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Synthesis, antimicrobial evaluation and theoretical studies of novel heterocycles from Poly (ethylene terephthalate) plastic waste

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Eco-friendly energy source was used for the degradation of Poly(ethylene terephthalate), which used as a versatile intermediate for the synthesis of a form of heterocyclic compounds. The structures of the newly synthesized compounds such as IR, mass, 1H and 13C NMR spectral data. Some of the new heterocyclic compounds exhibited promising antimicrobial activities. Computational study calculations at the B3LYP/6-31G level of theory have been carried out to investigate the equilibrium geometry of the pyrazolo[1,5-a]pyrimidine 16. The energy of the HOMO and LUMO and Mulliken atomic charges were also calculated.