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A Structural Perspective on Halogens in Protein Ligand Binding Mechanisms

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Editorial

Many rational medicinal chemistry applications in drug design have focused on halogen atoms. While fluorine and chlorine atoms are frequently used to improve physicochemical qualities, bromine and iodine are commonly used to improve selectivity. Quantum mechanics and statistical analysis have been used to investigate favourable halogen interactions such as the halogen bond. Although most research focus on halogen interaction through its-hole, hydrogen bonding plays an important role as well. We give an investigation of the halogen atoms' interaction environment in the context of protein ligands. Tendencies toward specific molecular interactions have been modified with account of structural redundancy in the PDB, and implications for rational drug design using halogens have been examined further. Finally, we emphasise the very rare occurrence of halogen bonding and discuss the additional functions of halogen in protein-ligand complexes, bringing the medicinal chemistry guide to rational halogen interactions to a close. The amount of publicly available structural data on Protein Data Bank1 (PDB) structures has expanded dramatically in recent years, from 47,000 to 134,000 in just ten years. Computer-aided drug design, for example, benefits from this richness of structural data by improving our understanding of small molecule binding. As a result, a variety of approaches for visualising, analysing, and comparing protein-ligand interactions have been developed. Numerous studies have detailed specific interactions, such as hydrogen bonds and sulfuroxygen interactions, over the years. Fluorine (F), Chlorine (Cl), Bromine (Br), and iodine has all been incorporated into designed drugs for different reasons: To improve selectivity by adding bromine or iodine, to increase ADME properties by adding chlorine and fluorine, or to reduce unwanted reactions like ring hydroxylation. While their many activities in medicinal chemistry have been investigated, their ability to create molecular contacts has also been investigated in order to better understand their role in improving binding affinity. On their equatorial sides, heavy halogen elements such as chlorine, bromine, and iodine have an anisotropic electron distribution, resulting in a positive outer region along their covalent bond called the σ-hole. Its size is determined by a variety of circumstances, including the presence of a heavier halogen or an electron-withdrawing scaffold, which results in a larger positive σ-hole. Fluorine has a region like this in uncommon circumstances, but due to its strong electronegativity, it is generally thought to σ-hole deficient. Molecular interactions involving halogens have primarily been investigated in the σ-region. The first noncovalent halogen interaction was described in the 1950s, and the term "halogen bonding" was coined in the late 1990s. Multiple nucleophiles, such as oxygen, sp3-hybridized nitrogen, aromatic ring, or sulphur, operate as halogen bond acceptors.

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