

Computational Studies of Antioxidant Activity

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Emotional stress and environmental pollution increase free radicals in our body beyond healthy levels. These very reactive species can damage proteins and other biomolecules in a variety of ways. Antioxidants counteract the effect of free radicals and depending on their mechanisms of action, they can be classified as either primary (radical scavengers), secondary (preventive), or tertiary (repairing) antioxidants.

Primary antioxidants can retard oxidation by capturing free radicals. Secondary antioxidants can sometimes act as chelators (usually of Cu^{2+} and Fe^{3+} ions) that bind and thus inactivate or reduce the activity of pro-oxidant metals whose reduction leads to the formation of very reactive $\cdot\text{OH}$ radicals. Tertiary antioxidants can repair an already damaged biomolecule. Some examples of our theoretical (kinetic and thermodynamic) studies of the primary, secondary and tertiary antioxidant activity will be illustrated.

