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ATOMISTIC INSIGHT INTO SOLVENT EFFECTS ON THE CHEMICAL STRUCTURE OF BETULONIC ACID

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Abstract. Contemporary scientific inquiry has underscored the tremendous potential inherent in natural substances and their semi-synthetic counterparts, emphasizing their pivotal role as a basis for the development of innovative drug candidates, poised to cater to an expansive array of biological and pharmacological requirements. In this pursuit, the focal point of our investigation centers on the elucidation of the chemical structures and conformations of betulonic acid within various solvent environments. Understanding these structural intricacies stands as a critical milestone in the rational design of betulonic acid derivatives tailored for medical applications. To study this issue, quantum chemical calculations were performed at the atomistic level using the PM6 method in the GAMESS software package. The outcomes of our rigorous study unveiled noteworthy transformations in the chemical structures and conformations of betulonic acid as a direct response to shifts in solvent types. These quantum chemical insights offer a profound glimpse into the dynamic nature of betulonic acid, providing important guidance for their bespoke design within the realm of medicine. This study provides a scientific basis for further development of research on betulonic acid and its derivatives. By uncovering the interaction between chemical structure and solvent dynamics, our study lays a scientific foundation for the rational design of new betulonic

acid derivatives. The results obtained may facilitate the further development of new betulonic acid derivatives and be used in the search for promising compounds for medical use. The practical significance of the study is that the obtained results can be used in the rational design of new betulonic acid derivatives and the prediction of their properties, which is of interest for further research in the field of medicinal chemistry and drug development.

Key words: betulonic acid, PM6 method, solvent effects, solvation model, atomistic modeling

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БЕТУЛОН ҚЫШҚЫЛЫНЫҢ ХИМИЯЛЫҚ ҚҰРЫЛЫМЫНА ЕРІТКІШТЕРДІҢ ӘСЕРІН АТОМИСТИКАЛЫҚ ТҮРҒЫДАН ЗЕРТТЕУ

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Аннотация. Табиғи заттар мен олардың жартылай синтетикалық туындылары жаңа биологиялық және фармакологиялық белсенді қосылыстарды әзірлеудің маңызды көзі болып табылады. Осы тұрғыдан алғанда, бетулон қышқылының әртүрлі орта жағдайларындағы құрылымдық ерекшеліктерін зерттеу оның медициналық мақсатта қолдануға перспективалы туындыларын ұтымды жобалау үшін маңызды. Зерттеудің мақсаты — әртүрлі еріткіштердің бетулон қышқылының молекулалық құрылымына, конформациясына және электрондық қасиеттеріне атомистикалық деңгейде әсерін анықтау. Кванттық-химиялық есептеулер GAMESS бағдарламалық кешенінде жүзеге асырылған жартылай эмпирикалық PM6 әдісімен жүргізілді. Еріткіш полярлығының молекуланың

құрылымдық және электрондық сипаттамаларына әсерін бағалау үшін бетулон қышқылы газ фазасында, суда және диметилсульфоксидте (DMSO) зерттелді. Есептеу нәтижелері молекулалық геометрияның, толық энергияның, сондай-ақ НОМО және LUMO шекаралық молекулалық орбитальдарының энергиясы мен кеңістіктік орналасуының еріткішке тәуелді өзгерістерін көрсетті. Суда және DMSO ортасында сольватация газ фазасымен салыстырғанда молекулалық жүйенің тұрақтануына әкелді, ал ең айқын энергетикалық әсер DMSO ортасында байқалды. Шекаралық молекулалық орбитальдардағы өзгерістер еріткіш ортаның бетулон қышқылының электрондонорлық және электронакцепторлық қасиеттеріне әсер ететінін көрсетті. Алынған нәтижелер еріткіш ортасы мен бетулон қышқылының құрылымдық-электрондық қасиеттері арасындағы байланысты атомистикалық деңгейде түсіндіруге мүмкіндік береді. Зерттеу нәтижелері бетулон қышқылының әртүрлі орталардағы мінез-құлқын болжауға және перспективалы фармакологиялық қасиеттері бар жаңа туындыларды ұтымды жобалауға теориялық негіз бола алады.

Түйін сөздер: бетулон қышқылы, PM6 әдісі, еріткіш әсерлері, сольватация моделі, атомдық модельдеу

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АТОМИСТИЧЕСКОЕ ИССЛЕДОВАНИЕ ВЛИЯНИЯ РАСТВОРИТЕЛЕЙ НА ХИМИЧЕСКУЮ СТРУКТУРУ БЕТУЛОНОВОЙ КИСЛОТЫ

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Аннотация. Природные вещества и их полусинтетические производные являются важным источником соединений для разработки новых биологически и фармакологически активных веществ. В этой связи изучение структурного поведения бетулоновой кислоты в различных средах имеет существенное значение для рационального конструирования её производных, перспективных

для медицинского применения. Цель исследования заключалась в установлении влияния различных растворителей на молекулярную структуру, конформацию и электронные свойства бетулоновой кислоты на атомистическом уровне. Квантово-химические расчёты выполнены полуэмпирическим методом PM6 с использованием программного комплекса GAMESS. Для оценки влияния полярности среды бетулоновую кислоту исследовали в газовой фазе, воде и диметилсульфоксиде (DMSO). Результаты расчётов выявили зависящие от растворителя изменения молекулярной геометрии, полной энергии, а также энергий и пространственной локализации граничных молекулярных орбиталей НОМО и LUMO. Сольватация в воде и DMSO приводила к стабилизации молекулярной системы по сравнению с газовой фазой, при этом наиболее выраженный энергетический эффект наблюдался в среде DMSO. Изменения характеристик граничных молекулярных орбиталей свидетельствуют о способности растворителя модифицировать электронодонорные и электроноакцепторные свойства бетулоновой кислоты. Полученные результаты позволяют на атомистическом уровне охарактеризовать взаимосвязь между природой растворителя и структурно-электронными свойствами бетулоновой кислоты. Они могут быть использованы для прогнозирования поведения соединения в различных средах и служить теоретической основой для рационального конструирования новых производных с потенциально значимыми фармакологическими свойствами.

Ключевые слова: бетулоновая кислота, метод PM6, влияние растворителей, модель сольватации, атомистическое моделирование

Introduction. Natural triterpenoids represent a large class of secondary metabolites with diverse chemical structures and a wide range of biological activities. Due to their antitumor, anti-inflammatory, antiviral, antioxidant, and antimicrobial properties, these compounds are considered promising candidates for the development of new drugs and biologically active substances (Abdullah et al., 2026; Orchel et al., 2025; Wimmer, 2025). Among the pentacyclic triterpenoids of the lupan series, betulonic acid, which is a product of betulin oxidation, is of particular interest. This compound serves as an important intermediate in the synthesis of many derivatives with improved physicochemical and pharmacological properties (Long et al., 2024; Li et al., 2021).

In recent years, research on betulonic acid has been aimed not only at obtaining new derivatives, but also at studying their biological activities. Betulonic acid derivatives have been shown to exhibit pronounced antitumor activity, inhibit the proliferation of various tumor cells, and have antibacterial and anti-inflammatory activities (Kraynova et al., 2025, Jalmakhanbetova et al., 2024; Bębenek et al., 2024). They are also considered promising compounds for the development of new drugs. However, the effectiveness of such compounds is determined not only by their chemical structure, but also by the characteristics of their electronic structure, which can vary significantly under the influence of the environment. It is known that solvents have a significant effect on the geometric and electronic characteristics of organic molecules. The polarity

of the medium, dielectric constant, electrostatic interactions and polarization processes can change the electron density distribution, dipole moment, energy parameters and reactivity of the compounds under study (Laurence et al., 2024; Paiva, 2022; Medved' et al., 2016). Water is the main medium for many biochemical processes, and dimethyl sulfoxide (DMSO) is widely used as a universal solvent in organic synthesis, pharmaceutical research and computational chemistry. Comparative analysis of the behavior of water and DMSO molecules allows us to assess the effect of different solvents on their structural and electronic properties (Paiva, 2022; Medved' et al., 2016).

Modern computational chemistry methods allow us to study the effect of the solvent on the molecular structure without complex experimental studies. Semiempirical methods occupy an important place among quantum chemical approaches due to their high computational speed and satisfactory accuracy in the study of large organic molecules. One of the most widely used semiempirical methods is PM6, which is successfully used to optimize geometry, calculate the total energy, the energies of the HOMO and LUMO frontier molecular orbitals, and other electronic characteristics of biologically active compounds (Haji et al., 2024, Stewart et al., 2023; Fedik et al., 2023).

Despite numerous studies on the synthesis and biological activity of betulonic acid, the effect of solvents on its molecular structure and electronic properties is still poorly understood. There are practically no works in the literature that have conducted a comparative study of betulonic acid in the gas phase, water, and DMSO using the semi-empirical PM6 method.

Literature review. Betulonic acid is a pentacyclic triterpenoid belonging to the lupane family. It is formed by the oxidation of betulin and is considered one of the most valuable derivatives of natural triterpenes due to its versatile chemical reactivity and broad biological activity. Chemically, betulonic acid is called 3-oxo-lup-20(29)-ene-28-oic acid and has the molecular formula $C_{30}H_{46}O_3$. The molecule consists of a rigid pentacyclic carbon skeleton typical of lupane triterpenoids. The molecular structure contains several chemically important functional groups. The carbonyl group at the C-3 position acts as a strong electron-withdrawing center, while the carboxyl group at the C-28 position promotes the formation of hydrogen bonds and acid-base interactions. These functional groups mainly determine the polarity of the molecule, intermolecular interactions, and reactivity towards nucleophilic and electrophilic reagents. In addition, the double bond located between C-20 and C-29 contributes to the conjugation characteristics and affects the frontier molecular orbitals.

Despite the presence of polar functional groups, betulonic acid remains largely hydrophobic due to its large hydrocarbon structure. Consequently, it has poor solubility in water, but is readily soluble in many organic solvents, such as DMSO, dimethylformamide, acetone, methanol, ethanol, chloroform, and tetrahydrofuran. The solvent environment has a major impact on its molecular geometry, electron distribution, dipole moment, and intermolecular interactions. These solvent-dependent

effects are particularly important when considering pharmaceutical formulations, drug delivery, and computational studies using implicit solvation models.

The electronic properties of betulonic acid are determined by the distribution of electrons in its frontier molecular orbitals. The energies of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) provide valuable information about molecular stability, chemical reactivity, electron donating and accepting abilities. The energy gap between the HOMO and LUMO is often used as an indicator of molecular kinetic stability and chemical toughness. Smaller energy gaps generally correspond to increased chemical reactivity, while larger gaps indicate increased molecular stability.

The solvent is one of the most important factors determining the physicochemical properties of organic compounds. In addition to providing a medium for chemical reactions, solvents significantly affect molecular geometry, electron density distribution, energy characteristics, spectral properties, and reactivity. These changes arise from various types of intermolecular interactions, including electrostatic forces, hydrogen bonds, dipole-dipole interactions, and dispersion forces. In recent years, the effects of solvents have been actively studied using quantum chemical methods, which allow for a detailed analysis of changes in the electronic structure of molecules under different solvent conditions (Becker, 2025; Garcia-Alvarez et al., 2024; Kramer et al., 2023).

Currently, semi-empirical methods are an effective tool for preliminary geometry optimization, electronic structure studies, and analysis of the effects of solvents on molecular properties (Elm et al., 2023)

Parametric Method 6 (PM6) was developed in 2007 by James J.P. Stewart as a further development of the PMx series of semi-empirical methods, including MNDO, AM1, and PM3. The main goal of PM6 was to improve the accuracy of describing molecular geometry, heats of formation, chemical bond lengths, dipole moments, and other molecular characteristics while maintaining high computational speed.

Unlike PM3, the development of PM6 has significantly expanded the parameterization databases and improved the description of interatomic interactions, including hydrogen-bonded systems, carbonyl compounds, and organic molecules containing oxygen, nitrogen, sulfur, and halogens (Christensen et al., 2016).

Current modifications of PM6 (e.g., PM6-D3H4, PM6-ORG) additionally take into account dispersion interactions and more accurately describe hydrogen bonds, which significantly expands the scope of the method in modeling biological systems and large organic molecules (Stewart et al., 2023).

One of the main advantages of the PM6 method is its high computational efficiency. While density functional theory (DFT) calculations for molecules with a few dozen atoms can take hours or even days, PM6 allows for similar optimizations to be performed in minutes. This is especially important when studying natural compounds with complex polycyclic structures.

The method reliably reproduces the main structural characteristics of large organic molecules, including optimized geometry, dipole moment, electron density distribution, HOMO and LUMO frontier molecular orbital energies, total electron energy, and other

parameters. Despite being slightly less accurate than state-of-the-art DFT methods, PM6 provides a good fit to experimental data for many organic compounds at a significantly lower computational cost (Řezáč et al., 2023).

Due to its optimal balance between speed and accuracy, PM6 is widely used for the calculation of molecules consisting of more than 100-300 atoms, as well as for the modeling of proteins, enzymes, ligand-receptor complexes and other biological objects (Stewart et al., 2023).

A review of the current scientific literature indicates that betulonic acid is one of the most promising naturally occurring pentacyclic triterpenoids. In recent years, research on this compound has been mainly focused on developing methods for its preparation, chemical modification, and synthesis of new derivatives with improved pharmacological properties.

Despite the considerable volume of published works, most of the research has been devoted to the experimental synthesis, biological activity, and molecular bonding of betulonic acid derivatives. Relatively little attention has been paid to the fundamental study of its electronic structure and physicochemical properties using computational chemistry methods.

The number of studies aimed at a comparative analysis of the behavior of betulonic acid in the gas phase and in polar solvents using modern continuous solvent models is particularly limited. There are practically no studies in the available scientific literature that simultaneously compare the electronic properties of betulonic acid in the gas phase, water, and DMSO.

However, these media are of greatest practical interest, since water is the main biological medium, and DMSO is widely used as a solvent in the study of natural compounds and in the development of drugs.

Furthermore, no studies have been found that investigate the influence of these solvents on the geometric and electronic properties of betulonic acid using the semi-empirical PM6 method. This method combines high computational efficiency with sufficient accuracy for modeling large organic molecules, making it particularly promising for studying natural triterpenoids. The use of PM6 allows for the assessment of changes in optimized geometry.

The solvent effect on molecular structure is a complex interplay between various factors, including electrostatic interactions, dispersion forces, and hydrogen bonding, among others. These interactions collectively contribute to changes in the solute's conformation, geometry, and energy. Therefore, a comprehensive understanding of how solvents influence the structural properties of betulonic acid can offer profound insights into its behavior in different physiological and chemical environments.

In the pursuit of gaining atomistic insights into the solvent effect on betulonic acid's chemical structures, this study aims to employ quantum chemical calculations. Quantum chemistry provides a robust framework for simulating molecular behavior at the atomic level, enabling the exploration of intricate details that are often inaccessible through experimental means alone. Specifically, we will utilize the semi-empirical PM6 method, a widely employed quantum mechanical approach known for its efficiency and

accuracy in the description of molecular properties. The calculations will be carried out using the freely available GAMESS software, a powerful computational tool renowned for its versatility in performing quantum chemical calculations.

Our primary objective is to elucidate how different solvent environments influence the conformational landscape and electronic structure of betulonic acid. We will systematically investigate the solvation effects by simulating betulonic acid in the presence of various solvents, representing a spectrum of polarity and hydrogen bonding capabilities. By doing so, we intend to unravel the dynamic responses of betulonic acid to changes in its surroundings, providing valuable insights into its behavior in physiological and chemical contexts. The outcomes of this study hold significant implications for a myriad of scientific disciplines. In the realm of drug design, understanding how betulonic acid's chemical structure adapts to different solvents can aid in the rational design of derivatives with optimized pharmacological properties. Moreover, the findings may shed light on the compound's behavior in biological systems, potentially guiding its application in the treatment of various diseases.

Herein, this research embarks on a journey to delve into the atomistic world of betulonic acid and its interaction with solvents. Through quantum chemical calculations and theoretical modeling, we aim to uncover the intricate nuances of how solvents shape the chemical structures of betulonic acid, offering valuable insights that have the potential to reshape the future of drug development and chemical research.

Materials and main methods. Betulonic acid was chosen as a model compound due to its known biological activity and its importance as a versatile precursor for the synthesis of biologically active triterpenoid derivatives. The initial molecular structure was constructed according to its published chemical structure and subsequently underwent full geometry optimization before calculating the electronic properties. All calculations were performed for the molecule in the gas phase and in two solvents to assess the effect of solvent polarity on the molecular structure and electronic properties.

Quantum chemical calculations were performed using the PM6 semi-empirical Hamiltonian (Parametric method 6). PM6 belongs to the NDDO (Neglecting Differential Overlapping of Diatomic Molecules) family of semi-empirical quantum mechanical methods and represents an improved parameterization compared to previous methods such as AM1 and PM3.

The PM6 method was chosen because it provides a favorable balance between computational efficiency and accuracy for medium-sized organic molecules. The betulonic acid molecule contains more than seventy atoms and has a complex five-ring skeleton, as well as oxygen-containing functional groups that can participate in intermolecular interactions. Density functional theory (DFT) calculations for molecules of this size require considerable computational resources, and the PM6 method has been shown to reproduce structural and electronic parameters with satisfactory accuracy for many classes of biologically active organic compounds. Therefore, the PM6 method is well suited for studying solvent-induced changes in molecular geometry and electronic structure.

All quantum chemical calculations were performed using the General Atomic

and Molecular Electronic Structure System (GAMESS). GAMESS is a widely used computational chemistry software. The effect of solvent was investigated by performing calculations in three different environments: in the gas phase, in water, and in DMSO. Since biological processes mainly occur in aqueous media, water was chosen as a representative, highly polar, protic solvent. DMSO was chosen as a highly polar solvent widely used in pharmaceutical research, molecular modeling, and biological analysis due to its ability to dissolve triterpenoid compounds. The solvent effect was characterized using the continuum solvation approach implemented in GAMESS, where the solvent is represented as a homogeneous dielectric medium surrounding the solute molecule. No molecular dynamics simulations were performed in this study; therefore, molecular-dynamics-specific parameters such as force field, temperature, pressure, and simulation time were not applicable. Instead, stationary structures were obtained by quantum-chemical geometry optimization.

After optimizing the geometry for each medium, a series of structural and electronic parameters were calculated to assess the solvent-induced changes in the molecular properties of betulonic acid. The 2D structures of above-mentioned compound is illustrated in Figure 1.

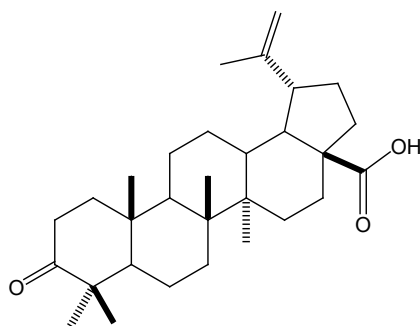


Figure 1 - 2D chemical structure of betulonic acid.

The designed simulation systems were illustrated in Table 1. As can be seen in Table 1, initially we did Quantum Chemical Calculation for pure betulonic acid in the gas phase. After that, we simulated betulonic acid in the presence of water. Then betulonic acid was modeled and simulated in the presence of DMSO.

Table 1 – The designed simulation system for study of betulonic acid in the presence of various solvents

Betulonic acid	Water	DMSO	Intended Purpose
1	-	-	Pure Betulonic acid
1	1	-	Effect of Water
1	-	1	Effect of DMSO

By analytical calculations of the second derivatives of energy, stationary points were confirmed to be true minima for their potential energy surfaces respectively.

Results. *Pure Betulonic acid.* Firstly, to study the quantum chemical properties for betulonic acid itself, we studied the betulonic acid in terms of optimized structures, molecular orbitals and energies. Now we began our Quantum Chemical Calculation analysis on betulonic acid structure as can be seen in Figure 2.

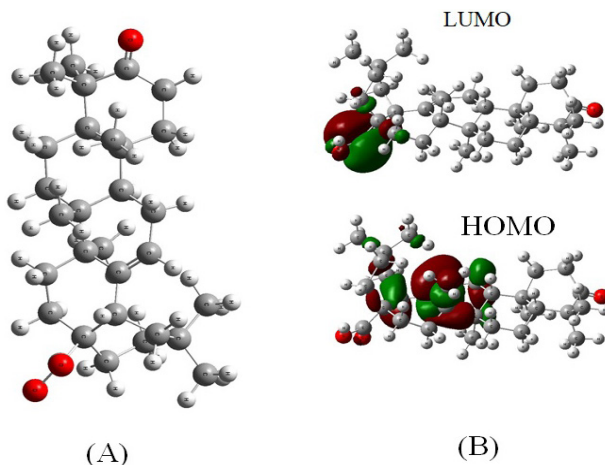


Figure 2 - Quantum chemical calculation based optimized structures of betulonic acid.

Betulonic acid in the presence of water. Secondly, to study the quantum chemical properties for betulonic acid in the presence of water, we studied the betulonic acid in terms of optimized structures, molecular orbitals and energies. Now we began our Quantum Chemical Calculation analysis on betulonic acid structure as can be seen in Figure 3.

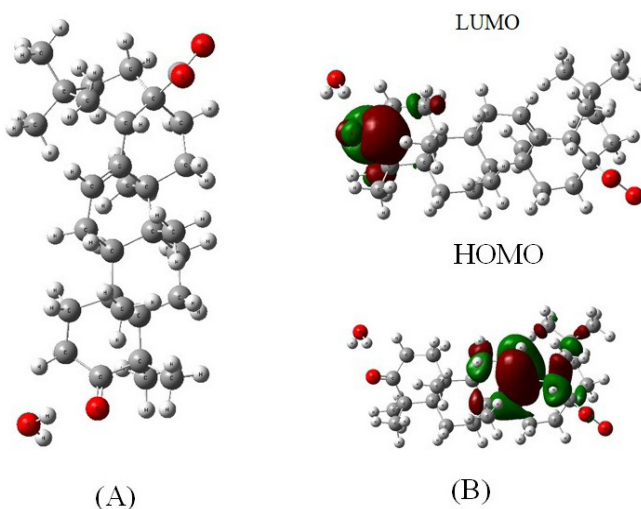


Figure 3 - Quantum chemical calculation based optimized structures of betulonic acid in the presence of water.

Betulonic acid in the presence of DMSO. Lastly, to study the quantum chemical properties for betulonic acid in the presence of DMSO, we studied the betulonic acid in terms of optimized structures, molecular orbitals and energies. We began our analysis with quantum chemical calculations of the structure of betulonic acid in the presence of DMSO, as shown in Figure 4.

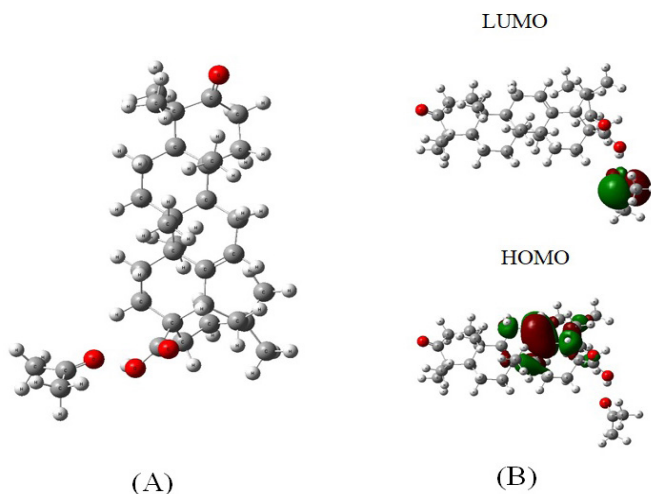


Figure 4 - Quantum chemical calculation based optimized structures of betulonic acid in the presence of DMSO.

Discussions. In this section, we delve into a comprehensive discussion of the gas phase optimization of betulonic acid's molecular structure and its subsequent optimization in the presence of two different solvents: water and DMSO. These computational investigations were carried out using the PM6 method within the GAMESS software package, providing valuable insights into the solvent effect on betulonic acid's structural and electronic properties.

Initially, we conducted a gas phase optimization of betulonic acid's structure to establish a baseline for its molecular properties. The optimized structure in the absence of solvents was characterized by an energy value of -798.55 kJ/mol. This energy value serves as a reference point, allowing us to assess the impact of solvation on the stability and energetics of betulonic acid.

The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies were also determined for the gas phase structure. The HOMO energy for betulonic acid was approximately -9.21 eV, while the LUMO energy value was approximately 0.66 eV. These values offer insights into the compound's electronic structure and reactivity. Notably, the HOMO orbitals were predominantly localized around the ring of betulonic acid, indicating regions of electron density suitable for nucleophilic attack or electron donation. Conversely, the LUMO orbitals were primarily distributed around the carboxylic groups of betulonic acid, suggesting potential sites for electrophilic interactions or electron acceptance.

To elucidate the influence of solvent environments on betulonic acid, we subsequently performed structural optimizations in the presence of water and DMSO.

In the presence of water, the optimized structure of betulonic acid exhibited an energy value of -1050.21 kJ/mol. Comparing this to the gas phase energy, it is evident that the solvation by water resulted in a more stable structure, indicating favorable interactions between betulonic acid and water molecules. The HOMO energy remained relatively consistent at approximately -9.25 eV, while the LUMO energy decreased slightly to around 0.40 eV. These subtle changes in the electronic energies signify that the presence of water affects the electronic structure of betulonic acid, albeit to a limited extent. The HOMO orbitals continued to be localized around the ring of betulonic acid, the LUMO orbitals were predominantly localized around the carbonyl (C=O) group of the betulonic acid skeleton, indicating that this region may serve as the primary electron-accepting site during intermolecular interactions.

Conversely, when betulonic acid was optimized in the presence of DMSO, the resulting structure exhibited an energy value of -1061.46 kJ/mol. This energy is notably lower than the gas phase value, indicating that DMSO has a more pronounced stabilizing effect on the molecule compared to water. However, it's essential to highlight that DMSO is a highly polar aprotic solvent known for its strong solvation capabilities. The HOMO energy was approximately -8.97 eV, and the LUMO energy value decreased significantly to around 0.04 eV. These considerable shifts in the electronic energies underscore the substantial impact of DMSO on the electronic structure of betulonic acid. Importantly, the HOMO orbitals retained their localization around the molecular ring, while the LUMO orbitals were now predominantly situated around the DMSO molecule itself.

The results of our computational study offer valuable insights into how solvents, specifically water and DMSO, influence the structural and electronic properties of betulonic acid. These findings have significant implications for various scientific disciplines, particularly in the fields of drug design and molecular biology.

Understanding the solvation effects on betulonic acid is essential for the rational design of derivatives with tailored pharmacological properties. Our observations suggest that different solvents can indeed modulate the electronic structure of betulonic acid, potentially affecting its reactivity and pharmacological behavior. Future studies could explore a broader range of solvents and extend these findings to guide the optimization of betulonic acid for specific therapeutic applications.

This computational exploration provides atomistic insights into the solvent effect on betulonic acid's chemical structures, offering a foundation for further research and the rational design of novel pharmaceutical agents. The dynamic interplay between betulonic acid and solvents represents a promising avenue for innovative advancements in chemistry and drug development.

Conclusion. In this study, we employed the PM6 method-based quantum chemical calculations using the GAMESS software to investigate the solvent effect on betulonic acid's chemical structures. By simulating betulonic acid in the presence of water and DMSO, we aimed to unravel the intricate interplay between this biologically relevant

compound and various solvents. The outcomes of our computational exploration have provided valuable insights into the solvent-induced changes in the quantum properties of betulonic acid. Our results revealed significant alterations in the molecular structures and electronic properties of betulonic acid in response to different solvent environments. Notably, variations in solvent polarity and hydrogen bonding capabilities played a pivotal role in shaping the conformational landscape of the compound. These changes in molecular structure were accompanied by shifts in the calculated electronic energy levels, in particular, the HOMO and LUMO energies showed solvent-dependent changes.

The implications of our findings extend beyond the realm of fundamental chemical research. Understanding how solvents impact the behavior of betulonic acid holds immense promise for practical applications. In drug design and pharmaceutical development, this knowledge can be harnessed to rationally design betulonic acid derivatives with tailored pharmacological properties. Furthermore, our insights into the solvation effect on betulonic acid provide a foundation for predicting its behavior in biological systems, potentially facilitating its application in the treatment of various diseases. This study has shed light on the atomistic responses of betulonic acid to changes in solvent environments. Our research has unveiled the dynamic nature of this compound and its adaptability to different solvents, underscoring the importance of considering solvent effects in both theoretical and practical investigations. As a future direction, we recommend further studies that explore the solvation effects on betulonic acid in even more diverse solvent systems and extend the application of this knowledge to the rational design of novel pharmaceutical agents and therapeutic strategies. The insights gained from this work pave the way for innovative advancements in the fields of chemistry, drug development, and molecular biology.

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