Yang Yi

Quantum chemical studies of selected compounds determined as active components of traditional Chinese medicine

Traditional Chinese medicine (TCM) is based on more than 2500 years of Chinese medical practice, including herbal medicine, acupuncture, massage, and recently also influenced by modern western medicine. It has been reported that Chinese patients of chronic obstructive pulmonary disease (COPD) are significantly increasing because China has been attacked by smog with a serious air pollution in recent years. Fine particles, especially $PM_{2.5}$, are significantly harmful to the human body. Clinically, antioxidants from traditional Chinese medicine are used for COPD patients to prevent their pathophysiological changes and it is believed that the curative effect of some Chinese herbal medicines is closely related to their antioxidative activities found in flavonoids, saponins, polysaccharides, organic acids, terpenes and so on. However, active compounds and pharmacological mechanism of traditional Chinese medicine are still not commonly recognized.

In the present work we investigated two Chinese plants known as Rheum palmatum and Radix puerariae. The theoretical work includes chemical properties such as molecular structure and thermodynamics of molecules, corresponding radicals and transition states, charge distribution and electron spin density (where applicable), molecular orbital structure, and vibrational spectra. The determined properties were used to study antiradical properties of active compounds found in plants of interest. The studies confirmed promising antioxidative behavior and extended the knowledge on antiradical mechanisms. Additionally, studies include experimental ^{1}H and ^{13}C NMR properties of spectra for emodin (Rheum palmatum component) and puerarin and daidzein (Radix puerariae components). The interpretation of determined spectra was enhanced by quantum-chemical calculations. Some initial studies were performed for molecular intercalation of active compounds with selected fragments of DNA to study their possible anticancer properties. Most of theoretical studies presented are based on the density functional theory methodology. The interpretation of experimental NMR data is based on the original approach developed by cooperators.