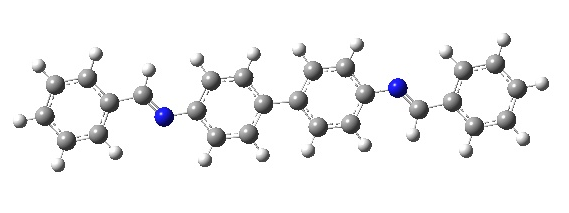
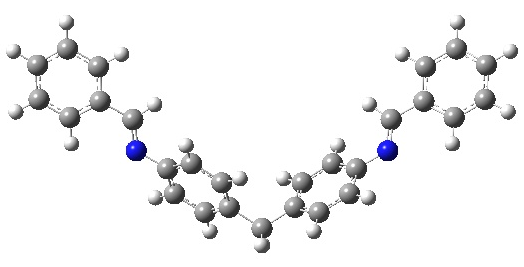


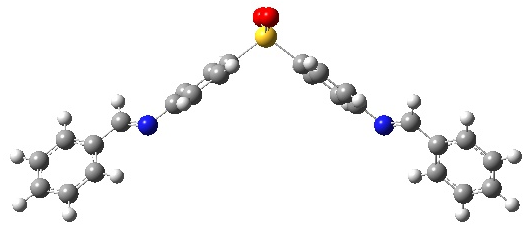
**Figure 1: Chemical molecular structures of the studied dianiline Schiff bases.**



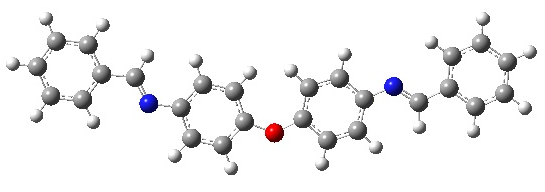
**DAA**



**MDAA**



**SDAA**

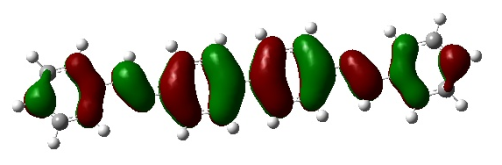
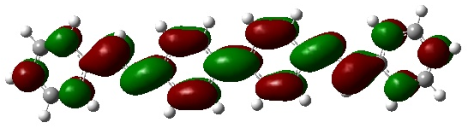


**ODAA**

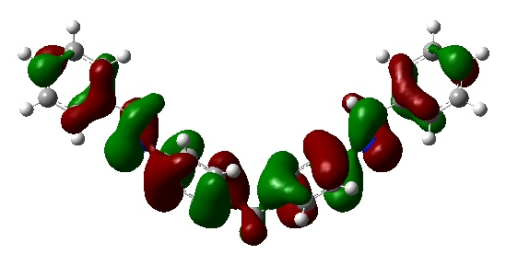
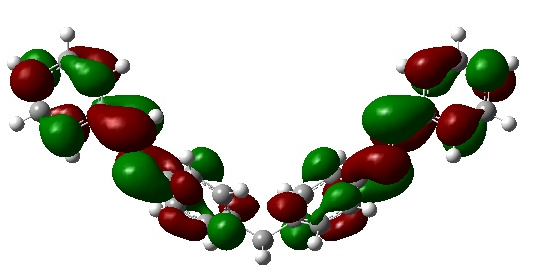
**Figure 2: Optimized molecular structures of non-protonated inhibitor molecules using B3LYP/6-31G calculation level.**

C:\Documents and Settings\HACHANI\Bureau\new planarity 2.tif

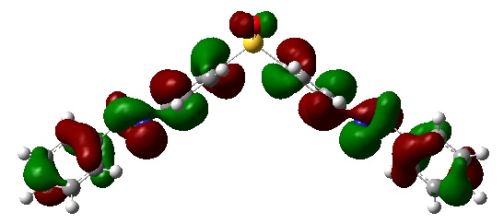
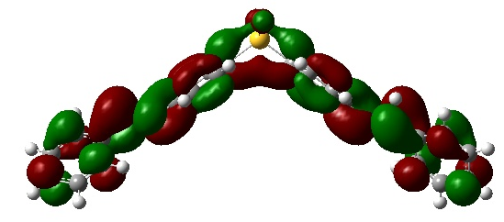
**Figure 3: Geometry planarity of the studied dianiline Schiff bases.**

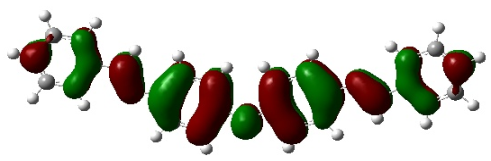
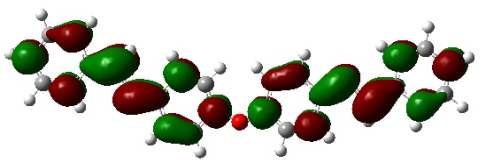
**DAA HOMO DAA LUMO**

**MDAA HOMO MDAA LUMO**

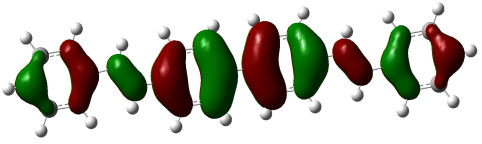
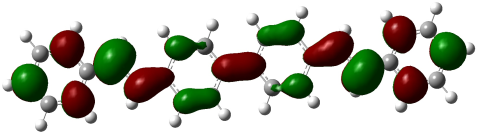
 

**SDAA HOMO SDAA LUMO**

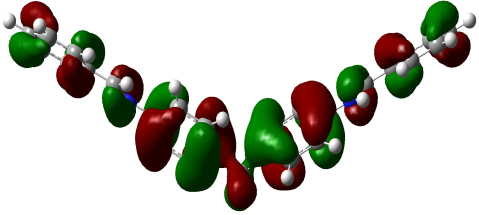
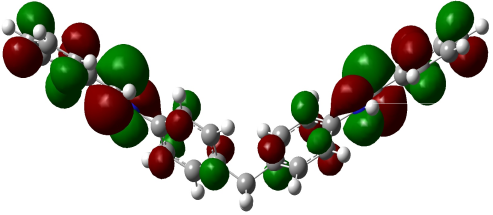
 

**ODAA HOMO ODAA LUMO**

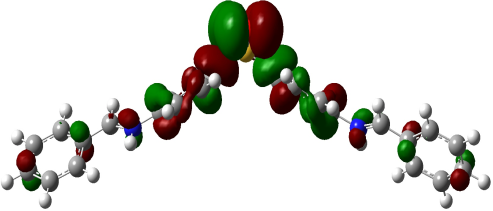
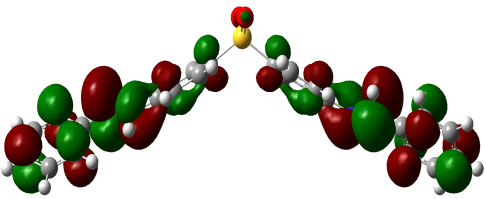
**Figure 4: HOMO and LUMO orbitals of non-protonated inhibitor molecules using B3LYP/6-31G calculation level.**

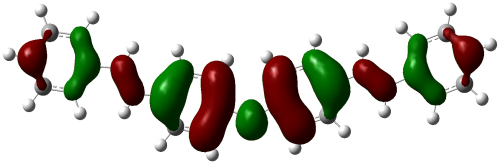
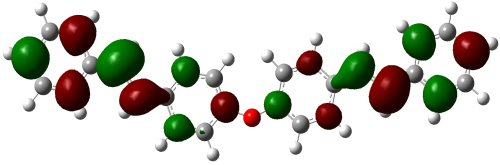
**Protonated DAA HOMO Protonated DAA LUMO**

**Protonated MDAA HOMO Protonated MDAA LUMO**

**Protonated SDAA HOMO Protonated SDAA LUMO**

**Protonated ODAA HOMO Protonated ODAA LUMO**

**Figure 5: HOMO and LUMO orbitals of the protonated inhibitor molecules at B3LYP/6-31G level.**