## Abstract

The IEDDA reaction of diene 2-oxo-2H-pyrido[1,2-*a*] pyrimidin-3(4*H*)-ylidiene acetic acid with various electron rich dienophiles in DMF medium yielded moderate to good yields in the presence of Lewis acid catalyst indium (III) chloride. FT-IR, $^{1}$H NMR, $^{13}$C NMR, and Mass Spectroscopy investigations were used to characterize and confirm the structures of all the synthesized adducts. Except for 3-butoxy-9-methyl-2,3,4,5-tetrahydropyrano[2,3-*d*]pyrido[1,2-*a*]pyrimidine-4-carboxylic acid **(5)** and Methyl-2-Oxo-1-Phenyl-1,2,3,3*a*,4,5-hexa hydropyrazolo[1,5-*b*]Pyrido[1',2':1,2]Pyrimido[5,4-*e*][1,2]Oxazine-4-Carboxylic Acid **(7)** which showed 1:1 and 6:4 ratio and for other adducts the ratio was found to be 6:1, supporting the *endo* rule. The analysis of the LUMO and HOMO energies of diene and dienophiles helped to prove the IEDDA reaction pathway. NBO charges computed using DFT techniques gave justification for the regioselectivity provided by the reaction. The synchronous nature of the transition states and intrinsic reaction coordinates of the reaction of diene 2-oxo-2H-pyrido[1,2-*a*] pyrimidin-3(4H)-ylidiene acetic acid with dienophiles butyl vinyl ether and 1-methyl-1-cyclohexene by DFT method explained the observed diastereoisomeric ratio of 1:1 and 6:1 *endo* and *exo* ratio respectively. All synthesized compounds were tested for antibacterial activity, which showed moderate activity, however the compound 3*a*-methyl-2-oxo-1-phenyl-1,2,3,3*a*,4,5-hexahydropyrazolo[1,5-*b*]pyrido[1',2':1,2]pyrimido[5,4-*e*][1,2]oxazine-4-carboxylic acid was shown to be more powerful in both *in-silico* and *in-vitro* investigations.