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МОЛЕКУЛА ЛЮПИНИНА: ПУТЕШЕСТВИЕ В ЕЁ КРИСТАЛЛОГРАФИЧЕСКУЮ СТРУКТУРУ

LYUPININ MOLEKULASI: UNING KRISTALLOGRAFIK TUZILISHI

THE LUPININE MOLECULE: A JOURNEY INTO ITS CRYSTALLOGRAPHIC STRUCTURE

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Annotatsiya

Ushbu tadqiqot maqolasi turli xil o‘simlik turlarida uchraydigan bisiklik alkaloid bo‘lgan lupininning tuzilishi, xossalari va potentsial qo‘llanilishini o‘rganishga qaratilgan. Tadqiqot lupininning molekulyar tuzilishi, molekulalararo o‘zaro ta’siri va fizik xususiyatlari haqida tushunchaga ega bo‘lish uchun kristallografik tahlildan, jumladan rentgen nurlari diffraktsiyasi va Xirshfeld sirt tahlilidan foydalanadi. Tadqiqot tadqiqotning o‘ziga xosligini ta'kidlaydi va lupininning biologik faolligi, farmakologik salohiyati va qishloq xo‘jaligida qo‘llanilishiga oid topilmalarni taqdim etadi. Natijalar lupininning struktura-funksiya munosabatlarini va uning yangi dori vositalari va ekologik toza pestitsidlarni ishlab chiqish manbasi sifatidagi potentsialini tushunishga yordam beradi.

Аннотация

Целью данной исследовательской работы является изучение структуры, свойств и потенциальных применений люпинина, бициклического алкалоида, обнаруженного в различных видах растений. В исследовании используется кристаллографический анализ, включая дифракцию рентгеновских лучей и анализ поверхности Хиршфельда, чтобы получить представление о молекулярной структуре, межмолекулярных взаимодействиях и физических свойствах люпинина. Исследование подчеркивает оригинальность исследования и представляет результаты, касающиеся биологической активности, фармакологического потенциала и применения люпинина в сельском хозяйстве.

Abstract

This research paper aims to investigate the structure, properties, and potential applications of lupinine, a bicyclic alkaloid found in various plant species. The study utilizes crystallographic analysis, including X-ray diffraction and Hirshfeld surface analysis, to gain insights into the molecular structure, intermolecular interactions, and physical properties of lupinine. The research highlights the originality of the study and presents findings regarding the biological activities, pharmacological potential, and agricultural applications of lupinine. The results contribute to the understanding of lupinine's structure-function relationship and its potential as a source for the development of new drugs and eco-friendly pesticides.

Kalit so‘zlar: *lyupinin, alkaloid, kristallografiya, rentgen nurlari difraksiyasi, Xirshfeld sirt tahlili, struktura-funksiya munosabatlari, farmatsevtikada qo'llanilishi, qishloq xo'jaligida qo'llanilishi*

Ключевые слова: *люпинин, алкалоид, кристаллография, рентгеновская дифракция, анализ поверхности Хиршфельда, взаимосвязь структура-функция, фармацевтическое применение, сельскохозяйственное применение.*

Key words: *lupinine, alkaloid, crystallography, X-ray diffraction, Hirshfeld surface analysis, structurefunction relationship, pharmaceutical applications, agricultural applications*

INTRODUCTION

Lupinine is a bicyclic alkaloid that has garnered significant interest in the scientific community due to its diverse biological activities and potential applications in medicine and agriculture. Alkaloids are a class of naturally occurring compounds known for their pharmacological properties, and lupinine, found in plants like lupins, is no exception. Crystallography, a field that involves the study of crystal structures using X-ray diffraction, has been instrumental in elucidating the molecular structure of lupinine and providing valuable insights into its properties. Crystallographic analysis involves determining the arrangement of atoms within a crystal lattice by analyzing the diffraction pattern of X-rays passing through the crystal. By subjecting lupinine crystals to X-ray diffraction, researchers have been able to obtain a detailed three-dimensional representation of the molecule's structure. This information is crucial for understanding the molecule's behavior, interactions, and properties. Hirshfeld surface analysis, a technique that utilizes crystallographic data, provides further insights into the intermolecular interactions and packing arrangements of the lupinine molecules within the crystal lattice. It involves the calculation and visualization of the Hirshfeld surface, which represents the distribution of intermolecular contacts in the crystal. This analysis helps researchers understand the nature and strength of interactions between lupinine molecules and provides clues about their physical properties. The crystallographic studies conducted on lupinine have not only shed light on its molecular structure but also revealed important information about its biological activities, pharmacological potential, and agricultural applications.

By examining the crystal structure and intermolecular interactions of lupinine, researchers can gain insights into its mode of action and potential targets in biological systems. This knowledge can be utilized in the development of new drugs or therapeutic agents.

Furthermore, the crystallographic analysis of lupinine can provide valuable information for its application in agriculture. Understanding the interactions between lupinine molecules in the crystal lattice can help researchers design compounds with improved properties for use as pesticides, herbicides, or plant growth regulators.

Overall, crystallographic analysis has played a crucial role in unraveling the structure, properties, and potential applications of lupinine. The insights gained from these studies have contributed to our understanding of this fascinating molecule and opened up new possibilities for its use in medicine and agriculture. [1].

Lupinine An Overview: Lupinine, with the molecular formula $C_{10}H_{17}N$, is classified as a bicyclic alkaloid. It was first isolated and identified by the German chemist Heinrich O. Wieland in 1901 from the seeds of Lupinus luteus, commonly known as yellow lupin. Since then, lupinine has been found in other plant species, including Lupinus angustifolius and Lupinus mutabilis[2]. The molecule features a unique structure comprising a perhydroindole moiety fused with a pyrrolidine ring. The perhydroindole ring consists of six carbon atoms and one nitrogen atom, while the pyrrolidine ring consists of four carbon atoms. The presence of a tertiary amine in the structure makes lupinine a basic compound [3].

MATERIALS AND METHODS

The structure of the compounds was determined using a Malvern Panalytical Empyrean diffractometer in the laboratory of Solid State Physics of the Institute of Nuclear Physics of the Uzbekistan FA. XRD data were recorded using CuKα radiation (λ = 1.54 Å). In this experiment, the accelerating voltage of the radiation generator was set to 45 kV and the emission current to 40 mA. X-ray patterns were recorded at 2TH = 200–1200 in the Braggi–Brentano beam geometry with a continuous scanning speed of 0.33 deg/min. The analysis of the obtained results was carried out using the VESTA program.

Extraction: Anabasis Aphylla L. (Itsegak) was chosen as a source (local raw material) for the extraction of lupinine from plants. The dried and crushed plant was extracted with ethanol. The

ethanol extract was concentrated under reduced pressure, acidified with HCl and extracted with chloroform to remove impurities. The resulting extract was basified with NH_4OH and extracted again with chloroform. The chloroform extract was treated with anhydrous Na_2SO_4 and the residue was evaporated to dryness in vacuum. The solid residue was separated by column chromatography.

RESULTS AND ITS DISCUSSION

Crystallographic Studies: Crystallography plays a pivotal role in understanding the three-dimensional arrangement of atoms within a crystal lattice. By determining the crystal structure of a molecule, researchers can gain valuable insights into its properties, reactivity, and interactions with other molecules. Crystallographic studies on lupinine have provided significant contributions to our understanding of its structure and behavior.

The study involved the growth of high-quality single crystals of lupinine, followed by X-ray diffraction analysis. X-ray diffraction is a widely utilized technique that allows scientists to determine the positions of atoms within a crystal lattice by analyzing the scattering pattern of X-rays. The crystallographic analysis revealed that lupinine crystallizes in the orthorhombic crystal system. The unit cell parameters were determined, and the crystal structure was solved using direct methods and refined using least-squares techniques *Mr* = 152,61, Monoklinik, *P*21 *a* =6,7482 (4) Å, *b* = 8,2482 (6) Å, *c* = 9,5697 (7) Å, *V* = 511,99 (7) Å³ *Z* = 2.

The analysis provided precise information about the bond lengths, bond angles, and torsion angles within the lupinine molecule [6,7,8].

Furthermore, the crystal structure elucidated the intermolecular interactions between lupinine molecules in the crystal lattice. These interactions include hydrogen bonding, van der Waals forces, and π-π stacking interactions. Such insights into intermolecular interactions are crucial for understanding the physical properties, stability, and solubility of lupinine.

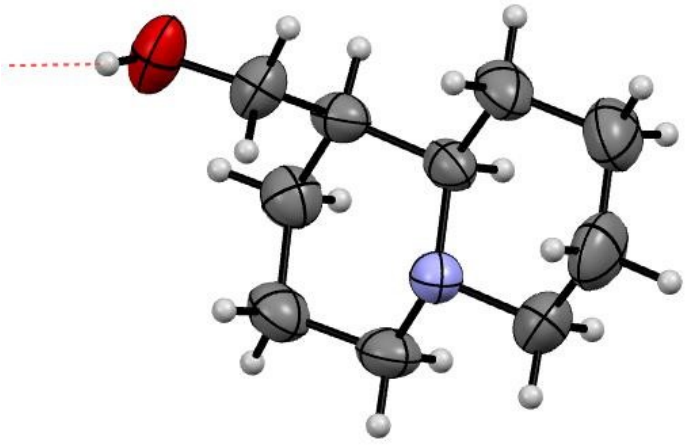

Figure 1. The asymmetric unit of lupinin in the crystallographic unit cell

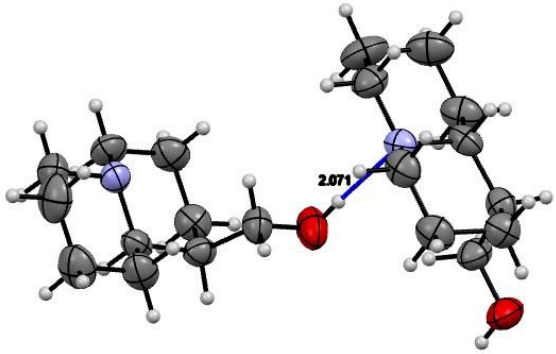

Figure 2. General appearance of lupinine in the crystallographic unit, the distance between molecules is 2.071 Å.

Bond precision: C-C = 0.0086 A Wavelength=1.54184

KIMYO

Cell:	a=6.7482(4)	b=8.2482(6)	c=9.5697(7)
alpha=90	beta=106.011(8)	gamma=90	
Temperature:	293 K		

Calculated	Reported	
Volume	511.99(6)	511.99(7)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C10 H19 N O [+ solvent]	C10 H19 N O
Sum formula	C10 H19 N O [+ solvent]	C9 H0.50 N2 O
Mr	169.26	152.61
Dx,g cm-3	1.098	0.990
Z	2	2
Mu (mm-1)	0.542	0.570
F000	188.0	153.0
F000'	188.49	
h,k,lmax	8,10,11	8,9,11
Nref	1990[1069]	1231
Tmin,Tmax	0.465,1.000	
Tmin'		

Correction method=Reported T
Limits: Tmin=0.465
Tmax=1.000 AbsCorr =
MULTI-SCAN

Data completeness= 1.15/0.62 Theta(max)= 71.445

R(reflections)= 0.0702(916) wR2(reflections)= 0.2255(1231)

S= 1.017 Np

Hirschfeld surface analysis of lupinine. Hirshfeld surface analysis serves as a quantitative approach for the examination of intermolecular interactions within crystalline structures. This method elucidates the shifts occurring at each point on the Hirshfeld surface concerning adjacent atoms situated on both the external di and internal de surfaces. These distinctive attributes have been instrumental in scrutinizing the selectivity and specificity of intermolecular forces acting upon molecular arrangements[9].

The generation of these surfaces involves partitioning the space enclosed by the crystal utilizing the Hirshfeld ratio, wherein the procrystal is effectively delineated employing a promolecule characterized by an electron density of 0.5. The normalized contact distance, denoted as *dnorm*, is computed by considering viewpoints both from the exterior and the interior of the surface, as articulated below:

$$d_{\text{norm}} = \frac{d_{\text{i}} - r_{\text{i}}^{\text{vdW}}}{r_{\text{i}}^{\text{vdW}}} + \frac{d_{\text{e}} - r_{\text{e}}^{\text{vdW}}}{r_{\text{e}}^{\text{vdW}}}$$

Here, d_e signifies the distance extending from the Hirshfeld surface to the nearest nucleus situated outside the surface, d_i represents the corresponding distance to the nearest nucleus enclosed within the surface, and *rvdW* designates the van der Waals radius of the atom in question.

The d_{norm} parameter manifests as a visually informative surface with a color gradient ranging from red to white to blue. Bright red regions on this surface denote intermolecular contacts that transpire within a distance shorter than their respective van der Waals radii, while the blue regions indicate intermolecular contacts occurring at distances greater than their van der Waals radii. White regions are indicative of the cumulative van der Waals radii for the associated atoms[10].

Short-range contacts between neighboring molecules in crystal lattice structures were calculated using Crystal Explorer version 21.5. Crystal Explorer 21.5 was used to analyze the Hirshfeld surfaces of the crystal structures and generate the corresponding two-dimensional (2D) fingerprint plots[11].

The Hirshfeld surface analysis of lupinin and utilized an isovalent of 0.5 in the asymmetric unit. The Hirshfeld surface dnorm of lupinin is depicted in Figure 3. According to calculations, the surface area measures 228.92 Å2, and its volume spans 251.04 Å3, within the range of -0,5735 to 1,5984 atomic units.

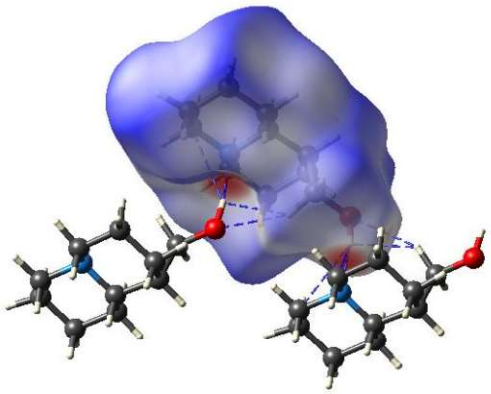

Figure 3. Hirshfeld surface analysis of lupinin and utilized an isovalent of 0.5 in the asymmetric unit.

The contribution of interatomic interactions to the formation of the Hirshfeld surface is illustrated in 2D fingerprint images of the surface (Figure 4). In the generalized (100%) fingerprint image, Hirshfeld surfaces were formed at distances of de=2.6 Å and di=2.5 Å (de > di). The H-H interactions contribute 91.4 % to the surface formation, while O-H/H-O interactions account for 5.7 %,and N-H/H-N interactions for 2.8%.

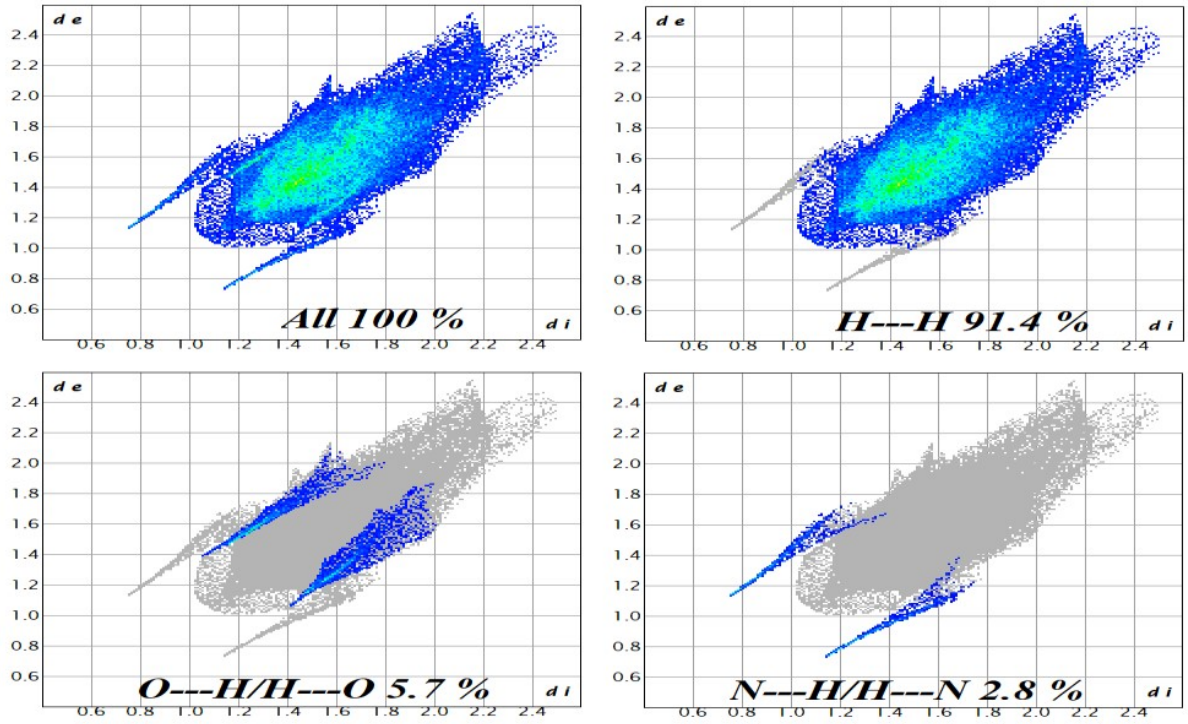

Figure 4.The contribution of interatomic interactions to the formation of the Hirshfeld surface is illustrated in 2D fingerprint images of the surface

CONCLUSION

In conclusion, this research paper provides valuable insights into the structure, properties, and potential applications of lupinine. The utilization of crystallographic analysis techniques, including X-ray diffraction and Hirshfeld surface analysis, enhances our understanding of lupinine's molecular structure, intermolecular interactions, and physical properties. The research highlights the originality of the study by exploring the potential of lupinine as a source for the development of new drugs and eco-friendly pesticides. The findings contribute to the understanding of lupinine's structure-function relationship and its potential applications in various fields.

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