

## Supplements

# Antioxidant and Cytoprotective Effects of the Di-O-Caffeoylquinic Acid Family: The Mechanism, Structure–Activity Relationship, and Conformational Effect

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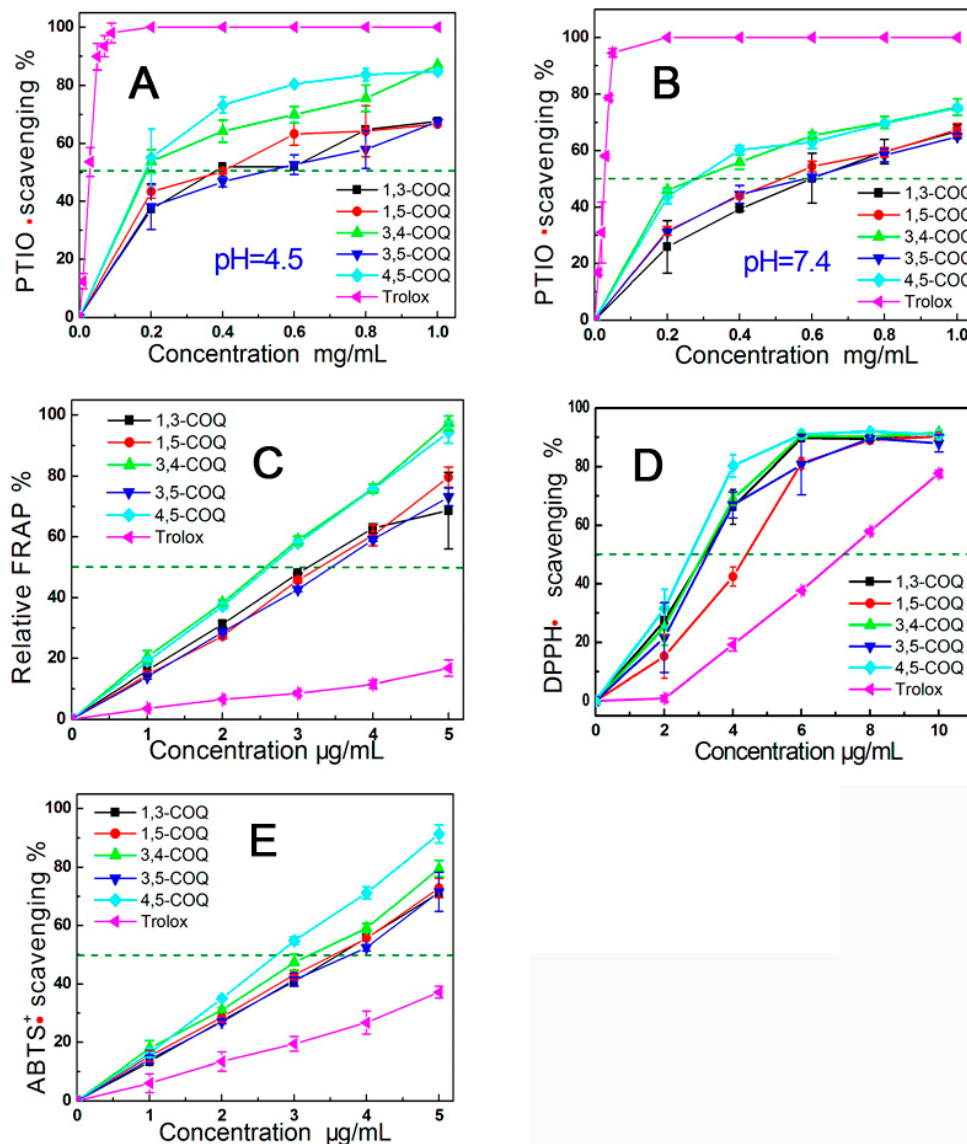
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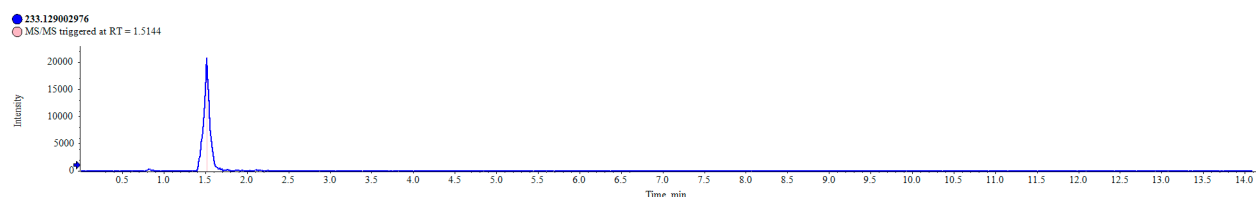
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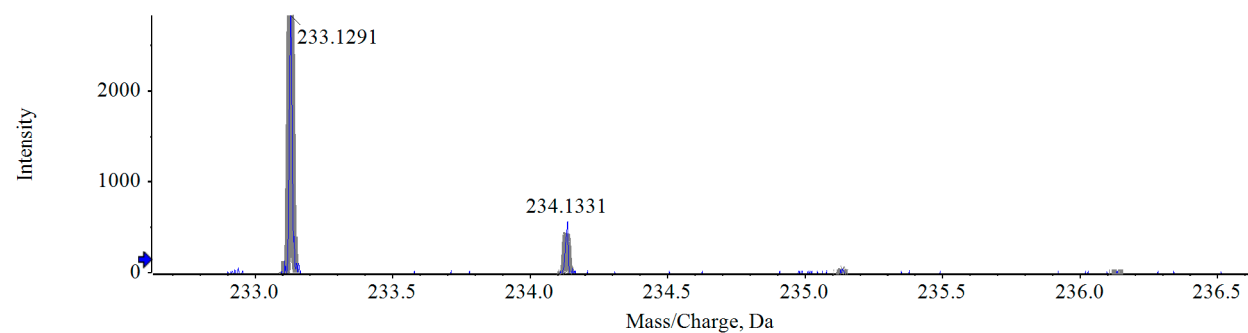
**Fig. S1.** Dose response curves of di-*O*-caffeoylquinic acids (**di-COQs**) in various antioxidant assays: (A) PTIO•-radical-scavenging assay (pH 4.5); (B) PTIO•-radical-scavenging assay (pH 7.4). (C) FRAP assay. (D) DPPH•-scavenging assay. (E) ABTS<sup>+</sup>•- scavenging assay.

Each value is expressed as the mean $\pm$ SD,  $n=3$ .

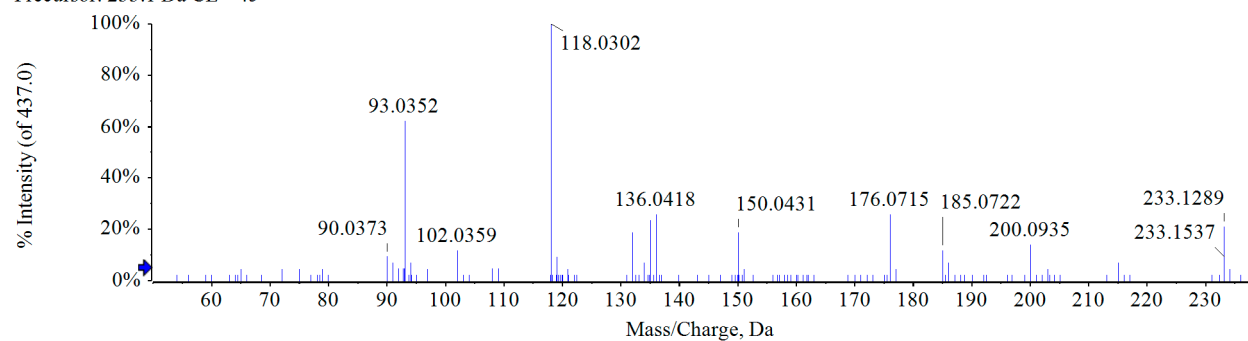
## Spectrum of PTIO.



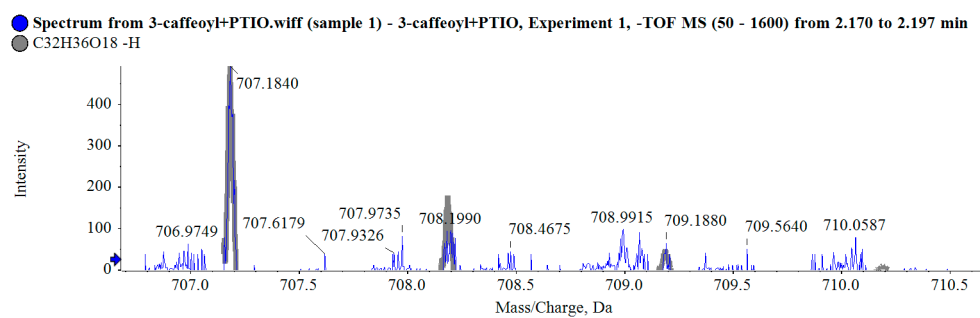
● Spectrum from 3-caffeoyl+PTIO.wiff (sample 1) - 3-caffeoyl+PTIO, Experiment 1, -TOF MS (50 - 1600) from 1.485 to 1.511 min  
● C13H17N2O2



Spectrum from 3-caffeoyl+PTIO.wiff (sample 1) - 3-caffeoyl+PTIO, Experiment 2, -TOF MS<sup>2</sup> (50 - 1600) from 1.514 min  
Precursor: 233.1 Da CE=-45



Spectrum of Dimer product in the mixture of chlorogenic acid with PTIO •



**Fig. S2** Original Data of UPLC-ESI-MS/MS analysis.