A Quantum-Chemical Approach to Develop Tetrahydroquinoxaline as Potent Ferroptosis Inhibitors

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Abstract

Ferroptosis is a recently characterized form of regulated necrosis with the iron-dependent accumulation of (phospho)lipid hydroperoxides (LOOH). It has attracted considerable attention for its putative involvement in diverse pathophysiological processes, such as cardiovascular disease and neurodegeneration. Here we describe the discovery of tetrahydroquinoxaline, a novel scaffold of ferroptosis inhibitors based on quantum chemistry methods. Tetrahydroquinoxaline deviates showed very good inhibition of ferroptosis, while being non cytotoxic for human cancer cells. And, the advantage of them is their small molecular weight (MW. = 148 Da) that can be coupled with other drugs to form multi-target drugs to better meet the treatment of complicated diseases.

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