

Chemical Structure Profile and Computational Descriptors of Fenbufen Butanamine by PubChem

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Abstract— Fenbufen Butanamine is a structural derivative of the non-steroidal anti-inflammatory drug (NSAID) Fenbufen, characterized by the addition of a butanamine group to its core structure. This modification is intended to improve the pharmacokinetic and pharmacodynamic properties of the parent compound, potentially enhancing its therapeutic efficacy. In this study, we conducted a detailed computational analysis of Fenbufen Butanamine's chemical structure and molecular descriptors using data retrieved from the PubChem database. The chemical identity was confirmed by its IUPAC name, InChI, InChIKey, and SMILES notation, which provide precise molecular characterization essential for database referencing and further computational modeling. Key computational descriptors, such as molecular weight, logP, topological polar surface area (TPSA), and the count of hydrogen bond donors and acceptors, were analyzed to assess drug-likeness and predict pharmacokinetic behavior. Our findings indicate that Fenbufen Butanamine possesses a biphenyl core that contributes to hydrophobic interactions, while the butanamine side chain introduces hydrophilic properties. This amphiphilic nature is likely to influence the compound's solubility, membrane permeability, and binding affinity to biological targets. The computed descriptors suggest favorable properties for oral bioavailability and potential interactions within biological systems. These results serve as a foundational step for in silico drug design and optimization of Fenbufen derivatives. Further experimental and pharmacological studies are warranted to validate these computational predictions and explore the therapeutic potential of Fenbufen Butanamine.

Keywords: Fenbufen, Butanamine, Computational Descriptors, Chemical Structure, PubChem.

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1. Introduction

Fenbufen is a compound derived from arylpropionic acid that is utilized as a non-steroidal anti-inflammatory drug (NSAID) [1]. It is widely recognized for its ability to inhibit the enzyme cyclooxygenase (COX), thereby decreasing the synthesis of prostaglandins, which are the primary mediators in the processes of inflammation and pain [2]. In recent decades, this compound has garnered significant attention in numerous pharmacological and medicinal chemistry studies due to its therapeutic effects and distinctive metabolic profile [3]. Its chemical structure, which comprises aromatic rings and carboxyl functional groups, offers significant potential for various molecular interactions, particularly through hydrogen bonding and π - π interactions with target proteins in the human body [4].

One of the structural derivatives currently under evaluation is Fenbufen butanamine, which is a

compound modified from fenbufen by the addition of a butanamine group to its core structure [5]. This modification has the potential to alter the pharmacokinetic and pharmacodynamic characteristics of the parent compound, including changes in lipophilicity, solubility, and affinity for biological targets [6]. In the modern approach to drug development, understanding the relationship between structure and activity (structure-activity relationship/SAR) is crucial [7]. Therefore, the use of data-driven computational approaches, such as chemical structure profiling and computational molecular descriptors, is extremely important for describing the characteristics of molecules in a more detailed and predictive manner [8].

PubChem, as a wide and reliable public repository, offers a variety of data regarding chemical structures, bioactivity, and computational properties of millions of compounds [9]. Through features such as computed descriptors, analysis of 2D and 3D structures, as well as predictions of toxicity and early pharmacokinetics, PubChem serves as a primary resource for exploration and initial modeling in computer-aided drug design (in silico approach) [10]. A study on Fenbufen butanamine through PubChem can reveal important descriptors such as polar surface area (PSA), logP, the number of hydrogen bond donors and acceptors, as well as molecular refractivity and polarizability, all of which play a significant role in predicting bioavailability, distribution, and drug interactions [11].

The mapping of computational properties can also be utilized in validating structures and making preliminary predictions regarding toxicity or the potential interactions of compounds [12]. In addition, the molecular structure information produced by this database can also be utilized for docking simulations or pharmacophore modeling in further research [13]. Therefore, a comprehensive understanding of the chemical structure and computational descriptors of Fenbufen butanamine is not only crucial for the fundamental science of pharmaceutical chemistry but also holds practical implications for the future design of drugs [14]. By understanding the potential for biological interactions and chemical stability based on this approach, the development of new derivatives of fenbufen can be directed more effectively and efficiently [15]. This research aims to outline the chemical structure profile and assess various molecular descriptors of the compound Fenbufen butanamine, which is available in the PubChem database [16]. This serves as a preliminary step for computational pharmacological and toxicological exploration [17].

2. Method

This research is a descriptive study based on secondary data, aiming to explore the chemical structure profile and computational descriptors of the compound Fenbufen Butanamine. The primary source of data utilized in this study is PubChem, an open chemistry database maintained by the National Center for Biotechnology Information (NCBI), which is part of the U. S. Department of Health and Human Services. United States National Library of Medicine. PubChem offers standardized molecular data, which includes chemical structures, physicochemical properties, molecular descriptors, and bioactivity information for a variety of chemical compounds that have been curated from numerous scientific and commercial sources.

The initial step in this method is to conduct a search for the compound entry using the keywords "Fenbufen Butanamine" on the PubChem search engine. If the compound is not found directly, an alternative approach is taken by searching for the parent compound "Fenbufen," followed by the identification of its derivatives based on structural modifications, particularly concerning the butyl amine group. Upon identifying the compounds, the 2D and 3D structure data are extracted in SDF (Structure Data File) and SMILES (Simplified Molecular Input Line Entry System) formats. The data structure was subsequently analyzed to obtain various molecular descriptors using the "Computed Descriptors" feature that is automatically available on the compound entry page in PubChem.

The computational descriptors examined include molecular weight, heavy atom count, polar surface area (PSA), the number of hydrogen bond donors and acceptors, logP, and rotatable bonds. The analysis also

includes an evaluation of tautomerism, stereochemistry, and the potential conformations of the compounds. Additionally, observations were made regarding the potential interactions of the compounds with biological targets based on the bioactivity prediction features available in the PubChem BioAssay Summary.

To ensure the accuracy and validity of the data, all parameters are compared with references from relevant organic chemistry and pharmaceutical literature. The results of the analysis are presented in the form of tables and graphical visualizations to illustrate the correlations between molecular properties. The process of data collection and analysis will take place from January to March 2025. The entire procedure is conducted *in silico* and does not require physical or experimental laboratory testing.

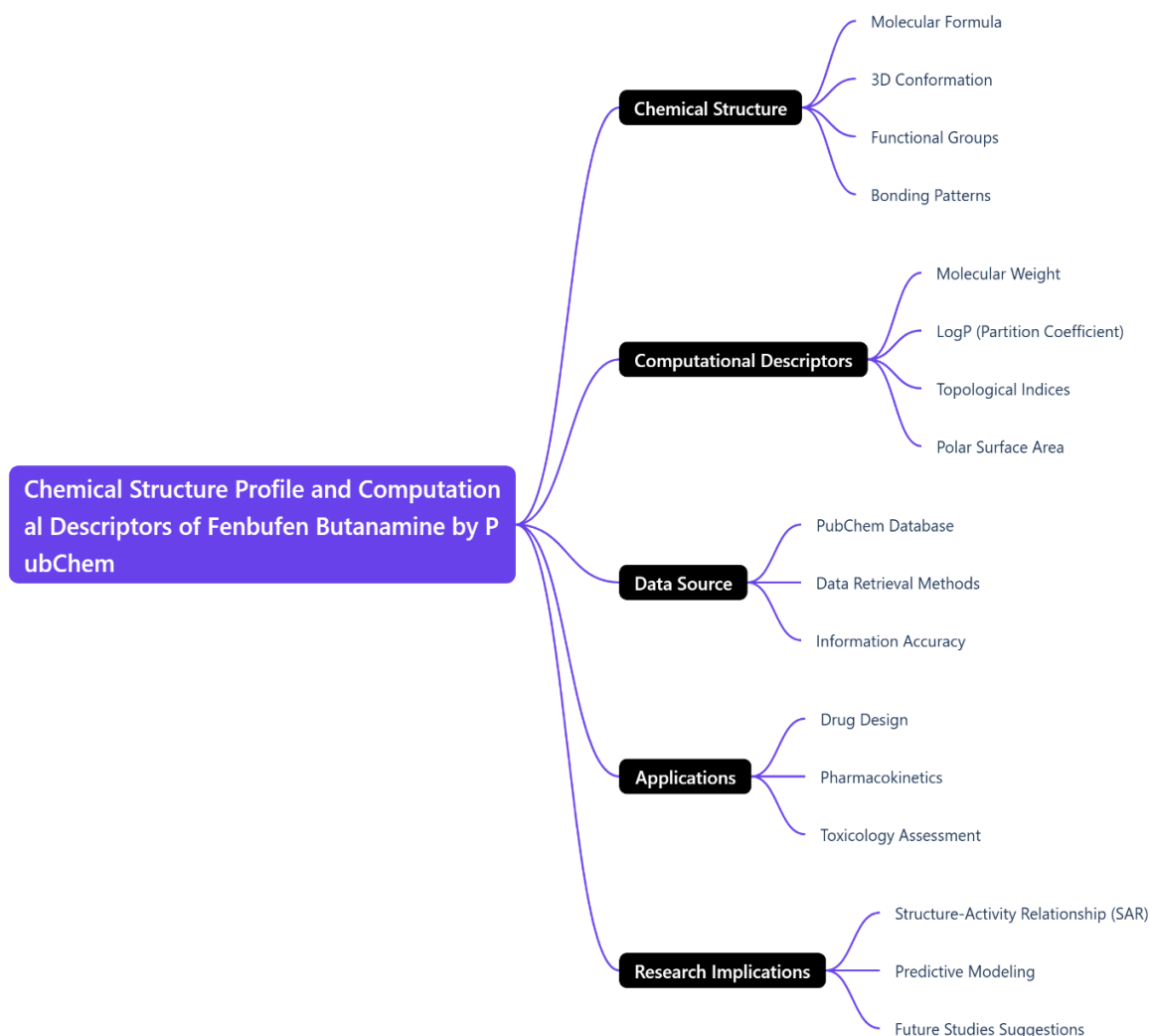


Figure 1. Mid Maps

3. Result and Discussion

Chemical Structure

Fenbufen Butanamine is a structural derivative of the parent compound Fenbufen, which is recognized as a non-steroidal anti-inflammatory drug (NSAID) that has the ability to inhibit the enzyme cyclooxygenase (COX). Fenbufen has a basic structure consisting of a biphenyl core connected to a butanoate chain that includes a carboxyl group and a ketone. The modification of the Fenbufen structure by adding a butylamine group leads to the creation of Fenbufen Butanamine, which is expected to have a pharmacokinetic and pharmacodynamic profile that differs from its parent compound.

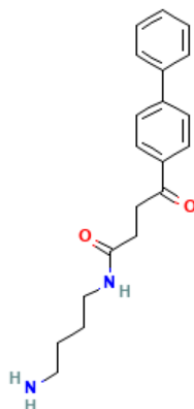


Figure 2. Chemical Structure Depiction

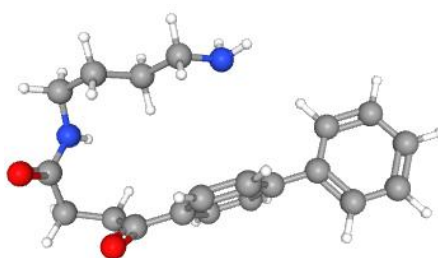


Figure 3. Interactive Chemical Structure Model

The chemical structure of Fenbufen Butanamine can be examined using representations such as SMILES (Simplified Molecular Input Line Entry System) and InChI (International Chemical Identifier) that are accessible in databases like PubChem. This representation allows for the visualization of 2D and 3D structures, as well as the calculation of various molecular descriptors that are important for predicting the biological activity and pharmacokinetic properties of compounds.

Structural analysis indicates that the addition of a butylamine group to the butanoate chain of Fenbufen can enhance the solubility of the compound in biological environments and influence interactions with target proteins through the formation of additional hydrogen bonds. Moreover, this modification can influence the logP value (the partition coefficient of octanol/water), which serves as an important indicator in predicting membrane permeability and oral bioavailability.

Another relevant descriptor includes the polar surface area (PSA), the number of hydrogen bond donors and acceptors, as well as the total count of rotatable bonds, all of which play a significant role in determining the pharmacokinetic and pharmacodynamic properties of compounds. This analysis is essential during the early stages of drug development, particularly in the *in silico* approach, which relies on computer predictions to identify potential compounds before laboratory testing is conducted.

By deeply understanding the chemical structure of Fenbufen Butanamine, including its structural modifications and their implications for physicochemical and biological properties, researchers can devise more effective and efficient drug development strategies. This involves optimizing the structure to enhance affinity for the biological target, reduce toxicity, and improve the stability and bioavailability of the compound.

Computational Descriptors of Fenbufen Butanamine

Fenbufen Butanamine is a structural derivative of the non-steroidal anti-inflammatory drug (NSAID) Fenbufen, modified by the addition of a butylamine group. This modification aims to enhance certain pharmacokinetic and pharmacodynamic properties, potentially improving its therapeutic efficacy. To

understand the implications of this structural alteration, computational descriptors provide valuable insights into the molecule's characteristics.

Table 1. Computed Descriptors of Fenbufen Butanamine

Descriptor	Value	Source
IUPAC Name	N-(4-aminobutyl)-4-oxo-4-(4-phenylphenyl)butanamide	Computed by Lexichem TK 2.7.0 (PubChem release 2025.04.14)
InChI	InChI=1S/C20H24N2O2/c21-14-4-5-15-22-20(24)13-12-19(23)18-10-8-17(9-11-18)16-6-2-1-3-7-16/h1-3,6-11H,4-5,12-15,21H2,(H,22,24)	Computed by InChI 1.07.2 (PubChem release 2025.04.14)
InChIKey	VEILLEFHLHRENO-UHFFFAOYSA-N	Computed by InChI 1.07.2 (PubChem release 2025.04.14)
SMILES	<chem>C1=CC=C(C=C1)C2=CC=C(C=C2)C(=O)CCC(=O)NCCCCN</chem>	Computed by PubChem (2025.04.14)

The IUPAC name of Fenbufen Butanamine is *N-(4-aminobutyl)-4-oxo-4-(4-phenylphenyl)butanamide*, as computed by Lexichem TK 2.7.0 in the PubChem release dated April 14, 2025. This nomenclature reflects the molecule's structural components, including the biphenyl moiety and the butanamide chain with an amino substituent.

The International Chemical Identifier (InChI) provides a textual representation of the compound's structure, facilitating database searches and interoperability. For Fenbufen Butanamine, the InChI is: InChI=1S/C20H24N2O2/c21-14-4-5-15-22-20(24)13-12-19(23)18-10-8-17(9-11-18)16-6-2-1-3-7-16/h1-3,6-11H,4-5,12-15,21H2,(H,22,24). The corresponding InChIKey, a hashed version of the InChI for easier web searches, is:VEILLEFHLHRENO-UHFFFAOYSA-N. The SMILES (Simplified Molecular Input Line Entry System) notation offers another linear representation of the molecule's structure: C1=CC=C(C=C1)C2=CC=C(C=C2)C(=O)CCC(=O)NCCCCN. Analyzing these descriptors reveals several key features of Fenbufen Butanamine. The molecule possesses a biphenyl core, contributing to its hydrophobic character and potential for π - π stacking interactions with biological targets. The butanamide chain, terminating with an amino group, introduces hydrophilic properties, potentially enhancing solubility and facilitating hydrogen bonding.

The presence of both hydrophobic and hydrophilic regions suggests amphiphilic behavior, which may influence the molecule's absorption, distribution, and interaction with biological membranes. Furthermore, the amino group could serve as a site for protonation under physiological conditions, affecting the molecule's charge state and, consequently, its pharmacokinetics.

Computational tools can further predict properties such as molecular weight, logP (octanol-water partition coefficient), topological polar surface area (TPSA), and the number of hydrogen bond donors and acceptors. These parameters are crucial for assessing drug-likeness and predicting oral bioavailability. For instance, a balanced logP value indicates favorable permeability and solubility, while an optimal TPSA suggests good intestinal absorption.

In summary, the computed descriptors of Fenbufen Butanamine provide a comprehensive understanding of its chemical structure and potential biological behavior. These insights are instrumental in guiding further pharmacological studies and drug development processes.

4. Conclusion

The computed descriptors of Fenbufen Butanamine provide essential insights into its chemical and

physicochemical properties, which are crucial for understanding its potential biological activity and pharmacokinetic behavior. The presence of a biphenyl core confers significant hydrophobic characteristics, which may facilitate strong interactions with biological targets through π - π stacking. Simultaneously, the butanamine side chain introduces hydrophilic elements, enhancing solubility and allowing for potential hydrogen bonding and protonation under physiological conditions. These amphiphilic properties suggest a balanced profile that may improve membrane permeability and bioavailability. The molecular descriptors, including the IUPAC name, InChI, InChIKey, and SMILES notation, confirm the unique structural identity of Fenbufen Butanamine and enable efficient database referencing and further computational modeling. This combination of hydrophobic and hydrophilic features, supported by computed physicochemical parameters, indicates that Fenbufen Butanamine holds promise as a drug candidate with favorable absorption and distribution profiles. Therefore, these computational findings provide a strong foundation for future experimental validation and pharmacological evaluation of Fenbufen Butanamine's efficacy and safety.

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