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Original Article

Bridging Tradition and Innovation: The Hail Desert Plant Database for Drug Discovery

Mohd Saeed[1,#,*], Sabiha Naaz[2,#], Munazzah Tasleem[3], Nawaf Alshammari[1], Arminder Kaur[2], Mohammad Jahoor Alam[1], Amir Saeed[4]

[1]Department of Biology, College of Science, University of Hail, Hail, SAUDI ARABIA.
[2]Department of Biotechnology, Sanskriti University, Mathura, Uttar Pradesh, INDIA.
[3]Department of Biochemistry, Jamia Hamdard, Delhi, INDIA.
[4]Department of Clinical Laboratory Sciences, College of Applied Medical Sciences, University of Hail, Hail, SAUDI ARABIA.
[#]These Authors Contributed Equally to this Work.

ABSTRACT

Introduction: The Hail Desert Plant Database serves as an extensive repository that has been created to consolidate and systematize information concerning medicinal plants that are native to the arid Hail region in Saudi Arabia. **Materials and Methods:** By conducting thorough literature mining from credible sources such as scientific articles and online databases, we systematically collected and organized data on more than 200 desert plant species. This comprehensive dataset includes botanical characteristics, phytochemical compositions, traditional applications, habitat preferences, documented medicinal uses, and the active compounds associated with these plants. In addition, we utilized molecular docking methodologies to perform computational investigations that aimed to elucidate the molecular interactions occurring between phytochemical compounds and target proteins that are known to be associated with the specific diseases traditionally treated by these plants. **Results:** The database, which has been meticulously crafted to feature a user-friendly interface, offers an indispensable resource for researchers and clinicians who are captivated by the therapeutic possibilities presented by these arid florae. The inclusion of three-dimensional structures of docked complexes in the database significantly enhances its research capabilities, enabling comprehensive investigations and assisting in the development of potential drug candidates derived from natural sources. **Conclusion:** The Hail Desert Plant Database serves as a crucial tool, facilitating progress in the field of drug discovery, investigations into structural biology, and the examination of alternative therapeutic agents derived from the diverse array of desert plants. The Hail Desert Plant Database is freely accessible at http://haildesertplants.com/.

Keywords: Desert plant database, Disease, Phytochemicals, Docked complex, Target protein.

Correspondence:
Dr. Mohd Saeed, Ph.D.
Associate Professor, Department of Biology, College of Science, University of Hail, Hail, SAUDI ARABIA.
Email: mo.saeed@uoh.edu.sa

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INTRODUCTION

The vast array of medicinal plants found in nature holds great cultural significance and plays a crucial role in the treatment of various ailments and the preservation of human well-being. In addition, these plants exhibit a high degree of productivity in terms of secondary metabolite production. These metabolites are synthesized as a response to environmental stress, thereby endowing the plants with a robust defense mechanism against diseases, organisms, and adverse conditions.[1,2] With a documented range of medicinal applications spanning 10,000 to 15,000 plant species on a global scale, it is noteworthy that only around 150-200 of these species have been incorporated into Western medicine.[3] This observation highlights the vast reservoir of therapeutic possibilities that the plant kingdom offers. It is noteworthy to observe that the global population continues to heavily rely on plants as primary sources of healthcare, as indicated by the World Health Organization's estimation, which suggests that approximately 80% of the world's population depends on them.[4] The long-standing association with plants serves as a driving force for ethnopharmacological investigations that examine their effectiveness, safety, and potential for discovering new drugs.[5]

Throughout history, medicinal plants have played a crucial role in traditional healing systems and persistently function as viable substitutes for synthetic pharmaceuticals.[6] Around 75% of the global population, particularly in developing nations, rely on plants for traditional medicine to fulfill their fundamental healthcare requirements.[7] Approximately 80,000 plant species have been acknowledged for their medicinal properties among

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the extensive range of plant species present on Earth.[8] These botanical specimens provide an intriguing foundation for the extraction of a wide array of biologically active plant compounds, encompassing alkaloids, terpenoids, polyphenolics, and other constituents.[9] The multifaceted roles of these bioactive compounds are indicative of their therapeutic potential, encompassing functions as antioxidants, antimicrobials, anti-inflammatories, anti-carcinogenic, and anti-diabetic agents.[10]

The pursuit of bioactive compounds derived from plants has remained a crucial undertaking in the field of drug discovery, as natural substances continue to serve as a source of inspiration and offer unique chemical entities for potential drug candidates.[11] Despite the inherent challenges in terms of time and financial resources associated with the process of drug discovery, it is noteworthy that a significant majority, specifically over 80%, of drug substances are sourced from or influenced by natural compounds.[12] The process of drug discovery is characterized by a protracted duration, necessitating substantial allocations of time and resources, frequently culminating in the identification of a small proportion of compounds suitable for clinical investigations.[13] Conventional animal trials, although necessary, exhibit suboptimal characteristics in terms of efficiency and toxicity assessment. The evident necessity for novel perspectives that facilitate the process of drug discovery, in accordance with the pharmaceutical principle of "fail fast, fail early," has been identified.[14] In the present context, the collaborative utilization of computational and experimental methodologies can significantly contribute to expediting the process of drug discovery and development.[15]

Contemporary scientific investigations conducted at the convergence of biology and natural compounds exemplify the persistent endeavor to unravel the latent capabilities harbored within substances derived from plants.[16] The utilization of advanced methodologies, sophisticated equipment, and automated processes has resulted in the comprehensive documentation of these organic substances, thereby enabling their examination and utilization.[17] Concurrently, the discipline of biology has witnessed significant growth, leading to enhanced comprehension of the diverse functions performed by these compounds. The interaction between nature and science plays a pivotal role in current investigations pertaining to naturally derived compounds.[18]

The Hail Desert Plant Database serves as an innovative and valuable tool that provides insights into the diverse array of plant species inhabiting the Hail region of Saudi Arabia. These plants are renowned for their noteworthy contributions to medicine and nutrition. The database in question offers users an extensive range of information, encompassing plant synonyms, genus classifications, habitats, phytochemical types, total phytochemical counts, PubChem IDs, diseases associated with these plants, the target proteins implicated in these diseases, and interaction of the target proteins and phytochemicals. The platform serves as a highly valuable tool, operating as a proficient search engine for researchers and clinicians who are committed to utilizing the potential of these plants to advance the development of more efficacious drugs and therapies. The database is situated at the intersection of conventional knowledge, contemporary science, and the boundless prospects of exploration and advancement.

MATERIALS AND METHODS

Literature Mining

The process of literature mining involves extracting and analyzing information from a wide range of published texts, such as scientific articles, and books, and online databases such as The International Plant Names Index (IPNI) (https://www.ipni.org/),[19] The Global Biodiversity Information Facility (GBIF) (https://www.gbif.org/),[20] PLANTS Database (USDA) (https://plants.usda.gov/home),[21] Jepson Herbarium-the University of California, Berkeley (https://ucjeps.berkeley.edu/),[22] IMPPAT: Indian Medicinal Plants, Phytochemistry And Therapeutics (https://cb.imsc.res.in/imppat/home),[23] PubChem (https://pubchem.ncbi.nlm.nih.gov/),[24] and RCSB Protein Data Bank (RCSB PDB) (https://www.rcsb.org/).[25] To compile a comprehensive database of desert plants in the Hail region of Saudi Arabia, an extensive literature-mining endeavor was undertaken. The main aim of our study was to gather valuable data concerning the medicinal and nutritional properties of these botanical specimens. To accomplish this objective, we systematically collected and examined a comprehensive selection of more than 100 published sources from various international and local academic journals, encompassing the period up to the year 2023. The sources contained a vast amount of information, rendering them an indispensable asset for our database.

The data on different aspects of these desert plants was extracted with great attention to detail. The provided information encompassed various aspects, such as the scientific names and synonyms of the plants, their phytochemical compositions, the specific plant parts traditionally used, details about their habitats, the sources of information, documented ailments associated with them, and the active compounds that have been identified within these plants. Furthermore, the plant's ability to cure diseases and its corresponding target protein structure were also obtained. The implementation of a comprehensive methodology for literature mining enabled the collection of a wide range of information, which formed the basis of our database.

Computational Analysis of Phytochemical-Target Protein Interactions

To enhance the utility of the Hail Desert Plant Database, we conducted molecular docking and interaction studies of phytochemical compounds extracted from the plants with their associated target proteins linked to specific diseases for which the plants are traditionally used in remedies. This advanced approach

aimed to shed light on the potential mechanisms by which these compounds exert their therapeutic effects and, in turn, support drug discovery efforts.

Phytochemical Selection

Phytochemicals were intensely selected from the database in preparation for docking investigations. The phytochemicals that were chosen exhibited a wide variety of secondary metabolites, including terpenoids and alkaloids, which have been documented or postulated to possess bioactive properties.

Target Proteins

The target proteins selected for the docking experiments were associated with the specific diseases traditionally treated with these desert plants. Three-dimensional protein structures were obtained from the RCSB Protein Data Bank.[25]

Molecular Docking

The docking simulations were conducted utilizing AutoDock Vina,[26] a molecular docking software that is widely acknowledged. The utilization of AutoDock Vina enabled us to forecast the modes of interaction and binding affinities that would occur between the phytochemical compounds and their corresponding target proteins. Electrostatic interactions, van der Waals forces, and other pertinent parameters were incorporated into the calculations to produce precise binding energy scores.

Database Preparation

The cornerstone of our endeavor lies in the development of a resilient and versatile database, ensuring seamless access and interaction for our users. To achieve this objective, we utilized an array of cutting-edge programming languages and web development tools.

Database Design and Programming Languages

The backbone of Web Application Development

The ASP.NET framework was utilized as the principal programming language in constructing the web application's backbone. This framework serves as the foundation for our web application, providing us with the ability to develop secure, responsive, and dynamic web applications.[27] This enhances the platform's resilience and scalability.

Enhancing User Interaction

JavaScript is utilized to incorporate interactive elements into the user interface. It effectively enhanced the overall user experience by promoting active engagement and facilitating smooth navigation across the database. Under the specific requirements of the project, we customized our web development approach by selecting Web Forms to create an interface that is both intuitive and user-friendly, thereby improving the accessibility and usability of the database. By capitalizing on the functionalities of JavaScript, we have enhanced the user interface with interactive elements, thereby augmenting the overall user experience, encouraging active participation, and facilitating smooth navigation.[28]

Structuring Web Content

The web content is structured using HTML5 within the application framework. It also ensured that information was presented in a manner that was straightforward to navigate, laying the groundwork for an efficient data presentation. HTML5, which is the current norm for structuring web content, serves as the foundational framework of our web application.[29]

Backbone for Back-end Development

C# serves as the fundamental building block for the back-end development methodology. Additionally, it implemented fundamental logic and functionality for the database, thereby enhancing security protocols, streamlining processes, and effectively overseeing data.[30] It guarantees that information is displayed in a clear and easily navigable fashion.

Styling and Layout

The implementation of CSS for styling and layout has been crucial in the development of visually captivating web pages, thereby augmenting the user experience through the provision of an aesthetically pleasing interface.[31]

Database Management Systems Utilized

Robust Relational Database Management

To bolster the dependability and effectiveness of our database, we opted for Microsoft SQL Server 2019, a reputable and robust relational database management system that ensures the integrity of data, facilitates retrieval, and streamlines database administration.[32]

Web Development Tools Employed

Hosting and Access Control

The web server, which is hosted on Internet Information Services (IIS), provides users with access to information in a secure and responsive environment.[33]

By combining literature mining with web development technologies, we have been able to construct the Hail Desert Plant Database, which is both resilient and intuitive for users. By integrating carefully selected data from a wide range of scholarly sources and web development tools, we demonstrate our dedication to furnishing researchers and clinicians who are intrigued by the potential medicinal and nutritional uses of these arid plants with indispensable resources.

RESULTS

The Hail Desert Plant Database signifies a substantial achievement in the field of medicinal plant research by utilizing sophisticated computational techniques to shed light on the potential therapeutic effects of phytochemicals against a wide range of pathogens, including enzymes, bacteria, viruses, and fungi. This resource, which is available to the public, is organized in a relational model consisting of seven tables. Each table provides significant insights into different aspects of medicinal plant data. The literature table functions as an all-encompassing repository of data, comprising botanical and scientific nomenclature, synonyms, genera, habitats, as well as an exhaustive compilation of scholarly articles and review articles pertaining to medicinal plants and their phytochemical components. The Habitat Table provides a comprehensive overview of the various habitats in which desert plants flourish, thereby offering a contextual comprehension of the environmental niches that are favorable for the development of these medicinal species. Table of Plant Parts Utilized, this table provides a practical aspect to the database by enumerating the diverse plant parts that are utilized for therapeutic purposes, thus delving into the practical applications of medicinal plants. The Phytochemicals Table is an essential element of the database as it contains an extensive collection of information, such as the names of phytochemicals, the classes they belong to (e.g., flavonoids, alkaloids), their PubChem CIDs, links to PubChem-CIDs, and molecular structures in ".sdf" format. Furthermore, it furnishes comprehensive details regarding the target proteins, including their PDB IDs, thereby facilitating a more profound comprehension of the molecular interactions. Table of Docked Complexes, this table presents the docked complexes, which illustrate the complex molecular relationships between phytochemicals and disease-associated proteins. Downloadable ".pdb" files are also available. Every entry is distinctively identified by its scientific name (plant), target disease (e.g., HCV, Dengue virus), and literature reference (PubMed-ID), thereby providing a comprehensive viewpoint on the effectiveness of the treatment. The genus table is a structured repository of distinct genus names. It serves as a vital reference point for phytochemicals and related information, improving the retrieval of data by ensuring its clarity and precision. An intuitive and user-friendly web interface is featured on the Hail Desert Plant Database. This feature enables users to effortlessly retrieve information regarding medicinal plants by utilizing simple queries, thus promoting accessibility and usability. The database is intentionally structured to be updated frequently, promising that the most recent research discoveries and supplementary information are seamlessly incorporated throughout its existence. This feature enhances the database's practicality and pertinence within the domain of medicinal plant research.

Database Interface: Enhancing Accessibility

The interface of the Hail Desert Plant Database was carefully designed to provide users with a smooth and intuitive experience while navigating through the vast repository. The design of the layout was optimized to enable efficient retrieval of essential information with minimal cognitive load. The interface exemplifies a design that prioritizes the needs and preferences of the user, incorporating fundamental navigational components such as Home, Plant Search, Advanced Search, Download, Guide, and Contact options. Every element fulfills a unique function, with the goal of accommodating a wide range of user needs and preferences. An interface titled "Find Your Plant" serves as an entry point, allowing users to conduct searches by entering plant names. This function is designed for convenience, presenting an alphabetical arrangement of plant names within the database. It offers a comprehensive list of available plants, ensuring easy access to specific plant profiles. The Advanced Search interface elevates the search experience by enabling users to explore the database using keywords. This sophisticated functionality extends beyond plant names, encompassing synonyms, habitats, parts used, types of phytochemicals, specific phytochemicals, diseases, and target proteins. This comprehensive search capability fosters detailed exploration, catering to the diverse needs of researchers and practitioners. Upon entering a plant name in the search box, users are presented with a detailed results page. This page offers an array of essential information including the plant name, synonym, habitat, parts used, types of phytochemicals present, specific phytochemicals, associated diseases, and target proteins. Clicking on a plant name opens a dedicated page with an exhaustive profile encompassing all the aforementioned details, ensuring a comprehensive understanding of each plant's attributes and medicinal potential.

Target-Centric Exploration

To facilitate research targeting specific diseases or proteins, the database allows users to input a target name from the available list. This action retrieves a curated set of plants associated with the specified target, listing plant names, synonyms, habitats, parts used, types of phytochemicals, specific phytochemicals, diseases, and target proteins. This feature expedites the exploration of potential therapeutic agents tailored to specific disease targets.

Data Retrieval

The database empowers users to download essential files in various formats. This includes the retrieval of docked complex files in pdb format, target proteins in pdb format, and PubChem IDs in sdf form. This flexibility in data retrieval enhances the usability of the database, allowing researchers to access and analyze data in formats compatible with their research methodologies. Expanding on these features not only provides a clearer picture of the database interface but also highlights its user-centric design and the multifaceted tools it offers to researchers and users

navigating the realm of medicinal plants and their therapeutic potential.

Hail Desert Plant Database Statistics

The statistical data provides a comprehensive representation of the extensive range of plant species and phytochemical compounds documented in the Hail Desert Plant Database. Furthermore, it is important to highlight the extensive investigation into molecular interactions, which demonstrates the wide range of protein targets and docked complexes that can be further explored for potential therapeutic applications. The Hail Desert Plant Database currently comprises a rich repository of medicinal plants, encompassing a total of 200 distinct desert plant species. Among these, the database showcases a diverse representation of 143 genera, signifying the breadth of botanical diversity encapsulated within. At present, the database houses an extensive collection of 1420 unique phytochemical compounds sourced from these desert plants. The database accounts for 49 distinct target proteins, signifying the breadth of therapeutic targets investigated. Additionally, it contains an impressive catalogue of 1300 docked complexes, showcasing the detailed molecular interactions between phytochemicals and disease-associated proteins.

Hail Desert Plant Database and Other Databases

In recent years, there has been a proliferation of databases pertaining to drug discovery and research on medicinal plants. Prominent databases such as PubChem,[24] Zinc,[34] ChEBI,[35] ChEMBL,[36] ChemBridge,[37] ChemSpider,[38] and DrugBank,[39] have emerged as extensive repositories housing millions of compounds with potential for drug development. Nevertheless, it should be noted that none of these databases has been specifically designed or customized for the purpose of medicinal plants. Several databases have been created specifically for medicinal plants, such as MAPS, Indian Medicinal Plants Database, Database on Medicinal Plants,[23] HerbMed,[40] MPDB 1.0,[41] GLOBinMED,[42] and MEDDB,[43] among others. Nevertheless, it is important to acknowledge that these databases possess certain limitations in terms of their functionalities. Certain databases provide limited options for interactive exploration, as they solely offer downloadable features. While there are various platforms that offer virtual screening, many of them lack the necessary specificity when it comes to screening medicinal plant extracts. There is a limited availability of databases that provide docked complexes, and certain databases lack comprehensive class and target information pertaining to phytochemicals. The Hail Desert Plant Database distinguishes itself from other databases by offering a wide range of specialized features that are specifically designed to cater to the needs of medicinal plants. The database provides comprehensive information pertaining to the classification, genus, phytochemical composition, targets, and extensive references from scholarly literature regarding medicinal plants. The topic of discussion pertains to the phytochemical's library and its application in the formation of docked complexes. This platform provides a distinctive collection of downloadable phytochemicals, as well as docked complexes, which can be utilized to explore the therapeutic capabilities against targets that have not been previously reported. This feature enhances and accelerates the process of investigating the effectiveness of medicinal plants against various targets. The Hail Desert Plant Database stands out due to its comprehensive collection of information specifically curated for medicinal plants. This database provides a distinct platform that encompasses a wide range of functionalities, including phytochemical libraries and docked complexes. This approach enables the effective and focused investigation in the field of medicinal plant research, encompassing both preliminary screening and comprehensive interaction analysis.

Experimental Procedure

Literature Mining and Database Development

The creation of the Hail Desert Plant Database required thorough examination of relevant academic literature and careful extraction of data from a wide range of scholarly resources. A comprehensive analysis was conducted on a collection of over 100 published texts, encompassing scientific articles, books, and esteemed online repositories such as The International Plant Names Index (IPNI), The Global Biodiversity Information Facility (GBIF), PLANTS Database (USDA), Jepson Herbarium - University of California, Berkeley, IMPPAT: Indian Medicinal Plants, Phytochemistry and Therapeutics, PubChem, and RCSB Protein Data Bank. The purpose of this scrutiny was to acquire significant knowledge regarding the medicinal and nutritional attributes of desert plants in the Hail region of Saudi Arabia.

Extracted Data Insights

The extracted data encompassed a wide range of information, comprising scientific names, synonyms, phytochemical compositions, traditional usage of plant parts, habitats, documented ailments, active compounds, properties related to the treatment of diseases, and associated target protein structures. The extensive methodology employed in literature mining has laid the essential foundation for our database, yielding a vast amount of invaluable information.

Computational Analysis of Phytochemical-Target Protein Interactions

In order to enhance the functionality of the database, molecular docking investigations were undertaken to elucidate the interactions between phytochemical compounds derived from desert plants and their respective target proteins associated with specific diseases traditionally addressed through the use of *in silico* approaches.

Phytochemical Selection

The selection of phytochemicals was conducted with regard to their occurrence in specific plant species and their significance in addressing common ailments traditionally treated by these plants. The compounds that were chosen exhibited a wide range of secondary metabolites, such as terpenoids and alkaloids, which are recognized or postulated to have bioactive characteristics.

Target Proteins and Molecular Docking

Target proteins, which are pertinent to the diseases targeted by these desert plants, were thoroughly selected. The three-dimensional protein structures of these target proteins were obtained from the RCSB Protein Data Bank. The utilization of AutoDock Vina in molecular docking enabled an estimation of interaction patterns and binding strengths between phytochemical compounds and their corresponding target proteins. The computation of binding energy scores was conducted with a high level of precision, considering both electrostatic interactions and van der Waals forces.

Database Development and Interface

The development of the Hail Desert Plant Database incorporated advanced programming languages and web development tools. A platform was developed using the ASP.NET framework, JavaScript, C#, HTML5, CSS, and Microsoft SQL Server 2019. This platform was designed to be resilient, secure, and user-friendly, enabling smooth access and interaction. The amalgamation of literature mining and advanced web development technologies has led to the creation of a user-friendly and all-encompassing tool for researchers and clinicians who are interested in exploring the medicinal and nutritional attributes of plants that thrive in arid regions (Figures S1-S4).

DISCUSSION

The Hail Desert Plant Database is a significant advancement in computational techniques for studying medicinal plants. It provides a comprehensive framework for exploring the therapeutic capabilities of phytochemicals. The database has profound consequences for pharmaceutical research and botanical exploration. The Plant Table is an intellectual hub that contains plant-related data and its reference research articles. It allows for comprehensive knowledge synthesis by integrating a wide range of botanical knowledge. This enables research to go beyond isolated studies and gain interconnected insights. The Genus Table establishes connections between phytochemicals and their botanical sources. It allows for accurate data retrieval and comparative analyses of medicinal plants and their components. The Habitat Table provide ecological context for the desert plants. It allows researchers to examine the relationship between medicinal plant attributes and the environment. This contextualization opens up opportunities for investigating how ecological factors impact bioactive compound synthesis. The Plant Part Used Table explores the practical applications of medicinal plants. It provides insights into established therapeutic customs and guides current pharmacological investigations. It bridges the gap between traditional wisdom and modern pharmaceutical advancements. The Phytochemicals and Docked Complexes Tables reveal the molecular interactions between phytochemicals and disease-associated proteins. This enhances our understanding of therapeutic mechanisms and informs the development of pharmaceuticals. The web interface of the database promotes data democratisation by making it user-friendly. It allows universal access to complex botanical and pharmacological data, fostering collaborations and empowering a wide range of users in the field of medicinal plant sciences.

The Hail Desert Plant Database advances the investigation of medicinal plants. By integrating computational capabilities with botanical expertise, this system facilitates the identification of potential pharmaceutical compounds in plants. The navigability of the database is user-friendly. The portal is equipped with distinct sections, namely Plant Search and Advanced Search, which facilitate efficient information retrieval for researchers. One illustrative instance is the "Find Your Plant" feature, which facilitates the retrieval of plants by their respective names in an organized manner, specifically in alphabetical order. The Advanced Search function facilitates the retrieval of information by allowing users to conduct searches based on specific botanical terms, such as habitats or utilized plant parts. Every individual plant within the database is accompanied by a comprehensive page containing a wide range of detailed information. The comprehensive content encompasses the nomenclature of the botanical specimen as well as its potential applications in the field of medicine. Additionally, it is possible to acquire files containing additional details regarding the interaction between plant chemicals and disease proteins through downloading. The database also provides information regarding the geographical distribution of these plants and the specific plant parts that are utilized for medicinal purposes. This information provides insights into the manner in which natural factors impact the synthesis of valuable phytochemicals in plants. The process can be compared to acquiring knowledge from the vast array of natural remedies found in the environment. Within the database, there exist distinct sections that elucidate the intricate mechanisms by which the chemical constituents present in plants engage in interactions with proteins implicated in the pathogenesis of various diseases. This aids scientists in elucidating the mechanisms by which plant-based medicines may exert their therapeutic effects against pathogenic microorganisms such as viruses or bacteria. The database undergoes continuous updates, rather than being one-time events. This facilitates the dissemination of scientific discoveries among researchers worldwide, thereby enhancing the collective knowledge base. In subsequent periods, there is potential for the incorporation

of an increased number of botanical specimens, scientific investigations, and diverse methodologies for their examination.

The evaluation of docking outcomes in the Hail Desert Plant Database provides valuable insights into the intricate dynamics of interaction between phytochemical compounds and their respective target proteins. This thorough investigation functions as a critical foundation in elucidating possible sites of binding and quantifying the intensity of these interactions, thus outlining hypothesized mechanisms of action. The incorporation of downloadable three-dimensional structures of the docked complexes into the database represents an important boost in value. These structures provide an illustration depiction, enabling scientists to utilize indispensable tools for further investigation into the molecular complexities of these interactions. By utilizing AutoDock for molecular docking and interaction studies, our database provides a platform to explore the therapeutic potential of phytochemical compounds derived from desert plants and enhances its research capabilities. The availability of PDB structures not only facilitates a comprehensive examination of these interactions but also acts as a catalyst in the pursuit of potential drug candidates derived from natural sources; this highlights the profound importance of the database in the fields of structural biology and drug discovery.

CONCLUSION

The Hail Desert Plant Database serves as a comprehensive repository that provides unrestricted access to a vast amount of information encompassing medicinal plants that are native to the arid environments of the Hail region in Saudi Arabia. Currently, this database is home to a comprehensive collection of more than 1400 phytochemicals derived from 200 plant species inhabiting desert regions, spanning across 143 different genera. It plays a crucial role as an indispensable source of information. The database enables comprehension of the therapeutic potential inherent in these plant species by providing information on botanical classifications, phytochemical compositions, traditional uses, and targets associated with various diseases. The existing version of the database offers extensive data and docking capabilities for investigating interactions between phytochemicals and proteins. However, future updates are being developed with the objective of improving its functionalities. Future iterations of the system are intended to include tools for drug profiling, thereby enhancing its usefulness in drug discovery efforts. Consistent updates and rigorous data management protocols are essential to maintain the currency and usability of the database, thereby creating an environment that facilitates advancements in drug design and discovery. The Hail Desert Plant Database is a valuable resource for researchers engaged in the study of medicinal plants and Computer-Aided Drug Design (CADD). It provides efficient and convenient access to essential information, thereby facilitating advancements in medicinal plant research and the development of innovative therapeutic agents. To gain unrestricted access to a vast collection of knowledge, the Hail Desert Plant Database can be conveniently accessed at http://haildesertplants.com/. It provides a comprehensive repository of invaluable information.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ABBREVIATIONS

WHO: World Health Organization; **IPNI:** International Plant Names Index; **GBIF:** Global Biodiversity Information Facility; **IMPPAT:** Indian Medicinal Plants, Phytochemistry and Therapeutics; **PDB:** Protein Data Bank; **HTML5:** Hypertext Markup Language 5; **ASP.NET:** Active Server Pages; **NET, CSS:** Cascading Style Sheets; **SQL:** Structured Query Language; **IIS:** Internet Information Services.

SUMMARY

The Hail Desert Plant Database is an extensive collection containing information on more than 200 native medicinal plants found in the arid Hail region of Saudi Arabia. This repository contains carefully selected information from reliable sources, including botanical characteristics, chemical compositions, traditional uses, and documented medicinal applications. Additionally, it includes molecular docking analyses that demonstrate the interactions between phytochemicals and proteins associated with diseases.

At present, it contains 1400 phytochemicals derived from 200 desert plant species belonging to 143 genera. This collection is highly valuable for researchers and clinicians who are interested in exploring the healing properties of these arid plants. The database's interface, which is easy for users to navigate, incorporates 3D structures of docked complexes. This integration improves the database's ability to conduct research and assists in the investigation of natural sources for potential drug candidates.

Although the current version already supports thorough investigations, future updates will focus on improving functionalities by adding tools for drug profiling. This will enhance drug discovery efforts. The continuous maintenance and updates of the database are crucial to ensure its current and

usable state, creating an environment that promotes progress in drug design and discovery.

The Hail Desert Plant Database is a crucial tool for researchers studying medicinal plants and practitioners using Computer-Aided Drug Design (CADD). It provides easy access to important information, which helps advance medicinal plant research and the development of innovative therapeutic agents.

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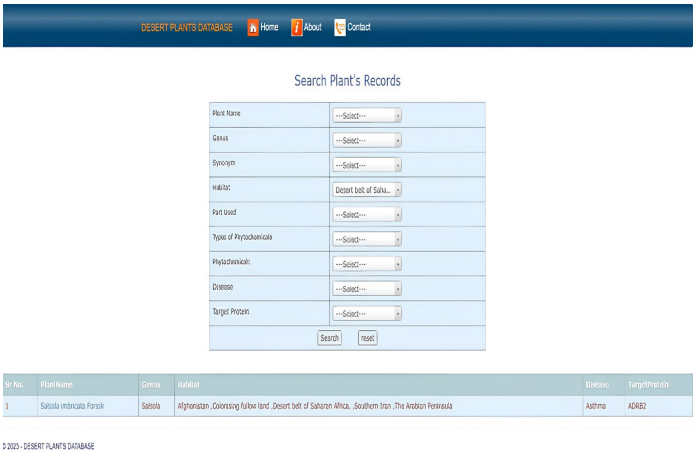

Figure S1: Screenshot displaying the user-friendly interface and advanced search features of the Hail Desert Plant Database, a comprehensive collection of native medicinal plants found in the arid Hail region of Saudi Arabia.

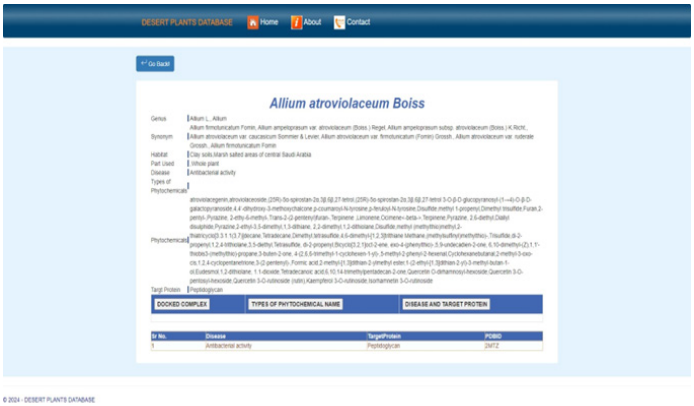

Figure S3: A snapshot from the Hail Desert Plant Database that provides an overview of plant data associated with specific diseases and target proteins. This image depicts the functionality of the interface, which grants users access to crucial information regarding the use of medicinal plants to treat particular diseases as well as downloadable PDB files of target proteins.

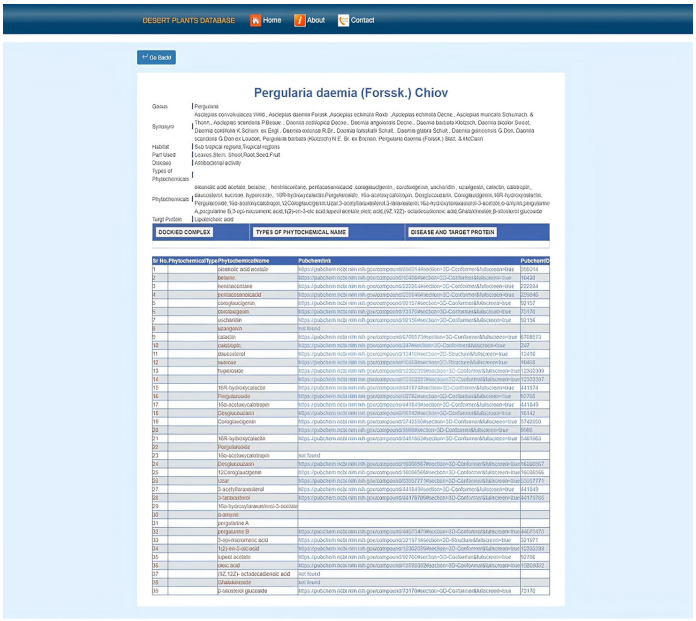

Figure S2: The provided snapshot showcases the user interface of the Hail Desert Plant Database, emphasizing its extensive collection of plant information and convenient access to detailed profiles through direct links.

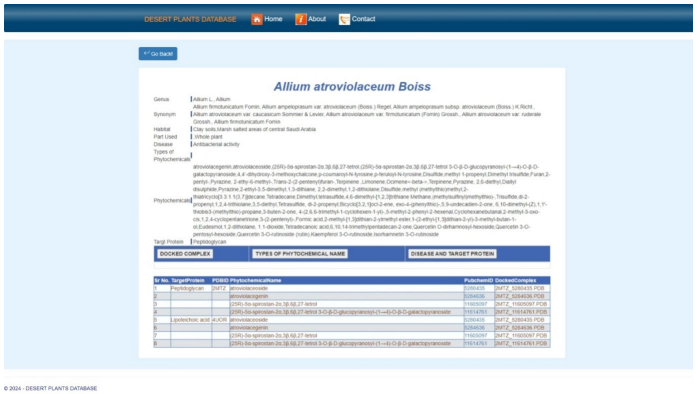

Figure S4: An excerpt from the Hail Desert Plant Database that presents plant data that is associated with docked complexes of phytochemical compounds, target proteins, and their corresponding PDB files. The availability of downloadable PDB files for target proteins facilitates structural analyses and research into drug development.