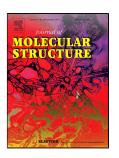
## **Accepted Manuscript**

Antimicrobial Activities, DNA Interactions, Spectroscopic (FT-IR and UV-Vis) Characterizations, and DFT Calculations for pyridine-2-carboxylic acid and its derivates



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#### **ACCEPTED MANUSCRIPT**

### **Highlights**

- The interaction of 4Mpic with DNA is superior than 4Cpic and pic
- 4Clpic is very active against to Gram (+) bacteria
- The optimizations of pic, 4Clpic and 4Mpic were performed by using B3LYP level
- FT-IR and UV-Vis spectral characterizations were made for pic, 4Clpic and 4Mpic
- The OCH<sub>3</sub> and Cl substituent increase charge asymmetry, leading to increase in β

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