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REHAN-LANEL INDICES OF ANTI-TUBERCULOSIS DRUGS

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Abstract

Tuberculosis (TB), caused by *Mycobacterium tuberculosis*, remains a major global health threat and continues to demand new, effective therapeutic agents. Chemical graph theory offers a powerful approach to studying molecular structures and predicting their physicochemical properties without the need for extensive laboratory experiments. In chemical graph theory, molecules are represented as graphs where atoms are vertices and covalent bonds are edges, allowing computation of numerical descriptors called topological indices that capture the structural and connectivity features of molecules. The objective of this study is to identify the selected Rehan–Lanel(RL) indices that are highly correlated with the physicochemical properties of anti-tuberculosis drugs and to use these indices to build regression models capable of predicting properties such as boiling point, flash point, molar refractivity, molar volume, and polarizability for anti-tuberculosis drugs, namely, amikacin, bedaquiline, clofazimine, delamanid, ethambutol, ethionamide, imipenem-cilastatin, isoniazid, levofloxacin, linezolid, moxifloxacin, and *p*-aminosalicylic acid. Chemical graphs of these anti-tuberculosis drugs were constructed, representing each atom as a vertex and each bond as an edge. The first, second, third, and fourth RL indices and corresponding Revan versions of these RL indices were calculated for each drug. Six physicochemical properties were compiled for the same set of compounds. Statistical analyses were performed to investigate the relationships between each topological index and each physicochemical property. The results revealed that different indices exhibited strong and highly significant correlations with specific properties. Certain Rehan–Lanel indices showed the highest correlations with molar refraction, molar volume, and polarizability, while specific Rehan–Lanel Revan indices correlated best with boiling point and flash point. This study demonstrates that chemical graph theory and topological indices provide an efficient, low-cost approach to predict physicochemical properties of anti-tuberculosis drugs, supporting early-stage drug screening and design. Future research may focus on integrating these indices or developing hybrid descriptors to simultaneously predict multiple properties, further enhancing their application in quantitative structure–property relationship studies and drug discovery.

Keywords*:* *Rehan-Lanel Indices, Tuberculosis, Chemical Graph Theory*