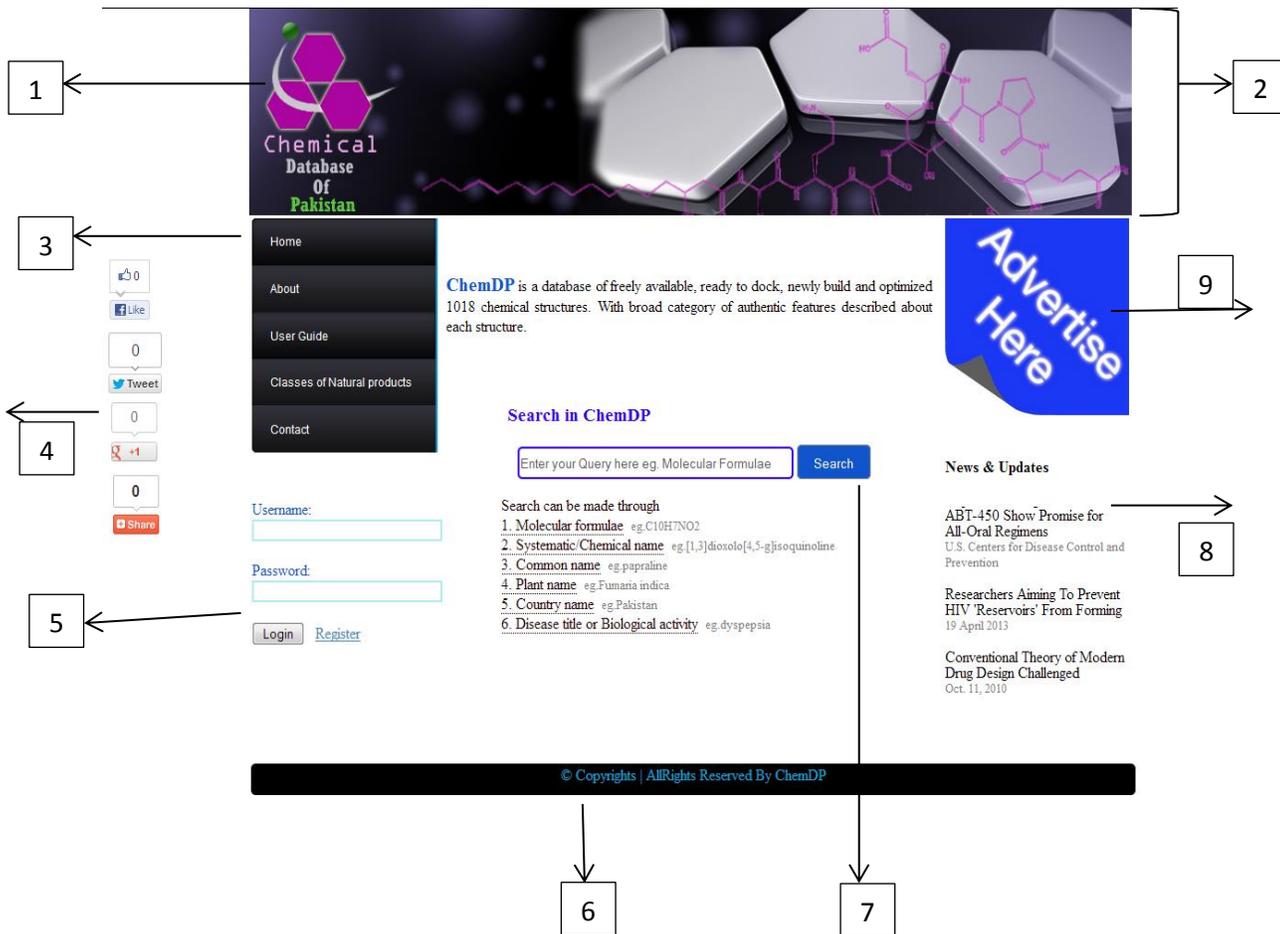


### **Structure of ChemDP:**

Chemical Database of Pakistan (ChemDP) comprises of over 1000 ready to dock chemical compounds from natural sources. Each compound contains over 100 datasets, which provide respective information about that particular compound. Interactive graphical user interface (GUI) provides user with ease of access to a broad category of information as well as optimized 2D and 3D structures for usage in computer-aided drug designing.

Figure shows a labeled image of the first page of the ChemDP, and further elaborates its contents.



1. Logo of ChemDP, explaining the nature of the database.
2. Header of ChemDP. Header contains the Chemical compound image and graphics relevant to the logic of database. At the left side of the header, the logo of ChemDP is placed. It is the registered logo copyrighted by ChemDP.
3. List of tabs shows that the following actions are available to perform by clicking them. The details of action of these tabs will be described in the next page.
4. These are the widgets to socialize the ChemDP through Facebook, Twitter and Google plus.
5. User login/register section. It allows users to register and login to access the functionality of database.
6. This sleek bar declares the authority of the contents of ChemDP.
7. This part of the database provides facility to access required chemical compounds and information regarding these chemical structures.
8. News and update session will keep the user updated about new happening in the world of chemical compounds.
9. This section is allocated for advertisement purposes. If a user/industry/company is interested to advertise something relevant to academia or industry etc, they are allowed to request ChemDP administration for a response with some conditions applied.

ChemDP is a database, developed by linking many activities on one place to facilitate users. There are different tabs that can be accessed from every page of the database. Each tab is described further with snapshot preview in next paragraphs.

### **Search in ChemDP:**

Search in ChemDP can be made with allowed queries, which could be a molecular formulae, systematic name, common name, plant name, country name, disease title or biological activity. Each search has been exemplified as well.

By clicking search or enter, a page will appear comprising of ChemDP-ID, Common Name and Molecular Formulae. Selecting Molecular Formulae or Common Name will lead to the page covering all information about query, ChemDP ID, 2D and 3D structures with interactive Jmol

plugin etc. The mol and mol2 files can also be downloaded from the same page. By expanding the boxes, they show extra information like properties and source of that compound. Assays tab includes the IC<sub>50</sub>, Ki and % inhibition of assays applied on that compound. Reference tab includes the reference to the source from where the whole data of that compound is taken.

### **About Tab in ChemDP:**

From the 'About' menu tab, one can get information about ChemDP, latest projects and team members of ChemDP.



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## ChemDP

Chemical Data Base of Pakistan is the chemical structure database. Chemical structures available in ChemDP are ready to use and ready to dock. ChemDP is preferentially designed to accommodate chemical structures of Pakistan, either the products are natural, synthetic, or derivatives of natural products. Compounds or substances produced by natural sources are called natural products. The source could be plants, fungi, small living organisms and animals. Plant kingdom is the most common source of natural products. Natural products are divided into many classes including alkaloids, terpenoids, polyphenols, nicotine, quinine, paclitaxel, morphine etc. All chemical structures available in ChemDP are prepared and built using ChemOffice and Chem3D. The structures are then optimized using latest PM7 semi empirical method with a convergence gradient ( $<0.1$ ). ChemDP has available structures with many facilities.

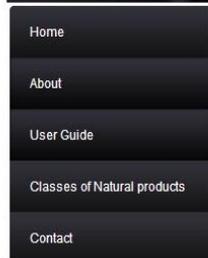
**2D structure:** mol file for a structure can be downloaded via a tab there.

**Images:** images for a structure can be "save as" to the required drive on your computer.

## Features

Features described for each structure includes the

- **Plant/Animal name:** This section includes the name of Plant or animal which is the source of that chemical compound.
- **Origin:** In this section name of places are described which is the origin of that chemical structure.
- **Class of Natural Products:** Chemical structure belongs to which class of natural products is described in this section.
- **Biological Activity:** This section includes the biological activities of that compound such as antioxidant, antitumor etc.



**Dr. M. Qaiser Fatmi** received his PhD degree in the field of computational chemistry and molecular modeling from the University of Innsbruck. Later on, he worked at the International Center for Chemical and Biological Sciences (ICCBS), University of Karachi as a Research Officer. He joined University of California, Riverside, USA to pursue his post doctoral research studies. He has been serving the Department of Biosciences, COMSATS Institute of Information Technology (CIIT). His research interests include molecular dynamics simulations of metal and protein complexes, structure and ligand based drug design, structural bioinformatics and computational chemistry. He came up with the idea to build a database of Natural products of Pakistan (ChemDP) which is novel in its category and supervised whole the research project.



**Dr. Habib Bukhari** is an Associate Professor and Chairperson of Biosciences department, COMSATS Institute of Information Technology Islamabad. He obtained his PhD degree in Microbiology from University of Glasgow UK. Dr. Bokhari has been awarded with post doc. positions at George Mason University USA and London School of Hygiene and Tropical Medicine London. He has won a number of research grants from local and international organizations. He is among the first few pioneer members to start the education program in Bioinformatics in Pakistan in 2003. His areas of interest include Genomics & Bioinformatics, Vaccines, Molecular epidemiology of infectious diseases and Nanotechnology based systems for control and identification of microbes. He supervised the whole research Project of ChemDP.



**Shahr Bano Mirza** is a MS student of Bioinformatics at COMSATS Institute of Information Technology. She had done her BS in Bioinformatics from Govt. Collage University Faisalabad. She carried out the work schema of ChemDP to action as a MS research Project, with chemicals, ligands preparation, optimization skills, whole the information, authentic reference gathering, and Database development for ChemDP.

**Special Thanks to.**



**Muhammed Rizwan Riaz** is a MS student of Bioinformatics at COMSATS Institute of Information Technology. He had done his BS in Bioinformatics from Govt. Collage University Faisalabad. He encouragingly helped in Database development with his Programming skills for ChemDP.

**Tab of Classes of Natural Products in ChemDP:**

Tab menu contain the tab 'Classes of Natural Products', it has the alphabetic search options to search for a required class of natural product, further selection could leads to the compounds of those classes and from molecular formulae, one can search for information about every member of that class. Go back tab can be used to get back to the alphabetic search.



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Alphabetic Search for Classes of Natural products:

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(a)



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Click on the Class of natural products for information about it. [Go Back](#)

**Classes of natural products**

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[Amides](#)

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[Acridones Alkaloids](#)

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[Acridone](#)

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[Anthocyanin](#)

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[AcyI Phenyl Alanine Derivative](#)

(b)

**Contact tab:**

One can contact to ChemDP team for any kind of assistance and help by visiting the 'Contact' page and filling the given form.

**Note:** One has to be registered and logged in to use all interactive session of ChemDP. All contents of the database are property of ChemDP, and all rights are reserved by ChemDP.



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