

**S1Table. LC-MS/MS data (S4 Fig.) of compounds present in SM6Met and subsequent fractions obtained during activity-guided fractionation.**

| Nr | t <sub>R</sub> <sup>a</sup> | λ <sub>max</sub>   | [M-H] <sup>-</sup> | Fragment ions                                | Compound  | Class                | Notes <sup>b</sup> | SM6Met         | PF             | NPF | F1 | F2 | F3  |
|----|-----------------------------|--------------------|--------------------|--|---|----------------------|--------------------|----------------|----------------|-----|----|----|-----|
| 1  | 2.7                         | 293                | 569                | 479, 449, 317, 287* <sup>c</sup>             | Iriflophenone-3-C-β-D-glucoside-4-O-β-D-glucoside | Benzophenone         | ID                 | x <sup>d</sup> | X <sup>e</sup> | x   | x  |    |     |
| 2  | 4.1                         | 259, 293           | 153                | No fragments observed                        | Protocatechuic acid                               | Hydroxybenzoic acid  | ID                 |                | X              |     | X  |    | X   |
| 3  | 5.6                         | 286                | 611                | 491, 431, 401, 371*                          | (S)-Eriodictyol-di-C-hexoside                     | Flavanone            | [3]                | x              | x              | x   | x  |    |     |
| 4  | 5.7                         | 286                | 611                | 491, 431, 401, 371*                          | (R)-Eriodictyol-di-C-hexoside                     | Flavanone            | [3]                | x              | x              | x   | x  |    |     |
| 5  | 5.8                         | 294                | 407                | 317, 287*, 257, 245, 215, 201, 193, 165, 125 | Iriflophenone-3-C-β-D-glucoside                   | Benzophenone         | ID                 |                | X              | x   | X  |    | X x |
| 6  | 7.3                         | 285                | 595                | 475, 415, 385*, 355                          | Naringenin-di-C-hexoside                          | Flavanone            | [3]                | x              | x              | x   | x  |    |     |
| 7  | 8.4                         | 239, 257, 317, 366 | 421                | 331, 301*, 271, 259                          | Mangiferin  | Xanthones            | ID                 |                | X              | x   | X  |    | X   |
| 8  | 8.8                         | 240, 255, 316, 365 | 421                | 331, 301*, 271, 259                          | Isomangiferin                                     | Xanthones            | ID                 |                | X              | x   | X  |    | X   |
| 9  | 9.0                         | 231, 270, 330      | 593                | 503, 473*, 383, 353                          | Vicenin-2 (apigenin-6,8-di-C-β-D-glucoside)       | Flavone              | ID                 | x              | x              | x   | X  | x  |     |
| 10 | 10.1                        | 281                | 449                | 287, 151*, 135                               | Eriodictyol-O-glucoside                           | Flavanone            | [3]                | x              |                | x   |    |    | X   |
| 11 | 11.2                        | 285                | 613                | 475, 433, 403, 373*, 361, 331, 209           | 3-Hydroxyphloretin-3',5'-di-C-hexoside            | Dihydrochalcone      | [3]                |                | X              | X   | X  | X  | x x |
| 12 | 11.3                        | 309                | 163                | No fragments observed                        | p-Coumaric acid                                   | Hydroxycinnamic acid | ID                 | x              | x              | X   |    |    | X   |
| 13 | 12.0                        | 283                | 595                | 287, 151*                                    | Eriocitrin (eriodictyol-7-O-rutinoside)           | Flavanone            | ID                 |                | X              | x   | X  | X  | X   |
| 14 | 13.0                        | 265, 348           | 593                | 285  | Scylloside (luteolin-7-O-rutinoside)              | Flavone              | ID                 |                | X              | X   | X  |    | x X |
| 15 | 13.3                        | 284                | 597                | 459, 417, 387, 357*, 345, 315                | Phloretin-3',5'-di-C-β-D-glucoside                | Dihydrochalcone      | ID                 |                | X              | X   | X  | X  | x x |
| 16 | 13.6                        | 254, 265, 348      | 447                | 285  | Luteolin-O-hexoside                               | Flavone              | NC                 | x              |                | x   |    |    | X   |
| 17 | 14.3                        | 282                | 579                | 271*, 151                                    | Naringenin-O-dihexoside                           | Flavanone            | [3]                | x              | x              | x   |    |    | X   |
| 18 | 15.0                        | 266, 337           | 577                | 269  | Isorhoifolin (apigenin-7-O-rutinoside)            | Flavone              | NC                 | x              | x              | x   |    |    | X   |
| 19 | 15.5                        | 283                | 609                | 301  | Hesperidin (hesperetin-7-O-rutinoside)            | Flavanone            | ID                 |                | X              | X   | X  | x  | X x |
| 20 | 15.8                        | 252, 265, 346      | 607                | 299*, 284                                    | Chrysoeriol-O-deoxyhexose-O-hexoside              | Flavone              | NC                 | x              | x              | x   |    |    | X   |
| 21 | 18.0                        | 259, 375           | 609                | 301  | Quercetin-O-deoxyhexose-O-hexoside                | Flavonol             | NC                 | x              |                |     |    | x  |     |
| 22 | 21.0                        | 252, 265, 348      | 285                | No fragments observed                        | Luteolin  | Flavone              | ID                 | x              |                | x   |    |    | X   |

<sup>a</sup> indicates the polyphenol retention time

<sup>b</sup> MS data from literature used to tentatively identify compounds

<sup>c\*</sup> indicates the major daughter ion

<sup>d</sup> Minor polyphenols in extract are represented by "x"

<sup>e</sup> Major polyphenols in extract are represented by "X"

ID refers to the fact that the compound was identified by means of an authentic reference standard

NC refers to the presence of a compound not identified before and further structure elucidation is required