Mulliken charge analysis on Pharmacodynamic activity of 7-Bromo-5-Chloro-8-Quinolinol using DFT

S. Ramalingam[a], S. Periandy[b]

[a] PG and Research department of Physics, A.V.C. College, Mayiladuthurai, Tamilnadu, India.

[b]Department of Physics, Kanchi Mamunivar Centre for PG studies, Puducherry, India.

Corresponding Author: ramalingam.physics@gmail.com

***ABSTRACT** In this case, Mulliken charge profile of 7-Bromo-5-Chloro-8-Quinolinol was displayed and simulated by performing DFT calculations. The enlarged charge displacement was keenly monitored by which the accumulation of nucleophilic and electrophilic chemical potential was identified. The process of Pharmacodynamic activity was noted and the suitable interpretation was drawn.*

***Key words:** 7-Bromo-5-Chloro-8-Quinolinol, DFT, nucleophilic, chemical potential, Pharmacodynamic activity.*

I.INTRODUCTION

Hydroxquinoline is most popular and versatile organic crystalline material that made up of coupled rings in which a phenol ring fused with pyridine ring. 8-Hydroxyquinoline and its derivatives have found an enormous multifunctional applications ranging from pharmacological and pharmaceutical agents[1-2]. In medicinal field, 8hydroxyquinoline derivatives can be used as insecticides, antibacterial, fungicidal, neuroprotective, and anti HIV agents [3-5].

Recently, after screening the literature, no computational investigation was made on the compound; 7-Bromo-5-Chloro-8-Quinolinol to study the molecular charge locations for creating nodal regions for generating antibacterial so far. Hence, in this work, the Pharmacodynamic analysis related to Mulliken charge distributions have been carried out on present compound.

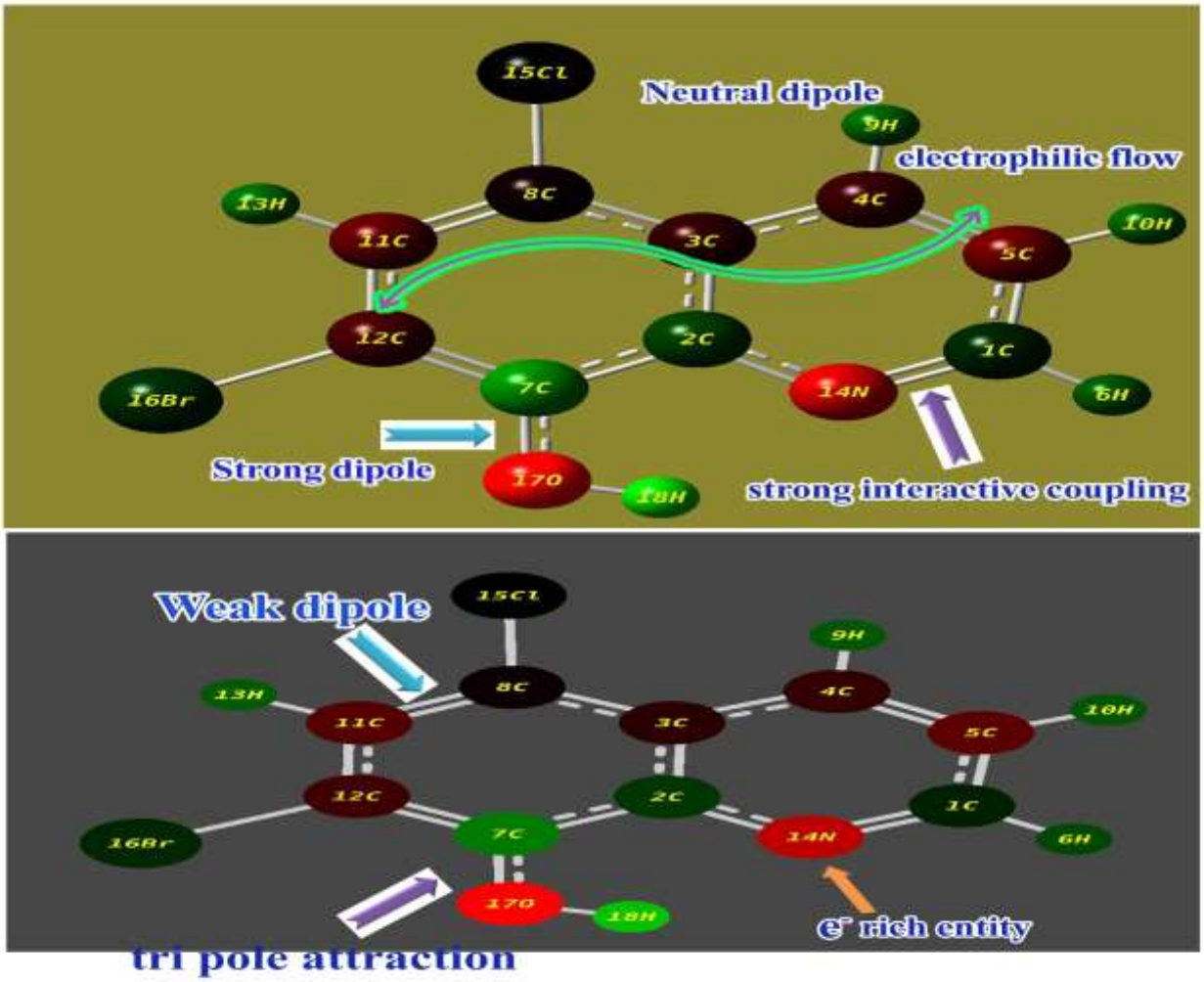
II.RESULTS AND DISCUSSION

The Charge-transfer complexes are an electron donor/electron acceptor association for which an intermolecular electronic charge-transfer transition is observed. When combining base compound with substitutions, it is supposed that a stable charge-transfer complex has formed between the components of the mixture [6]. In the complex, some chemical entities are formed with electrophilic and nucleophilic boundaries in which the electron cloud is oriented asymmetrically and the molecule would have an uneven distribution of charge regions and these charge dispensations that allowed leads electrostatic interaction to occur between different electron donor (HOMO) and electron acceptor (LUMO) among the orbitals and the interaction energy making effective unique chemical property on compound [7-8].

The Mulliken charge distribution levels presented in the following table and its diagram was depicted in the following Figure. Here, the electron cloud was observed to be oriented on core C of top moiety of the quinoline ring in which the electron cloud delocalization started from Br atom corresponding to C of ring. The deficiency of electrons in Br atom, it becomes positive entity (appeared to be green). The electronic charges were accumulated from C12 to C5 of ring (electrophilic flow). Here, the Cl atom and its corresponding C of the ring changed as neutral atom since the electron cloud was completely exchanged on par with C-Cl bond. In the hydroxyl group, the strong dipole bond was formed to enhance its activity on the ring and except N, the C of the bottom moiety of the ring was appeared to be positive. Generally, the formation of imine group in CT complex produces antibiotic and antipyretic property [8]. In this case, the presence of imine group in quinoline ring generates the energy sufficient to produce antibiotic character. In addition to that, the negative charge inducement in the C of the top moiety of ring stimulate anti bactericidal activity for tuberculosis.

Table: Mulliken Charges of 7-Bromo-5-Chloro-8-Quinolinol

Atom Position	Charge level
C1	0.086
C2	0.143
C3	-0.109
C4	-0.128
C5	-0.239
C7	0.315
C8	-0.034
C11	-0.215
C12	-0.158
N14	-0.488
15Cl	0.006
16Br	0.102
O17	-0.651
H6	0.191
H9	0.227
H10	0.218
H13	0.237
H18	0.499



Mulliken charge distribution

III.CONCLUSION

The Pharmacodynamic activity was studied by performing Mulliken charge analysis. The molecular charge displacement was noted in the figure and accordingly, the nodal charge regions were found for observing the accumulation of chemical potential. The addition of ligands dislocates the charge levels and thereby various chemical boundaries in different entities were found. The change of drug activity by attaching active ligands in suitable positions was studied by analyzing the asymmetric charge delocalization in different entities. The molecular orbital interaction formation found to be favoured for the chemical process to produce desirable drug property was predicted. The chromophores reactivity on the base compound causing the electrophilic and nucleophilic shift was discussed in detail.

References

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