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Abstract: The development of reactivity descriptor based on DFT has provided the scientific community with a formal framework for the understanding of many empirical chemical concepts. The Fukui function is a local reactivity descriptor that supplies information about the reactive sites of a molecule, thus predicting the region where a molecule is more prone to suffering an electrophilic, nucleophilic or radical attack. TAFF is a program that carries out the topological analysis of the Fukui function in a fast, simple and efficient way; acting as a pipeline between the user and the external Multiwfn software, with the aim of making easy the analysis of a selected molecule.

Conflicts of Interest

The authors declare no conflict of interest.