Supplementary Information

Structural Study of Phenolic Acids by Triple Quadrupole Mass Spectrometry with Electrospray Ionization in Negative Mode and H/D Isotopic Exchange

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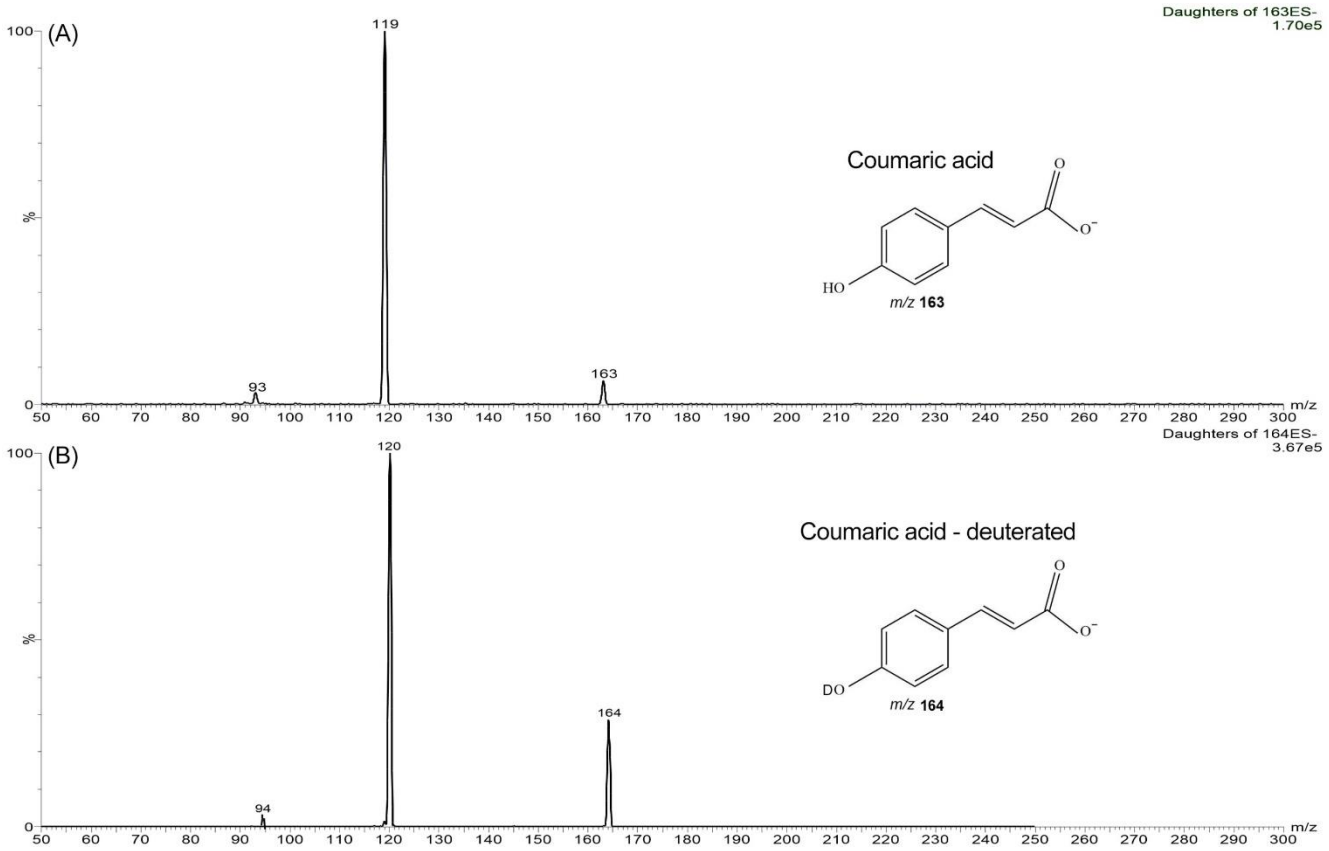


Figure S1. Triple quadrupole mass spectrometry by electrospray ionization in negative ionic mode (ESI(–)-MS/MS) spectra of (A) *p*-coumaric acid *m/z* 163 and (B) *p*-coumaric-deuterated acid *m/z* 164.

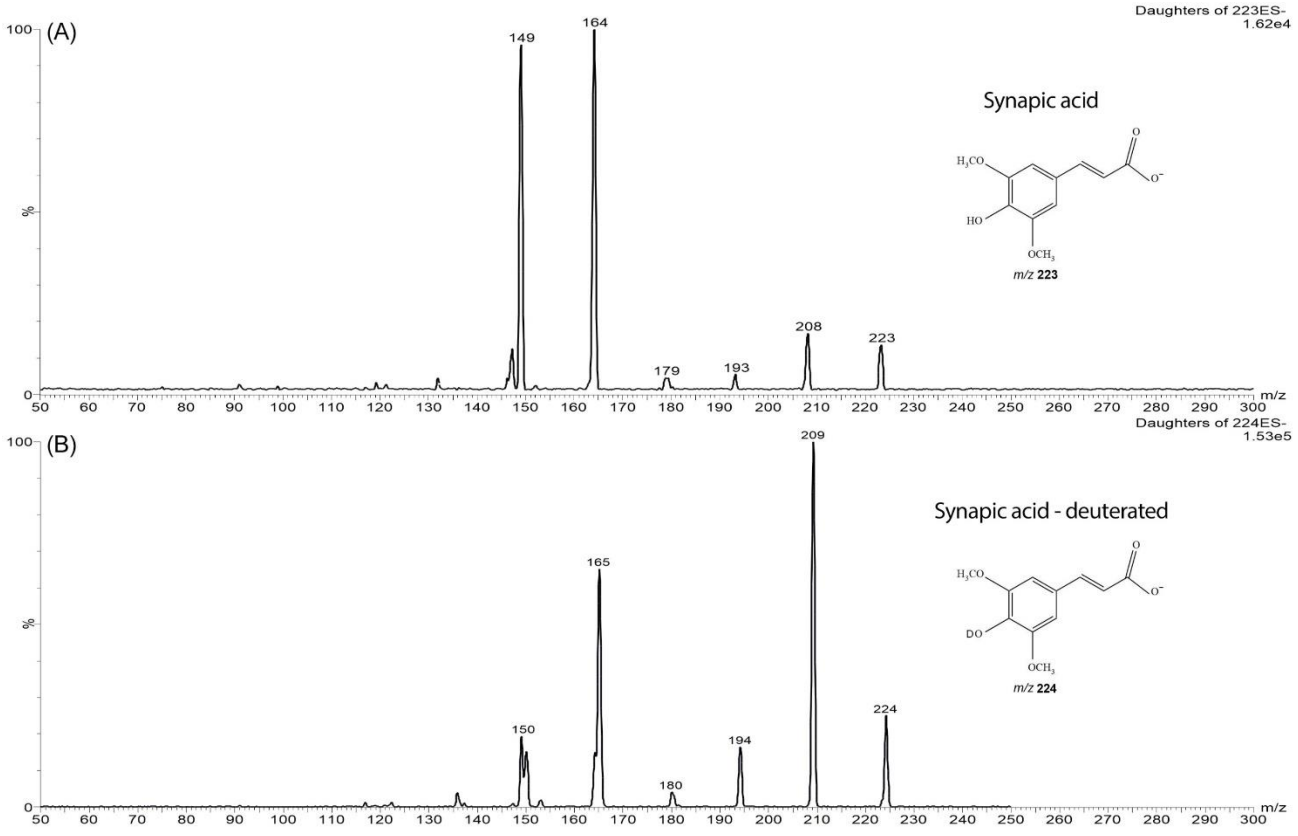


Figure S2. ESI(–)-MS/MS spectra of (A) synapic acid *m/z* 223 and (B) synapic-deuterated acid *m/z* 224.

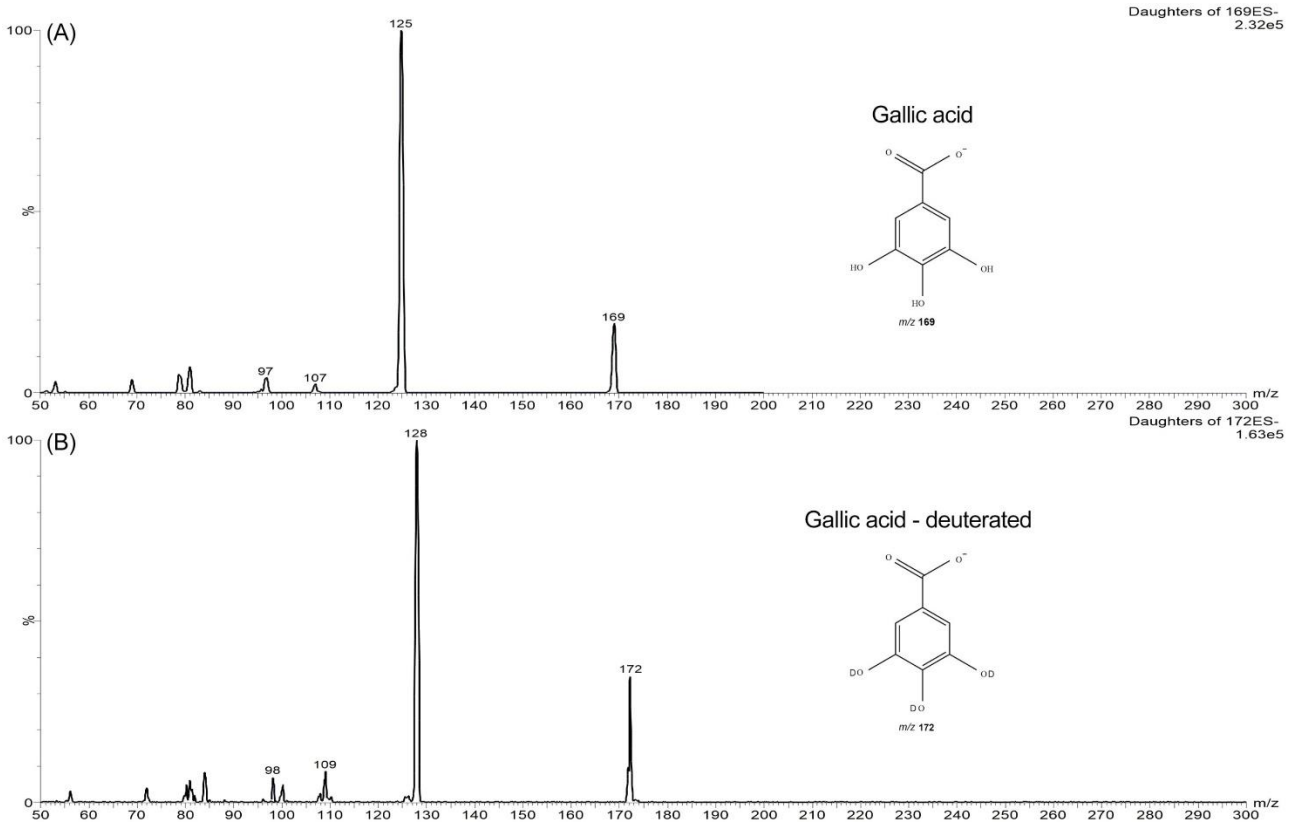


Figure S3. ESI(−)-MS/MS spectra of (A) caffeic acid *m/z* 179 and (B) caffeic-deuterated acid de *m/z* 181.

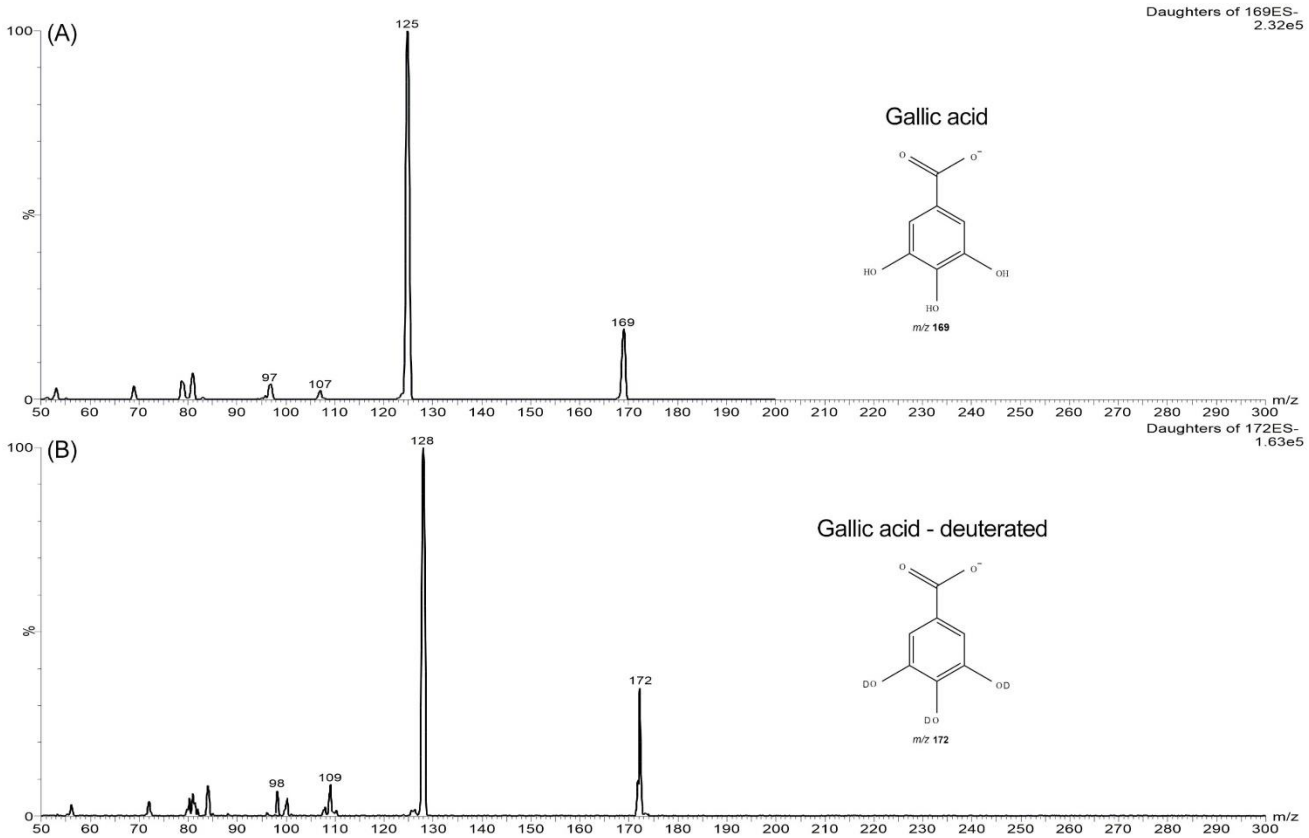
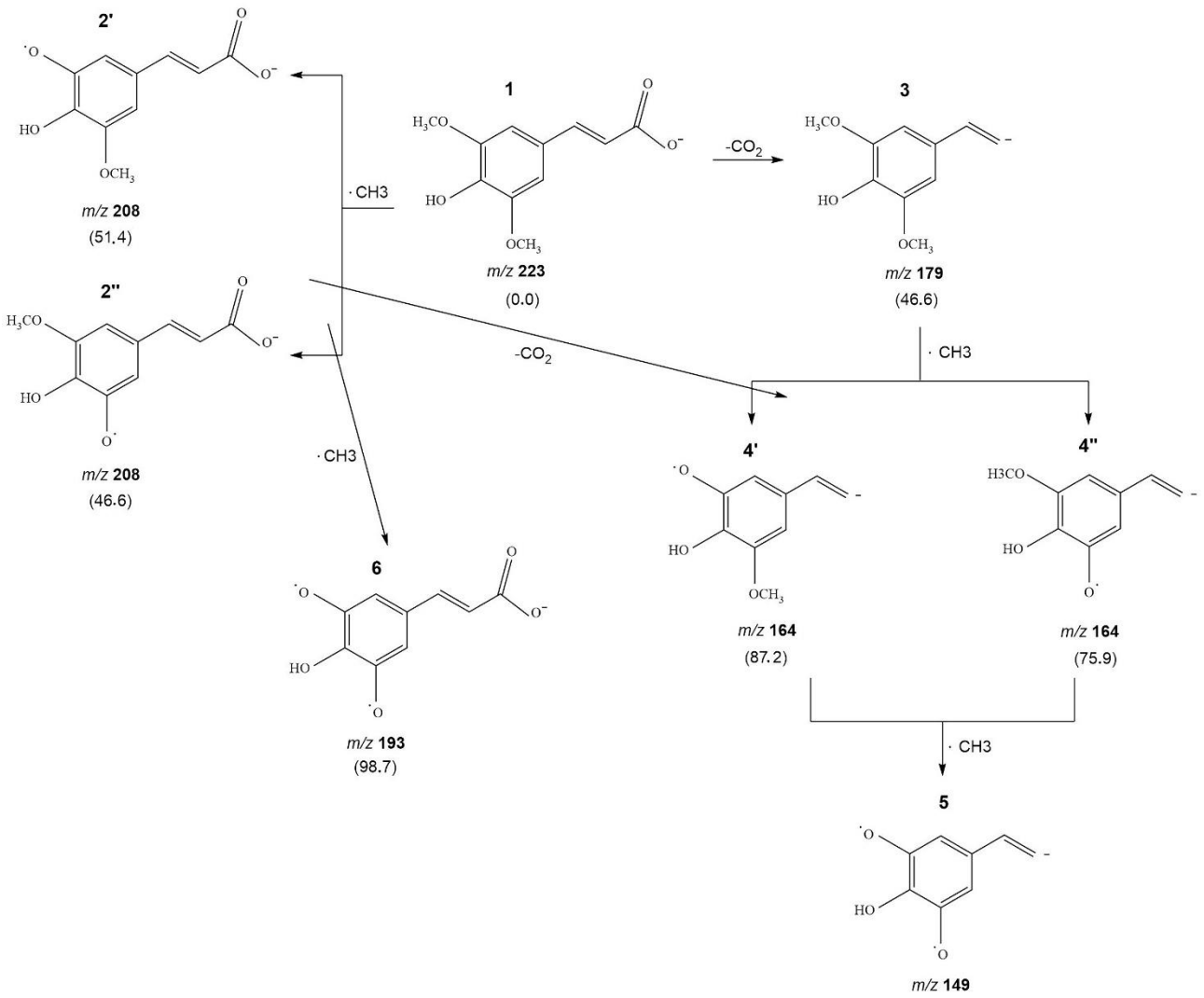
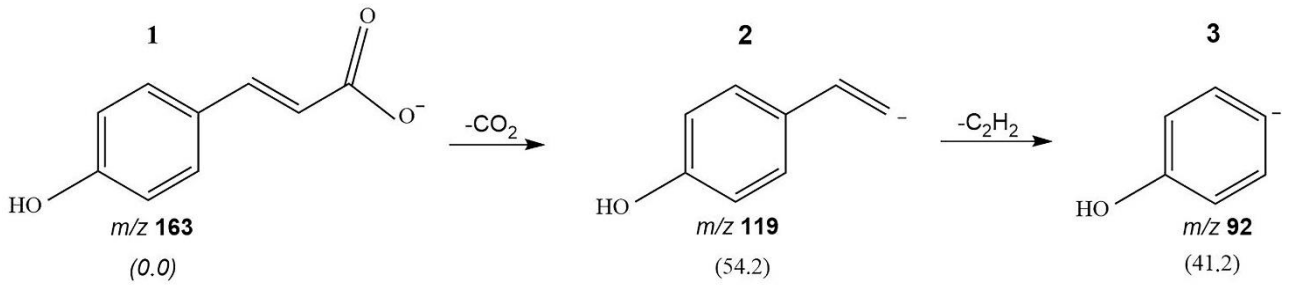


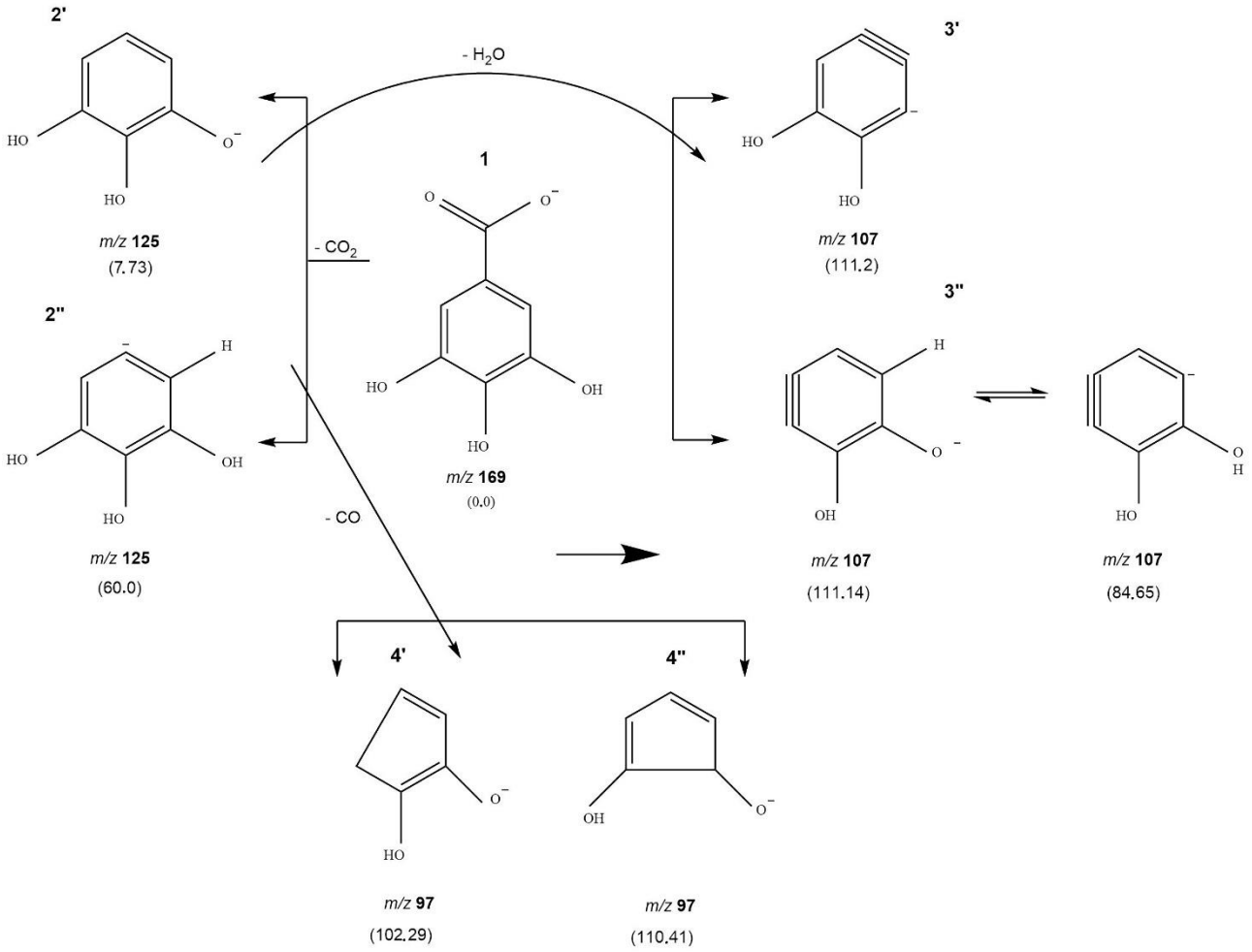
Figure S4. ESI(−)-MS/MS spectra of (A) gallic acid *m/z* 169 and (B) gallic-deuterated acid *m/z* 172.



Scheme S1. Fragmentation mechanisms for deprotonated synapic acid. Values between parentheses are relative potential energies in kcal mol^{-1}, obtained at the theory level B3LYP/6-311+G**.



Scheme S2. Fragmentation mechanisms for deprotonated *p*-coumaric acid. Values between parentheses are relative potential energies in kcal mol^{-1}, obtained at the theory level B3LYP/6-311+G**.



Scheme S3. Fragmentation mechanisms for deprotonated gallic acid. Values between parentheses are relative potential energies in kcal mol^{-1}, obtained at the theory level B3LYP/6-311+G**.