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M-POLYNOMIAL ANALYSIS OF DEGREE-BASED TOPOLOGICAL INDICES IN GONORRHEA DRUG MOLECULES

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Mathematical Chemistry is a fascinating field that blends mathematics and chemistry. Topological indices are numerical descriptors derived from molecular structures using a molecular graph. It describes the molecular structure in which the atoms and bonds are treated as vertices and edges, respectively, and all multiple bonds were treated as multi-edges, and all hydrogen atoms were included in the molecular graph. This is an enhanced method that has been newly incorporated in this study when computing topological indices to reduce assumptions of traditional computing techniques using molecular graphs of compounds. This method gives more reliable results when analysing drugs for diseases using degree-based numerical descriptors. Gonorrhea is a sexually transmitted disease, known as venereal disease, caused by the bacterium *Neisseria gonorrhoeae*, which is estimated at 82.4 million new cases among adults aged 15 – 49 worldwide. In this study, structures of important drugs, including Ceftriaxone, Cefixime, Cefotaxime, Probenecid, Spectinomycin, Cefpodoxime, Ciprofloxacin and Ofloxacin, used to treat gonorrhea were investigated. The objective of this study was to compute degree-based topological indices for the selected drugs for the disease using a polynomial approach. *M*-polynomial is a generalised algebraic polynomial used to derive degree-based topological indices, and this polynomial approach provides closed forms for topological indices formulae, which help further studies. In this research, the first, second, and third Zagreb indices, the forgotten index, the hyper Zagreb index, the atom-bond connectivity index, the product connectivity index, the sum connectivity index, the harmonic index, and the geometric-arithmetic index were selected for the computations using the suggested enhanced method. The highest values of indices reflect greater branching on the molecular structure. These findings assist in designing novel drugs for the treatment of analysing the physicochemical and the biological properties of drugs using the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies.

Keywords: Gonorrhea, Mathematical Chemistry, *M*-polynomial, Topological indices