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# Electronic structure of phenolic anti-oxidant trihydroxybenzoic acid using combined XPS and NMR spectroscopy

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Gallic acid (GA, 3,4,5-trihydroxybenzoic acid) and derivatives have been found in a number of phytomedicines with diverse biological and pharmacological activities, including radical scavenging, interfering with the cell signalling pathways and apoptosis of cancer cells. GA exhibits both antioxidant as well as prooxidant characteristics [1]. The chemical properties of phenolic hydroxyls are significantly different from those of the aliphatic-OH in glucose. As result, it is important to understand the properties of phenolic acids such as GA at molecular level. The present study uses theory and experiment, which combines state of the art XPS and NMR techniques to reveal detail of gallic acid. Our accurate quantum mechanical calculations connect the measured XPS and NMR spectra to the structure of GA, revealing the nearly-equivalent atoms in GA which are unable to differentiate by XPS nor NMR. Certain structural correlation between the XPS and NMR signals indicates that the para-position, C(5) as indicated, to the carboxyl group -COOH of GA, contains interesting information. In addition, the present quantum mechanical calculation is able to decompose the valence orbital contributions to the binding energy spectrum based on their orbital symmetry.

References

1. B. Badhani, N. Sharma and R. Kakkar, RSC Adv., 2015,5, 27540-27557.

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