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Similarity of the Disposition of the Electrostatic Potential of Tetrazole and Carboxylic Group to Investigate Their Bioisosteric Relationship

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Abstract : Bioisosteres are functional groups that can be interchangeably used without affecting the potency of the drug. Bioisosteres have similar pharmacological properties. Bioisosterism is useful for modifying the physicochemical properties of a drug while obeying the Lipinski's rules. Bioisosteres are key in optimizing the pharmacokinetic and pharmacodynamics properties of a drug. Tetrazole and carboxylate anions are non-classic bioisosteres. Density functional theory was used to obtain the wavefunction of the molecules and the optimized geometries. The quantum theory of atoms in molecules (QTAIM) was used to uncover the similarity of the average electron density in tetrazole and carboxylate anions. This similarity between the bioisosteres capped by a methyl group was valid despite the fact that the groups have different volumes, charges, energies, or electron populations. The biochemical correspondence of tetrazole and carboxylic acid was also determined to be a result of the similarity of the topography of the electrostatic potential (ESP). The ESP demonstrates the pharmacological and biochemical resemblance for a matching "key-and-lock" interaction.

Keywords : bioisosteres, carboxylic acid, density functional theory, electrostatic potential, tetrazole
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