

Table S1. Non-targeted analysis of methanolic extract of *A. sinensis* flower using LC-QToF.

| # | RT (min) | Compound Name | Mol. formula | <i>m/z</i> [M+H] ⁺ | Fragment ions | <i>m/z</i> [M-H] ⁻ | Major Fragment ions |
|----|----------|---|---|--|--|-------------------------------|---|
| 1 | 1.8 | Malic acid | C ₄ H ₆ O ₅ | - | - | 133.0140 (133.0142) | - |
| 2 | 2.6 | Succinic acid | C ₄ H ₆ O ₄ | - | - | 117.0193 (117.0193) | 73.0306 |
| 3 | 4.34 | Phenylalanine | C ₉ H ₁₁ NO ₂ | 166.0857 (166.0863)* | 103.0510, 77.0368 | - | - |
| 4 | 5.4 | Procatechuic acid (3,4-dihydroxybenzoic acid) | C ₇ H ₆ O ₄ | - | - | 153.0191 (153.0193) | 109.0292 [M-H-CO ₂] ⁻ |
| 5 | 8.5 | Iriflophenone 3-C-glucoside | C ₁₉ H ₂₀ O ₁₀ | 409.1128 (409.1129) | 247.0610 [M+H-Glc] ⁺ | 407.0989 (407.0984) | 245.0456 [M-H-Glc] ⁻ |
| 6 | 8.8 | Iriflophenone 3,5-di-C-β-D-glucopyranoside | C ₂₅ H ₃₀ O ₁₅ | 571.1655 (571.1657) | 247.0613 [M+H-2Glc] ⁺ | 569.1515 (569.1512) | 407.0961 [M-H-Glc] ⁻ 245.0461 [M-H-2Glc] ⁻ |
| 7 | 11.2 | Mangeferin/isomangeferin | C ₁₉ H ₁₈ O ₁₁ | 423.0926 (423.0922) 445.0737 (445.0741) [M+Na] ⁺ | 405.0815 [M+H-H ₂ O] ⁺ | 421.0779 (421.0772) | 403.0681 [M+H-H ₂ O] ⁺ |
| 8 | 11.75 | | | | 387.0711 [M+H-2H ₂ O] ⁺ | | |
| | | | | | 369.0589 [M+H-3H ₂ O] ⁺ | | |
| | | | | | 327.0492 [M+H-96] ⁺ | | |
| | | | | | 303.0503 [M+H-120] ⁺ 273.0412 [M+H-150] ⁺ | | |
| 9 | 13.9 | Iriflophenone 2-rhamnoside | C ₁₉ H ₂₀ O ₉ | 393.1176 (393.118) | 247.0611 [M+H-Rha] ⁺ | 391.1034 (391.1035) | 245.0461 [M-H-Rha] ⁻ |
| 10 | 15.4 | Iriflophenone 2- <i>O</i> - <i>α</i> -L-(4"-acetyl)-rhamnopyranoside /Aquilarinenoside E | C ₂₁ H ₂₂ O ₁₀ | 435.1285 (435.1286) | 247.0611 | 433.1137 (433.1140) | 245.0453 |
| 11 | 17.2 | | | | | | |
| 12 | 17.7 | | | | | | |
| 13 | 20.6 | | | | | | |
| 14 | 18.7 | kaempferol-3- <i>O</i> -β-D-glucopyranoside | C ₂₁ H ₂₀ O ₁₁ | 449.1077 (449.1078) | 287.055 [M+H-Glc] ⁺ | 447.0931 (447.0933) | 285.0395 |
| 15 | 23.1 | Kaempferol dihexoside | C ₂₇ H ₃₀ O ₁₆ | 611.1589 (611.1607) | 287.055 [M+H-2Glc] ⁺ | 609.1451 (609.1461) | 285.0402 [M-H-2Glc] ⁻ |
| 16 | 24.5 | Aquilarisinine | C ₂₅ H ₃₀ O ₁₄ | 555.1701 (555.1708) | | 553.1559 (553.1563) | |
| 17 | 24.8 | Kaempferol (<i>p</i> -coumaroyl-glucoside)/ Kaempferol (<i>p</i> -coumaroyl-galactoside) | C ₃₀ H ₂₆ O ₁₃ | 595.1449 (595.1446) | 287.055 [M+H-coumaroyl-Glc or Gal] ⁺ | 593.1307 (593.1301) | 285.0399 |

| | | | | | | | |
|----|-------|--|---|------------------------|---|------------------------|--------------------------------|
| 18 | 25.3 | | | | 147.0444 [coumaroyl+H] ⁺ | | |
| 19 | 25.2 | Isorhamnetin coumarylglucoside | C ₃₁ H ₂₈ O ₁₄ | 626.1555 (625.1552) | 317.0656 147.0441 [coumaroyl+H] ⁺ | 623.1403 (623.1406) | 315.0505 |
| 20 | 26.9 | Kaempferol | C ₁₅ H ₁₀ O ₆ | 287.0555 (287.0550) | - | 285.0410 (285.0405) | - |
| 21 | 31.2 | Genkwanin | C ₁₆ H ₁₂ O ₅ | 285.0745 (285.0757) | | 283.0606 (283.0612) | |
| 22 | 17.1 | Aqulaside B | C ₂₂ H ₂₂ O ₁₂ | 479.1181 (479.1184) | 247.0609 | 477.1039 (477.1038) | 245.0453 |
| 23 | 18.73 | Aqulaside C (Iriflophenone derivative) | C ₂₅ H ₂₈ O ₁₃ | 537.1601 (537.1603) | 247.0599 | 535.1446 (535.1437) | 245.0457 |
| 24 | 24.6 | Aqulaside A | C ₂₈ H ₂₆ O ₁₂ | 555.1491 (555.1497) | 247.0606 | 553.1354 (553.1351) | 245.0459 |
| 25 | 15.04 | Unk-1 | C ₁₉ H ₂₆ O ₁₀ | 415.1591 (415.1599) | | 413.1460 (413.1453) | 311.1139, 269.1030, 99.0452 |
| 26 | 12.8 | Unk-2 | C ₂₂ H ₃₈ O ₁₂ | - | | 493.2297 (493.2316) | 391.1967, 349.1862, 99.0451 |
| 27 | 19.2 | Unk-3 (Iriflophenone derivative) | C ₁₈ H ₃₀ O ₁₀ | - | | 405.1766 (405.1766) | 245.0447 |

*calculated accurate mass

Figure S1: MS and MS-MS spectra of mangiferin in positive ion mode using LC-QToF

