The College of Graduate Studies and the College of Science Cordially Invite You to a

Master Thesis Defense

Entitled

TOPOLOGICAL INDICES AND THEIR APPLICATIONS IN DESIGNING DRUGS

by

Fedaa Ismail AbuNawa

Faculty Advisor

Dr. Muhammad Imran, Department of Mathematical Sciences

College of Science

Date & Venue

11:00 AM

Wednesday, 5 June 2024

Room 2022, F1 Building

Zoom link:

https://uaeu-ac-ae.zoom.us/j/89351402328?pwd=OsX62EEGesojrGXxMjaDdYWnLo74au.1

Abstract

This research delves into the use of indices, in the field of drug design with a specific focus on anticancer medications. Topological indices, values derived from representations of chemical structures provide meaningful connections to the physical and chemical characteristics of molecules. These indices act as tools for predicting behavior playing a vital role in crafting therapeutic drugs. The study primarily delves into topological indices like the Sombor index, Randić index, and Atom Bond Connectivity (ABC) index. These indices are calculated for structures and their relationships with physical properties such as molar volume, refractive index, and flash point are explored using statistical methods like linear regression and correlation analysis. Noteworthy discoveries from this investigation reveal that topological indices can accurately forecast the properties of anticancer medications assisting in optimizing their structures for improved therapeutic effectiveness.

The thesis not emphasizes the aspects of these indices but also showcases their practical utility in pharmaceutical sciences by offering fresh insights into drug molecule design and analysis. In summary, this research adds to the realm of chemistry by presenting an indepth examination of how topological indices can be leveraged to predict and control the physicochemical attributes of chemical compounds, for targeted drug development.

Keywords: Topological index, Sombor index; drug design