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ABSTARCT

Coumarins (1, 2-benzopyrone) or α-benzopyrone and its derivatives are a subject of concern due to their interesting photophysical properties. Coumarin, the parent molecule of coumarin derivatives is the simplest compound of a large class of naturally occurring phenolic substance made up of fused benzene and α-pyrone ring. Coumarins are naturally occurring substance which can be synthesized in the laboratory as well. The growing interest is due to their chemical reactivity, biological compatibility and a number of applications associated with them. Coumarins establish a family of laser dyes which emit in blue-green region in the electromagnetic spectrum. These have also have applications as optical brightener, fluorescent probe, widely used for the preparation of liquid crystals and act as sunburn preventive. Coumarin derivatives are used in dye sensitized solar cells (DSSC. In the present research work we have investigated the UV/VIS and IR spectroscopy of coumarin derivatives. Effects of different substituents on the spectroscopic properties of couamarin were investigated from the point of view to determine the dipole moment in ground and excited state and their interaction with Bovine Serum Albumin (BSA).

The thesis comprises of six chapters, **chapter 1** presents a brief introduction of coumarin and their applications. The general introduction of coumarins, their occurrence in nature and synthesis processes molecular structure, various phenomenon related to spectroscopic and photophysical properties of coumarin e.g. molecular spectroscopy, emission, fluorescence and phosphorescence has been discussed. **Chapter 2** describes the basic principle and working of UV/VIS

spectrophotometer (Shimazdu UV-2450), spectrofluorophotometer (Shimazdu RF-5301 PC) and FTIR (Perkin Elmer BXII Spektrum) spectrometer. In **chapter 3** a brief mathematical formulation of Molecular modeling, Semi-empirical, ab initio and Density Functional Theory (DFT) is discussed. Using these methods we have calculated different structural and spectroscopic parameters e.g. bond length, HOMO-LUMO energies and natural bonding orbitals (NBO) analysis for coumarin derivatives. Apart from this we have computed the IR spectra of the coumarin derivatives so as to strengthen our experimental findings. **Chapter 4** presents the dipole moments of ground and excited state and their difference of five coumarin dyes; 7-diethylamino coumarin (7DEAC); 7-diethylamino-4-methyl coumarin (7DEA4MC); 7-hydroxy-4-trifluoromethyl coumarin (7H4TFMC); 7-methoxy-4-trifluoromethyl coumarin (7M4TFMC); 6, 7-dihydroxy-4-trifluoromethyl coumarin (67DH4TFMC) has been estimated by using the following four different methods; i) Bakhsiev method, ii) Lippert-Mataga, iii) McRae, iv) Molecular microscopic solvent polarity parameter E_T^N.Our results shows that the excited state dipole moment is 1.6 times than the ground state dipole moment, which suggests that, the excited state are more polar than the ground state. It has also been observed that on increasing the polarity of the solvent the absorption and emission spectra show a red shift suggesting $\pi \rightarrow \pi^*$ transitions. We have studied the absorption and emission spectra of coumarin derivatives in a large number of polar and non-polar solvents in order to observe the excited state dipole moment, which was limited to only a few solvents in the previous reported works. For calculation of different parameters i.e. ΔE (HOMO-LUMO gap), charge density distribution and binding energies of these coumarins, here we have applied the high level ab initio quantum mechanical methods for optimization. On the basis of the above calculations it has been observed that HOMO-LUMO gap of 67DH4TFMC is smaller than the other two which is why it is more reactive than the other two studied systems. **Chapter 5** presents the interaction of coumarin derivative (7-diethyl-amino-4-mehyl coumarin) with Bovine Serum Albumin (BSA) which is a commonly used protein. Results showed that coumarin bind with BSA and quenched the intrinsic fluorescence of BSA. In, **Chapter 6** we have summarizes the results obtained in the present investigations on structural and spectroscopic properties of different coumarin derivatives and their potential applications. The scope of future work has also been discussed in this chapter.