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REVIEW article

Bridging the gap: A strategic review of natural product databases and the proposal for the Libyan Natural Products Database

Abdelkarim N. Sasi [*], **Ali M. Rafieda**, **Sezar M. Jouda**
Yacoub M. Amer, and **Fathi M. Khalifa**

Faculty of Pharmacy, Misurata University, Misurata, Libya
[*] Author to whom correspondence should be addressed

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Abstract: Natural products are a vital source of therapeutic agents due to their diverse chemical structures and wide range of biological activities. With the advancement of computational technologies, natural product databases have become essential tools in drug discovery, offering organized access to chemical structures, biological properties, and biosynthetic information. These databases support various stages of drug development, from target identification to lead optimization. This review outlines the essential features of Natural Products Databases and introduces the framework for the first Libyan Natural Products Database, a project designed to harness Libya's unique biodiversity. This foundational work involves a detailed review of existing natural product databases to identify their core components, data architectures, and user interface designs. While acknowledging challenges such as data standardization, limited resources, and long-term sustainability, the creation of the Libyan Natural Products Database is expected to enhance local scientific capacity and contribute meaningfully to the global drug discovery landscape. This positions the Libyan Natural Products Database to play a foundational role in advancing pharmaceutical research and drug discovery.

Introduction

Natural product (NP) databases are essential tools in drug discovery, offering extensive information on bioactive compounds, including chemical structures, biological activities, pharmacokinetics data, molecular descriptors, and drug likeness. These databases support in silico screening and aid in identifying promising drug candidates. At the same time, some databases focus on regional or traditional medicine systems, others compile global datasets [1]. Despite its rich biodiversity and strong herbal medicine tradition, Libya remains underrepresented in this field and lacks a comprehensive national NP database. Establishing such a resource would document Libya's natural heritage and integrate traditional knowledge with modern research, enabling virtual screening and drug development [2, 3]. A Libyan Natural Products Database (LibNPDB) would also contribute to global biodiversity representation, particularly for North Africa [4]. However, challenges persist, including data quality, accessibility, sustainability, and reliable sourcing. In addition, Libya faces unique hurdles like limited infrastructure, scarce funding, and the need for international collaboration to ensure successful integration with global platforms [1].

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Types of NP databases: NP databases can be broadly classified based on their accessibility and thematic focus. Open-access NP databases are freely available for public use and often allow bulk downloads, while others require subscription-based access (**Table 1**). These resources support a wide range of research efforts, from pharmacology and medicinal chemistry to biodiversity conservation. Within this broader classification, databases are further organized by their specific content and purpose. Some databases focus on geographical or ecological sources, others on spectral or biological activity data, and many are developed with a thematic emphasis, such as traditional medicine or drug-likeness evaluations [1, 5].

A key distinction among NP databases lies in their geographic focus. Some are region-specific, highlighting compounds derived from natural sources within particular continents or countries. For example, the African Natural Products Database (AfroDb) [6] and the Latin American Natural Products Database (LANaPDB) [7] serve as continent-level repositories. In contrast, country-level examples include the South African Natural Compound Database (SANCDB) [8] and the Peruvian Natural Products Database (PeruNPDB) [9]. These collections are instrumental in capturing the unique phytochemical diversity of specific locations. In contrast, generalist databases like the Collection of Open Natural Products (COCONUT) [10] and LOTUS [11] take a broader approach, aggregating compounds from global sources without restriction to any particular geography. Another important category is spectral databases, which house experimental data such as Nuclear Magnetic Resonance (NMR) and mass spectrometry spectra crucial for compound characterization and structural elucidation. Additionally, some databases are curated with thematic intentions, such as those centered on traditional medicine, drug-likeness profiling, or ecosystem-specific biodiversity [1].

Table 1: Summary of the most common (open-access) databases

Database Name	Abbreviations	Size	Type	
Collection of Open Natural Products	COCONUT	695130	Global NPD	General
LOTUS	LOTUS	750000	Global NPD	General
Natural Products Atlas	NP Atlas	32552	Global NPD	General
The Natural Product Activity and Species Source Database	NPASS	96481	Global NPD	General
Latin American Natural Product Databases	LANaPDB	13578	Regional NPD	Latin American
The Peruvian Natural Products Database	PeruNPDB	280	National NPD	Peru
African Natural Products Database	ANPDB	6515	Regional NPD	Africa
Northern African Natural Products Database	NANPDB	4500	Regional NPD	Africa
Natural products from African sources	AfroDb	1000	Regional NPD	Africa
The Eastern Africa Natural Products Database	EANPDB	1870	Regional NPD	Africa
South African Natural Compound Database	SANCDB	1012	National NPD	South African
The Cameroonian Natural Products Database	CamMedNP	2500	National NPD	Cameroon
Traditional Chinese Medicine	TCM	61000	National NPD	Taiwan
Indian Medicinal Plants, Phytochemistry and Therapeutics	IMPPAT	17967	National NPD	India
Zinc Database	Zinc	230 m	Global CDB	General
The ChemSpider Database	ChemSpider	130 m	Global CDB	General
The PubChem Database	PubChem	119 m	Global CDB	General

Among the generalist databases, several stand out for their scale and features. COCONUT is one of the most comprehensive open-access NP databases, initially launched in 2021 by aggregating a wide array of public NP datasets. It offers detailed information on chemical structures, names, synonyms, species origins, geographical distribution, and literature references, all accessible via various search functionalities including structure and substructure queries. Building on similar principles, the LOTUS database focuses on structure-organism pairs, systematically referencing over 750,000 such connections corresponding to more than 250,000 unique compounds. While COCONUT and LOTUS provide broad, inclusive datasets, other databases offer specialized collections [10, 11]. The Natural Products Atlas (NP Atlas) targets microbial natural products and contains over 32,000 curated compounds [12]. In a different but complementary direction, the Natural Product

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Activity and Species Source Database (NPASS) connects closely 100,000 compounds to experimentally determined bioactivity data and source species [13]. Together, these databases COCONUT, LOTUS, NP Atlas, and NPASS, provide powerful, yet distinct, tools for NP research. COCONUT offers a vast, community-curated resource; LOTUS excels in referencing structure-source pairs; NP Atlas specializes in microbial compounds; and NPASS bridges chemical structure with biological function. Despite differences in scope and focus, they share a commitment to open access and data-driven drug discovery, often functioning as complementary tools in research workflows [1, 5, 14].

Region-specific databases play a critical role in documenting the phytochemical wealth of Africa. AfroDb compiles over 1,000 compounds from medicinal plants across the continent [6]. SANCDB, by contrast, focuses on South African biodiversity, initially offering 600 compounds and now exceeding 1,000 entries [8]. This curated and referenced database includes both planetary and marine natural products. NANPDB, representing Northern Africa, is a larger and more diverse resource, documenting about 4,500 compounds from plants, fungi, bacteria, endophytes, and even marine organisms like corals. Spanning literature from 1962 to 2016, it includes computed physicochemical properties, predicted toxicity, and known biological activities for many entries. NANPDB is the most extensive in terms of compound count and includes data types not found in the others, such as predicted toxicities and mode of action annotations [1, 4].

Country-specific databases further emphasize national biodiversity and traditional knowledge systems. The Cameroonian Natural Products Database (CamMedNP) contains over 2,500 compounds from 224 medicinal plants, including some semi-synthetic derivatives [15]. In East Asia, the Traditional Chinese Medicine (TCM) Database@Taiwan stands as one of the largest non-commercial repositories of TCM-derived compounds. With over 20,000 pure compounds from 453 ingredients, it supports searches based on molecular features, substructures, specific TCM herbs, and traditional classifications of therapeutic action. This integration of chemical and ethnomedical data enables researchers to explore the pharmacological basis of TCM systematically [16, 17, 18]. Similarly, India's IMPPAT 2.0 is a major expansion of its predecessor and is based on over 100 books and numerous research articles. It catalogs 17,967 phytochemicals from 4,010 Indian medicinal plants, linked to 1,095 therapeutic uses. A distinguishing feature is its mapping of phytochemicals to specific plant parts and their uses, allowing more granular analysis. Despite differences in size and feature sets, each of these databases aims to bridge traditional knowledge with modern drug discovery tools, offering valuable resources for the identification of novel drug candidates through in-silico methodologies [19-23].

Practical applications and techniques of NPDBs in drug discovery: All these NPDBs play a pivotal role in modern drug discovery by providing comprehensive, searchable datasets that integrate chemical, biological, and ethnopharmacological information. These platforms are equipped with advanced molecule search functionalities that greatly enhance their accessibility and usability for researchers [1, 5, 14]. A key feature is the ability to search for compounds by name using IUPAC names, common names, or synonyms, allowing efficient retrieval of relevant molecules. In addition, these databases support searches using SMILES, InChI, and InChIKey identifiers. The use of SMILES, InChI, and InChIKey in databases offers significant advantages by providing standardized and searchable identifiers that facilitate data management, integration, and exchange within the chemical community. Moreover, each compound in an NP database typically has a unique compound identifier (CID), enabling direct access to individual entries [1, 10, 11]. This varied search options name-based, structure-based, structure similarity, and physicochemical properties, are designed to accommodate different research needs, ranging from broad exploration to precise targeting. As a result, these platforms enable researchers to explore the therapeutic potential of natural products efficiently [5, 14, 21]. By bridging traditional knowledge with cutting-edge computational tools, these databases not only accelerate drug development but also promote biodiversity conservation and sustainable exploration of natural resources [1, 24, 25], **Figure 1**.

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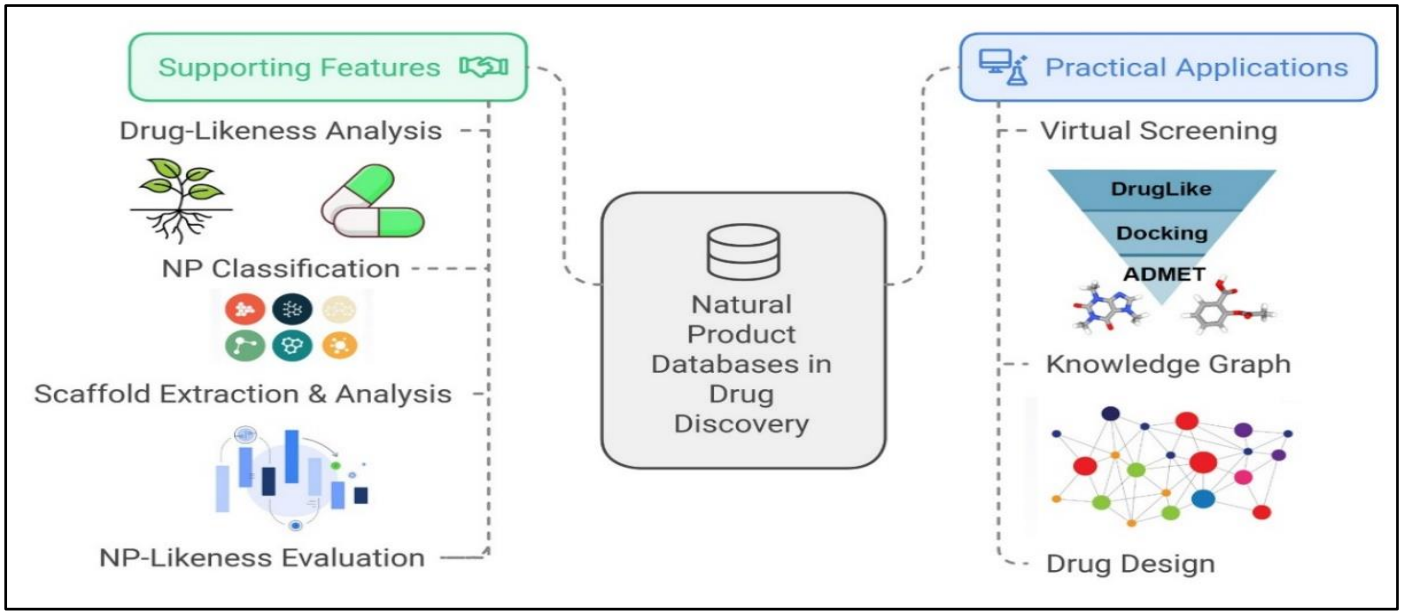

Figure 1: The role of natural product databases in drug discovery, highlighting supporting features like drug-likeness analysis, and practical applications such as virtual screening

NPDBs provide essential tools for drug discovery. These databases provide essential chemical diversity for virtual screening, molecular docking, and pharmacophore modeling to identify potential drug leads. Furthermore, NPDBs' structural data is essential for structure-based drug design (SBDD), enabling the optimization of candidates against biological targets for improved efficacy and safety. NPDBs also underpin bioactivity prediction models, which use chemical structures alone to forecast biological activity, streamlining early-stage exploration. These techniques, often enhanced by artificial intelligence and visualized through knowledge graphs integrating biological annotations, significantly accelerate the identification and repurposing of bioactive compounds [26]. The tangible success of this approach is validated by numerous NP derived drugs, including the anticancer agent Paclitaxel from the Pacific yew [27], the antimalarial Artemisinin from sweet wormwood [28], the antiviral Oseltamivir synthesized from a precursor in star anise, and the hepatitis C cure Sofosbuvir inspired by natural nucleotides [29]. These examples underscore how NPDBs bridge traditional knowledge and advanced computation to deliver vital therapeutics. Despite their transformative potential, NPDBs face challenges such as ensuring data quality, maintaining accessibility, and sustaining regular updates [10, 11].

Libya's biodiversity: A treasure trove for drug discovery: Libya's rich biodiversity and deep-rooted traditions in herbal medicine offer significant, yet largely untapped, potential for modern scientific exploration and drug discovery [2]. The current absence of a dedicated LibNPDB severely restricts the systematic utilization of these resources, as traditional knowledge often remains scattered in non-digitized formats, limiting its accessibility for contemporary research [30]. Existing regional databases contain minimal entries from Libya, highlighting a critical information gap. For instance, as shown in **Figure 2**, the African Natural Products Database (ANPDB) lists only 89 compounds from Libyan sources, compared to 3,668 from Egypt out of 6,515 total entries [4]. This disparity highlights the urgent need for a Libyan NPDB to document and organize the country's unique natural resources. The LibNPDB aims to address this gap by digitizing and standardizing information, making it accessible for modern research and drug discovery [8, 9, 15, 31]. Developing a specific LibNPDB would address this by digitizing and centralizing chemical structures, biological activities, and ethnopharmacological data, making it readily available for global research efforts, including computational drug discovery techniques [10, 11]. This initiative is vital not only for bridging traditional Libyan medicinal knowledge with modern pharmaceutical science but also for fostering national and international collaboration.

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By overcoming data collection and accessibility challenges, establishing a LibNPDB would help preserve Libya's unique botanical heritage amidst threats like climate change and overexploitation, empower local researchers, and position Libya as a valuable contributor to global scientific innovation and drug development [1, 5, 14]. Libya's unique challenges include limited digital infrastructure and fragmented data sources. Strategies for overcoming these challenges include adopting open-access policies, leveraging artificial intelligence for data curation, and fostering international collaborations to enhance database utility [7, 24, 31].

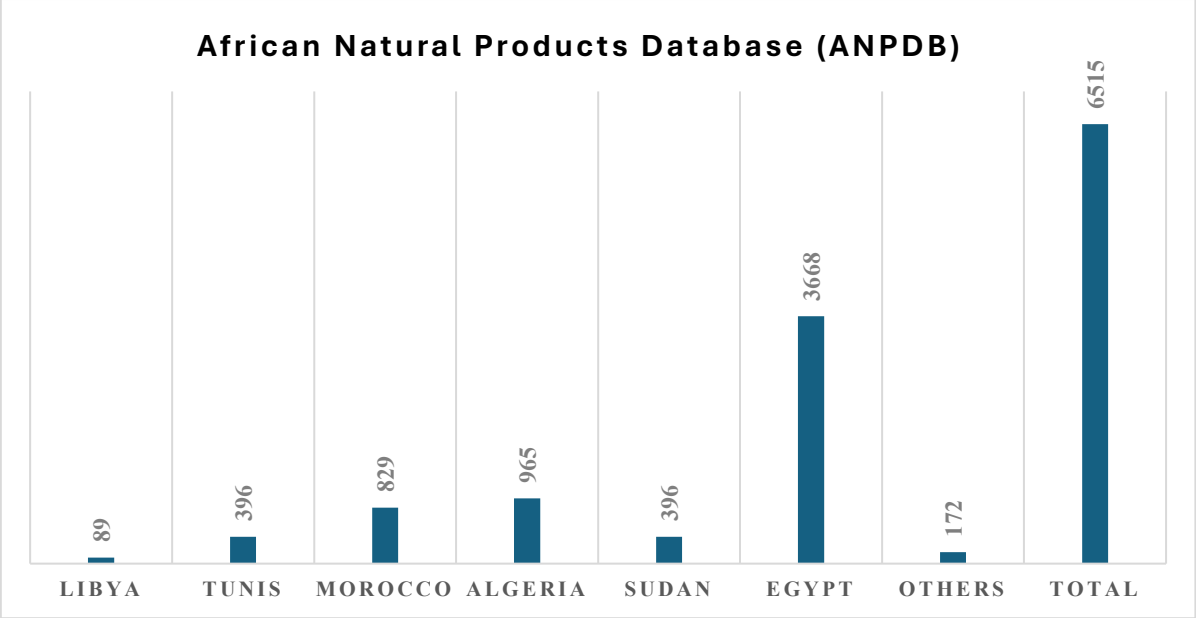

Figure 2: Comparison of the number of natural product compounds from Libya, Egypt, and other countries as listed in the ANPDB. Libya is underrepresented with 89 compounds, compared to 3,668 from Egypt out of 6,515 total entries

Future directions and innovations in NPDBs: Future developments in NPDBs focus on integrating advanced computational methods, expanding the coverage of natural products, and improving user interfaces to enhance both accessibility and analytical capabilities [26]. Innovations such as artificial intelligence, machine learning (ML), and cross-database connectivity are set to transform NPDB functionality, fostering global collaboration and improving research outcomes [32]. Deep learning models trained on natural product data can more accurately predict molecular properties, structure-activity relationships, and therapeutic targets, thereby accelerating the drug discovery pipeline [32, 33]. In addition, collaboration and cross-database connectivity enable the seamless integration of data across multiple platforms, providing researchers with comprehensive resources to explore chemical diversity and bioactivity [11]. These interconnected networks promote interdisciplinary research, improve the reproducibility of scientific findings, and increase the visibility of databases, such as LibNPDB [1]. To meet modern research needs, NPDBs must incorporate user-friendly interfaces, advanced search functions, and interactive analytical tools to support efficient data mining and analysis. By automating data extraction and bioactivity prediction, these tools can streamline drug discovery workflows. Furthermore, establishing a robust framework for international collaboration can position the LibNPDB as a pivotal resource, contributing meaningfully to regional and global health initiatives [5, 34].

Ongoing and future perspective: The development of the LibNPDB is structured into three stages. This study forms a part of the first stage, which involves data structure, data mining, cataloguing, and digitizing Libya's medicinal biodiversity. By the submission date, over 350 entries have been successfully catalogued. The second stage will focus on creating a freely accessible online platform to facilitate research and drug discovery through in silico screening while continuing to expand the database with new compounds. The third stage aims to integrate advanced functionalities, including enhanced search capabilities and online drug discovery

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tools, further solidifying LibNPDB as a valuable resource for scientific and medical research. These efforts collectively aim to position LibNPDB as a cornerstone for pharmaceutical innovation locally and globally. To ensure the effectiveness and longevity of the LibNPDB, it is recommended that the database incorporate rigorous data validation protocols and undergo regular updates through active collaboration with both local and international partners. Furthermore, promoting open access will help democratize its benefits and increase its visibility within the scientific community. The integration of predictive tools for physicochemical properties calculations, Pharmacokinetic profiling, and biological target identification, along with the adoption of advanced computational methods such as artificial intelligence and machine learning, will further enhance its analytical capabilities and streamline the drug discovery process. These strategies will position the LibNPDB as a valuable and sustainable resource for researchers worldwide.

Conclusion: Natural product databases are essential to modern drug discovery, serving as bridges between traditional knowledge and computational approaches to identify novel therapeutic agents. This study highlights the importance of establishing the first LibNPDB to harness Libya's unique biodiversity and support local and international research initiatives. Despite existing challenges such as data standardization, limited resources, and concerns regarding long-term sustainability, the creation of LibNPDB is expected to enhance local scientific capacity and contribute meaningfully to the global drug discovery landscape.

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Author contribution: AENS conceived and designed the study and data analysis. All authors contributed to data collection. AENS performed the analysis and interpreted data, drafted and revised the manuscript. All authors approved the final version of the manuscript and agreed to be accountable for its contents.
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Author declarations: The authors confirm that they have followed all relevant ethical guidelines and obtained any necessary IRB and/or ethics committee approvals.