

**Supplementary Table S7.** Retention times of compounds, ESI polarity, precursor ions, product ions and collision energy.

| Compound Name           | Retention time (min) | ESI polarity | Precursor Ion (m/z) | Product Ion (m/z) | Collision Energy (V) |
|-------------------------|----------------------|--------------|---------------------|-------------------|----------------------|
| <i>L</i> -ascorbic acid | 2.79                 | negative     | 174.99              | <b>115.0</b>      | 10                   |
|                         |                      |              |                     | 87.0              | 18                   |
| Ferulic acid            | 11.68                | negative     | 192.99              | <b>134.0</b>      | 14                   |
|                         |                      |              |                     | 149.0             | 10                   |
|                         |                      |              |                     | 177.9             | 10                   |
| Sinapic acid            | 11.61                | negative     | 222.99              | <b>192.9</b>      | 22                   |
|                         |                      |              |                     | 93.0              | 38                   |
|                         |                      | positive     | 225.01              | <b>207.0</b>      | 6                    |
|                         |                      |              |                     | 65.0              | 54                   |
|                         |                      |              |                     | 91.0              | 34                   |
|                         |                      |              |                     | 118.9             | 22                   |
| Kaempferol              | 14.53                | negative     | 284.99              | <b>93.0</b>       | 38                   |
|                         |                      |              |                     | 65.0              | 70                   |
|                         |                      |              |                     | 117.0             | 50                   |
|                         |                      | positive     | 287.01              | <b>152.9</b>      | 38                   |
|                         |                      |              |                     | 68.9              | 58                   |
| Quercetin               | 13.71                | negative     | 300.99              | <b>151.0</b>      | 22                   |
|                         |                      |              |                     | 65.0              | 50                   |
|                         |                      |              |                     | 121.0             | 30                   |