

Supplementary Table 4

CHARACTERIZATION OF HAENKENIUM EXTRACT

Characterization was performed by UPLC-QTOF, after extracting the sample in methanol. A representative chromatogram is reported in Figure 5a, while the characterization results are shown in this Table.

| RT (min) | m/z | Fragments (MS/MS) | Identification | Ion type | % w/w * |
|----------|----------|-------------------------------------|------------------------------------|-------------------------------------|-------------|
| 9.2749 | 637.1194 | 285.0399 175.0387 151.0387 | Luteolin diglucuronide | [M-H] ⁻ | 0.55 |
| 7.9191 | 315.0499 | 151.0288 | Isorhamnetin | [M-H] ⁻ | 0.48 |
| 7.2652 | 401.1238 | 211.0828 | Nobiletin | [M-H] ⁻ | 0.38 |
| 6.8429 | 461.0719 | 285.0396 151.0024 133.0283 | Luteolin glucuronide | [M-H] ⁻ | 0.59 |
| 5.8229 | 593.1515 | 473.1082 383.0767 353.0662 | Elatin | [M-H] ⁻ | 0.32 |
| 8.6852 | 329.0661 | 314.0421 299.0188 | 3,7-Dimethylquercetin | [M-H] ⁻ | 0.21 |
| 8.7185 | 577.1924 | 285.0393 | Prenyleriodictyol | [M-H] ⁻ | 0.21 |
| 8.4595 | 285.0397 | 175.0388 151.0027 133.0285 107.1270 | Luteolin | [M-H] ⁻ | 0.15 |
| 9.1078 | 591.1715 | 301.1163 | Hesperetin 7-neohesperidoside | [M-H ₂ O-H] ⁻ | 0.11 |
| 8.0571 | 533.1647 | 371.1120 | Phellatin | [M-H] ⁻ | 0.09 |
| 6.9794 | 463.0874 | 301.0336 | Quercetin-glucoside (isoquercetin) | [M-H] ⁻ | 0.07 |
| 9.9239 | 299.0551 | 284.0316 256.0352 | Diosmetin | [M-H] ⁻ | 0.05 |
| 9.2643 | 593.1502 | 285.0387 | Luteolin-7-O-rutinoside | [M-H] ⁻ | 0.04 |
| 5.5006 | 609.1447 | 301.0269 | Rutin | [M-H] ⁻ | 0.02 |
| 9.2690 | 285.0399 | 255.0289 227.0346 | Kaempferol | [M-H] ⁻ | 0.02 |
| | | | Total identified flavonoids | | 3.29 |
| | | | | | |
| 7.8315 | 403.1399 | 357.1332 163.0388 151.0389 | Pinosresinol # | [M+FA-H] ⁻ | 7.29 |
| 7.3855 | 359.0767 | 197.0450 179.0343 161.0239 | Rosmarinic acid | [M-H] ⁻ | 4.92 |

| | | | | | |
|---------|----------|-------------------------------------|---|-------------------------------------|--------------|
| 7.3855 | 719.1615 | 359.0766 161.0236 | Sagerinic acid | [M-H] ⁻ | 2.58 |
| 8.0107 | 553.2286 | 521.2021 507.2228 465.1761 419.1968 | Ssioriside | [M-H] ⁻ | 1.9 |
| 8.7593 | 515.1188 | 353.0874 | Di-caffeoylquinic acid | [M-H] ⁻ | 0.92 |
| 7.9846 | 627.2288 | 581.2233 401.1595 59.0123 | Lyoniresinol 9-glucoside [#] | [M+FA-H] ⁻ | 0.58 |
| 8.5969 | 567.1147 | NA | Chrysophanol 8-(6-galloylglucoside) | [M-H] ⁻ | 0.58 |
| 6.5666 | 717.1464 | 537.2167 519.0921 475.1023 | Salvianolic acid L | [M-H] ⁻ | 0.64 |
| 8.3924 | 515.1184 | 179.0339 | Dicaffeoylquinic acid | [M-H ₂ O-H] ⁻ | 0.92 |
| 6.7077 | 373.1285 | NA | 8-Hydroxypinoresinol [#] | [M-H] ⁻ | 0.44 |
| 7.3945 | 161.0235 | 179.0338 | Caffeic acid | [M-H ₂ O-H] ⁻ | 0.43 |
| 6.8777 | 555.1128 | 313.0718 | Salvianolic acid K | [M-H] ⁻ | 0.07 |
| | | | Total identified phenols and lignans [#] | | 21.26 |
| | | | | | |
| 5.6685 | 387.1651 | 225.0790 207.1017 | beta-D-Glucopyranosyl-11-hydroxyjasmonic acid [§] | [M-H] ⁻ | 3.92 |
| 13.6175 | 571.2884 | 409.2351 | Phosphatidylinositol [§] | [M-H] ⁻ | 0.19 |
| 15.8469 | 455.3522 | 437.3423 411.3579 | Ursolic acid | [M-H] ⁻ | 0.24 |
| 9.5309 | 347.1860 | 329.1734 317.1751 | 2 α ,16-Dihydroxy-4 β -carboxy-O- β -D-glucopyranosyl-19-nor-totarol | [M-H] ⁻ | 0.13 |
| 13.9808 | 455.3528 | NA | Oleanolic acid | [M-H] ⁻ | 0.16 |
| 8.7593 | 389.1596 | NA | Rosmic acid | [M-H] ⁻ | 0.1 |
| 11.5745 | 331.1911 | 287.2020 | Carnosic acid | [M-H] ⁻ | 0.05 |
| 15.7777 | 471.3474 | 453.3380 | Corosolic acid | [M-H] ⁻ | 0.05 |
| 12.3086 | 487.3429 | NA | Salvin A | [M-H] ⁻ | 0.05 |
| 16.7308 | 730.5480 | 568.4941 | Araliacerebroside [§] | [M-H] ⁻ | 0.07 |
| 16.0299 | 461.3632 | 415.1462 149.0967 | beta-Tocopherol | [M+FA-H] ⁻ | 0.05 |
| 12.4451 | 471.3476 | NA | Maslinic acid | [M-H] ⁻ | 0.05 |
| 6.4211 | 369.0827 | 207.0285 | 5-Hydroxy-6-methoxycoumarin 7-glucoside [§] | [M-H] ⁻ | 0.02 |
| | | | Total identified terpenes and others [§] | | 5.08 |

* Flavonoids amounts are expressed as rutin equivalents; phenols as chlorogenic acid equivalents; terpenes as oleanolic acid equivalents; glycerides and fatty acid derivatives as lecithin equivalents; coumarins as coumarin equivalents.

