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Original article

LibNPDB: The First Freely Accessible Database of Libyan Natural Products

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Abstract
Libya's rich flora is a significant but untapped resource for natural products research. A lack of accessible digital information has limited progress in this area. To address this gap, we systematically collected data on bioactive compounds from Libyan plants, gathering information from various local records and existing online databases. This effort resulted in the Libyan Natural Products Database (LibNPDB), the first free, web-based repository for Libyan natural products. It currently holds 1,047 entries from scientific literature, covering 562 unique chemical compounds. As a powerful tool, LibNPDB allows users to search in multiple ways, such as by compound name, plant part, or plant source, and other parameters, providing researchers with a user-friendly interface to find data. Beyond being a comprehensive reference, the database aims to increase the global visibility of Libyan natural product research. Future developments include expanding the data on plant phytochemicals, adding more information on Libyan medicinal plants, improving the search filtrations and analysis tools, and enabling users to download data in bulk. These planned improvements will make the database more useful for advanced applications like virtual screening, molecular docking, and drug discovery. Ultimately, the LibNPDB (available at https://www.libnpdb.ly) is an essential resource for unlocking the scientific and economic potential of Libya's natural resources while encouraging collaboration and innovation within the global research community.
Keywords. Chemoinformatics, Phytochemicals, Data Mining, Libyan Natural Product, Database.

Introduction

Natural products, the structurally diverse small molecules synthesized by living organisms, are invaluable to pharmacology and other industries, historically serving as a primary source of novel drug candidates [1], [2]. To support *in silico* drug discovery, over 120 natural product (NP) databases and collections have been published since 2000. Among the most well-established are the Traditional Chinese Medicine (TCM) and the Chinese Natural Product Database (CNPD), which together contain nearly 80,000 unique chemical structures. More recently, the Collection of Open Natural Products (COCONUT) database was released, aggregating data from over 120 sources to provide more than 400,000 non-redundant, freely accessible entries with broad regional coverage [3].

As part of this global effort, countries worldwide are systematically cataloging their native NPs. In Africa (Table 1), this has led to the creation of several key databases, including the Cameroonian Natural Products Database (CamMedNP) and the Congolese Natural Products Database (ConMedNP) for Central African flora, the Northern African Natural Products Database (NANPDB) for North Africa, the African Natural Products Database (AfroDb) for continental Africa, and the South African Natural Compound Database (SANCDB) for South Africa [3, 4]. These initiatives are crucial as they complement each other to reveal region-specific structural diversity and bioactivity profiles. This, in turn, advances drug discovery by highlighting the unique chemical landscapes of different biogeographical zones.

Table 1. Selected major natural product databases in Africa.

Database Name	Abbreviations	Size
African Natural Products Database	ANPDB	6515
Northern African Natural Products Database	NANPDB	4500
Natural products from African sources	AfroDb	1008
The Eastern Africa Natural Products Database	EANPDB	1871
South African Natural Compound Database	SANCDB	1012
The Cameroonian Natural Products Database	CamMedNP	2500
The Congo Natural Products Database	ConMedNP	3200

Libya's diverse ecosystems, which range from a temperate Mediterranean coast to an arid desert, sustain a uniquely adapted flora. Researchers have documented 2,103 species across 155 plant families and 856 genera, with approximately 450 possessing medicinal properties. Of these, 208 are actively used in traditional medicine by local communities. The country's varied topography, including the Al-Jabal Al-Akhdar and Jabal-Nafousa mountain ranges, creates distinct habitats that contribute to this rich biodiversity. This botanical heritage is not only a cornerstone of traditional healthcare for nearly one-third of Libyans but also a vital cultural asset [3, 5, 6]. However, despite the clear therapeutic and cultural value of Libya's endemic plants, natural product research in the country faces significant challenges [3, 7, 8].

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Prior to this work, the primary obstacle was the absence of a comprehensive national database, which hindered the systematic documentation and dissemination of information related to the country's rich biodiversity and traditional herbal medicine. This deficiency is compounded by the poor accessibility of existing knowledge, as critical resources like university theses and local scientific articles are often not digitized or available in global repositories. Furthermore, a lack of sustained government programs to support innovation has limited research and documentation efforts. The development of the Libyan Natural Products Database (LibNPDB) is therefore a critical undertaking, aimed at overcoming these challenges by collecting, verifying, and digitizing this scattered information [3, 9].

There is an urgent need to advance research initiatives focused on collecting specimens, isolating compounds, and progressing drug discovery from Libya's medicinal plant flora [3, 10, 11]. Establishing a unified, open-access compound database is a foundational step in this process. By integrating all available data into a single, comprehensive resource, the LibNPDB is expected to make significant contributions to natural product-based drug discovery, both within Libya and on a global scale. This study details the construction of the first comprehensive Libyan Natural Product Database, a vital tool for unlocking the scientific and economic potential of the nation's unique botanical resources [3].

Methods

All computational and data management tasks were performed using commercial and open-source tools alongside public web services. Chemical structures were drawn and standardized in ChemOffice 2019, and initial records were compiled in Excel 2019 using custom VBA-powered forms for streamlined data curation. Bibliographic and phytochemical information was enriched by querying PubMed, Google Scholar, ScienceDirect, and Wikipedia. The public-facing database is a lightweight client-side application built with HTML5, CSS3, and JavaScript (ES6), with all assets versioned on GitHub and real-time chemoinformatic enrichment achieved through PubChem's PUG-REST API. Python 3.12 was used for statistical analyses and served as the primary computational environment, employing RDKit for molecular descriptor calculations and drug-likeness evaluations, Pandas for data management, and NPClassifier for hierarchical structural [6, 12, 13, 14].

Data Mining and Collection Strategy

The search strategy for data collection in the Libyan Natural Products Database (LibNPDB) involved an extensive and systematic approach across multiple sources (Figure 1). A thorough literature review was conducted, focusing on journal articles, theses, and textbooks that documented the extraction of compounds from Libyan plants and marine organisms. The collection of theses from Libyan universities proved particularly valuable, albeit challenging, especially when locating locally published articles that were not available online or included in existing local databases. Key databases such as PubMed, ScienceDirect, Google Scholar, and other Databases were extensively utilized to identify relevant publications. Additional literature was uncovered through targeted Google searches and by tracing references cited in previously discovered materials. All collected data were then organized in an Excel worksheet [3,15,16].

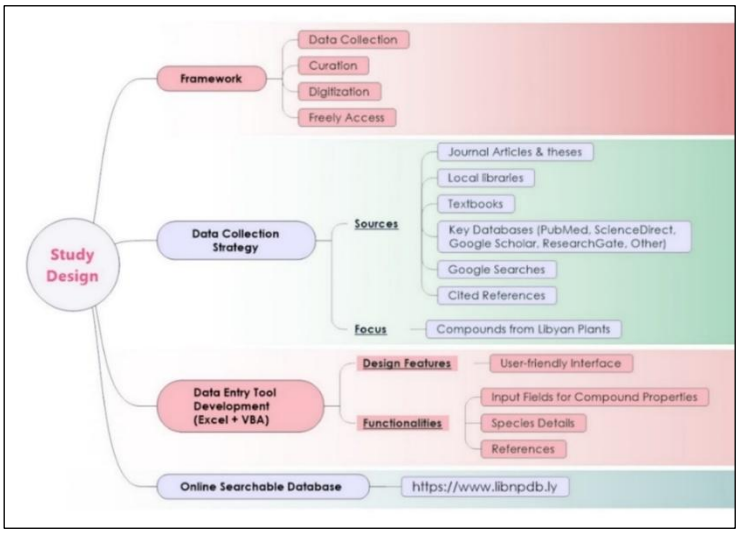

Figure 1. Flowchart illustrating the LibNPDB development workflow

Database Structure and Comparative Analysis

The development of the data entry tool and database structure was initiated by creating a dedicated "Data" worksheet in Excel. The headers were precisely defined to capture all essential fields. These headers include essential data points such as Compound Name, PubChem CID, SMILES Strings, InChIkey Code, Compound Class, Species Name, Family, Known Uses, Biological Activity, Mode of Action, Source Country, GPS,

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Collection Date, Authors, and Reference information [3]. A fundamental principle guiding the development of LibNPDB was linking all data to at least one referenced source. This ensured that reference information was captured before any other details were added. To streamline data input, a user-friendly interface was developed using a Visual Basic for Applications (VBA) UserForm, which organized input fields into three logical frames: Compound, Plant, and Reference. To visualize the distribution and overlap of LibNPDB collected compounds across five African databases, a 5-way Venn diagram was constructed using a custom Python script. This analytical visualization was implemented through the specialized Venn module, enabling the quantitative assessment of both unique compounds specific to individual databases and shared compounds occurring across multiple database systems. This approach provided valuable insights into the comprehensiveness and redundancy patterns within the regional chemical database landscape [17, 18].

Structural Classification

The structural classification of compounds within the LibNPDB was accomplished using NPClassifier, a deep neural network-based tool designed for the categorization of natural products. This system organizes compounds into a three-tiered hierarchy consisting of pathway, superclass, and class levels. To effectively visualize the distribution of dominant chemical structures across each of these three hierarchical categories, pie charts were generated using the Python programming language (version 3.12), providing a clear quantitative representation of the structural diversity within the database [14, 18].

Visual representation of chemical space

To enable high-throughput analysis, a custom Python script was developed to calculate key ADME (Absorption, Distribution, Metabolism, and Excretion) and drug-likeness metrics from chemical structures. The tool leverages the Pandas library for data management and RDKit to compute six molecular physicochemical descriptors [19]. Drug-likeness was evaluated using Lipinski's Rule of Five, which predicts good oral bioavailability when no more than one of the following criteria is violated: MW $\leqslant$ 500 Da, SlogP $\leqslant$ 5, HBD $\leqslant$ 5, and HBA $\leqslant$ 10. Compounds meeting at least three of these four criteria were classified as drug-like [17, 20]. Violin plots visualize the distribution of each property, highlighting drug-likeness thresholds. Additionally, Chemical space visualization was performed using dimensionality reduction techniques implemented in Scikit-learn (version 1.3.0) [18, 21]. Principal Component Analysis (PCA) and t-Distributed Stochastic Neighbour Embedding (t-SNE) were performed to visualize local structural similarities [22]. This pipeline supports comparative analysis of Natural Products across African databases that include AfroDb, SANCDB, ANPDB, NANPDB, LibNPDB, and two reference datasets: COCONUT and FDA-approved drugs [18].

Development of LibNPDB Platform

In constructing the LibNPDB, the website uses a client-side architecture with HTML5 for structure, CSS3 for responsive styling, and ES6 JavaScript for interactivity and data handling. This enables dynamic compound rendering in the browser without a back-end server, simplifying deployment and maintenance while ensuring fast, responsive performance. All source code, including the HTML templates and the curated JSON files in which compound metadata are stored, will be hosted in a public GitHub repository. This arrangement guarantees version control, facilitates collaborative editing of both code and data, and enables automated publication through GitHub Pages [15, 16].

To enrich each database entry in real time, the client-side script will call free chemical web services, principally PubChem's PUG-REST API, which returns canonical SMILES strings, InChIKeys and selected bioactivity annotations. Furthermore, PubChem's PUG-REST service can convert a SMILES string of a compound as input and return either a 2D or a 3D image. Because these requests are executed directly in the browser, the platform avoids server overhead entirely [23]. New compounds can therefore be added simply by appending a record to the JSON dataset and committing the update; once the changes are merged, GitHub Pages will redeploy the site automatically, ensuring rapid, reproducible expansion of LibNPDB.

Statistical Analysis

All statistical analyses were performed using Python 3.12 with Scikit-learn (version 1.3.0) and SciPy libraries. Six molecular descriptors (MW, SlogP, TPSA, Rb, HBA, and HBD) were calculated using the RDKit cheminformatics toolkit to compare physicochemical properties between LibNPDB and other African natural product databases. Database overlap was visualized using matplotlib-venn, while violin plots and statistical graphics were generated with Matplotlib and Seaborn to illustrate descriptor distributions across datasets. Statistical significance of distribution differences was assessed using the non-parametric Kruskal-Wallis test with significance thresholds set at $p < 0.05$. For chemical space analysis, dimensionality reduction was conducted through (PCA) with standard scaling, extracting components until exceeding 95% cumulative variance, and (t-SNE) with perplexity = 30, learning rate = 200, and 1,000 iterations, enabling visualization of structural similarity patterns between LibNPDB, COCONUT, and FDA-approved drug collections [17, 18, 22].

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Results and discussion

Database Overlap and Compound Uniqueness

The comparative analysis of African natural product databases is illustrated in (Figure 2). Panel A presents a Venn diagram that delineates the distribution and overlap of unique compounds among five major databases: LibNPDB, AfroDb, ANPDB, SANCDB, and NANPDB [4,18]. The diagram reveals a high degree of exclusivity, with a substantial number of compounds (374) being unique to a LibNPDB database. In contrast, 188 compounds (33.45% of LibNPDB, 562 unique compounds) are shared with at least one other database. This visualization underscores the complementary nature of these repositories and highlights the value of integrating them to achieve a more exhaustive catalogue of the continent's natural product diversity. On the other hand, (Figure 2B) explores the relationship between the number of natural products and the corresponding plant species documented within the Libyan Natural Products Database (LibNPDB). The bar chart demonstrates a positive correlation between the abundance of natural products and the diversity of plant species across various Libyan regions. Notably, certain locations exhibit a pronounced richness in both natural product counts and plant species, reflecting the influence of local biodiversity on the breadth of chemical entities catalogued. Together, (Figures 2A and 2B) provide critical insights into both the distribution of compounds at a continental scale and the ecological factors shaping chemical diversity within a regional context.

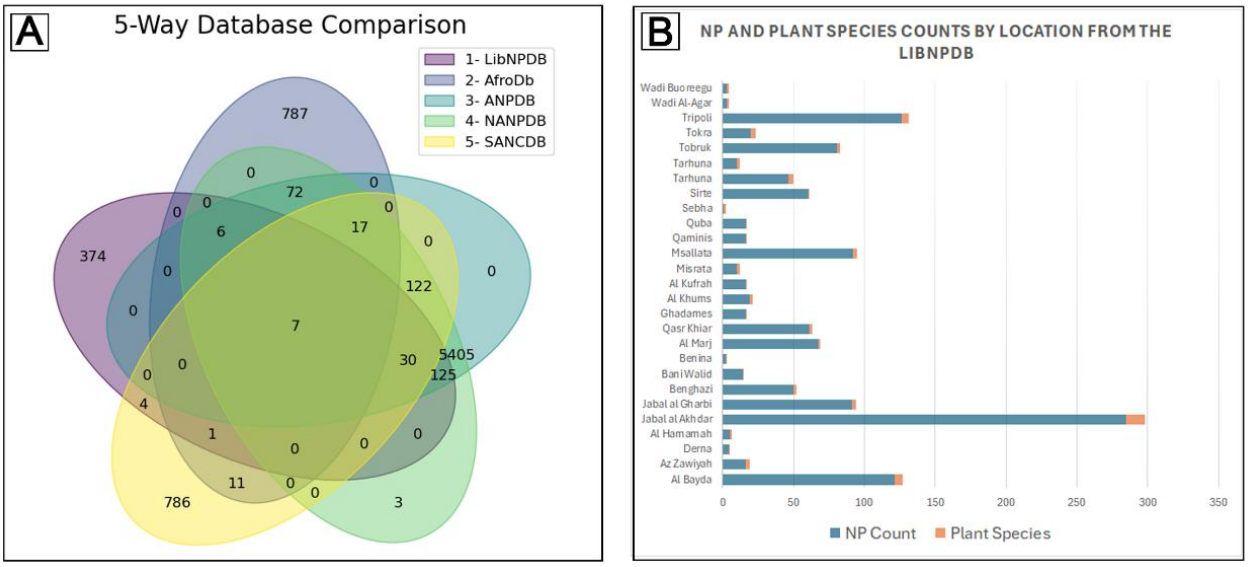

Figure 1. (A) Venn diagram showing the distribution and overlap of unique compounds among African natural product databases: LibNPDB, AfroDb, ANPDB, NANPDB, and SANCDB. The numbers indicate the count of unique compounds specific to each database or shared between them. (B) Correlation between the number of natural products and plant species recorded in the (LibNPDB).

Structural Classification

As shown in (Figure 3), the analysis of the LibNPDB compound library reveals a distinct distribution across various biochemical classifications [3, 10]. The compounds were classified into a total of six different pathways, thirty-two superclasses, and one hundred and three classes, with data highlighting a significant concentration in a few major categories. The classification by biosynthetic pathway shows that a vast majority of the compounds originate from three predominant pathways: terpenoids, which represent the largest group at 46.5%; shikimates and phenylpropanoids at 31.4%; and fatty acids at 17.7%. At the superclass level, this distribution is mirrored, with the main subclasses being monoterpenoids (19.3%), sesquiterpenoids (16.1%), and flavonoids (13.4%). The classification becomes more granular at the class level, where the most prevalent classes are cinnamic acids and derivatives (5.87%), menthane monoterpenoids (5.68%), hydrocarbons (5.58%), and flavones (5.19%).

LibNPDB mirrors the typical spectrum of plant metabolites. Terpenoids dominate, reflecting their vast structural diversity, with monoterpenoids and sesquiterpenoids strongly represented. The next largest group shikimates and phenylpropanoids, aligns with the high levels of flavonoids and cinnamic acids found in the LibNPDB database.

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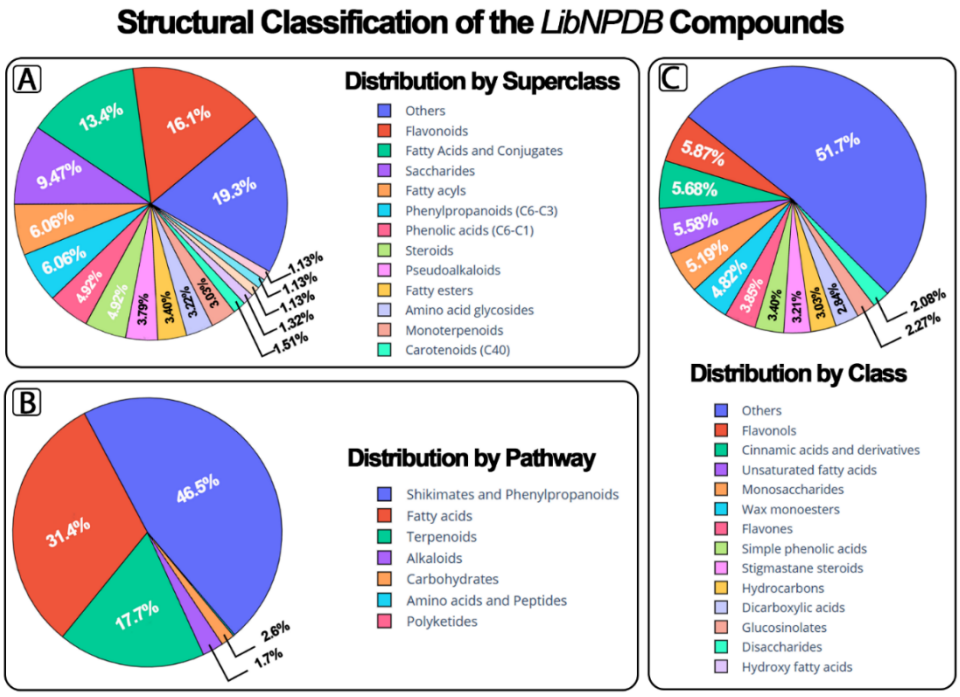

Figure 2. Distribution of LibNPDB compounds across three classification levels: Distribution by (A) Superclasses, (B) Pathways, and (C) Chemical classes

Physicochemical Properties

To evaluate its potential for drug discovery, the physicochemical properties of the Libyan Natural Product Database (LibNPDB) were analysed and benchmarked against four other African databases (AfroDb, ANPDB, NANPDB, and SANCDB). This comparative assessment utilized six key molecular descriptors: MW, SlogP, TPSA, Rb, HBA, and HBD to validate LibNPDB utility as a high-quality screening library, referencing established thresholds like Lipinski's Rule of Five [9,18]. As shown in (Figure 4), the findings demonstrate that LibNPDB compounds are predominantly situated within a drug-like chemical space. A significant majority adhere to the criteria of Lipinski's Rule of Five: 92.88% meet the MW requirements, 79.18% meet SlogP thresholds, 92.35% fall within the HBA range, and 88.97% comply with the HBD limits. The collection also shows strong compliance with Veber's rule [24], which suggests compounds are more likely to be orally bioavailable if they have ten or fewer rotatable bonds and a topological polar surface area (TPSA) of 140 Å² or less, with 85.59% falling within the Rb range and 88.61% satisfying TPSA limits. These high compliance rates indicate a strong alignment with parameters favourable for oral bioavailability and membrane permeability, underscoring the database's enrichment with molecules suitable for orally administered drug development [24, 25]. Crucially, the physicochemical properties are remarkably consistent across all databases, validating that LibNPDB is a representative and high-quality collection comparable to other major African natural product libraries [17, 18].

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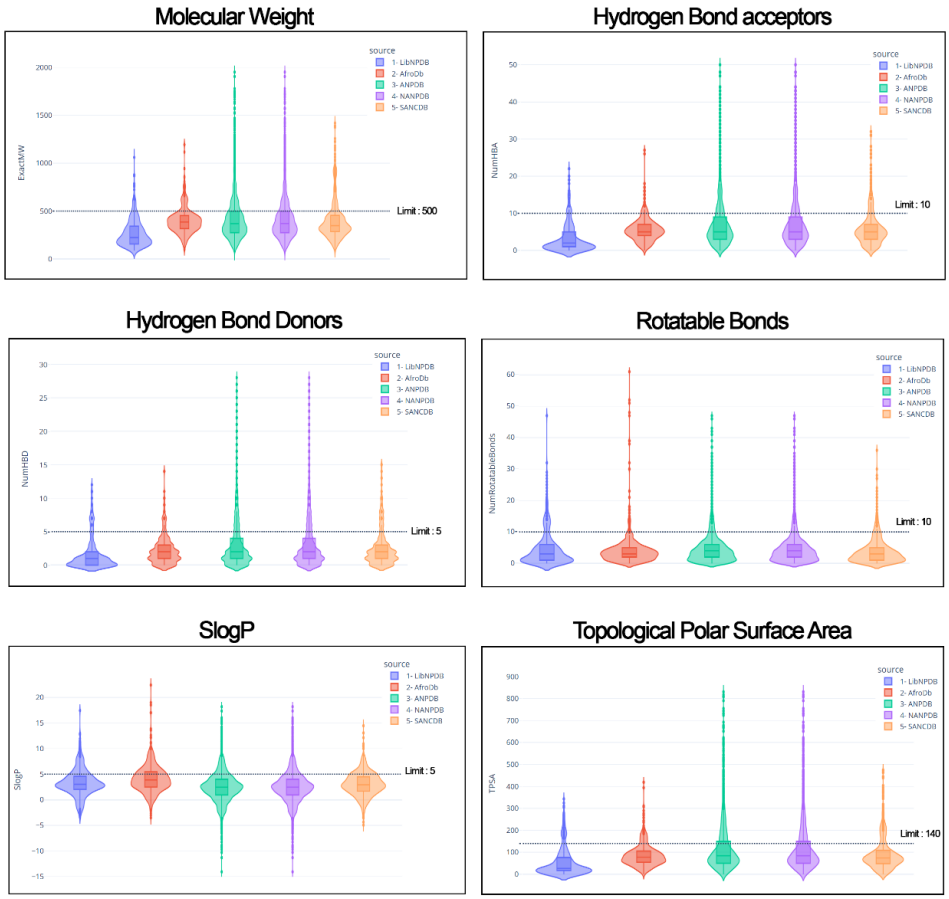

Figure 3. Violin plots comparing six key physicochemical properties of natural products collected from five African-focused databases: LibNPDB, AfroDb, ANPDB, NANPDB, and SANCDB

Chemical space was explored by applying PCA and t-SNE dimensionality reduction to six molecular descriptors [22]. For comparative context, LibNPDB compounds were analysed alongside the COCONUT database and FDA-approved drugs [18]. The PCA effectively simplifies the dataset's complexity, with the first two principal components (PC1 and PC2) accounting for a significant 93.1% of the total variance (60.3% and 32.8%, respectively). This substantial overlap indicates that compounds within the LibNPDB collection share structural characteristics with established medications. The results indicate that many LibNPDB compounds occupy chemical space similar to FDA-approved drugs, suggesting their suitability for in silico screening. However, chemical similarity alone does not confirm biological activity; experimental validation will be needed for true lead identification. The t-SNE analysis complements the PCA by visualizing local structural similarities [22]. It reveals a dense, intermixed cluster, demonstrating substantial overlap between the natural product libraries (LibNPDB and COCONUT) and FDA-approved drugs. These highlights shared chemical features, reinforcing the pharmacological relevance of the natural product databases for drug discovery [9, 18].

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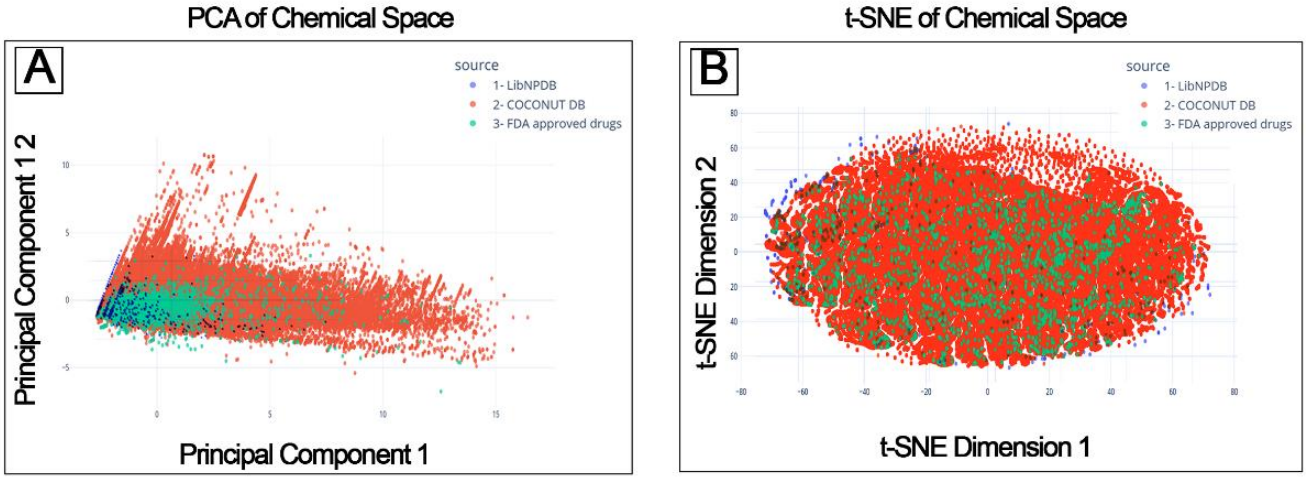

Figure 4. Chemical space analysis of the LibNPDB, COCONUT, and FDA-approved drug databases. (A) PCA plot, where the first two principal components explain 93.1% of the total variance (PC1: 60.3%, PC2: 32.8%. (B) t-SNE plot, which visualizes local similarities among compounds.

The First Libyan Natural Products Database (LibNPDB) Platform

The LibNPDB platform represents an important advancement in the documentation and exploration of Libya's rich biodiversity, particularly for drug discovery. This initiative has produced the first national database of natural products for Libya. This initiative aims to systematically collect, analyse, and make accessible information on natural products derived from Libyan flora. A key contribution of the LibNPDB project is the consolidation of fragmented data on Libyan natural products. By centralizing information previously dispersed across disparate and often inaccessible sources, the database establishes a single, invaluable platform for the national and international scientific communities, enhancing research accessibility and efficiency [3]. The initial release of the LibNPDB catalogues a total of 1047 compound entries. This collection corresponds to 562 chemically unique compounds, each identifiable by a distinct LibNPDB ID. The database utilizes multiple entries for a single compound to document each reported isolation from different literature sources, thus providing a comprehensive record of its existence.

LibNPDB facilitates data exploration through two distinct yet complementary interfaces. For broad, relational discovery, the "Browse" page allows users to navigate interconnected information. Clicking a compound name reveals its comprehensive details, including molecular structures and geographical origin, while selecting a plant name lists all its known phytochemicals. This feature enables an intuitive exploration of chemo diversity and compound distribution across various botanical sources. Complementing this exploratory approach, the "Search" page offers a streamlined tool for targeted inquiries. Its minimalist design is optimized for rapid lead compound identification. Beyond simple retrieval, users can download molecular structures in multiple formats (e.g., SDF, JSON) and, notably, perform real-time calculations of molecular descriptors and drug-likeness parameters directly within the platform. This dual functionality supports both extensive investigation and focused queries, creating a versatile and powerful resource accessible to researchers with diverse expertise.

The LibNPDB platform integrates a powerful chemical toolkit, creating a seamless workflow for molecular analysis across three interconnected modules. The system facilitates bidirectional molecular representation, allowing users to either generate 2D and 3D structures from SMILES notation or utilize an interactive sketcher to draw molecules and obtain their corresponding SMILES strings. This functionality feeds directly into the subsequent drug-likeness calculator. Leveraging the RDKit library [19]This advanced tool accepts the generated SMILES to compute critical molecular descriptors and evaluate drug-likeness using multiple filters, including Lipinski's Rule of Five and the Quantitative Estimate of Drug-likeness (QED) score [26]. This cohesive system establishes a complete pipeline, enabling researchers to progress efficiently from molecular visualization to a sophisticated in silico pharmacological assessment, all within a single, unified environment [4, 13, 16].

Despite significant challenges, including limited funding and access to local sources, the LibNPDB has successfully established a vital foundational resource. Looking forward, the planned second phase aims to build directly upon this groundwork by addressing these initial limitations [3]. A primary objective is to substantially expand the dataset by systematically incorporating compounds from previously inaccessible local publications and traditional knowledge repositories. This expansion will be complemented by enriching entries with comprehensive biological activity and pharmacological data. Technologically, the platform will be significantly enhanced with advanced in silico tools, including integrated molecular docking for virtual screening and robust similarity search functionalities. These upgrades are designed to transform LibNPDB

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into a more powerful source for drug discovery, underscoring the need for sustained investment to realize its full scientific potential and accelerate the development of new therapeutics [4].

Conclusion and recommendations

The Libyan Natural Products Database (LibNPDB) has been successfully established as the first and only freely accessible, web-based repository of chemical compounds isolated from Libyan plants. LibNPDB functions as more than a static, literature-referenced catalogue by providing a robust and user-friendly chemoinformatic environment. This dynamic platform empowers researchers with versatile search capabilities to efficiently identify molecules of interest. This resource is vital for accelerating scientific discovery. Building upon the initial release, a major update (version 2.0) is planned to substantially expand the database scope and analytical capabilities. Future improvements will focus on enriching the content by expanding the compound collection and integrating data on the traditional medicinal uses of Libyan plants. Furthermore, the database will be enhanced with deeper data, such as additional computed molecular descriptors and comprehensive stereochemical information for each entry. Functionality will also be upgraded with an improved user interface and bulk data download capabilities to support large-scale computational analyses. These planned upgrades will significantly elevate the visibility of Libyan natural product research on a global scale. Ultimately, by empowering scientists with this valuable data, LibNPDB will become an essential tool for advanced applications in virtual screening, molecular docking, and drug discovery. This will help unlock the full scientific and economic potential of Libya's natural resources while encouraging international collaboration.

Conflicts of Interest

The authors declare no conflicts of interest.

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