# CHAPTER 4

## Conclusions

In summary, the geometry optimizations of HBQ and its derivatives are carried out at B3LYP/TZVP level. The distances of O···N, N···H, and C1···N are found to be shortened in the $S_1$ state, indicating that intramolecular hydrogen bonds become strengthen in the $S_1$ state. The O–H stretching modes of all compounds are shifted to lower frequencies in $S_1$ state compared with the $S_0$ state, which confirms that the hydrogen bonding interaction is strengthened in the S state. The calculated absorption and emission spectra of HBQ are in good agreement with experimental data, indicating that TD-B3LYP/TZVP is reliable. The frontier molecular orbitals show that upon photoexcitation, ESIPT is triggered by the charge distribution and intramolecular charge transfer between proton donor and proton acceptor. The ESIPT can occur via O–H···N intramolecular hydrogen bond because this bond becomes strengthen in $S_1$ state, supported by shorter of N···H, O···N, and C1···N distances and also the red-shifted of O–H vibrational mode. Furthermore, PECs of PT reaction coordinate reveals that PT is mostly like to occur in the excited-state but not in the ground state. From the dynamics simulation, the ESIPT processes of all systems occur through a hydrogen bonded network in ultrafast timescale within 100 fs depending on geometry change of HBQ derivatives. After ESIPT is complete, the profoundly twisted skeleton behavior found in PDP and PRP has initiated the internal conversion, leading to lower intensity of tautomer emission.