

Synthesis, Characterization, and Antimicrobial Assessment of Some Computationally Bioactive 1,2-Oxazole Derivatives¹

M. Arshad^{a,*}

^a Department of Basic Sciences, College of Medicine Al-Dawadmi, Shaqra University, Saudi Arabia
*e-mail: m.arshad@su.edu.sa; mohdarshad1985@gmail.com

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Abstract—1,2-Oxazole derivatives **1–6** were designed and evaluated computationally to calculate the physicochemical properties and the bioactivity score by Mol-inspiration, and were determined to possess very good activity score. 1,2-Oxazoles were then synthesized, characterized by FT-IR, ¹H NMR and mass spectroscopy, and tested for antibacterial activity against the pathogens (*Staphylococcus aureus*, *Staphylococcus epidermidis*, *Escherichia coli*, and *Proteus mirabilis*). The antibacterial therapeutic effect strongly supported the prior computational results. Four synthesized compounds **2, 4–6** demonstrated antibacterial potential higher than the standard drug Ciprofloxacin.

Keywords: 1,2-oxazole, computational properties, synthesis, characterization, antibacterial screening

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