

**Table. S4. The detail data for Venn diagram.**

| No. | Compounds                                | Formula   | Class I        | Class II       | CAS        | LF-OMTMS-D_vs_MF-OMTMS-D | LF-OMTMS-D_vs_HF-OMTMS-D | MF-OMTMS-D_vs_HF-OMTMS-D | LF-OMTMS-D-1 | LF-OMTMS-D-2 | LF-OMTMS-D-3 | MF-OMTMS-D-1 | MF-OMTMS-D-2 | MF-OMTMS-D-3 | HF-OMTMS-D-1 | HF-OMTMS-D-2 | HF-OMTMS-D-3 |
|-----|--|-----------|----------------|----------------|------------|--------------------------|--------------------------|--------------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| 1   | Quercetin-3-O-glucoside (Isoquercitrin)* | C21H20O12 | Flavonoids     | Flavonols      | 482-35-9   | TRUE                     | TRUE                     | TRUE                     | 421057.313   | 446645.47    | 263769.876   | 1212120.92   | 1032665.45   | 1402252.61   | 3713237.53   | 3512582.88   | 4708750.8    |
| 2   | Quercetin-4'-O-glucoside (Spiraeoside)*  | C21H20O12 | Flavonoids     | Flavonols      | 20229-56-5 | TRUE                     | TRUE                     | TRUE                     | 450519.092   | 426162.926   | 320578.55    | 1018447.34   | 1006256.02   | 1102172.2    | 2888189.87   | 2889136.48   | 4055777.68   |
| 3   | Hesperetin-5-O-glucoside                 | C22H24O11 | Flavonoids     | Flavanones     | 69651-80-5 | TRUE                     | TRUE                     | TRUE                     | 455748.531   | 529312.347   | 341796.548   | 1028142.43   | 1008044.13   | 1111913.27   | 2688568.49   | 2834596.69   | 3880119      |
| 4   | Quercetin-7-O-glucoside*                 | C21H20O12 | Flavonoids     | Flavonols      | 491-50-9   | TRUE                     | TRUE                     | TRUE                     | 452057.822   | 445017.272   | 272312.892   | 892933.843   | 826908.124   | 1180745.7    | 2491273.46   | 2507147.37   | 3691012.63   |
| 5   | Kaempferol-7-O-glucoside*                | C21H20O11 | Flavonoids     | Flavonols      | 16290-07-6 | TRUE                     | TRUE                     | TRUE                     | 303188.176   | 305734.892   | 247274.819   | 698574.801   | 638674.174   | 732649.002   | 1596767.78   | 1743625.48   | 2301864.76   |
| 6   | Kaempferol-3-O-galactoside (Trifolin)*   | C21H20O11 | Flavonoids     | Flavonols      | 23627-87-4 | TRUE                     | TRUE                     | TRUE                     | 321004.479   | 305908.575   | 213722.393   | 686313.416   | 615340.738   | 761976.392   | 1627863.71   | 1528297.64   | 2264533.45   |
| 7   | Chrysoeriol-5-O-glucoside                | C22H22O11 | Flavonoids     | Flavones       | -          | TRUE                     | TRUE                     | TRUE                     | 83106.0587   | 77629.9028   | 66624.5139   | 175186.703   | 142297.016   | 183497.46    | 414026.924   | 412310.032   | 508464.314   |
| 8   | Quercetin-3-O-arabinoside                | C20H18O11 | Flavonoids     | Flavonols      | 22255-13-6 | TRUE                     | TRUE                     | TRUE                     | 3838.1627    | 17635.6479   | 9095.33105   | 34482.5626   | 26288.4918   | 34445.9846   | 136090.317   | 121103.935   | 198967.017   |
| 9   | 3-O-p-Coumaroylshikimic acid             | C16H16O7  | Phenolic acids | Phenolic acids | -          | TRUE                     | TRUE                     | TRUE                     | 170082.597   | 154794.44    | 177883.278   | 87644.4679   | 95962.3411   | 58961.5481   | 35573.319    | 22103.8375   | 20459.1898   |

\* represents the presence of an isomer of the compound.