

Metrological aspects of a gas-phase DFT/B3LYP quantum-chemical approach to prioritize radical scavenging activity among a group of olive oil phenols

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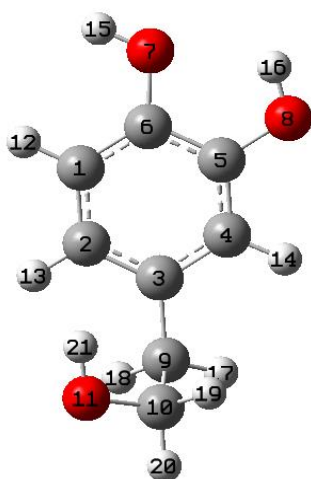
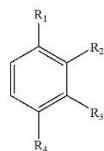
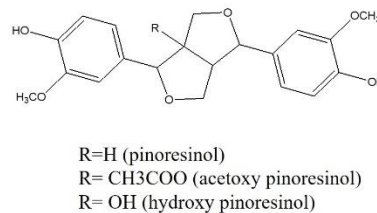
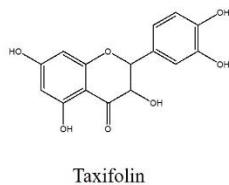
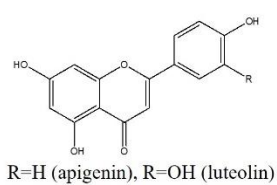


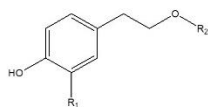
Figure S1. Atom numbering in hydroxytyrosol structure

No.	Hydroxybenzoic acid	Substitution pattern			
		R ₂	R ₃	R ₄	R ₅
1	4-Hydroxy-benzoic acid	H	H	OH	H
2	3-Hydroxy-benzoic acid	H	OH	H	H
3	4-Hydroxy-3-methoxy-benzoic acid	H	OCH ₃	OH	H
4	4-Hydroxy, 3,5-dimethoxy-benzoic acid	H	OCH ₃	OH	OCH ₃
5	3,4-Dihydroxy-benzoic acid	H	OH	OH	H
6	2,5-Dihydroxy-benzoic acid	OH	H	H	OH
7	3,4,5,-Trihydroxy-benzoic acid	H	OH	OH	OH

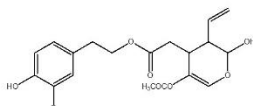
Figure S2. Structure of test group-2 phenols



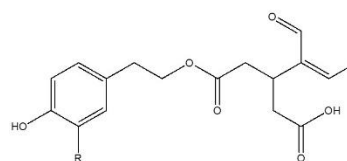
R₄=OH, R₃=R₂=H, R₁= -CH₂COOH (4-hydroxy phenyl acetic acid)
R₄=OH, R₃=OH, R₂=H, R₁= -CH₂COOH (3,4-dihydroxy phenyl acetic acid)
R₄=OH, R₃=R₂=H, R₁= -CH=CH-COOH (4-hydroxy cinnamic acid, p-coumaric acid)
R₄=H, R₃=H, R₂=OH, R₁= -CH=CH-COOH (2-hydroxy cinnamic acid, o-coumaric acid)
R₄=OH, R₃=OCH₃, R₂=H, R₁= -CH=CH-COOH (4-hydroxy, 3-methoxy cinnamic acid, ferulic acid)
R₄=OH, R₃=OH, R₂=H, R₁= -CH=CH-COOH (3,4-dihydroxy cinnamic acid, caffeic acid)



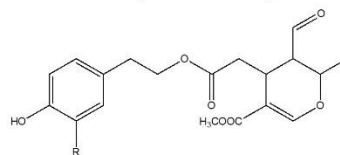
R₁=H, R₂=OCOCH₃ (tyrosol acetate)
R=OH, R₂=OCOCH₃ (hydroxytyrosol acetate)
R=OH, R₂=C₁₈H₃₃O (hydroxytyrosol oleate)
R=OH, R₂=C₁₈H₂₉O (hydroxytyrosol linolenate)



R=H (Ligstroside aglycone)
R=OH (Oleuropein aglycone)



R=H (oleocanthalic acid)
R=OH (Oleaceinic acid)



R=H (Ligstroside aglycone monoaldehyde)
R=OH (Oleuropein aglycone monoaldehyde)

Figure S3. Structure of diverse virgin olive oil phenols under study