Generalized Edge Metric Codes for Molecular Graphs of Fungal Treatment Drugs

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Abstract

The increasing prevalence of Invasive Fungal Infections (IFIs) and the limitations of current antifungal therapies necessitate the development of drugs with novel mechanisms of action, such as those that target specific fungal pathways or enhance the immune response against fungal pathogens. Graph-theoretic descriptors play a crucial role in representing molecular structures in cheminformatics. In this work, antifungal drug molecules are modeled as graphs in which atoms correspond to vertices and chemical bonds correspond to edges. We study the edge fault-tolerant metric dimension, which ensures the unique identification of vertices even after the deletion of any edge in the graph. Exact values of this parameter are obtained for the molecular graphs of several antifungal drugs, including paclobutrazol, tebuconazole, flutriafol, myclobutanil, propiconazole, prothioconazole, epoxiconazole, triadimefon, cyproconazole, flusilazole, hexaconazole, fluconazole, and voriconazole. The results provide precise structural characterizations of these molecular graphs and highlight the usefulness of edge fault-tolerant metric dimensions for robust molecular encoding.

Keywords: Edge fault-tolerant metric dimension; Chemical graph theory; Molecular graph modeling; Antifungal drug structures.

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