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Important role of the position of a functional group in isomers for Photophysical and Antibacterial Properties: A case study with Naphthalenemaleonitrile Positional Isomers.

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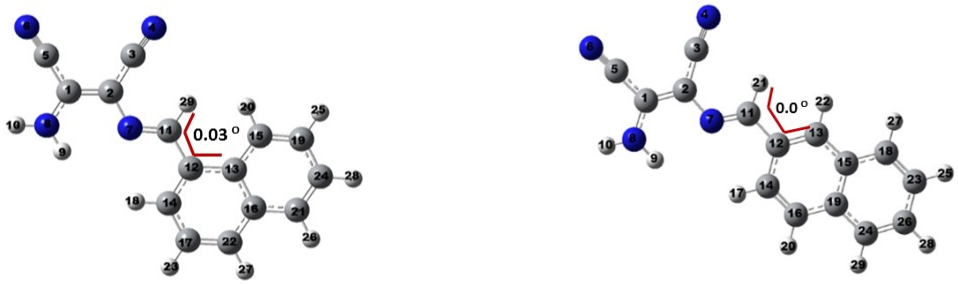

1N **2N**

Figure S1: The optimization geometry of **1N** with dihedral angle $D_{H29\text{-}C11\text{-}C12\text{-}C13}$ (0.03 °) and **2N** with dihedral angle $D_{H21\text{-}C11\text{-}C12\text{-}C13}$ (0.0 °) showing the numbering scheme of atoms.

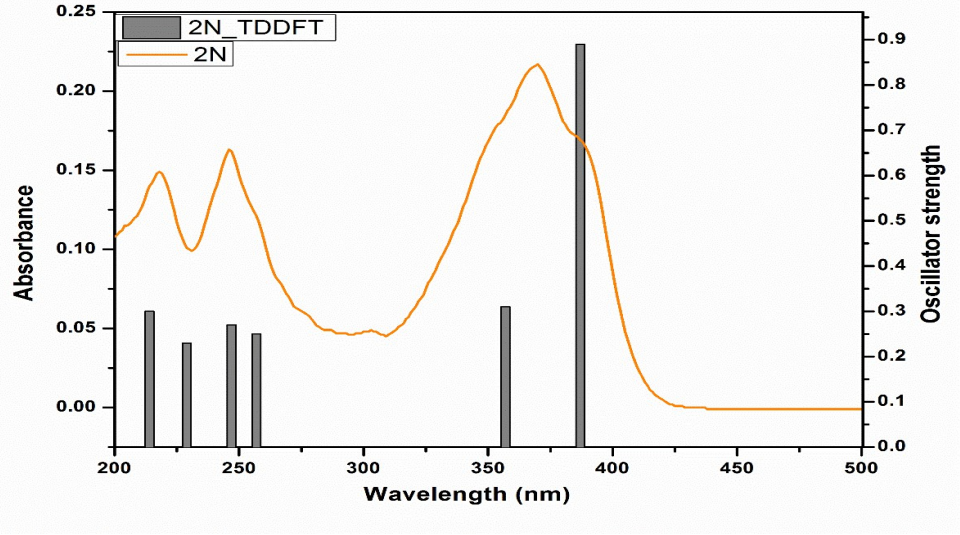

Figure S2: Computed absorption spectra in ACN for **2N** (bar graph) compared to experimental absorption spectra in ACN.

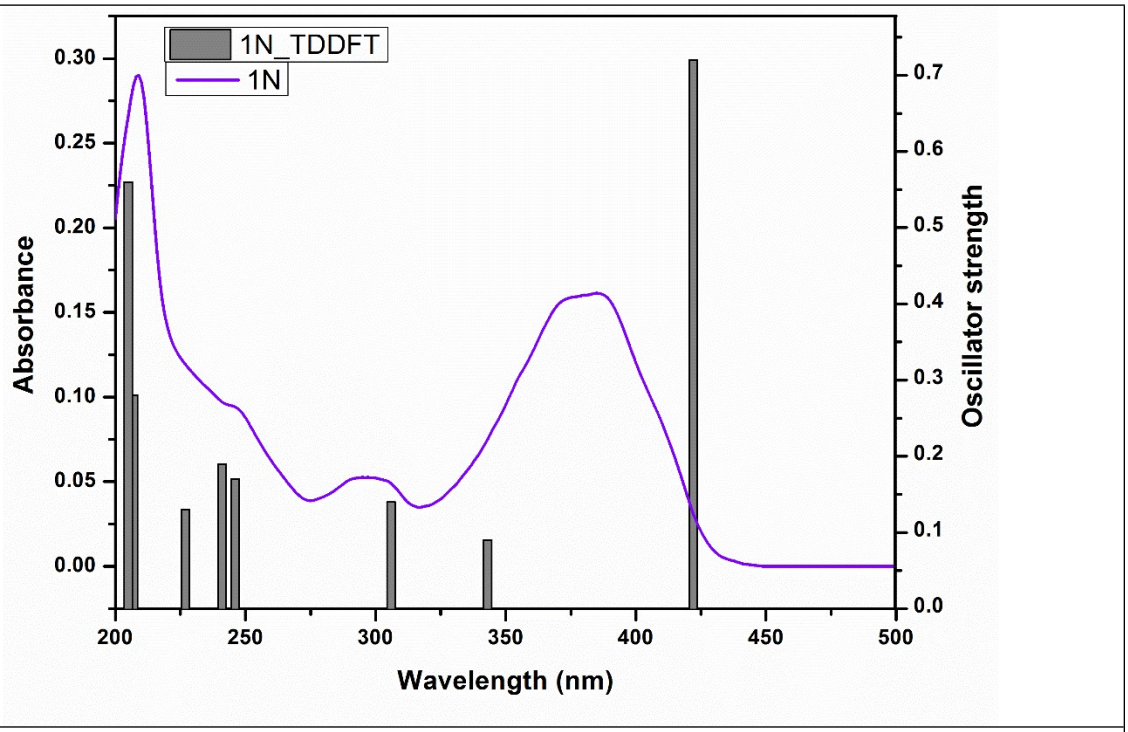

Figure S3: Computed absorption spectra in ACN for **1N** (bar graph) compared to experimental absorption spectra in ACN.

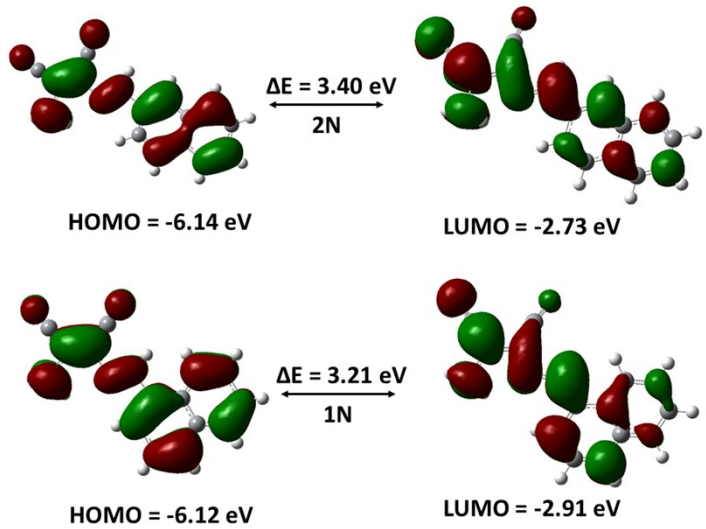

Figure S4: HOMO and LUMO energy level of **1N** and **2N**.

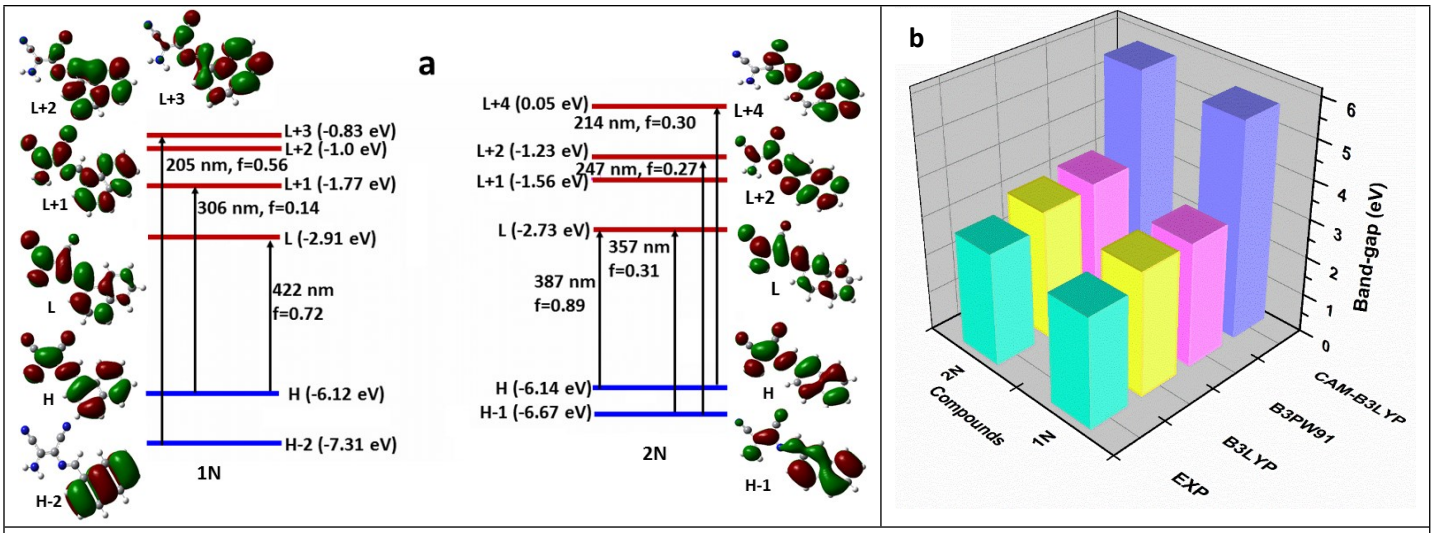

Figure S5. (a) Molecular orbitals of **1N** and **2N** involved in electronic transitions through TD-DFT calculations performed in ACN via CPCM model. (b) Showing the band gap through different level of theory.

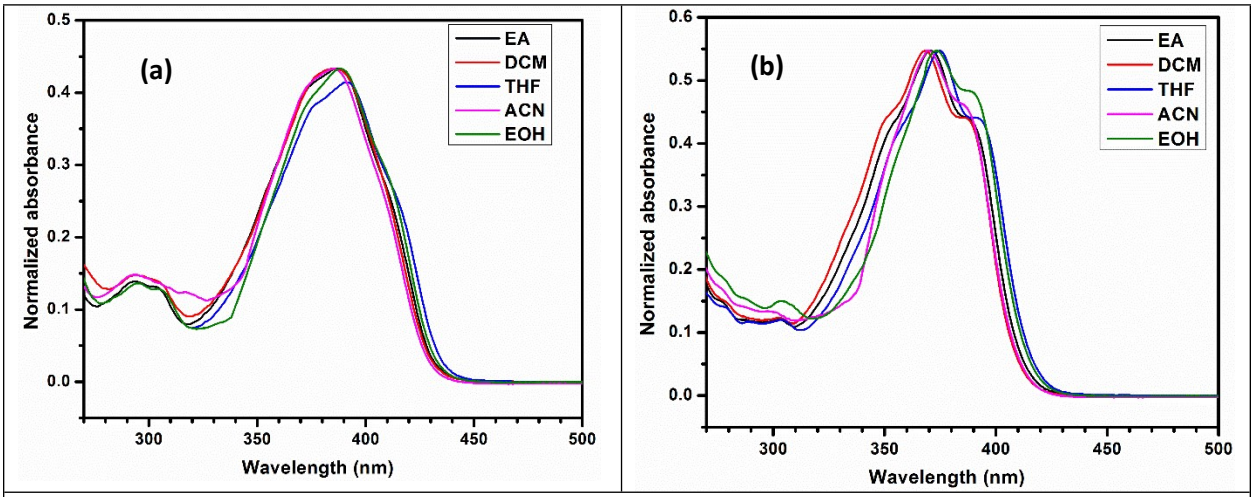

Figure S6: Normalized absorption spectra of (a) **1N** and (b) **2N** in different solvent at room temperature (10^{-5} mol/L concentration)

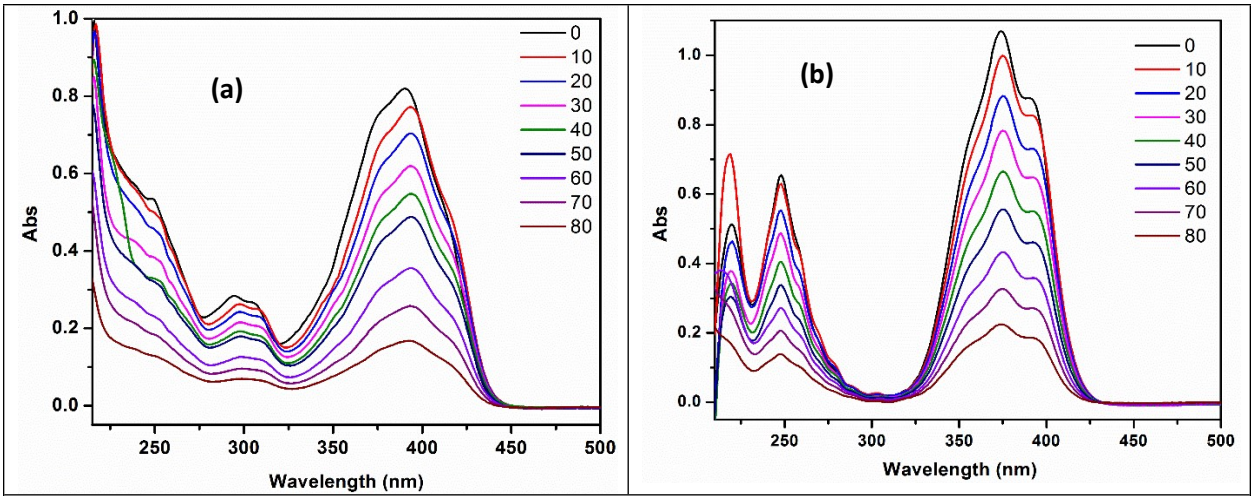

Figure S7: UV-vis absorption spectra of **1N** (a) and **2N** (b) in THF/H2O mixtures with different fractions of water. Concentration: 1×10^{-5} mol/L.

Cyclic voltammetry (CV) studies were carried out in mollimolar solution of compound 1N and 2N in anhydrous acetonitrile.

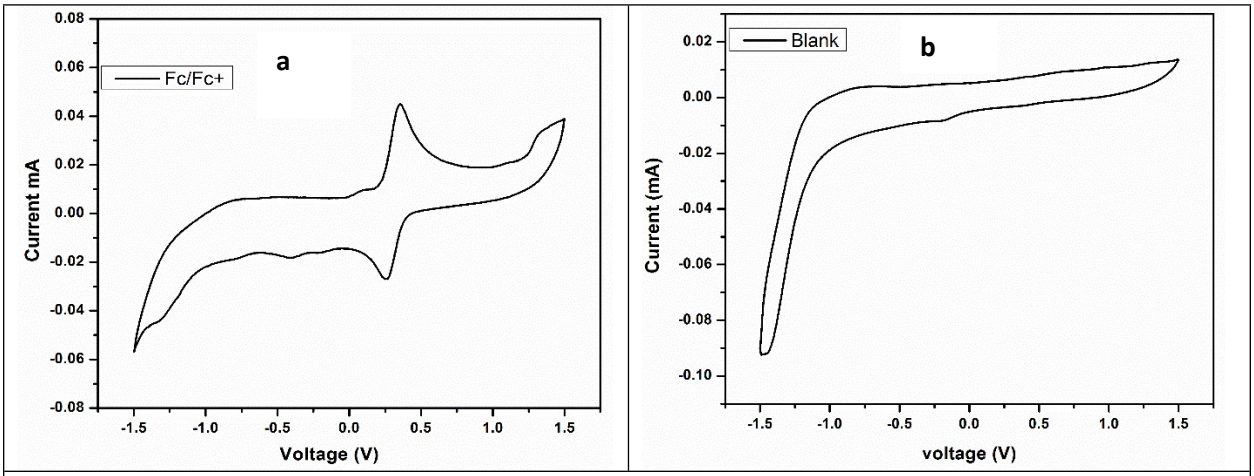

Figure S8: (a) Cyclic voltammogram of ferrocene in anhydrous ACN solution of TBAP (tetrabutyleammonium perchlorate) with 0.1M concetration. (b) Cyclic volammogram of blank in anhydrous ACN solution at a scanning rate 100 mV/s .

E_{red} and E_{oxd} were found to be -0.684, -0.390 and 0.50, 0.864 V for 1N and 2N respectively. The half-wave potential of the ferrocene/ferrocenium (F_c/F_c^+) redox couple was found to be 0.302 V by the following relation.

$$(E_{1/2,\ Fc/Fc^+}) = (E_{\text{anodic peak potential}} + E_{\text{cathodic peak potential}})/2 = (0.352+0.252)/2 = 0.302\ V$$

The band gap was calculated using the following relation:

$E_{HOMO} = -(_{Eoxd,onset}\text{-}E1/2,F_c,F_c^+ + 4.8)eV$

$E_{LUMO} = -(_{Ered,onset}\text{-}E1/2,F_c,F_c^+ + 4.8)eV$

$\Delta E_g = E_{HOMO} - E_{LUMO}$