

| Metabolite                        | Standard for quantification | MRM     | Declustering Potential (V) | Collision Energy (eV) |
|-----------------------------------|-----------------------------|---------|----------------------------|-----------------------|
| 4-O-methyl gallic acid (4OMG)     | 4OMG                        | 183>168 | -30                        | -15                   |
| 4-O-methyl gallic acid sulphate   | 4OMG                        | 263>183 | -30                        | -15                   |
| trimethyl gallic acid glucuronide | 4OMG                        | 387>211 | -30                        | -15                   |

Supplementary Table S1: MRM condition and transitions of identified metabolites