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DEGREE-BASED TOPOLOGICAL INDICES OF LEPROSY DRUGS USING THE *M*-POLYNOMIAL APPROACH

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Abstract

The *M*-polynomial is a generalized algebraic polynomial utilized to derive a wide range of topological indices. Topological indices are the numerical parameters that can be used to describe the structural and chemical properties of a molecular graph, where atoms are treated as vertices and chemical bonds are treated as edges. In this study, an enhanced method is used to compute topological indices where all multi-bonds were treated as multi-edges, and all hydrogen atoms were included in a molecular graph. It helps to reduce assumptions of traditional computing techniques using molecular graphs of compounds. The most popular and studied type of topological indices is the degree-based topological indices. In drug design, these indices assist physicochemical properties without laboratory experiments. Leprosy is a chronic disease, also referred to as Hansen's disease that is caused by the bacterium *Mycobacterium leprae*. It is spread through droplets from an infected person's nose and mouth, but it does not spread through casual contact. Here, we investigated important leprosy drugs, including Clarithromycin, Clofazimine, Dapsone, Minocycline, Moxifloxacin, Ofloxacin, Rifampicin and Sparfloxacin. The objective of this study is to compute degree-based topological indices for the selected leprosy drugs using a polynomial approach, since the polynomials provide closed forms for topological indices formulae. We computed 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 for selected leprosy treatment drugs. These computed values from the *M*-polynomials approach are approximately close to the values computed from standard topological indices formulae. The results of this study assist in analyzing physicochemical and biological properties of drugs using quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies.

Keywords*:* *Leprosy, M-polynomials, Topological Indices*