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The Molecular Structure of Chemical Compounds by using Quantitative Calculations in Chemistry

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Abstract

Computational chemistry traces its origins back to the late 1920s when theoretical physicists first attempted to solve the Schrödinger equation using mechanical calculators. These pioneering efforts confirmed that the equation's solutions accurately replicated experimentally observed properties of fundamental systems, such as helium atoms and hydrogen molecules. By providing both exact solutions for simple models and approximations for more complex structures, scientists gained deeper insight into molecular spectra, structural configurations, and chemical reactivity. The advent of electronic computers during World War II revolutionized scientific calculations, and by the 1950s, chemists began leveraging these machines to approximate molecular behaviors numerically. This marked the birth of computational chemistry as a distinct discipline, driven by efforts to quantitatively describe molecular interactions through computer-aided solutions of quantum mechanical equations. The field has since flourished, fueled by significant advancements in computational speed, reductions in hardware costs, and the development of sophisticated algorithms. Today, computational chemistry enables researchers to tackle large-scale chemical problems that were once beyond reach. The concept of using quantum computers to simulate molecular systems has been envisioned since the 1980s, and modern advancements are bringing this vision closer to reality. Chemists anticipate that quantum computing could pave the way for groundbreaking discoveries in areas such as catalysis, high-temperature superconductors, and advanced materials design, revolutionizing the future of molecular science.

Keywords: Chemical calculation, analysis, data, structure, molecular structure

INTRODUCTION

The graphical representation of numerical results allows us to directly see molecular properties, such as the distribution of electron density [1-5], thus enhancing our ability to predict the nature of molecular interactions between the host and the guest [6]. Chemistry software has become widely used to calculate the chemical properties of many materials in purely scientific fields, such as thermal and electrical properties [7] and calculations related to the electronic distribution of some materials, as well as in practical fields such as the manufacture and design of medicines, in environmental and atmospheric chemistry, in nanotechnology and in materials science [8-11].

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Using Quantitative Calculations in Chemical Pollution

Given international efforts to preserve the environment, several global trends have called for attention to the environment, which has led to the need to work on developing new branches of chemistry. Green chemistry has emerged, which is one of the new branches in chemistry, which

focuses on producing and manufacturing new materials free of pollutants and which follows a new approach to reducing the dangers that threaten humans and the environment. Scientific centers specialized in research have been established in the fields of converting traditional chemical processes into green chemical processes [12-15] as scientists have seen the need to replace all materials and products that produce harmful waste and waste with materials that are environmentally friendly and do not cause negative effects on humans and the surrounding environment. To keep pace with these global trends, it has become necessary to develop awareness of the concepts of green chemistry among learners [16-18]. Therefore, it has become important to develop the content of the chemistry subject in a manner that is consistent with these trends so that the learner has knowledge and awareness of the principles of green chemistry and its various applications, so that the learner is able to acquire scientific concepts in addition to developing his environmental values [19-21], Figure (1).

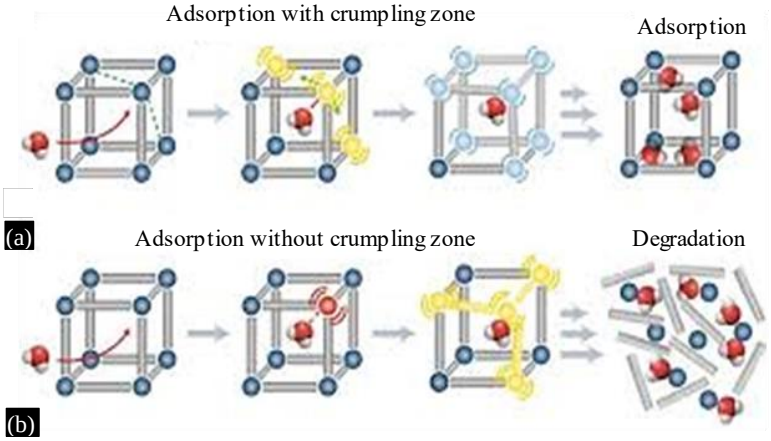

Figure 1. Computational Chemistry in Determination of Structures.

Computational Chemistry Applications

It calculates properties of molecules such as total energy, dipole and quadrupole moments, vibrational frequencies, reactivity and other properties, spectroscopy quantities and cross sections of molecular collisions with molecules of different atomic and subatomic diameters [22-25]. Qualitative analyses give values close to theoretical quantitative calculations for chemical applications, so these calculations are used to achieve accurate measurements. Their applications include:

- Calculating bond lengths and angles in a molecule.
- Distributing charge on atoms in a molecule.
- Calculating dipole moment.
- Calculating potential energy for rotation.
- Calculating vibrational patterns
- Calculating electronic spectra
- Calculating chemical shifts and coupling constants in NMR spectra
- Calculating reaction rate constants (kinetics).
- Calculating enthalpy, entropy, Caps energy and heat capacities (thermodynamics chemistry).
- Studying inter- and inter-hydrogen bonding, transition states and torsions.

Estimating the efficacy of chemical drugs in biotherapeutics

Identifying the efficacy of chemical drugs in biotherapeutics through virtual screening: Drug discovery involves in silico screening of molecules docked into protein pockets, ranking their similarities, and identifying potential drugs. It's like a Tinder for molecules [26-29]. Identifying the efficacy of chemical drugs in biotherapeutics through virtual screening: Drug discovery involves in silico screening of molecules docked into protein pockets, ranking their similarities, and identifying potential drugs. It's like a Tinder for molecules Identifying the efficacy of chemical drugs in biotherapeutics through virtual screening: Drug discovery involves in silico screening of molecules docked into protein pockets, ranking their similarities, and identifying potential drugs. The theory of

drug design is based on the idea that a drug is a chemical compound subject to the laws and properties of chemicals, and therefore entering all the chemical equations and laws [30,36] into an intelligent computer program means that it can predict the interactions of the drug.

Computational Chemistry

There are many computer software programs used in computational chemistry, some of which are used to analyze chemical data and predict chemical properties, and others are used to model molecules and chemical reactions [37-39]. Common software programs in this field include:

1. *Gaussian:* This program is used to calculate and analyze the chemical and physical properties of molecules and chemical reactions using quantitative calculation methods.
2. *ChemDraw:* It is used to draw and generate chemical structures in 3D.
3. *AutoDock:* It is used to model chemical interactions between molecules and predict potential drugs.
4. *PyMOL:* It is used to analyze and visualize structural data of molecules and proteins.
5. *VMD:* It is used to analyze and visualize structural data of molecules, proteins, and other biological materials.
6. *Open Babel:* It is used to convert molecular data between different formats and perform chemical extraction and analysis operations.

Drug Design in Chemistry Techniques

After researchers spent months or years testing drugs, it has become easier thanks to the use of computers in this field. German scientists say that they have made great progress in the field of drug design using computer programs, and they confirmed that "they are about to reach a near-complete design for drugs used in the treatment of cancer, rheumatism, acquired immunodeficiency syndrome, and other diseases." Drug design using computers is the use of computers in developing and improving drugs. In the past, experts used to design a very large group of similar compounds, then manufacture them and conduct many very expensive analyses and experiments [40]. After a long time of trouble, these efforts may not bear fruit. Figure (2).

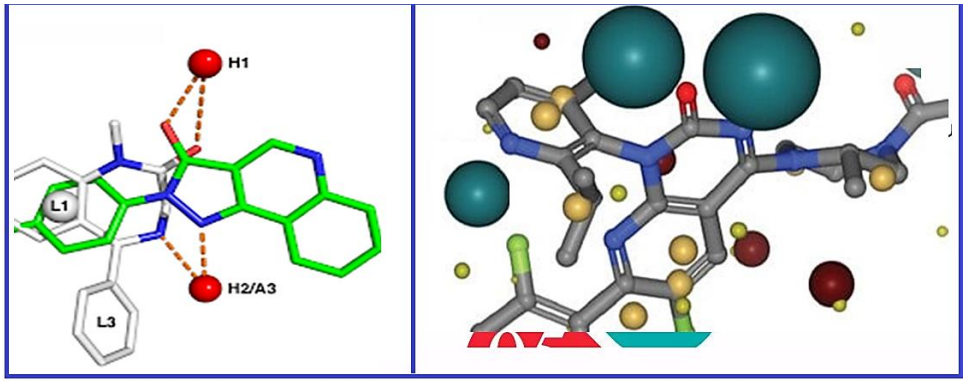

Figure 2. Designation of Chemical Drugs Via Chemical programs.

The technological development, many technologies and tools have emerged that help pharmacists, drug designers and teachers perform their jobs more easily and effectively. The most important of these tools currently are applications that they can install on their smartphones or tablets to help them easily deliver information to students and improve their performance. Chemistry is one of the practical subjects that requires in-depth study and many tools to help explore chemical reactions, understand chemical elements, molecules and compounds. Here comes the role of applications that allow chemistry teachers to help students with interactive activities and experiments with the ability to access element tables such as the periodic table and many other sources to enhance their learning of chemistry. There are many applications dedicated to chemistry teachers and their use in the classroom adds a whole new dimension to student learning and helps them participate in addition to easy access to them both inside and outside the classroom [41,42].

Designation of Chemical Compounds via Quantum Chemistry

Designing new drug candidates using molecular modeling techniques such as docking, pharmacophore modeling, and de novo design. These techniques can help identify potential binding sites, optimize the shape and charge of drug molecules, and generate new scaffolds or moieties that can interact with the target. Predicting the activity and selectivity of drug candidates using quantitative structure-activity relationship (QSAR) models, molecular dynamics simulations, and free energy calculations. These methods can help estimate the binding, selectivity, and specificity of drug molecules, as well as their conformational flexibility, solubility effects, and entropic contributions. These methods can help evaluate the pharmacokinetics, bioavailability, stability, metabolism, transport, and toxicity of drug molecules, as well as their interactions with other drugs or biomolecules., Optimize the manufacturing and formulation process of candidate drugs using reaction prediction, retrosynthesis analysis, and solubility prediction. These methods can help find the most efficient and economical synthetic routes, identify the best synthetic precursors, and determine the ideal solvents and excipients for drug molecules [43], Figure(3).

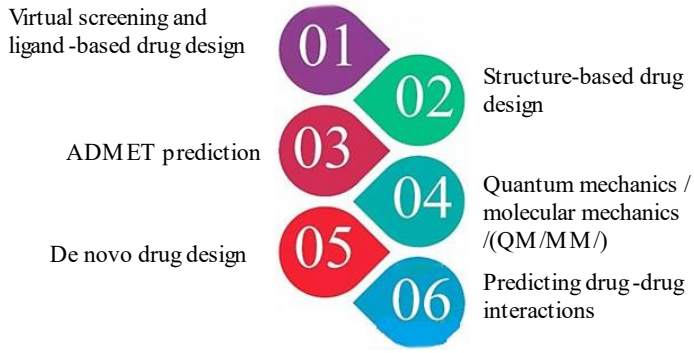

Figure 3. Uses of Chemical Programs.

For example, it can be used to predict the binding pose and affinity of a drug candidate for a protein target, or to explore the conformational space of a flexible molecule.

Quantum mechanics: This approach solves the Schrödinger equation for a molecular system, using mathematical approximations and numerical techniques. It can describe the electronic structure and properties of molecules, such as bond lengths, angles, charges, dipole moments, and energies. It is more precise than it, but it also requires more computational data and requires more input data. It is often used for small molecules, such as drug fragments, cofactors, or metal ions, or for specific regions of interest in larger molecules, such as active sites, reaction centers, or binding pockets. For example, it can be used to calculate the electronic properties and reactivity of a drug molecule, or to model the catalytic mechanism of an enzyme [42,43].

Molecular Docking

In this section, we will discuss some examples of successful drug discovery projects that have incorporated computational chemistry at various stages, such as target identification, target specification, lead optimization, and preclinical development. We will highlight the challenges, solutions, and outcomes of these projects, as well as the role of computational chemistry in addressing them. Computational chemistry has been involved in the discovery of PARP inhibitors in cancer cells through structure-based drug design, virtual screening, molecular docking, and fragment-based drug design. These techniques have helped identify novel binding patterns, improve selectivity and efficacy, and overcome inhibitor drug resistance. Several PARP inhibitors, such as olaparib, niraparib, and talazoparib, have been approved for clinical use and have shown significant benefits in patients with ovarian, breast, prostate, and pancreatic cancer. These techniques can enhance the efficiency and accuracy of computational chemistry methods by learning from large and complex datasets, generating new hypotheses, and automating workflows. For example, machine learning can be used to predict ligand-receptor binding affinities, compound toxicities, or molecular synthesis pathwaysn. However,

machine learning and AI also pose some challenges, such as the need for high-quality and diverse data, the interpretability and explainability of models, and the ethical and legal implications of their use. Multiscale and multidisciplinary modeling: Computational chemistry can benefit from integrating different levels of complexity and precision, from quantum mechanics to systems biology, and from different disciplines, such as chemistry, physics, biology, and pharmacology [43,44]. This can provide a more comprehensive and realistic picture of the drug discovery process and enable the exploration of new phenomena and interactions. For example, multiscale modeling can be used to study the effects of drug molecules on the structure and dynamics of biomolecules, membranes, cells, tissues, and organs. Multidisciplinary modeling can also facilitate the translation of computational results into experimental validation and clinical application. However, multiscale and multidisciplinary modeling also requires some challenges, such as developing efficient and accurate algorithms, integrating and harmonizing heterogeneous data, and collaboration and communication, Figure(4).

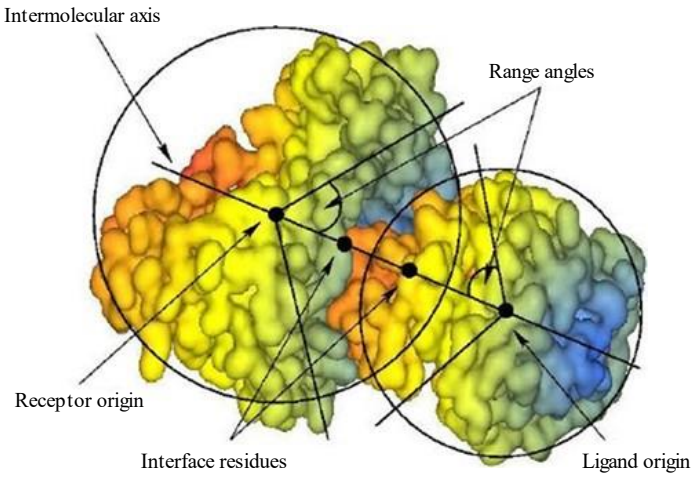

Figure 4. Mechanism of Molecular Docking.

CONCLUSIONS

As technology advances, computational chemistry is expected to become increasingly important in biochemistry. Through the use of artificial intelligence and machine learning, more discoveries can be expected in areas such as gene therapy and immunotherapy. These innovations will have a significant impact on how diseases are treated, and healthcare is improved.

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