

SUPPLEMENTARY INFORMATION

Protonation of the imino nitrogen deactivates the excited state of imidazolin-5-one in the solid state

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Figure S1 represent the one dimensional arrangement of compound **I** through hydrogen bonding between C(1)-H(1A)···O(3) (2.58 Å), C(12)-H(01C)···O(3) (2.56 Å) and C(3)-H(3)···O(5) (2.48 Å) (dotted red line). Color code: carbon: yellow; oxygen: red; nitrogen: blue; hydrogen: black, chlorine: light green.

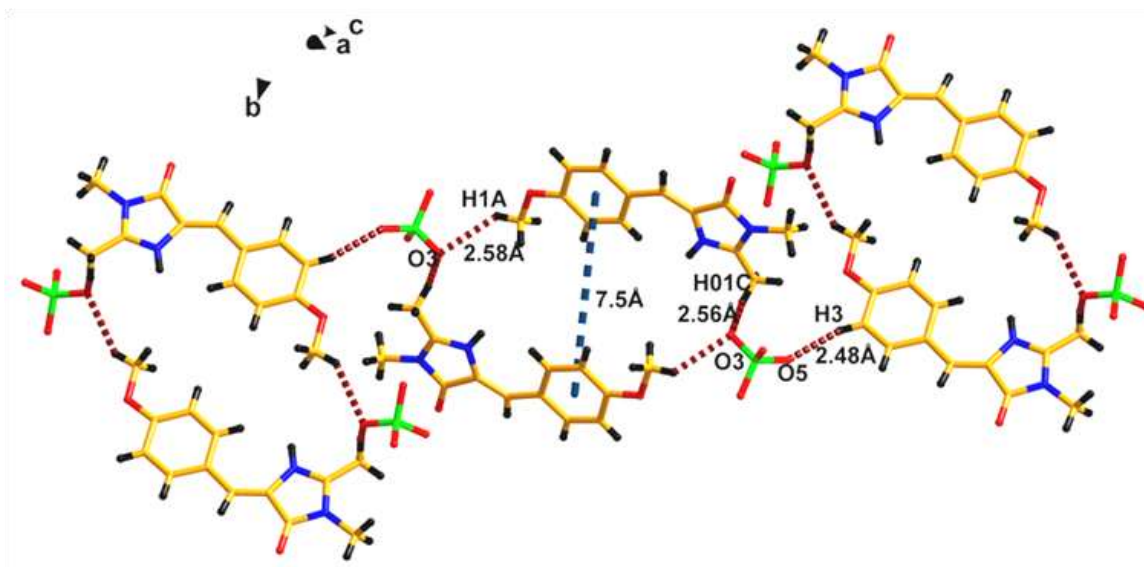


Figure S2:- IR spectra of compound **II**, in acetonitrile solvent (above) and in solid state (below). In solid state, N-H peak of the imidazolinone ring appears at 3477 cm^{-1} (highlighted region).

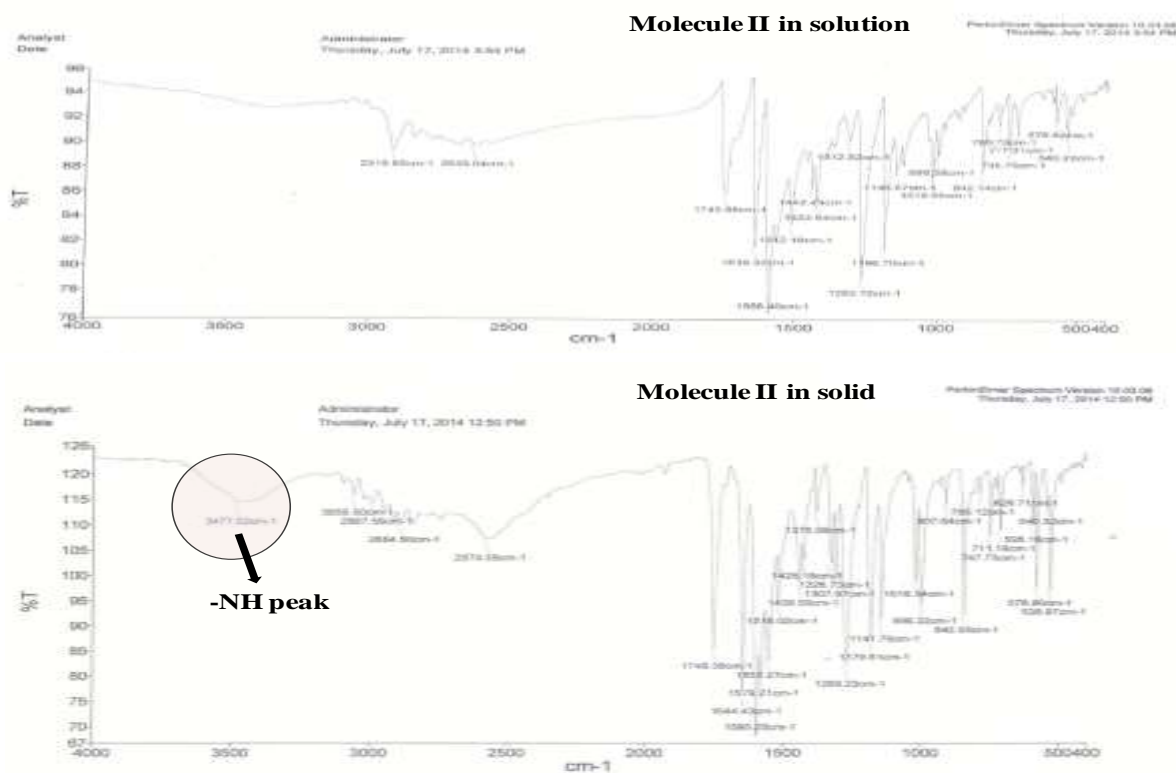
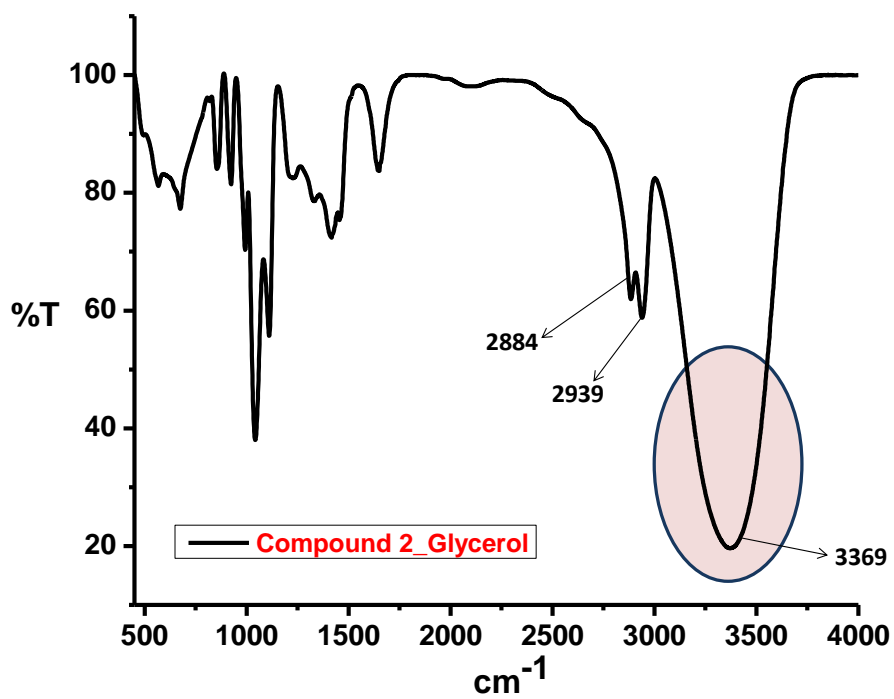
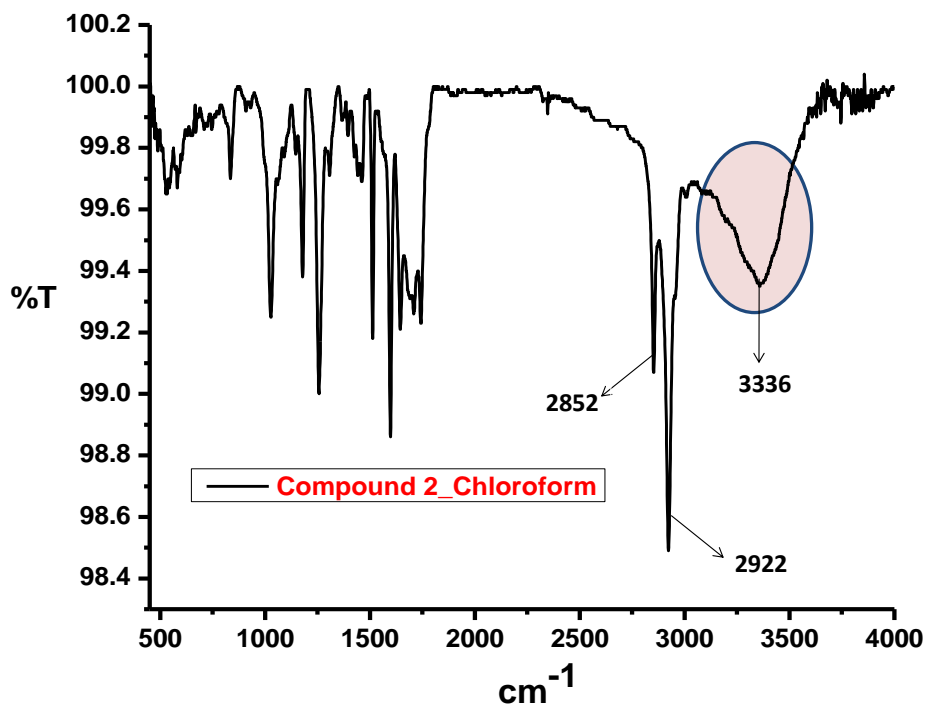


Figure S3: IR spectra of compound **II** in Chloroform (above) and in Glycerol (below). The N-H peak is highlighted.



Characterization of ligand and compound I-II: - The ^1H NMR of the molecule **I** and **II** was similar to the *p*-MBDI (ligand). Therefore, here we are reporting the Mass spectra and CHN analysis of molecule **I** and **II**.

(Z)-4-(4-methoxybenzylidene)-1,2-dimethyl-1H-imidazol-5(4H)-one (pMBDI) (ligand):

Yellow solid compound. Yield: 70%; M.p.: 130-132 °C; R_f 0.4 (40% Ethyl acetate: Petroleum ether), IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3078, 2997, 2837, 1703, 1636, 1596, 1427, 1253, 1176. ^1H NMR (CDCl_3 , 500 MHz): δ 2.36 (s, 3H, $-\text{CH}_3$), 3.17 (s, 3H, $-\text{NCH}_3$), 3.84 (s, 3H, $-\text{OCH}_3$), 6.93 (d, $J/\text{Hz} = 8.55$, 2H, $-\text{ArH}$), 7.07 (s, 1H, $=\text{CHAr}$), 8.10 (d, $J/\text{Hz} = 8.55$, 2H, $-\text{ArH}$), ^{13}C -NMR (CDCl_3 , 125 MHz): δ 15.7, 26.7, 55.4, 114.3, 127.1, 126.6, 134.1, 136.7, 161.3, 161.4, 170.7. ESI-MS+ m/z Calcd. for $[\text{C}_{13}\text{H}_{14}\text{N}_2\text{O}_2]$: 230.1055 $[\text{M}+\text{H}]^+$, found 231.1133.

(Z)-4-(4-methoxybenzylidene)-1,2-dimethyl-5-oxo-4,5-dihydro-1H-imidazol-3-ium

perchlorate (compound I):- ESI-MS+ m/z Calcd. for $[\text{C}_{13}\text{H}_{15}\text{N}_2\text{O}_2]\text{ClO}_4$: 231.1134 $[\text{M}^+]$, found 231.1137. Anal. Calcd for $\text{C}_{13}\text{H}_{15}\text{N}_2\text{O}_6\text{Cl}_1$: C, 47.21; H, 4.57; N, 8.47. Found: C, 47.26; H, 4.42; N, 8.55.

(Z)-4-(4-methoxybenzylidene)-1,2-dimethyl-5-oxo-4,5-dihydro-1H-imidazol-3-ium chloride

(compound II):- ESI-MS+ m/z Calcd. for $[\text{C}_{13}\text{H}_{15}\text{N}_2\text{O}_2]\text{Cl}$: 231.1134 $[\text{M}^+]$, found 231.1130. Anal. Calcd for $\text{C}_{13}\text{H}_{15}\text{N}_2\text{O}_2\text{Cl}_1$: C, 58.54; H, 5.67; N, 10.50. Found: C, 58.46; H, 5.72; N, 10.64.

Figure S4: ^1H and ^{13}C spectra of (Z)-4-(4-methoxybenzylidene)-1,2-dimethyl-1H-imidazol-5(4H)-one (ligand):

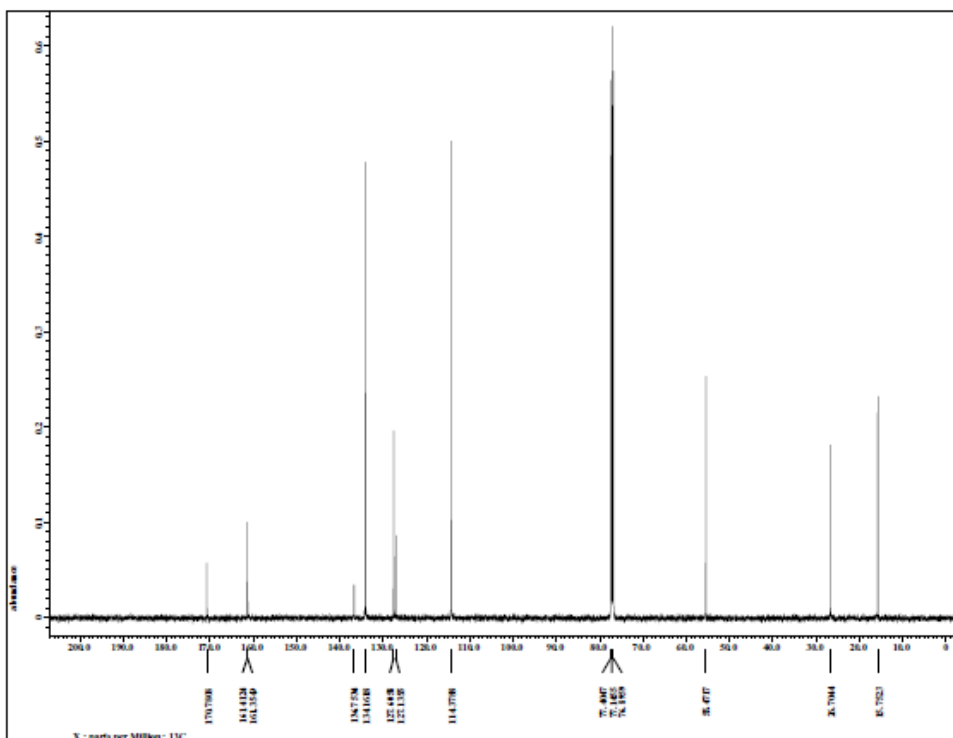
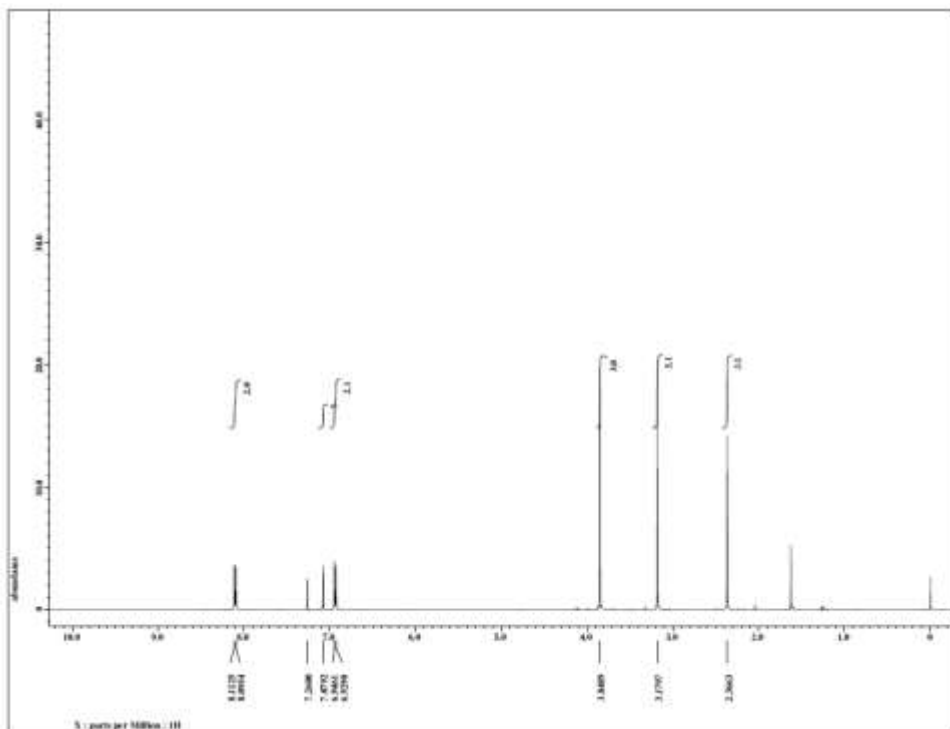


Figure S5: Mass Spectra of (Z)-4-(4-methoxybenzylidene)-1,2-dimethyl-5-oxo-4,5-dihydro-1H-imidazol-3-ium perchlorate (compound I)

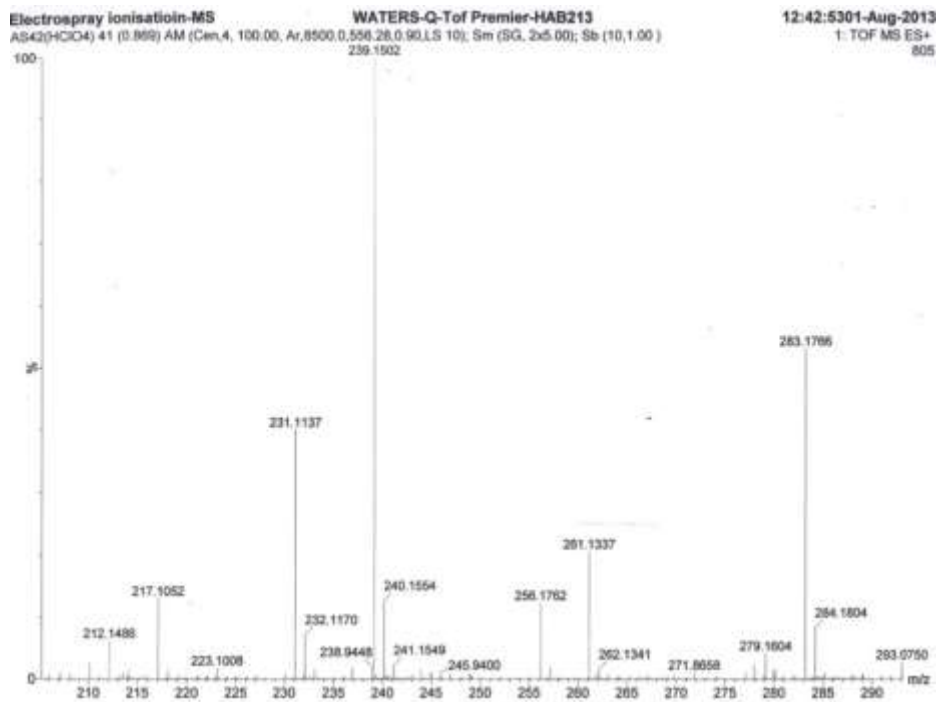


Figure S6: Mass spectra of (Z)-4-(4-methoxybenzylidene)-1,2-dimethyl-5-oxo-4,5-dihydro-1H-imidazol-3-ium chloride (compound II)

