Prediction of the Performance of Natural Hydroxybenzaldehydes and Corresponding Phenolic Acids upon Bulk Oil Oxidation using DFT Calculations in the Liquid Phase

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The present study focuses on understanding the activity trend derived for some common hydrohybenzaldehydes namely, protocatechuic aldehyde **1**, syringaldehyde **2**, vanillin **3**, *p*-hydroxybenzaldehyde **4** and salicylaldehyde, **5** and their corresponding acids (**1'**-**5'**) when tested under accelerated oxidation conditions of purified olive oil (Rancimat, 120 ^{o}C, air flow 20L/h) with regard to that based on bond dissociation enthalpy values (BDE) computed with density functional theory (DFT) and B3LYP exchange correlation functional. BDE values, characterizing the scavenging activity of the tested compounds via hydrogen atom donation, were calculated in the liquid phase (benzene) to simulate bulk oil. On the basis of protection factor (PF) values the experimental activity trend was **1'**>**1**>>**2'**~**2** whereas, **3**-**5** and **3'**-**5'** were found inactive. BDE values led to a similar trend only when computations included hydroxyl group at C-3 for **1** and **1'**. Similar activity of syringol derivatives (**2**, **2'**) was justified by similar BDE values (80.8 and 81.2 kcal/mol respectively) and inactivity of **3**-**5** and **3'**-**5'** was assigned to BDE values higher than that of phenol (85.2 kcal/mol).

The results support further that computed molecular descriptors facilitate efficient antioxidant selection through "green chemistry" processes and may provide insight to the mechanism of action of phenolic compounds in lipid substrates [1, 2].

References

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