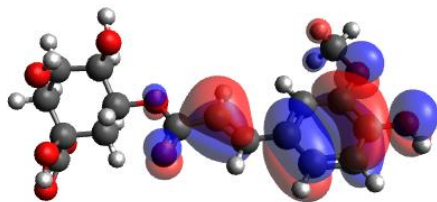
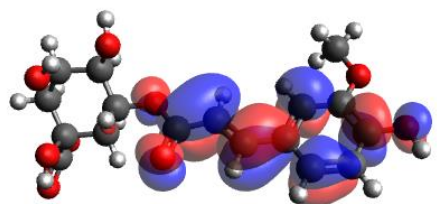


Figure S2. The frontier orbital HOMO and LUMO of selected quinic acid derivatives.

5-O-feruloylquinic acid

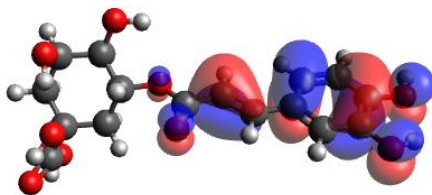


HOMO -5.648

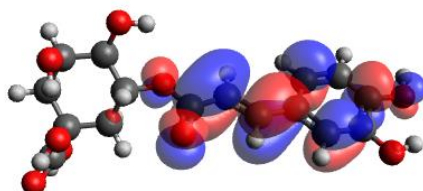


LUMO -1.517

chlorogenic acid

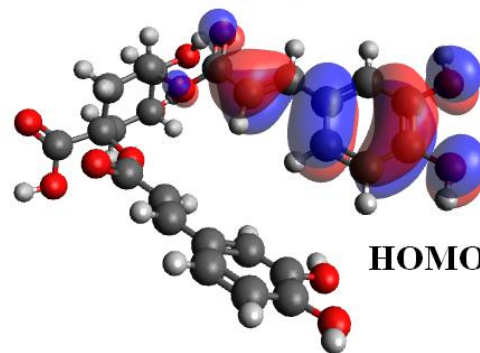


HOMO -5.888

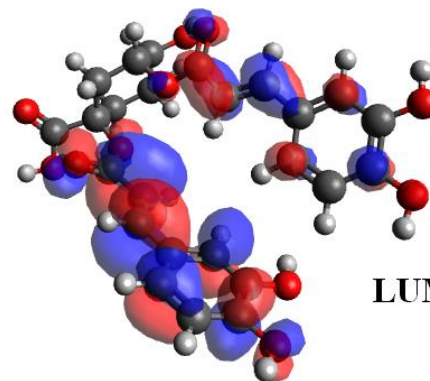


LUMO -1.728

1,5-dicaffeoylquinic acid



HOMO -5.484



LUMO -1.937