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Amphithéâtre P. Glorieux, CERLA
University of Lille, Faculté des Sciences et Technologies

14:00

Free Radical Scavenging Activity of Natural-based Terpene Compounds: A Computational Point of View

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Free radical chemistry has been widely studied for various applications such as drugs discovery, food processing, atmospheric reactions, combustion, etc. Among the common free radical categories, reactive oxygen species (ROS) such as superoxide oxygen (O2●), hydroxyl (HO●) and peroxyl radicals (ROO●) generally contribute to oxidative stress (OS) that concerns with numerous diseases and has dangerous consequence to human health. Thus, evaluating the ROS scavenging activities of the chemical compounds acted as antioxidant becomes crucial in different applications and subject of a huge number of scientific publications in recent decades.

This presentation resumes our recent studies on the free radical scavenging activities of natural-based terpene compounds which consists in one of the most extensive compounds occurring in the essential oils extracted from various parts of plant. The antioxidant capacities of the naturally occurring terpenes such as oxygenated monoterpenes, oxygenated sesquiterpenes and diterpenes present in the extract of various biological sources in Vietnam have been studied by employing density functional theory (DFT) approaches. Several reaction mechanisms with reactive oxygen species have been evaluated: formal hydrogen transfer (FHT, including hydrogen atom transfer – HAT or proton coupled electron transfer – PCET), radical adduct formation (RAF), single electron transfer (SET), sequential proton loss electron transfer (SPL-ET) and sequential electron proton transfer (SEPT).

The identification of chemical compounds with the highest activity under different conditions could help in the design of efficient pharmacological strategies against oxidative stress.