, 241.0468 | ND | Luteolin-7-O-β-D-glucuronide [c] | Flavonoids | HQ | [19] |
| 62 | $C_{21}H_{18}O_{11}$ | 19.26 | 447.0904 （-3.5） | 445.0745 （-6.8） | 447.0885$[M+H]^+$, 271.0583$[M+H-C_6H_8O_6]^+$, | 445.0727$[M-H]^-$, 269.0439$[M-H-C_6H_8O_6]^-$, | Baicalin [a] | Flavonoids | HQ, GC | |
| 63 | $C_{21}H_{22}O_9$ | 19.28 | 419.1324 （-3.1） | 417.1166 （-5.9） | 419.1321$[M+H]^+$, 257.0797$[M+H-Glc]^+$, 137.0224 | 417.1147$[M-H]^-$, 297.0711$[M-H-C_4H_8O_4]^-$, 255.0650$[M-H-Glc]^-$, 148.0163, 135.0082 | Isoliquiritin [a] | Flavonoids | GC | |
| 64 | $C_{42}H_{68}O14$ | 19.47 | ND | 795.4515 （-2.7） | ND | 841.4527$[M+COOH]^-$, 795.4515$[M-H]^-$, 633.4030$[M-H-Glc]^-$, | 21β-Hydroxysaikosaponin b2 | Triterpenoid saponin | CH | [20] |
| 65 | $C_{21}H_{22}O_9$ | 19.69 | 419.1322 （-3.5） | 417.1159 （-7.7） | 419.1338$[M+H]^+$, 257.0800$[M+H-Glc]^+$, 147.0424, 137.0234 | 417.1153$[M-H]^-$, 255.0656$[M-H-Glc]^-$, 135.0089, 119.0498 | Neoisoliquiritin | Flavonoids | GC | [11] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 66 | $C_{35}H_{36}O_{15}$ | 19.77 | 697.2121 （-0.9） | 695.1939 （-2.9） | 697.1801<br>257.0770$[M+H-C_{20}H_{25}O_{11}]^-$<br>167.0331 | 695.1927<br>549.1573$[M-H-C_9H_7O_2]^-$,<br>255.0639$[M-H-C_{20}H_{25}O_{11}]^-$ | Licorice glycoside B | Flavonoids | GC | [6] |
| 67 | $C_{15}H_{10}O_4$ | 20.24 | 255.0646（-2.3） | 253.0498 （-3.4） | 255.0642$[M+H]^+$<br>137.0227$[M+H-C_8H_6O]^+$ | 253.0495$[M-H]^-$,<br>135.0083$[M-H-C_8H_6O]^-$,<br>117.0345$[M-H-C_7H_4O_3]^-$, | 4′,7-Dihydroxyflavone | Flavonoids | GC | [21] |
| 68 | $C_{15}H_{12}O_5$ | 20.25 | 273.0747（-2.4） | ND | 273.0745$[M+H]^+$,<br>169.0115$[M+H-C_8H_8]^+$,<br>131.0472$[M+H-C_6H_4O_4]^+$, | ND | Dihydrobaicalein | Flavonoids | HQ | [22] |
| 69 | $C_{21}H_{20}O_{11}$ | 20.26 | 449.1057 （-4.7） | 447.0898 （-7.9） | 273.0748$[M+H-C_6H_8O_6]^+$<br>169.0124 | 447.0891$[M-H]^-$,<br>271.0597$[M-H-C_6H_8O_6]^-$, | Naringenin-7-O-Glu acid | Flavonoids | HQ | [23] |
| 70 | $C_{31}H_{40}O_{15}$ | 20.4 | ND | 651.2254 （-6.2） | ND | 651.2247$[M-H]^-$,<br>475.1895$[M-H-C_6H_8O_6]^-$,<br>175.0422 | Epimeredinoside A [c] | Glycosides | HQ | |
| 71 | $C_{21}H_{20}O_{11}$ | 20.62 | 449.1043 （-5.0） | 447.0898 （-7.1） | 449.0977$[M+H]^+$,<br>273.0736$[M+H-C_6H_8O_6-C_8H_8]^+$,<br>169.0121 | 447.0895$[M-H]^-$,<br>271.0606$[M-H-C_6H_8O_6]^-$,<br>243.0661$[M-H-C_6H_8O_6-CO]^-$, | 5,6,7-Trihydroxy flavanone (Dihydroxybaicalein)-7-O-glucuronide | Flavonoids | HQ | [5,24] |
| 72 | $C_{21}H_{18}O_{11}$ | 20.75 | 447.0905 （-3.2） | 445.0745 （-6.3） | 447.0912$[M+H]^+$,<br>271.0597$[M+H-C_6H_8O_6]^+$, | 445.0738$[M-H]^-$,<br>269.0444$[M-H-C_6H_8O_6]^-$, | Baicalein 6-O-glucuronide | Flavonoids | HQ | [23] |
| 73 | $C_{22}H_{20}O_{12}$ | 20.92 | 477.1007 （-4.2） | 475.0846 （-4.9） | 477.1019$[M+H]^+$,<br>301.0696$[M+H-C_6H_8O_6]^+$,<br>286.0462$[M+H-C_6H_8O_6-CH_3]^+$ | 475.0858$[M-H]^-$,<br>299.0560$[M-H-C_6H_8O_6]^-$,<br>284.0311$[M-H-C_6H_8O_6-CH_3]^-$,<br>175.0241$[M-H-C_{16}H_{12}O_6]^-$ | 5,7,8-Trihydroxy-6-methoxyflavone-7-O-glucuronide | Flavonoids | HQ | [5,16] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 74 | $C_{22}H_{22}O_{10}$ | 21.06 | 447.0904 （-3） | ND | 447.0913$[M+H]^+$, 285.0745$[M+H-Glc]^+$, 271.0596$[M+H-C_6H_8O_6]^+$, | ND | Wogonin 7-glucoside | Flavonoids | HQ | [5,24] |
| 75 | $C_{31}H_{40}O_{15}$ | 21.2 | ND | 651.2257 （-5.8） | ND | 651.2244$[M-H]^-$, 351.0559$[M-H-C_9H_{11}O_2-C_9H_9O_2]^-$, 175.0394$[M-H-C_9H_{11}O_2-C_{12}H_{20}O_{10}]^-$ | Isomartynoside | Glycosides | HQ | [5] |
| 76 | $C_{15}H_{12}O_4$ | 21.31 | 257.0808 （-0.2） | 255.0656 （-2.8） | 257.0801$[M+H]^+$, 147.0425$[M+H-C_6H_5O_2]^+$, 137.0218$[M+H-C_8H_7O]^+$, | 255.0669$[M-H]^-$, 219.8440$[M-H-2H_2O]^-$, 201.8325$[M-H-3H_2O]^-$, 135.0082$[M-H-C_8H_7O]^-$, 119.0498$[M-H-C_7H_5O_3]^-$, 91.0199$[M-H-C_7H_5O_3-C_2H_4]^-$, | Liquiritigenin [a, c] | Flavonoids | GC | [15] |
| 77 | $C_{22}H_{20}O_{11}$ | 21.37 | 461.1064 （-3.2） | 459.0904 （-6.3） | 461.1058$[M+H]^+$, 285.0745$[M+H-C_6H_8O_6]^+$, 270.0518$[M+H-C_6H_8O_6-CH_3]^+$, | 459.0884$[M-H]^-$, 283.0599$[M-H-C_6H_8O_6]^-$, 268.0369$[M-H-C_6H_8O_6-CH_3]^-$, 175.0240, 113.0234 | Oroxyloside (Oroxylin A-7-O-glucuronide) | Flavonoids | HQ | [23] |
| 78 | $C_{42}H_{64}O_{16}$ | 21.42 | 825.4241 (-0.2) | 823.4093 (-3.5) | 825.4147 649.3935 455.3506$[M+H-C_{12}H_{16}O_{13}]^+$, | 823.4092 | Licorice saponin J2 | Triterpenoid saponin | GC | [5] |
| 79 | $C_{22}H_{20}O_{12}$ | 21.64 | 477.1010 （-3.7） | 475.0848 （-6.4） | 477.1020$[M+H]^+$, 301.0701$[M+H-C_6H_8O_6]^+$, 286.0472$[M+H-C_6H_8O_6-CH_3]$ | 475.0853$[M-H]^-$, 299.0554$[M-H-C_6H_8O_6]^-$, 284.0313$[M-H-C_6H_8O_6-CH_3]^-$, | 5,6,7-Trihydroxy-8-methoxyflavone-7-O-glucuronide | Flavonoids | HQ | [6] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 80 | $C_{42}H_{70}O_{14}$ | 21.94 | 799.4790 （-6） | 797.4646 （-2.9） | ND | 843.4675[M+COOH]$^-$, 797.4646[M-H]$^-$, 635.4054[M-H-Glc]$^-$ | Hydroxysaikosaponin A | Triterpenoid saponin | CH | [5,24] |
| 81 | $C_{16}H_{12}O_5$ | 22.31 | 285.0746 （-2.6） | 283.0589 （-1） | 285.0750[M+H]$^+$, 270.0512[M+H-$CH_3$]$^+$, | 283.0587[M-H]$^-$, 268.0364[M-H-$CH_3$]$^-$, 163.0043[M-H-$CH_3$-$C_7H_5O$]$^-$, | Isomer of wogonin | Flavonoids | HQ | [20] |
| 82 | $C_{22}H_{20}O_{11}$ | 22.32 | 461.1062 （-3.1） | 459.0900 （-6.2） | 461.1048[M+H]$^+$, 285.0744[M+H-$C_6H_8O_6$]$^+$, 270.0514[M+H-$C_6H_8O_6$-$CH_3$]$^+$, | 459.0900[M-H]$^-$, 283.0598[M-H-$C_6H_8O_6$]$^-$, 268.0363[M-H-$C_6H_8O_6$-$CH_3$]$^-$, 175.0249 113.0241 | Wogonoside [a] | Flavonoids | HQ | |
| 83 | $C_{15}H_{10}O_7$ | 22.4 | 303.0502 （0.8） | 301.0354 （0） | ND | 301.0299[M-H]$^-$, 178.9955[M-H-$C_6H_4O_3$]$^-$, 151.0064[M-H-$C_8H_6O_3$]$^-$, | Quercetin [a] | Flavonoids | CH | |
| 84 | $C_{48}H_{72}O_{21}$ | 22.69 | 985.4640 （0.1） | 983.4446 （-4.4） | 985.4612 809.4258[M+H-$C_6H_8O_6$]$^+$, 647.3756[M+H-$C_6H_8O_6$-$C_6H_{10}O_5$]$^+$, 615.3866[M+H-$C_6H_8O_6$-$C_6H_8O_7$]$^+$ 453.3352[M+H-$C_6H_8O_6$-$C_6H_{10}O_5$-$C_6H_8O_7$]$^+$ | 983.4468 | Licorice saponin A3 | Triterpenoid saponin | GC | [6] |
| 85 | $C_{42}H_{62}O_{17}$ | 24.21 | 839.4021 （-4.6） | 837.3871 （-4.7） | 839.4033[M+H]$^+$, 663.3747[M+H-Glc]$^+$, 469.3297[M+H-2Glc-$H_2O$]$^+$, | 837.3855[M-H]$^-$, | Uralsaponin N | Triterpenoid saponin | GC | [6] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 86 | $C_{16}H_{12}O_6$ | 24.71 | 301.0699 （-0.4） | 299.0547 （-4.6） | 301.0713<br>286.0472$[M+H-CH_3]^+$,<br>168.0128$[M+H-CH_3-C_8H_6O]^+$ | 299.0550<br>284.0303$[M-H-CH_3]^-$,<br>136.9875 | Trihydroxy-methoxyfavone | Flavonoids | HQ | [12] |
| 87 | $C_{15}H_{10}O_5$ | 25.54 | 271.0594 （-2.5） | 269.0444 （-3） | 271.0599$[M+H]^+$,<br>169.0133$[M+H-C_8H_6]^+$ | 269.0446$[M-H]^-$,<br>225.0537$[M-H-CO_2]^-$,<br>197.0606$[M-H-CO_2-CO]^-$,<br>171.0433 | Norwogonin | Flavonoids | HQ | [5,15] |
| 88 | $C_{48}H_{78}O_{17}$ | 25.61 | 927.5252 （-1.7） | 925.5058 （-3.2） | 927.5343$[M+H]^+$,<br>747.4375$[M+H-C_6H_{11}O_6]^+$,<br>603.4330$[M+H-C_6H_{11}O_5-C_6H_{11}O_4-CH_3]^+$,<br>421.3416$[M+H-2C_6H_{11}O_5-C_6H_9O_5-H_2O]^+$,<br>309.1190 | 971.5080$[M+COOH]^-$,<br>925.5058$[M-H]^-$ | Saikosaponin c [a] | Triterpenoid saponin | CH | [5] |
| 89 | $C_{16}H_{12}O_6$ | 25.7 | 301.0699 （-2.6） | 299.0544 （-4.8） | 301.0698$[M+H]^+$,<br>286.0459$[M+H-CH_3]^+$,<br>183.9985$[M+H-CH_3-C_8H_6]^+$, | 299.0547$[M-H]^-$,<br>284.0312$[M-H-CH_3]^-$,<br>153.9900$[M-H-CH_3-C_9H_6O]^-$ | 5,7,8-Trihydroxy-6-methoxyflavone | Flavonoids | HQ | [25] |
| 90 | $C_{15}H_{10}O_5$ | 26.17 | 271.0595 （-2.2） | 269.0442 （-3.6） | 271.0592$[M+H]^+$<br>123.0068$[M+H-H_2O-C_9H_6O]^+$, | 269.0435$[M-H]^-$,<br>169.0656$[M-H-C_8H_6]^-$, | Baicalein [a] | Flavonoids | HQ | [26] |
| 91 | $C_{42}H_{62}O_{17}$ | 26.2 | 839.4060 （0.1） | 837.3867 （-5.1） | 839.3984$[M+H]^+$,<br>663.3678$[M+H-Glc]^+$,<br>487.3388$[M+H-2Glc]^+$,<br>469.3286$[M+H-2Glc-H_2O]^+$, | 837.3866$[M-H]^-$, | Yunganoside K2 | Triterpenoid saponin | GC | [6] |
| 92 | $C_{48}H_{80}O_{17}$ | 26.44 | 929.5457 （-1.2） | 927.5261 (-4.2) | 929.5431<br>767.4906$[M+H-Glc]^+$, | 973.5311$[M+COOH]^-$<br>927.5261$[M-H]^-$ | Saikosaponin f | Triterpenoid saponin | CH | [6] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | 471.1678[M+H-Glc-$C_6H_{11}O_4$-$C_5H_8O_5$]$^+$,<br>441.3737[M+H-2$C_6H_9O_6$-$C_6H_{11}O_4$]$^+$,<br>423.3608[M+H-2Glc-$C_6H_{11}O_4$-2$H_2O$]$^+$, | | | | | |
| 93 | $C_{42}H_{62}O_{17}$ | 26.99 | 837.3871<br>（-2.7） | 837.3871<br>（-5.2） | 839.4016[M+H]$^+$,<br>663.3718[M+H-Glc]$^+$,<br>487.3405[M+H-2Glc]$^+$,<br>469.3302[M+H-2Glc-$H_2O$]$^+$, | 837.3869[M-H]$^-$, | Licorice saponin G | Triterpenoid saponin | GC | [25] |
| 94 | $C_{16}H_{12}O_6$ | 27.07 | 301.0709<br>（0.9） | 299.0551<br>（-3.5） | 301.0702<br>286.0478[M+H-$CH_3$]$^+$,<br>168.0050 | 299.0534<br>284.0319[M-H-$CH_3$]$^-$,<br>137.9952 | Hispidulin | Flavonoids | HQ | [6,12] |
| 95 | $C_{42}H_{62}O_{17}$ | 27.37 | 839.4023<br>（-4.3） | 837.3874<br>（-4.6） | 839.4030[M+H]$^+$,<br>645.3597[M+H-Glc-$H_2O$]$^+$,<br>487.3383[M+H-2Glc]$^+$,<br>469.3294[M+H-2Glc-$H_2O$]$^+$, | 837.3872[M-H]$^-$, | Licorice saponin G2 | Triterpenoid saponin | GC | [27] |
| 96 | $C_{15}H_{12}O_4$ | 27.6 | 257.0805<br>（-1.3） | 255.0655<br>（-2.9） | 257.0806[M+H]$^+$,<br>147.0424[M+H-$C_6H_5O_2$]$^+$,<br>137.0219[M+H-$C_8H_7O$]$^+$, | 255.0659[M-H]$^-$,<br>219.8439[M-H-2$H_2O$]$^-$,<br>201.8345[M-H-3$H_2O$]$^-$,<br>135.0078[M-H-$C_8H_7O$]$^-$,<br>119.0497[M-H-$C_7H_5O_3$]$^-$,<br>91.0179[M-H-$C_7H_5O_3$-$C_2H_4$]$^-$, | Isoliquiritigenin [a, c] | Flavonoids | GC | [6] |
| 97 | $C_{42}H_{62}O_{16}$ | 27.74 | 823.4069<br>（-4.8） | 821.3922<br>（-5.3） | 823.4046[M+H]$^+$,<br>647.3737[M+H-$C_6H_9O_6$]$^+$,<br>453.3321[M+H-$C_6H_9O_6$-$C_6H_8O_7$]$^+$, | 821.3885[M-H]$^-$, | Glycyrrhizic acid [a] | Triterpenoid saponin | GC | |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 98 | $C_{16}H_{12}O_4$ | 27.88 | 269.0807 （-0.5） | 267.0649 （0.8） | 269.0802$[M+H]^+$, | 267.0647$[M-H]^-$, 252.0428$[M-H-CH_3]^-$, | Formononetin [a,c] | Flavonoids | GC | |
| 99 | $C_{42}H_{68}O_{13}$ | 28.74 | 781.4694 （-5.0） | 779.4536 （-6.5） | 781.4638$[M+H]^+$, 745.4519$[M+H-2H_2O]^+$, 619.4267$[M+H-Glc]^+$, 455.3498$[M+H-Glc-H_2O-Fuc]^+$, 437.3397$[M+H-Glc-2H_2O-Fuc]^+$, 419.3331$[M+H-Glc-3H_2O-Fuc]^+$, | 779.4585$[M-H]^-$, 617.4278$[M-H-Glc]^-$, | Saikosaponin a [a] | Triterpenoid saponin | CH | |
| 100 | $C_{42}H_{64}O_{15}$ | 28.77 | 809.4039 （-1.2） | 807.4125 （-5） | 809.4331 633.3988$[M+H-C_6H_9O_6]^+$, 457.3668$[M+H-C_6H_9O_6-C_6H_8O_6]^+$, 439.3576$[M+H-C_6H_9O_6-C_6H_8O_6-H_2O]^+$, | 807.4097 351.0550 | Licorice saponin B2 | Triterpenoid saponin | GC | [6] |
| 101 | $C_{30}H_{46}O_3$ | 28.99 | 455.3501 （-4.1） | ND | 455.3469$[M+H]^+$, 437.3337$[M+H-H_2O]^+$, 419.3270$[M+H-2H_2O]^+$, 407.3309$[M+H-H_2O-2CH_3]^+$, | ND | Betulonicacid [c] | Terpenoids | CH, DZ | [6,28,29] |
| 102 | $C_{42}H_{68}O_{13}$ | 29.01 | 781.4689 （-5.6） | 779.4550 （-4.7） | 763.4559$[M+H-H2O]^+$, 619.4174$[M+H-Glc]^+$, 455.3496$[M+H-Glc-H_2O-Fuc]^+$, 437.3399$[M+H-Glc-2H_2O-Fuc]^+$, 419.3257$[M+H-Glc-3H_2O-Fuc]^+$, | 779.4516$[M-H]^-$, 617.4070$[M-H-Glc]^-$, | Saikosaponin $b_2$ [a] | Triterpenoid saponin | CH | [28,29] |
| 103 | $C_{42}H_{62}O_{16}$ | 29.06 | 823.4065 （-5.2） | 821.3917 （-5.7） | 823.4081$[M+H]^+$, 647.3743$[M+H-C_6H_9O_6]^+$, 453.3335$[M+H-C_6H_9O_6-C_6H_8O_7]^+$, | 821.3874$[M-H]^-$, | Uralsaponin B | Triterpenoid saponin | GC | [6] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 104 | $C_{21}H_{20}O_6$ | 29.41 | 369.1323 （-2.6） | 367.1162 （-6.8） | 369.1289$[M+H]^+$, 313.0713$[M+H-C_3H_4O]^+$, 271.0602$[M+H-2CH_2O-2H_2O]^+$ | 367.1171$[M-H]^-$, 309.0395$[M-H-2CH_2O]^-$ | Curcumin [c] | Phenolic acids | SJ | [6] |
| 105 | $C_{48}H_{76}O_{19}$ | 29.48 | 957.5049 （-0.5） | 955.4845 （-6.1） | 957.5024 811.4426$[M+H-C_6H_{10}O_4]^+$, 599.3877$[M+H-C_6H_{10}O_4-C_6H_8O_6-2H_2O]^+$, 441.3682$[M+H-C_6H_{10}O_4-2C_6H_8O_6-2H_2O]^+$, 423.3613$[M+H-C_6H_{10}O_4-2C_6H_8O_6-3H_2O]^+$, 353.0702$[C_{12}H_{16}O_{12}]$ | 955.4848 | Yunganoside A1 | Triterpenoid saponin | GC | [6] |
| 106 | $C_{30}H_{46}O_3$ | 30.14 | 455.3499 （-4.6） | ND | 455.3491$[M+H]^+$, 437.3347$[M+H-H_2O]^+$, 419.3246$[M+H-2H_2O]^+$, | ND | Isomer of Betulonic acid [c] | Terpenoids | CH | [6] |
| 107 | $C_{44}H_{70}O_{14}$ | 30.33 | 823.4813 （-3.1） | 821.4613 （-4.8） | 823.4805$[M+H]^+$, 647.3682 455.3512$[M+H-C_2H_2O$-Glc-Fuc-$H_2O]^+$, 437.3386$[M+H-C_2H_2O$-Glc-Fuc-$2H_2O]^+$, | 867.4665$[M+COOH]^-$, 821.4613$[M-H]^-$, 779.4516$[M-H-C_2H_2O]^-$, 761.4461$[M-H-C_2H_2O-H_2O]^-$, 617.3947$[M-H-C_2H_2O$-Glc$]^-$ | 2″-O-Acetyl-Saikosaponin a | Triterpenoid saponin | CH | [20] |
| 108 | $C_{42}H_{64}O_{16}$ | 30.5 | 825.4259 （-1） | 823.4073 （-5.8） | 825.4260$[M+H]^+$, 455.3499$[M+H-2C_6H_8O_6-H_2O]^+$, 437.3416$[M+H-2C_6H_8O_6-2H_2O]^+$ | 823.4065 351.0539[M-H-2Glc]$^-$ | Uralsaponin C | Triterpenoid saponin | GC | [20] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 109 | $C_{30}H_{46}O_3$ | 30.58 | 455.3498 （4.8） | ND | 455.3504$[M+H]^+$, 407.3294$[M+H-H_2O-2CH_3]^+$, | ND | Isomer of betulonic acid [c] | Terpenoids | CH | [25] |
| 110 | $C_{42}H_{68}O_{13}$ | 30.65 | 781.4696 （-4.6） | 826.4630 （-9.6） | 763.4532$[M+H-H_2O]^+$, 601.4086[M+H-Glc-H2O]$^+$, 455.3492[M+H-Glc-H2O-Fuc]$^+$, 437.3391[M+H-Glc-2H2O-Fuc]$^+$, 419.3282[M+H-Glc-3H2O-Fuc]$^+$, | 826.4621$[M+COOH]^-$, 780.4575 618.4015[M-Glc]$^-$, | Saikosaponin b1 [a] | Triterpenoid saponin | CH | |
| 111 | $C_{44}H_{70}O_{14}$ | 30.75 | 823.4762 （-5.6） | 821.4645 （-5.2） | 823.4070$[M+H]^+$, 805.4739$[M+H-H_2O]^+$, 611.3492 455.3484$[M+H-C_2H_2O$-Glc-Fuc-$H_2O]^+$ , 453.3362$[M+H-C_2H_2O$-Glc-Fuc-$2H_2O]^+$ | 867.4697$[M+COOH]^-$, 821.4645$[M-H]^-$, 779.4562$[M-H-C_2H_2O]^-$, 761.4430$[M-H-C_2H_2O-H_2O]^-$, | 2″-O-Acetyl-Saikosaponin b2 | Triterpenoid saponin | CH | [20] |
| 112 | $C_{16}H_{12}O_5$ | 31.14 | 285.0750 （-2.8） | 283.0599 （-2.4） | 285.0745$[M+H]^+$, 270.0511$[M+H-CH_3]^+$, | 283.0602$[M-H]^-$, 268.0362$[M-H-CH_3]^-$, 163.0029$[M-H-CH_3-C_7H_5O]^-$, | Wogonin [a, c] | Flavonoids | HQ | [20] |
| 113 | $C_{36}H_{58}O_8$ | 31.31 | ND | 617.3953 (-4.3). | ND | 663.4081$[M+COOH]^-$, 617.3593$[M-H]^-$, | Prosaikogenin F | Triterpenoid saponin | CH | [20] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 114 | $C_{42}H_{62}O_{15}$ | 31.44 | 807.4110 （-6.4） | 805.3977 （-4.4） | 807.4176<br>631.3825$[M+H-C_6H_8O_6]^+$,<br>455.3489$[M+H-C_{12}H_{16}O_{12}]^+$,<br>437.3404$[M+H-C_{12}H_{17}O_{13}]^+$,<br>419.3287$[M+H-C_{12}H_{17}O_{13}-H_2O]^+$ | 805.3985<br>351.0542$[M-H-C_{30}H_{45}O_3]^-$ | Licorice saponin $C_2$ | Triterpenoid saponin | GC | [25] |
| 115 | $C_{17}H_{14}O_6$ | 31.47 | 315.0855 （-2.5） | ND | 315.0843$[M+H]^+$,<br>300.0611$[M+H-CH_3]^+$,<br>285.0385$[M+H-2CH_3]^+$,<br>282.0518$[M+H-CH_3-H_2O]^+$,<br>182.9911$[M+H-C_9H_8O]^+$,<br>154.9966{$M+H-C_{10}H_8O_2]^+$, | ND | 5,7-Dihydroxy-6,8-dimethoxyfavone | Flavonoids | HQ | [6] |
| 116 | $C_{15}H_{10}O_4$ | 31.59 | 255.0649 （-1.3） | 253.0497 （-3.7） | 255.0645$[M+H]^+$,<br>153.0159 | 253.0494$[M-H]^-$,<br>209.0600$[M-H-CO_2]^-$,<br>143.0500 | Chrysin [a] | Flavonoids | HQ, GC | [5,24] |
| 117 | $C_{19}H_{18}O_8$ | 31.71 | 375.1060 （-3.9） | 373.0903 （-6.9） | 375.0809$[M+H]^+$,<br>345.0586$[M+H-2CH_3]^+$,<br>327.0477$[M+H-2CH_3-H_2O]^+$,<br>197.0074$[M+H-C_{10}H_{10}O_3]^+$, | 373.0906$[M-H]^-$,<br>358.0668$[M-H-CH_3]^-$,<br>343.0435$[M-H-2CH_3]^-$,<br>328.0199$[M-H-3CH_3]^-$,<br>300.0228$[M-H-3CH_3-CO]^-$,<br>151.9756$[M-H-C_{11}H_{11}O_5]^-$, | Skullcapflavone II (Neobaicalein) | Flavonoids | HQ | [5] |
| 118 | $C_{16}H_{12}O_5$ | 32.24 | 285.0750 （-2.7） | 283.0601 （-3.9） | 285.0752$[M+H]^+$,<br>270.0517$[M+H-CH_3]^+$,<br>168.0048 | 283.0588$[M-H]^-$,<br>268.0365$[M-H-CH_3]^-$, | Oroxylin A | Flavonoids | HQ | [5] |
| 119 | $C_{44}H_{70}O_{14}$ | 32.35 | 823.4798 （-4） | 821.3890 （-4.9） | 823.4716$[M+H]^+$,<br>805.4647$[M+H-H_2O]^+$,<br>455.3489$[M+H-C_2H_2O$-Glc-Fuc-$H_2O]^+$ ,<br>437.3394$[M+H-C_2H_2O$-Glc-Fuc-$2H_2O]^+$ , | 821.4589$[M-H]^-$,<br>779.4503$[M-H-C_2H_2O]^-$,<br>761.4277$[M-H-C_2H_2O-H_2O]^-$,<br>617.4114$[M-H-C_2H_2O$-Glc$]^-$ | 3″-O-Acetyl-Saikosaponin b2 | Triterpenoid saponin | CH | [15,30] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | 419.3278[M+H-$C_2H_2O$-Glc-Fuc-$3H_2O$]$^+$ | | | | | |
| 120 | $C_{42}H_{68}O_{12}$ | 32.45 | ND | 763.4553 （-4.6） | ND | 809.4574[M-H+HCOOH]$^-$, 763.4553[M-H]$^-$, 601.4477[M-H-$C_6H_{10}O_5$]$^-$ | Saikosaponin m | Triterpenoid saponin | CH | [20] |
| 121 | $C_{20}H_{18}O_6$ | 32.71 | 355.1162 （-3.9） | 353.1008 （-6.4） | 355.1161 299.0565[M+H-$C_4H_7$]$^+$ | 353.1004 285.1101[M-H-$C_5H_9$]$^-$ , 163.0011[M-H-$C_5H_9$-$C_6H_4O_3$]$^-$ , | Licoisoflavone A | Flavonoids | GC | [25] |
| 122 | $C_{21}H_{20}O_6$ | 32.84 | 369.1330 （-0.6） | 367.1166 （-5.8） | 369.1313 313.0691[M+H-$C_4H_7$]$^+$, 285.0744[M+H-$C_5H_9$-$CH_3$]$^+$, 271.0583[M+H-$C_5H_9$-$CH_3O$]$^+$ 243.0587 | 367.1175 309.0390[M-H-$C_3H_6$-$CH_3$]$^-$, 297.0398[M-H-$C_5H_9$]$^-$ , 284.0287[M-H-$C_5H_9$-$CH_3$]$^-$ | Glycycoumarin | Phenylpropanoids | GC | [6] |
| 123 | $C_{36}H_{58}O_8$ | 32.85 | ND | 617.4028 （-6.9） | ND | 663.4065[M+COOH]$^-$, 617.4246[M-H]$^-$ | Prosaikogenin D | Triterpenoid saponin | CH | [6] |
| 124 | $C_{42}H_{68}O_{12}$ | 33.08 | ND | 763.4554 （-3.8） | ND | 809.4136[M+COOH]$^-$, 763.4554[M-H]$^-$, 601.4007[M-H-$C_6H_{10}O_5$]$^-$ | Saikosaponin e | Triterpenoid saponin | CH | [25] |
| 125 | $C_{36}H_{58}O_8$ | 33.34 | ND | 617.3950 （-3.8） | ND | 663.4025[M+COOH]$^-$, 617.4454[M-H]$^-$ | Prosaikogenin G | Triterpenoid saponin | CH | [25] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 126 | $C_{20}H_{16}O_6$ | 33.48 | 353.1018 （-0.4） | 351.0849 （-5.5） | 353.1016<br>153.0175$[M+H-C_{13}H_{12}O_2]^+$ | 351.0847<br>321.0396$[M-H-2CH_3]^-$,<br>203.0367$[M-H-C_7H_4O_4]^-$, | Licoisoflavone B | Flavonoids | GC | [25] |
| 127 | $C_{44}H_{70}O_{14}$ | 33.66 | 823.4827 （-1.4） | 821.4650 （-4.4） | 823.4812$[M+H]^+$,<br>805.4756$[M+H-H_2O]^+$,<br>641.4089<br>455.3510$[M+H-C_2H_2O$-Glc-Fuc-$H_2O]^+$ ,<br>437.3392$[M+H-C_2H_2O$-Glc-Fuc-$2H_2O]^+$ ,<br>419.3276$[M+H-C_2H_2O$-Glc-Fuc-$3H_2O]^+$ , | 867.4648$[M+COOH]^-$,<br>821.1650$[M-H]^-$, | 4″-O-Acetyl-Saikosaponin A | Triterpenoid saponin | CH | [6] |
| 128 | $C_{44}H_{70}O_{14}$ | 34.04 | 823.4815 （-2.9） | 821.4648 （-4.6） | 823.4805$[M+H]^+$,<br>805.4653$[M+H-H_2O]^+$,<br>787.4477<br>455.3505$[M+H-C_2H_2O$-Glc-Fuc-$H_2O]^+$ ,<br>437.3398$[M+H-C_2H_2O$-Glc-Fuc-$2H_2O]^+$ , | 867.4702$[M+COOH]^-$,<br>821.4648$[M-H]^-$, | 4″-O-Acetyl Saikosaponin B2 | Triterpenoid saponin | CH | [20] |
| 129 | $C_{46}H_{72}O_{15}$ | 34.61 | 865.4934 （-1.2） | 863.4714 （-5.2） | ND | 909.4688$[M+COOH]^-$,<br>863.4714$[M-H]^-$,<br>821.4593$[M-H-C_2H_2O]^-$,<br>761.4691$[M-H-2C_2H_2O-H_2O]^-$,<br>617.3882$[M-H-2C_2H_2O$-Glc$]^-$, | Diacetyl Saikosaponin A | Triterpenoid saponin | CH | [20] |
| 130 | $C_{20}H_{18}O_6$ | 34.89 | 355.1174 （-0.6） | 353.1008 （-5.8） | 355.1134<br>299.0543$[M+H-C_4H_7]^+$ | 353.1011<br>285.1110$[M-H-C_5H_9]^-$ ,<br>125.0236$[M-H-C_5H_9-C_9H_6O_3]^-$ | Gancaonin L | Flavonoids | GC | [20] |
| 131 | $C_{20}H_{20}O_4$ | 36.08 | ND | 323.1273 （-4.6） | ND | 323.1259$[M-H]^-$,<br>201.0920$[M-H-H_2O]^-$,<br>135.0451$[M-H-C_{12}H_{12}O_2]^-$, | Glabridin [c] | Flavonoids | GC | [6] |

| No. | formula | $t_R$, min | $[M+H]^+$ (error, ppm) | $[M-H]^-$ (error, ppm) | Major fragment ions in positive mode (m, z) [b] | Major fragment ions in negative mode (m, z) [b] | identification | Structure type | Source | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| 132 | $C_{21}H_{22}O_5$ | 37.92 | 355.1517 （-6.6） | 353.1380 （-4） | 355.1069<br>189.0923$[M+H-CH_3-C_8H_6O_3]^+$<br>153.0529$[M+H-C_{13}H_{14}O_2]^+$ | 353.1358<br>338.1126$[M-H-CH_3]^-$<br>150.0316$[M-H-CH_3-C_{12}H_{13}O_2]^-$ | Licochalcone D | Flavonoids | GC | [20] |
| 133 | $C_{30}H_{46}O_4$ | 39.82 | 471.3454 （-3.1） | 469.3278 （-8.5） | 471.3442$[M+H]^+$, | 469.3279$[M-H]^-$,<br>425.3379$[M-H-CO_2]^-$, | Glycyrrhetinic acid （enoxolone）[a, c] | Triterpenoid saponin | GC | [6] |

Footnote:“a” Compared with reference standards; “b” The losses are: Glc= glucose moiety, Fuc= fructose；ND=not detect；“c” Confirmation in comparison with mass spectral library (Natural Products HR-MS, MS Spectral Library, Version 1.0; AB Sciex, Foster City, USA).

CH：Bupleuri Radix，HQ：Scutellariae radix，SJ：Zingiberis rhizoma recens，JBX：Pinelliae rhizoma praeparatum cum zingibere et alumine，DZ：Jujubae fructus，DS：Codonopsis radix，GC：Glycyrrhizae Radix.

**Table S3** Results of calibration curve and content for the determination of 9 compounds

| **Name** | **Regression equation** | **$R^2$** | **Linear range (μg/ml)** | **Contents (mg/g)** |
|---|---|---|---|---|
| baicalin | y = 6.7581x + 0.4186 | 0.9961 | 0.53~4.74 | 3.25 |
| baicalein | y = 4.8933x + 9.445 | 0.9999 | 1.24~11.20 | 0.34 |
| Wogonin | y = 6.8079x + 0.4146 | 0.9983 | 6.32~61.97 | 0.2 |
| Wogonoside | y = 5.5312 x + 3.6203 | 0.9990 | 9.77~87.89 | 2.8 |
| quercetin | y = 6.3909x + 0.4414 | 0.9991 | 0.08~0.72 | 0.01 |
| Saikosaponin B1 | y = 3.8802x + 0.4141 | 0.9994 | 0.86~7.73 | 0.2 |
| Saikosaponin B2 | y = 3.854x + 0.4052 | 0.9998 | 0.89~7.97 | 0.25 |
| glycyrrhizic acid | y = 5.0736x + 8.023 | 0.9974 | 1.15~10.34 | 2.05 |
| Liquiritin | y = 4.8287x + 0.9097 | 0.9955 | 1.10~9.82 | 0.54 |

**Table S4** The active ingredients of XCHG

| Name | chemical compound |
|---|---|
| X1 | Glycyrrhetinic Acid |
| X2 | 5,7,8-Trihydroxy-6-methoxyflavone |
| X3 | Aspartic acid |
| X4 | Baicalein |
| X5 | Betulonic acid |
| X6 | Curcumin |
| X7 | Desaminotyrosine |
| X8 | Formononetin |
| X9 | Glabridin |
| X10 | Glycyrrhizic acid |
| X11 | Isoliquiritigenin |
| X12 | Licoisoflavone A |
| X13 | Licoisoflavone B |
| X14 | Licoricesaponin G2 |
| X15 | liquiritigenin |
| X16 | Liquiritin |
| X17 | Proline |
| X18 | Quercetin |
| X19 | Saikosaponin A |
| X20 | Saikosaponin B1 |
| X21 | Saikosaponin B2 |
| X22 | Saikosaponin C |
| X23 | Valine |
| X24 | Wogonin |
| X25 | Wogonoside |
| X26 | Dihydrobaicalein |
| X27 | Baicalin |
| X28 | Neobaicalein |
| X29 | Adenosine |
| X30 | Lobetyolin |

**Table S5** Enriched KEGG signaling pathway/GO biological process of XCHG-fever targets

| **Biological functional modules** | **Type** | **GO biological process/ KEGG signaling pathway** | ***p*-value** |
|---|---|---|---|
| Inflammation/Immune | KEGG | NF-kappa B signaling pathway | 9.72E-10 |
| | KEGG | TNF signaling pathway | 2.55E-15 |
| | GO | inflammatory response | 1.38E-16 |
| Neuromodulation | KEGG | Neuroactive ligand-receptor interaction | 1.94E-04 |
| | KEGG | Serotonergic synapse | 1.98E-07 |
| | KEGG | Inflammatory mediator regulation of TRP channels | 8.70E-05 |
| | GO | calcium-mediated signaling | 1.17E-05 |
| Vasodilatory | KEGG | Relaxin signaling pathway | 1.79E-10 |
| | GO | positive regulation of nitric oxide biosynthetic process | 1.73E-13 |
| | GO | response to muscle stretch | 3.97E-07 |
| Metabolism | KEGG | Endocrine resistance | 2.13E-20 |
| | KEGG | cAMP signaling pathway | 2.22E-08 |
| | GO | glucose metabolic process | 6.51E-06 |
| | GO | positive regulation of cholesterol efflux | 4.98E-05 |
| | GO | positive regulation of prostaglandin secretion | 7.06E-04 |

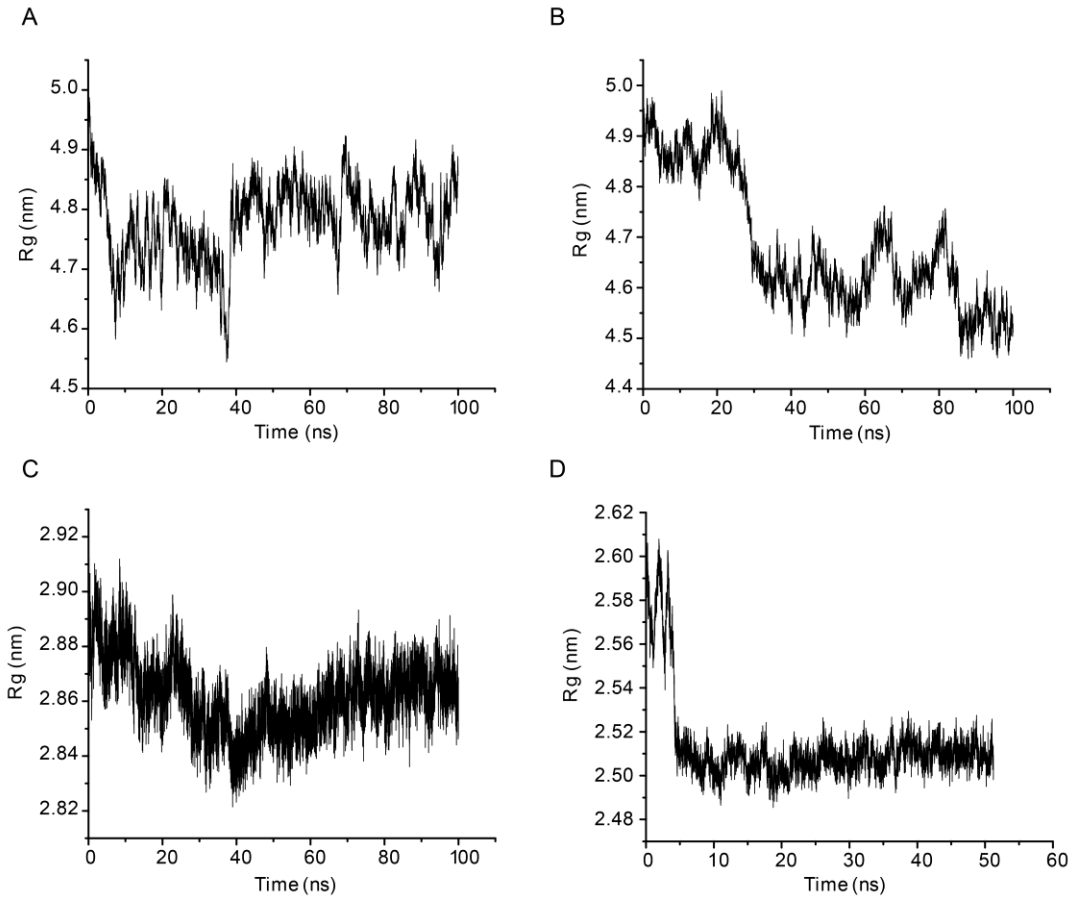


**Figure S1.** Radius of gyration (Rg) values of indicated complexes: GABBR2-saikosaponin C (**A**), GABBR2-baicalin (**B**), NFKBIA-glycyrrhizicacid (**C**) and PTGS2-lobetyolin (**D**) from the data of 100 ns MDs trajectories.

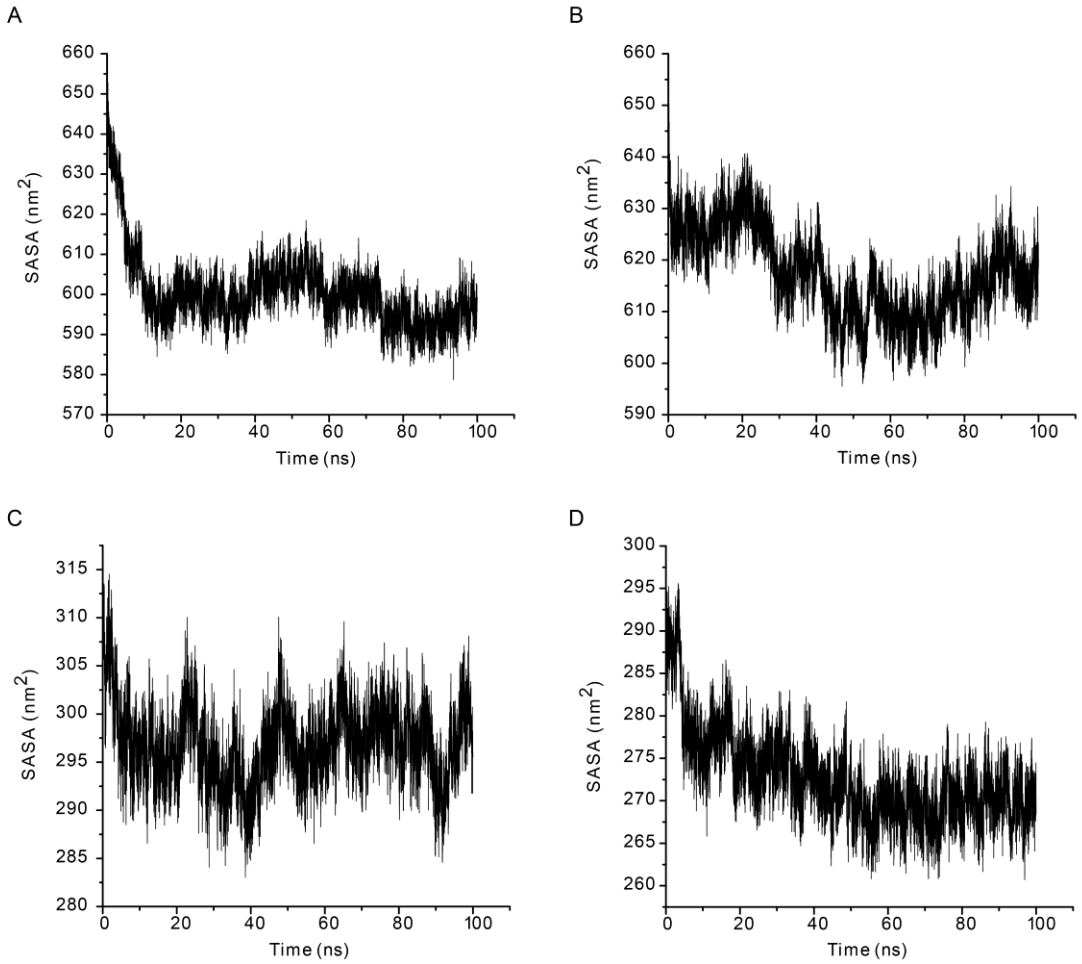


**Figure S2.** Solvent accessible surface area (SASA) values of indicated complexes: GABBR2-saikosaponin C (**A**), GABBR2-baicalin (**B**), NFKBIA-glycyrrhizicacid (**C**) and PTGS2-lobetyolin (**D**) from the data of 100 ns MDs trajectories.

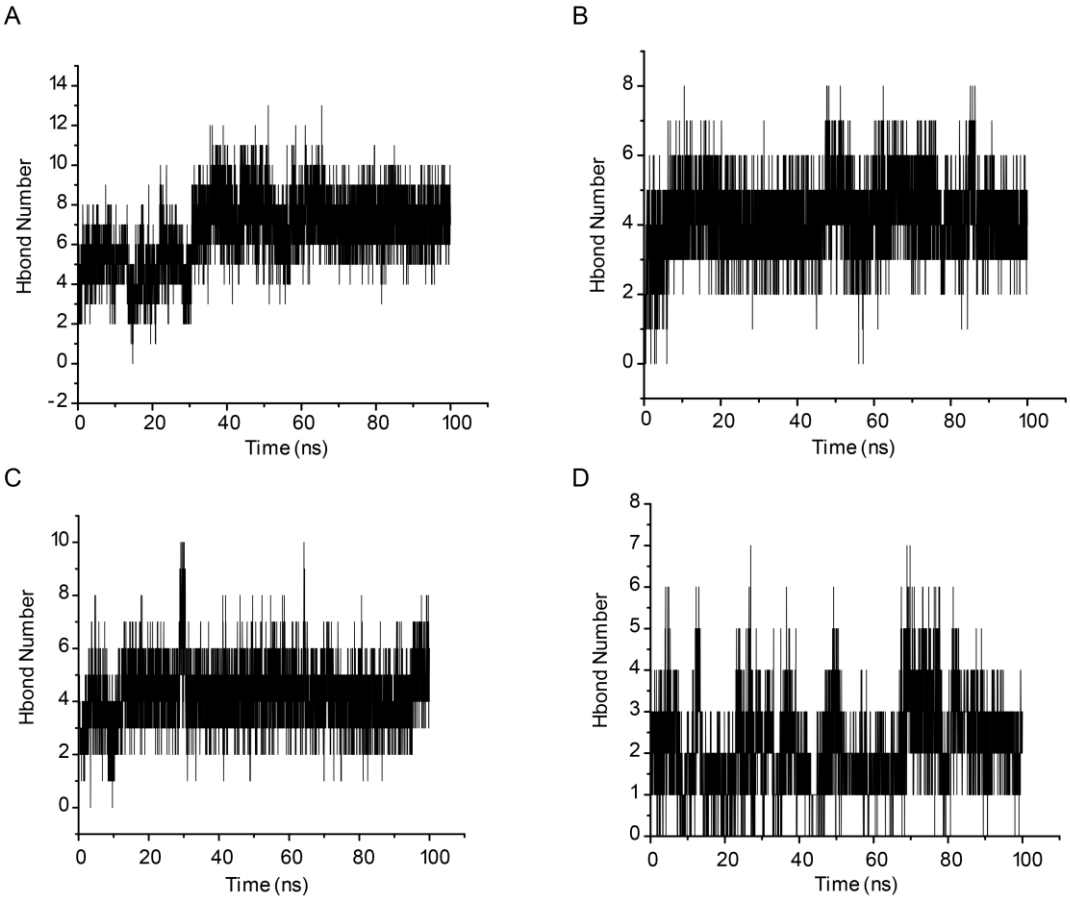


**Figure S3.** Hydrogen bond (Hbond) numbers of indicated complexes: GABBR2-saikosaponin C (**A**), GABBR2-baicalin (**B**), NFKBIA-glycyrrhizicacid (**C**) and PTGS2-lobetyolin (**D**) from the data of 100 ns MDs trajectories.

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