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Editorial

Introducing Structural Symmetry and Asymmetry Implications in Development of Recent Pharmacy and Medicine

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1. Introduction

Structural symmetry, anti-symmetry, or asymmetry represent a foundational property that, for chemical compounds, often determines their chemical and biological activity.

Symmetric objects can be material, such as a crystal [1], a molecule [2], a cluster [3], or a person [4], or can be an abstract structure such as a mathematical equation [5] or a software code [6].

Symmetry refers to the identification and use of invariants to any various transformations for any paired dataset and characterizations associated with it (such as on series systems in [7] and on wavelet filters in [8]). Symmetry may work as a powerful tool for problem reduction and solving; [5,9–12] are typical recent examples in this regard. Chirality in chemistry [13,14], crystallography in materials science [15,16], taxonomy in biology [17,18], and bilateral symmetry in medicine [19,20] are important manifestations of symmetry integration in sciences.

The symmetry of compounds is diverse and can be considered at various levels of structural organization; for geometrical vs. topological symmetry, please see [21–23]. Symmetry, asymmetry, and anti-symmetry play important roles in numerous biological compounds, such as proteins, saccharides, and nucleic acids; the presence of centers, planes, or axes of symmetry, which determine the structure of numerous chemical systems such as metal complexes of organic compounds [24] and crystal lattices of compounds exhibiting pharmacological potential [25] up to nanomaterials [26].

The investigation of structural correlations with the biological activity of compounds has become a large area of research, with important practical implications in developing novel materials, targeted therapies, and drug design [27].

The aim of Structural Symmetry and Asymmetry Implications in Development of Recent Pharmacy and Medicine was to bring together recent contributions on structural symmetry and asymmetry with implications in the development of modern chemistry, pharmacy, and medicinal chemistry.

2. Contributions

Structural Symmetry and Asymmetry Implications in Development of Recent Pharmacy and Medicine presents a collection of four articles.

Cell division protein kinase 2 (CDK2, enzyme-encoded by the CDK2 gene in humans) is critical to the abnormal growth processes of cancer cells [28]. Indirubin and its analogs are potent inhibitors of cyclin-dependent kinases [29]. In this context, Dr. Czelen led a research study regarding the immobilization of oxindole derivatives and the results are communicated in [30]. Its computation results allowed a group of substituents and substitution sites to be selected, providing the most stable complexes for creating new nanocarriers for (Z)-3-(2-(3-(methylamino)-5-(trifluoromethyl)phenyl)ethylidene)-2-oxo-N-((2-oxo-2,3-dihydro-1H imidazol-1-yl)methyl)indoline-5-carboxamide and (Z)-3-(2-(5-(4-aminophenethylcarbamoyl)-2-oxoindolin-3-ylidene)ethyl)benzoic acid.

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Moving from another direction with the same aim, the development of platinum-based anticancer compounds has been focused on the synthesis and evaluation of complexes that obey structure–activity relationships set forth in the 1970s [31], some of the most commonly used and active chemotherapy drugs utilized by oncologists today [32]. In this context, Dr. Szefler led a research study regarding the immobilization of oxindole derivatives and the results are communicated in [33]. The computation helped to find potential nanocarriers for lobaplatin, heptaplatin, oxaliplatin, and nedaplatin molecules.

Humans and other animals must ingest histidine or histidine-containing proteins since their body is not synthesizing them [34], despite the fact that it is an essential aminoacid, and it participates in essential enzymatic centers, such as catalytic triads [35]. Dr. Panek and coworkers studied the modeling of the change in molecular properties between the gas phase and solution using microsolvation models of histidine in its three protonation states, microsolvated with 1:6 water molecules [36]. An important finding of their computational study is that even with microsolvation, polarization induced by the presence of implicit solvent is significant.

Medicine has made major progress in recent years; let us take, for instance, the development of the mRNA vaccines [37]. The COVID threat has shown how important it is to shorten the time to develop a new therapy. Typically, the pilot study of a new treatment is grounded on a statistical experiment, as compared with standard treatment, and the outcomes are assessed in terms of cured or not cured, and occurrence and non-occurrence of side effects [38]. Let us take the case of the sample (x, m) from a known population of n, and let us go directly to the example of a family doctor with a known (and more or less fixed) list of patients. He/she may want to study the prevalence of COVID, for instance. Then, x from m can be used to assert about y from n or even more, about what is happening in one country or another. This is a distinct experimental design case, and in [39], confidence intervals are provided. By arguing that the preventive measures may be different from one country to another, even from one district to another, in the opinion of the author, the confidence in the results should be expressed in terms of the analyzed sample and not of the population or in terms of the population of the world, because it may simply be not true.

3. Perspectives

Structural symmetry and asymmetry can be further exploited in research studies across a broad area of scientific fields. Recent communications are related to the identification of planar structures [40]; the characterization of planar graphs [41] and boron nitride layers [42]; and the design of nanoscale transistors [43], catalytic [44] and ferroelectric [45] materials, and solid solutions [46] and polymers [47]. Even more is employed in emerging fields, such as in nanoarchitectonics [48].

We should emphasize in our perspective the important connection between Lie algebra and its representations and symmetry, since Lie groups appear as symmetry groups of physical systems, and their Lie algebras (e.g., tangent vectors near the identity) may be thought of as infinitesimal symmetry motions [49–53].

Contingency tables, very important in survey research, business intelligence, engineering, and medical research, by their design, give another use for symmetry [54], while experimental medicine focuses more on the identification of asymmetries rather than of symmetries [55–58] and [59] collection, while medical imaging seeks better and faster storage, retrieval, and processing methods [60].

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