

MS32-P06 | IDENTIFICATION OF NON-COVALENT INTERACTIONS BY HIRSHFELD SURFACE AND ENERGY FRAMEWORKS IN CHALCONE-FLAVANONE ISOMERS

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Chalcones and flavanones are members of flavonoid class, which is one of the most important family of natural products. Chalcones and their derivatives have displayed numerous synthetic applications and have attracted much interest due to their multitarget and broad-spectrum biological activities. They exhibit, among others, antioxidant, antimicrobial, cancer-preventive activity, neuroprotective and hepatoprotective effects.

ortho-Hydroxychalcone and flavanone are examples of a molecular switching, these molecules are capable of predictable and reversible conformational changes. Such compounds have become increasingly desirable targets for organic synthesis.

The aim of the study is to analyze non-covalent interactions via Hirshfeld surface approach and pairwise model energy calculations together with energy frameworks visualization for 7 pairs chalcone-flavanone isomers. What is more the electron structure descriptors are also examined in order to find relationship between energetic parameters and structural descriptors.