

Figure 1. (a) Fragmentation patterns and full scan product ion mass spectra of [M+H]<sup>+</sup> ion of kaempferol standard.



Figure S-1 (b) Fragmentation patterns and full scan product ion mass spectra of [M+H]<sup>+</sup> ion of quercetin standard.



Figure S-1 (c) Fragmentation patterns and full scan product ion mass spectra of [M+H]<sup>+</sup> ion of ferulic acid standard.



Figure S-1 (d) Fragmentation patterns and full scan product ion mass spectra of [M+H]<sup>+</sup> ion of apigenin standard.



Figure S-1 (e) Fragmentation patterns and full scan product ion mass spectra of [M+H]<sup>+</sup> ion of baicalein standard.



Figure S-1 (f) Fragmentation patterns and full scan product ion mass spectra of [M+H]<sup>+</sup> ion of caffeic acid standard.



Figure S-2. Recovery of six compound in AR, calculated from the solvent-based standards, with different SPE cartridges using the optimized clean-up step. Data presented as mean  $\pm$  standard error from 3 replicates (n=3). Bars with the different letters showed statistically significant difference (P < 0.05). The small letters mean that the recovery of same compounds compared with the different SPE columns.



Figure S-3. Recovery of six compound in AR, calculated from the solvent-based standards, with the different concentration of formic acid (FA) extraction solution and salt-out step (0.1% NaOH). Data presented as mean  $\pm$  standard error from three replicates (n=3) Bars with the different letters showed statistically significant difference (P < 0.05). The small letters mean that the recovery of same compounds compared with the different extraction conditions.





Figure S-4-G-C, UV and MS-SIM chromatograms of the six compounds in Chinese green AR. 1: Caffeic acid, 2: Quercetin, 3: Apigenin, 4: Ferulic acid, 5: Baicalein, 6: Kaempferol

NL: 6.35E4 UV\_VIS\_1 UV 6



7 8

5

6

4

9



RT: 20.57 MA: 342728

21 22

23 24 25

SNt 2

20

Figure S-4-G-N, UV and MS-SIM chromatograms of the six compounds in New Zealand AR. 1: Caffeic acid, 2: Quercetin, 3: Apigenin, 4: Ferulic acid, 5: Baicalein, 6: Kaempferol

Time (min)

13

10 11 12

14 15

16 17 <u>1</u>8 19

RT: 0.00 - 25.00

35000-30000-25000-

20000-

15000-10000-5000-0-

Ó

2

3

2



Figure S-4-P-C, UV and MS-SIM chromatograms of six compounds in Chinese purples AR. 1: Caffeic acid, 2: Quercetin, 3: Apigenin, 4: Ferulic acid, 5: Baicalein, 6: Kaempferol



Figure S-4-P-NZ, UV and MS-SIM chromatograms of six compounds in New Zealand purple AR. 1: Caffeic acid, 2: Quercetin, 3: Apigenin, 4: Ferulic acid, 5: Baicalein, 6: Kaempferol