Molecular Property Diagnostic Suite Compound Library (MPDS-CL): A Structure based Classification of the Chemical Space

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Research Article

Keywords: Chemical Space, Structural classification, Compound library, Aadhar card, MPDS

Posted Date: August 10th, 2023

DOI: https://doi.org/10.21203/rs.3.rs-3236523/v1

Additional Declarations: No competing interests reported.

Version of Record: A version of this preprint was published at Molecular Diversity on October 30th, 2023. See the published version at https://doi.org/10.1007/s11030-023-10752-1.

Abstract

Molecular Property Diagnostic Suite-Compound Library (MPDS-CL), is an open-source galaxy-based cheminformatics web-portal which presents a structure-based classification of the molecules. A structure-based classification of nearly 150 million unique compounds, which are obtained from 42 publicly available databases were curated for redundancy removal through 97 hierarchically well-defined atom composition-based portions. These are further subjected to 56-bit fingerprint-based classification algorithm which led to a formation of 56 structurally well-defined classes. The classes thus obtained were further divided into clusters based on their molecular weight. Thus, the entire set of molecules was put in 56 different classes and 625 clusters. This led to the assignment of a unique ID, named as MPDS-*Aadhar card*, for each of these 149 169 443 molecules. *Aadhar card* is akin to the unique number given to citizens in India (similar to the SSN in US, NINO in UK). MPDS-CL unique features are: a) several search options, such as exact structure search, substructure search, property-based search, fingerprint-based search, using SMILES, InChIKey and key-in; b) automatic generation of information for the processing for MPDS and other galaxy tools; c) providing the class and cluster of a molecule which makes it easier and fast to search for similar molecules and d) information related to the presence of the molecules in multiple databases. The MPDS-CL can be accessed at http://mpds.neist.res.in:8086/.

Introduction

Chemical space is quite vast and finding a molecule with the desired property is arguably the most formidable challenge. In general, structurally similar compounds are expected to have similar properties. In drug/molecular design, the structural similarity is of paramount importance and any effort which structurally and systematically divide the chemical space will be of outstanding interest [1–5]. The need for developing new chemical libraries is of fundamental importance in the current scenario to systematize the process of covering huge chemical space and tapping its potential in multifarious applications in science and technology [6–10]. Such an effort will help to qualitatively and quantitatively estimate and assess the structural similarity and chemical diversity which will be of utility in mining the chemical/biological property space [11–13]. The ability to synthesize molecules has remarkably enhanced due to the pioneering efforts by experimental chemists, which resulted in the synthesis of huge number of molecules of diverse structural scaffolds and features [1]. However, in practice only a very small fraction of such synthesized molecules is of utility, which highlights the limitations of exploratory approaches, and emphasize the need to adopt rational design. Therefore, in recent years, the focus was shifted from “how to synthesize” to “what to synthesize”.

While there are extensive studies made on chemical space, most of them are devoted to explore the property space and very few of them focus on structure-based classification. One of the pioneering attempts was made by Waldmann’s group in attempting to a structural classification of natural products (SCONP), which is thus limited to only natural products [4, 14]. The focus was on heterocycles and the occurrence of those compounds in natural products. Other approaches are based on theoretical generation of molecules, and explore the size of the chemical space [1–5, 15–18]. Fragment based approaches also have played a very important role, and a number of methods were developed especially in the area of medicinal chemistry directed drug discovery [19–21].

Compound libraries are developed with the objective of enumeration, analysis, and extrapolation of the chemical space for various applications in chemistry, biology, and allied sciences. The curation of the chemical data is also concerned with the cleaning of molecules to remove any salts, and mixtures, normalization of various chemotypes, de-duplication of redundant molecules, etc. Besides, the manual and automated curation applied to the big chemical data, the lack of rigorous standardization methods in the chemical reaction, transformations are still one of the problems faced by chemists and the role of informatics and Artificial Intelligence (AI) is valuable in removing the barriers and deriving novel insights from the vast molecular space [22–28].

Finding druglike and non-druglike molecules through various means of theory and experimentation is the prime motto of drug discovery projects. While there are a large number of databases depicting the chemical structures, to our knowledge attempts towards the structural classification of compounds are scarce. The recent progress made in the synthesis and the growing need for novel chemical entities together push for an urgent need to scale up the existing methods and design new methods in developing elegant technologies for making the best use of deciphering the structure-property relationships from the chemical space [8–12]. The ultimate goal in all these attempts is to find out the molecule(s) with most desirable properties, e.g., drugs, catalysts, agrochemicals, etc. [13, 14].

The Galaxy based MPDS was an initiative made towards strengthening the open-source computational drug discovery, by providing access to most of the available open-source, custom designed indigenously developed scripts, programs and software packages [29–34]. Galaxy platform supports both the web and the standalone version which can be implemented on a Linux server. The Toolshed of Galaxy, which are periodically updated, is populated with a wide range of programs that can be directly imported and installed on users' Galaxy portals [30, 31, 35]. It also offers the advantage of adding several user-developed programs which are incorporated into the Galaxy directory and are programmatically called to the front interface through an XML file. Several virtual machine images of Galaxy instances [30] are also made available online so that they can be used for various hands-on and other training sessions for data-intensive biology and chemistry applications. MPDS-CL in specific and other chemical libraries in general; its development, scalability, and automation techniques will be essential in deriving novel insights for drug discovery by comprehensively assessing the chemical space and finding out various ways of prioritizing the lead molecules for drug discovery projects [36–40]. Ensuring the unique molecules along with creating a structurally well-defined chemical data library was taken as the paramount significance in creating the MPDS-CL.

Genesis of Galaxy based MPDS

MPDS is an indigenous initiative that is developed to strengthen computational drug discovery and is an attempt to address the pressing issues of drug discovery. As it is developed on the Galaxy platform, the features like cloud-based accessibility, reproducibility, and various data-driven methods are also made available. The MPDS suites of disease-specific web portals include proprietary libraries, machine learning models, and other relevant open-source tools and resources essential for drug discovery solutions. The compound library has been the most important component of the data library module of MPDS, which was initially integrated into the $MPDS^{TB}$ web portal. At that time, using the 6 most popular and abundant chemical databases, around 110 million unique non-redundant set of compounds, with 31 classes, was reported. Over the period of time, various disease-specific MPDS portals including $MPDS^{TB}$ [15], $MPDS^{DM}$ [34], $MPDS^{COVID-19}$[41] were developed, and other portals like $MPDS^{NAFLD}$ and $MPDS^{HIV}$ are under development. The modules in MPDS are categorized into (i) data library (that consists of information on genes and targets specific to a disease or disorder, a molecular repository, druglike fragments, literature, etc.,) (ii) data processing (computation of molecular descriptors/fingerprints, file format converter) (iii) data analysis (QSAR, docking, drug-likeness filter, and visualization tool), (iv) Advanced modules (which include various predictive modules for disease–disease interaction, big data analysis, and machine learning tools). MPDS is also equipped with a workflow management system that enables the users to easily integrate multiple tools from the available modules and customize the existing workflows as per the requirements [32–34, 41]. The utility and scope of open-source packages are well documented in the literature [42–43].

The current MPDS-CL was developed into a new full-fledged web portal, and not as one of the modules of MPDS and in that respect it is vastly different from the earlier module, which was presented as one of the modules of $MPDS^{TB}$ about 6 years ago. The MPDS-CL is an independent web portal, which is well positioned to integrate with Galaxy and MPDS web portals. The classification of close to 150 million molecules and redundancy removal techniques employed are different and much more efficient, compared to those employed in $MPDS^{TB}$ six years ago (Fig. 1). This module enables comprehensive structural analysis, assigns a unique *Aadhar* ID to each molecule, offers descriptor analysis tools, fragment library, and screening tools.

Materials and methods

The public domain chemical databases, 42 of them, have been considered in making the current compound library (Table S1), while the erstwhile compound library module of $MPDS^{TB}$ has taken 6 databases (PubChem, KEGG, ZINC, DrugBank, ASINEX, and NCI). However, two types of databases were excluded: a) large databases of hypothetical molecules and b) some commercial/inaccessible databases (Table S2).

The databases considered here may be categorized as general and specialized database based on the type of molecules it contains. The bioactivity libraries constitute repositories like PubChem and ChEMBL. While other categories of databases include drugs and molecules of biological importance such as Therapeutic Target Database, DrugCentral, SuperDrug2, DrugBank, PharmGKB, GRAC, SMPDB, KEGG compound database, HMDB, and ChEMBL-DNDi. Other libraries include molecules extracted from patent and general literature (SureChEMBL, BindingDB), GPCR ligand database, GPCR decoy database, a database of lipid-like molecules (LipidBank), a database of the crystal structure of organic and inorganic, metal-organics and other minerals (Crystallography-open database), Natural product database (InterBioScreen, UNPD), and database with lead-like molecule and useful fragments (ASINEX and ChemDiv) (Table S1). The methodology described in the further sections essentially deals with various open-source cheminformatics packages and the python programs developed for chemical data analysis.

Retrieval of molecules

The molecules used for developing the compound library were retrieved from various public domain chemical databases in multiple file formats like SMILES, SDF, and MOL. The molecules that were not in the SMILES format, were converted to the canonical SMILES to maintain a unique representation for all the molecules in the database. The canonicalization algorithm as implemented in the OpenBabel3 [44] was used for the conversion of all the SMILES formats into the canonical format. Few of these databases are updated over a specific period while others like PubChem, SureChEMBL are populated with new molecules every other day. In the current study, we have retrieved the molecules till July 2023 and all analysis was performed using this dataset. The chemical databases offer a wide range of information about the molecules that include their structural, physicochemical, reaction profiles, analytical data, etc. The molecules which were obtained from public domain chemical databases are mentioned in Table S1 in which each database and its statistics of update is indicated. The work summarized here mainly consists of the structural information in the form of SMILES, which were parsed into the SMARTS pattern for subsequent processing and analysis of the dataset. Linux-based expressions, such as AWK, sed, along with a set of python packages were employed to obtain a unique non-redundant 97 atom-based portions (Table S3). The process of retrieving data from each database differs and retrieval is dependent on the type and number of new molecules included in the database. In the case of PubChem, molecules included within a specific duration were retrieved using the file transfer protocol (FTP) method whereas for ChEMBL, a web resource client that is a python-based library, as well as a bulk download option, was used. In the case of SureChEMBL, the quarterly updated molecules were retrieved in bulk. ZINC database has the option to retrieve specific subsets, “Tranch” according the molecule’s type, its reactivity, purchasability, etc., While there are a large number of molecules in ZINC, we considered only the “Standard + In-Stock” subset. From all the remaining databases, the molecules were retrieved as ‘bulk download (Fig. 2). Some region-specific natural products and phytochemicals-based databases are also available and some of them are developed in our group [45, 46], and if new molecules are found they will be added to MPDS-CL periodically, during the half-yearly updates.

Schema for redundancy removal and structural classification

Each database was classified into 97 hierarchically well-defined atom-based portions (Fig. 3). As the classification is hierarchical, those portions which were not considered for further classification were labelled as ‘terminal portions’, and the rest as ‘open portions’. The classification has been carried out in five distinct classification steps, which are called layers (Fig. 3). The first layer of classification was based on molecular weight (MW) and atom composition. Thus, Portions 1–3 were assigned as terminal portions for the first layer of classification, and all remaining portions were further classified in the second layer. The second layer of classification was based on molecular topology (acyclic or cyclic), and all those molecules that were categorized as acyclic were considered as terminal portions, while cyclic molecules were further classified as alicyclic and aromatic molecules in the third layer.

In the third layer of classification, both alicyclic and aromatic portions that contain Te, Se, Ge, As, Sb (Portions 12–13), B & Si (Portions 14–19), Phosphorus (Portions 20–21), and hydrocarbons (Portions 22–25), were assigned as terminal portions, and the remaining portions were considered for further classification. The fourth layer of classification is based on the count of heteroatoms, which generate portions that were specifically categorized as sulphur, oxygen, and nitrogen containing. These were subjected for further classification as no terminal portions were identified in this layer. The open portions obtained from the fourth layer were used for classification in the fifth layer, and it was based on the position of the heteroatom in a molecule that can be inside or outside the ring. For example, if a molecule consists of sulphur inside a ring, then it was classified into a separate portion, and if the molecule doesn't have any sulphur atom inside the ring, it was classified into a different portion. Likewise, the oxygen and nitrogen-containing molecules were classified into their respective portions. In this way, all the open portions of the fourth layer were completely classified as terminal portions in the fifth layer, and hence a total of 97 different atom-based portions were obtained.

As among the file formats InChIKey [47] appear to be the gold standard for unambiguously identifying the molecule, it has been used for redundancy removal in the compound library. For all the molecules, the standard InChIKey was computed using OpenBabel3 [44]. InChIKey is a string of 27 characters built on the SHA-256 encoding algorithm applied on the InChI and the abstract notation consisting of hashed information for molecular skeleton and isomerism. It was primarily developed for indexing purpose but is very useful for text-based mining and searching in chemical databases, as well as for removing redundancy.

All programs used to classify the molecular space were coded in python3 and extensive use of SMARTS patterns was utilized [48]. The validation of SMARTS patterns was done rigorously so as to avoid any misclassification of molecules. For atoms-based classification, the SMARTS pattern consisting of the acronym of individual atoms or corresponding atomic number was used, while the next level of classifying the cyclic and acyclic molecules was done by identifying the atoms in rings and outside the rings. The structural classification of molecules was primarily carried out on all the cyclic portions to identify the structural diversity of molecules. The algorithm used to classify the molecules first parses the SMILES string and converts it to the SMARTS pattern by calling the 'pybel function'of the OpenBabel package. This pattern is then searched in the parsed SMILES, and based on the presence/absence or position of specific atoms, molecules are classified (Fig. 4). The programs developed for structural classification has extensively made use of the SMARTS pattern parsed through both OpenBabel and RDkit modules [49], and individual SMARTS based expression was created and validated for each class.

Each of these SMARTS patterns act as substructure queries for identifying specific structural feature in a molecule from the large chemical space, and thus aid in classifying the molecules with matched features. Particular syntax such as presence of rings, ‘n-’ring-membered type, ring systems (fused / non-fused / connected) and other complex structural features, all were used to screen and efficiently identify molecules from large space.

Results and discussion

After obtaining an unambiguous set of 149 169 443 molecules, structural classification of them into 56 classes was achieved by employing a series of scripts and tools, as described in the foregoing sections (Table 1). The 56 classes presented in the Table 1, are carefully carved to group and enumerate molecules with such features into distinguishable groups.

Table 1
List of 56 classes and population of molecules belonging to each class.

Class	Description	Population
1	Acyclic (saturated / unsaturated)	3 455 531
2	Pure inorganic molecules	12 630
3	Monocyclic 3 membered saturated ring	333 466
4	Monocyclic 3 membered unsaturated ring	5 711
5	Monocyclic 4 membered saturated ring	249 354
6	Monocyclic 4 membered unsaturated ring	9 553
7	Monocyclic 5 membered saturated ring	1 224 146
8	Monocyclic 5 membered unsaturated ring	153 678
9	Monocyclic 5 membered aromatic ring	2 708
10	Pyrrole (Free)	171 154
11	Furan (Free)	288 279
12	Thiophene (Free)	604 404
13	Monocyclic 6 membered saturated ring	2 452 169
14	Monocyclic 6 membered unsaturated ring	405 431
15	Monocyclic 6 membered aromatic ring	77 290
16	Benzene (Free)	26 496 311
17	Pyridine (Free)	5221 873
18	Monocyclic ≥ 7 membered saturated ring	620 637
19	Monocyclic ≥ 7 membered unsaturated ring	118 401
20	Multiple (≥ 2) main group elements in a ring	16 304 254
21	Bicyclic connected rings	30 111 865
22	Bicyclic fused 3+’n’ membered	211 041
23	Bicyclic fused 4+’n’ membered	365 491
24	Bicyclic fused 5 + 5 membered [A + A]	216 117
25	Bicyclic fused 5 + 5 membered [A + NA]	168 626
26	Bicyclic fused 5 + 6 membered [A + A]	5 300 636
27	Indole (Free)	1 631 787

Class	Description	Population
28	Bicyclic fused 5 + 6 membered [A + NA]	1 079 827
29	Bicyclic fused 5 + 6 membered [NA + A]	3 620 404
30	Bicyclic fused 5+(5/6/≥7) membered [NA + NA]	1 962 058
31	Bicyclic fused 5 + ≥ 7 membered [A + NA]	167 017
32	Bicyclic fused 6 + 6 membered [A + A]	4 729 630
33	Bicyclic fused 6 + 6 membered [A + NA]	3 658 454
34	Bicyclic fused 6 + 6 membered [NA + NA]	885 091
35	Bicyclic fused 6 + ≥ 7 membered	709 655
36	Bicyclic fused ≥ 7 + ≥ 7 membered	16 923
37	Bicyclic spiro	1 133 303
38	Tricyclic connected (1 ring aromatic)	715 276
39	Tricyclic connected (2 rings aromatic)	3 448 581
40	Tricyclic connected (3 rings aromatic)	1 115644
41	Tricyclic connected (no aromatic rings)	52 924
42	Tricyclic fused (1 ring aromatic)	809 585
43	Tricyclic fused (2 rings aromatic)	1 257 912
44	Tricyclic fused (3 rings aromatic)	609 406
45	Tricyclic fused (no aromatic rings)	579 092
46	Tricyclic fused-connected [Any combinations]	11 066 401
47	Tetracyclic connected [Any combinations]	873 036
48	Tetracyclic fused [Any combinations]	1 167 417
49	Tetracyclic fused + connected [Any combinations]	4 559 512
50	Complex ring systems up to tetracyclic	1 013 766
51	Pentacyclic & above	3 962 984
52	1 transition metal in a molecule	56 796
53	2 transition metals in a molecule	1 871
54	≥ 3 transition metals in a molecule	303
55	Mol.wt. =750.00-1200.99 Da	2 973 899

Class	Description	Population
56	Mol.wt. ≥1201.00 Da	730 133
Total		**149 169 443**
A- Aromatic; NA- Non aromatic		

One need to consider that a molecule may belong to multiple classes, but the sole idea of structural classification is to identify or designate a molecule on the basis of the core moiety or a principal structural feature responsible for rendering a specific activity, that again depends on its structure-property based relationship. In literature various studies were reported [1–10] which focuses on various hierarchical levels of structural classification such as topological, skeleton, atomic connectivity, formulae, and biological role. However, the current classification scheme is based on identifying and profiling molecules based on a chemically well-defined structural motif, termed as a '*class*'.

In this manuscript, the entire molecular structure was considered for enumerating various types of molecules existing in this portion of chemical space. Two cyclic molecules combine in various ways, a) edge sharing, which is called fused, b) vertex sharing, which is spiro, c) connected by a bond, which may be called connected, or d) connected by a linker, which are called disconnected (Fig. 5). As seen in the Table 1, Class 21 (Bicyclic connected rings) was found to have the largest population of molecules, i.e., 30.11 million, which clearly indicates that this class consists of large number of molecules that have ring connected via a non-ring bond and absence of fused ring systems. The presence of connected rings systems offers stability and rigidity to the molecules in addition which may responsible for their higher synthetic accessibility. Classes 10–12, 16–17, and 27 were designed to group specific molecules where free forms of Pyrrole, Furan, Thiophene, Benzene, and Pyridine can be identified. This is also done with an interest to identify molecules with medicinally relevant rings exhibiting their unique functional role as valuable building block in drug design, optimizing certain therapeutic effects with respect to a drug, etc. Classes 22–37 are different forms of bicyclic fused ring systems, which are intended to group molecules with varied bicyclic scaffolds in terms of ring size, and combination of aliphatic and aromatic patterns. These classes combinedly constitutes 25.85 million molecules, showing their immense contribution in the therapeutic chemical space, with a large population representing the terpenes, alkaloids, and other molecules belonging to pharmaceutically important natural products. The tricyclic molecules are grouped from classes 38–46, each class depicting the molecules with notable topological variations in association of different ring systems. Tetracyclic and polycyclic classes are arranged from 47–51, with a special class designated for large complexed fused rings up to tetracyclic group in class 50, while classes 52–54 are exclusively designed for molecules constituting transition metals, and classes 55–56 are designated for large MW (≥ 750.00 Da) molecules.

Table 2 illustrates the various possible combinations as explained between the two cyclic moieties, by taking a simple ring system. Molecules which contain both five and six membered rings simultaneously represent the largest chunk, 66.16 million, which represent more than 44% of all chemical space.

Therefore, 4 out of 10 molecules have both 5 and 6 membered rings in them. The next best combination is three and six membered rings with a total number of 2.59 million molecules. Among the, classes the three or more transition metal containing molecules class 54, with a population of only 303 represent the least abundant class in the chemical space. The least population (1,445) of molecules is obtained from those constituting both eight and ≥ 9 membered ring systems.

Table 2
Pairwise distribution of ‘n’ membered rings as observed in MPDS-CL.

	3	**4**	**5**	**6**	**7**	**8**
4	30 581					
5	641 651	404 334				
6	2 597 353	1 668 516	66 169 215			
7	22 867	15 344	312 595	1 699 025		
8	4 931	2 598	29 430	165 032	2 013	
≥ 9	8 460	2 870	65 248	391 692	1 587	1 445

Property space for cyclic and acyclic molecules

While the molecules are classified as cyclic and acyclic systems, the general property distribution in the chemical space between these varieties was examined and the results are depicted in Fig. 6. The molecular descriptors like molecular weight, hydrogen bond donor/acceptor, number of rotatable bonds, polar surface area, number of heavy atoms, and logP were computed for all the acyclic and cyclic non-redundant molecules. The distribution of descriptors is used to understand the property space of the molecules (Fig. 6), and thereby aid in estimating the druglikeness of the given chemical space. Concerning molecular weight, the highest number of molecules in acyclic space covers a range of 100.00-500.00 Da with a peak at 250.00 Da, while in the case of cyclic molecules, a progressive increase in the population of molecules is observed in the range of 150.00-750.00 Da, with the peak population between 300.00–350.00 Da. Figure 6 illustrates the distribution observed in, both cyclic and acyclic molecules with respect to their properties: a) molecular weight, b) molar refractivity, c) hydrogen bond donor, d) hydrogen bond acceptor, e) no. of heavy atoms, f) rotatable bonds, g) logP, and h) topological polar surface area. The prototypical 8 parameters considered for comparing and contrasting the chemical space distribution in cyclic and acyclic molecules reveal the following trends. Similar trends were observed in the distribution of hydrogen bond donor, hydrogen bond acceptor, logP and topological polar surface area for acyclic and cyclic molecules. While it has been observed that there is a slight broadening for cyclic molecules in the case of the distribution of molecular weight, molar refractivity and the no. of heavy atoms. In contrast, in the case of rotatable bonds the distribution is sharper in cyclic molecules compared to acyclic. Thus, as expected the trends reveal higher diversity in the case of cyclic molecules and less flexibility compared to their acyclic counterparts.

Cheminformatics tools

Galaxy is a publicly available web server that provides open-source web-based platform for a wide range of bioinformatics, cheminformatics, genomics, proteomics and other analysis [29, 30, 50, 51]. Another major strength of Galaxy is the workflow system, which allows a very effective and automated execution of large projects involving multiple steps. Further, the ease with which one can write scripts, programs and develop software in any programming language to the already existing webservers based on Galaxy such as MPDS makes it highly desirable.

The chemical space in MPDS integrates various Galaxy chemical tools for the structural analysis. Bray et al., developed the Galaxy ChemicalToolbox which provide the large assembly of tools for drug discovery and cheminformatics [31]. MPDS-CL provides access to the Galaxy ChemicalToolbox, as well as a host of other tools. These tools are PaDEL [52], CDK [53], Rdkit [49], Mordred [54], file format converters, JMol [55] editor and molecular visualizer for drawing and visualizing molecules along with a variety of search options (as described in Table 3 and Fig. 7). BCS classification, toxicity filter, drug likeness and natural product likeness filter are some other tools that are currently available and it is our quest to continually augment more filters like these. Efforts to add several of the in-house developed machine learning tools based on the property of the molecule, such as the antiviral, toxicity, and susceptibility of failure in clinical trials, blood brain barrier prediction are in the pipeline [56–59].

Table 3
Description of different modules available in MPDS−Compound Library.

Modules	Description
Get Data	Locally upload data/files of different file formats
Chemical structure editor	Draw a molecule (using Jmol editor) and export the SMILES
MPDS Aadhar ID search	A molecule from the MPDS-CL can be searched in various ways in addition to MPDS Aadhar ID card based search
Exact structure search	User can upload/draw structure and search
Sub structure search	Search with sub structure based on the user defined fragments
Properties based search	Screening the molecules based on molecular properties
Fingerprint based search	Identifying the structural features from the canonical SMILES
Fragmenter	Split a molecule to smaller fragments based on predefined rules (i.e., RECAP rules)
Fragment based search	Searching the MPDS fragment library based on nature of fragments
File format conversion	Small molecules file format converter (i.e., pdb, sdf, pdb, mol) for different chemoinformatics operation
3D coordinates generation	Adding hydrogen atom to the molecule and convert the structure from 2D to 3D
Descriptors calculation	Calculation of different descriptors based on "*PaDEL*", "*CDK*", "*RDkit*", "*Mordred*"
Physico-chemical properties calculation	Calculating the physico-chemical properties for a set of molecules
Estimation of drug-likeness	Calculation of different drug-like rules, using DruLiTo, Lipinski's rule, Ghose filter, etc.
BCS classification	Classifying the query molecule based on Biopharmaceutical Classification System (BCS)
Toxicity filter	Identifying the toxicophores for the given molecule
Natural product likeness calculator	Calculation of the natural-product likeness score for the user given molecule

The search methods and options

The search methods provided in the MPDS-CL is the way to navigate through the chemical space by employing various search such as exact structure, sub-structure, fingerprint, and molecular property-based search. The idea of exact structure search is to generate the exact molecule as provided by the user. Whereas the substructure search is employed to identify series of molecule with the desired query.

The substructure search is essentially employed to check for molecules that is build up with other scaffolds and in a way to explore the synergistic effects of different building blocks while interaction with the biological receptors. The results of substructure search in MPDS-CL can be performed by providing a query molecule in .sdf/.mol/.smi format, which on search will result in giving the series of molecules with the substructure match in independently existing form. The fingerprint search is a search option to explore the molecules through specific classes. All classes are categorized under the main category viz., monocyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic and a few special classes. The idea behind this search, is to provide an understanding of the 56 classes, without asking the user to explicitly search for a specific molecule. Next in the line, is the search option based on molecular properties, where the user can search for molecules belonging to a range of properties as well as it comes with multiple filters to efficiently look for molecules with desired properties.

Each of these search methods is designed to cater to a wide range of research objectives, allowing users to perform targeted searches as per their interests. The diverse search functionalities provided by the MPDS-CL enhance its utility as a valuable resource for researchers from various disciplines, empowering them to explore the chemical space, discover novel molecules, and gain valuable insights into compound properties (Fig. 7).

MPDS- Aadhar card

The name *Aadhar card* is inspired by a thought process of comparing the molecules to human beings. See, for example, if one wants to get a particular work done, we need to find the right person. Similarly, when you look for a specific property, you need to find a right molecule. As every human is unique and so are the molecules, and our endeavour is to keep the full profile of molecule and its properties can be explored and thus assigning a unique id, which traces its structural identify is useful.

Each of these unique features have been clearly defined and they have chosen to represent a “class” and thus 56 classes were designated in MPDS-CL. As molecules can have multiple features, we employed priority rules and the number of a class is arranged in the ascending order. The 56-bit vector available in the *Aadhar card* reveal the other features of a molecule, i.e., if a molecule belongs to class 45, but also contain the features of class 34, 23, and 8, then the 56-bit vector is 00000001000000000000001000000000010000000000100000000000.

The *Aadhar card* of each existing molecule in the MPDS-CL is intended to provide all the information of a given molecule in a sequential fashion. The first page provides the critical details, which are common and computable to all the molecules in the chemical space, and it is generated on the fly by MPDS-CL (Fig. 8). However, molecules will have a varying detail of information and the subsequent pages of *Aadhar card* can be custom designed to populate and use and as this information is specific to a given molecule and as such will not be generated on the fly.

Conclusions

MPDS-CL is a non-redundant chemical library, represent about 150 million unique molecules, which was built by compiling a large dataset of molecules obtained from 42 publicly available chemical databases. It is an attempt to systematically classify the chemical space by infusing the structural-chemical insights which helps in the design of molecules. The scheme of dividing molecules into 56 classes has been arrived methodically exploring various ‘structural features’ which determine the identity of a given molecule and all these molecules already available or easily accessible synthetically. The MPDS-CL provides various search options driven by MPDS *Aadhar* ID search, exact structure search, sub-structure search and fragment-based search, which helps in elegantly exploring the chemical space. The study has employed various cheminformatics, and other informatics methods to systematically analyse the chemical space and aid in rational design of molecules with a desired property.

If one were to describe any effort for the design of a molecule, it is finding the right molecule for performing a given task. In the quest to discover a drug, catalyst or any special property of a molecule, it is all about hitting the right spot in the realm of chemical space. Further, understanding of various structural and topological diversity of molecules and establishing various data-oriented analytics for structure-property and activity relationships, is a topic of outstanding importance in molecular design. Thus, when molecules are grouped in structurally similar categories, it unlocks newer possibilities for finding repurposable spectrums of varied interest and applications. Thus, the present work may be exploited in various fields, such as drug discovery, smart materials design, finding environmentally friendly pesticides, herbicides, petrochemicals, and other broad applications of chemical molecules.

Declarations

Acknowledgements

DBT is thanked for the financial support in the form of Centre of Excellence in Advanced Computation and Data Sciences (Ref. No: BT/PR40188/BTIS/137/27/2021).

Author Contributions

The entire project is conceived and designed by GNS. Bulk of the data collection and consolidation was done LJ, SN, HJM, NK, and AK. Analysis, validating the webserver, manual preparation was done by SV, AK, EJ, LP along with all others. The website design and validation are done by SV, HJM, SN, and LJ. First draft is prepared by LJ and LP. The manuscript was verified by all authors. The suggestion for the final draft was collected and a pre-final draft was made by LJ, LP, SN, and HJM. GNS has corrected and finalised the manuscript.

Data availability All the data can be obtained from the open-source platform provided in the article.

The authors have no conflict of interest.

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Figures

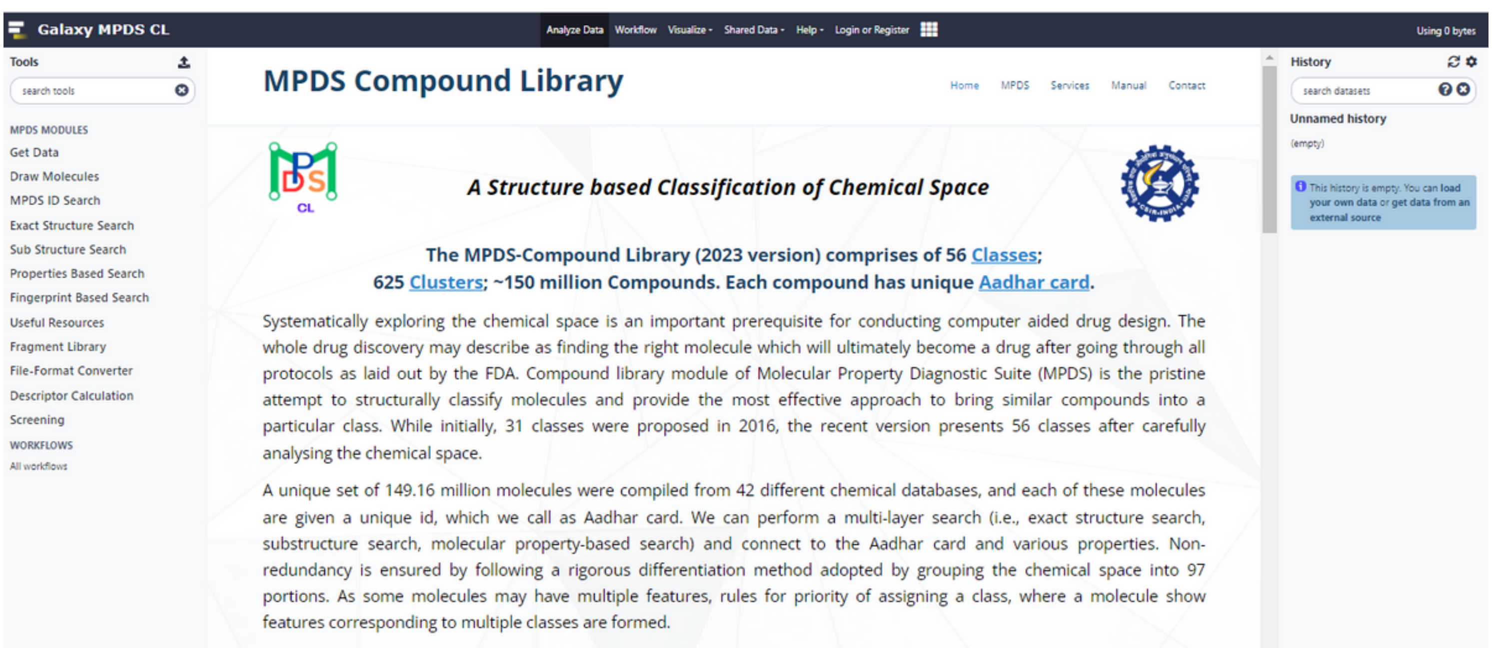


Figure 1

Home page of MPDS Compound Library (MPDS-CL) accessible at http://mpds.neist.res.in:8086/. The left panel consists of various search options and cheminformatics tools incorporated in the portal. The right-side panel displays the uploaded data and the calculations results.

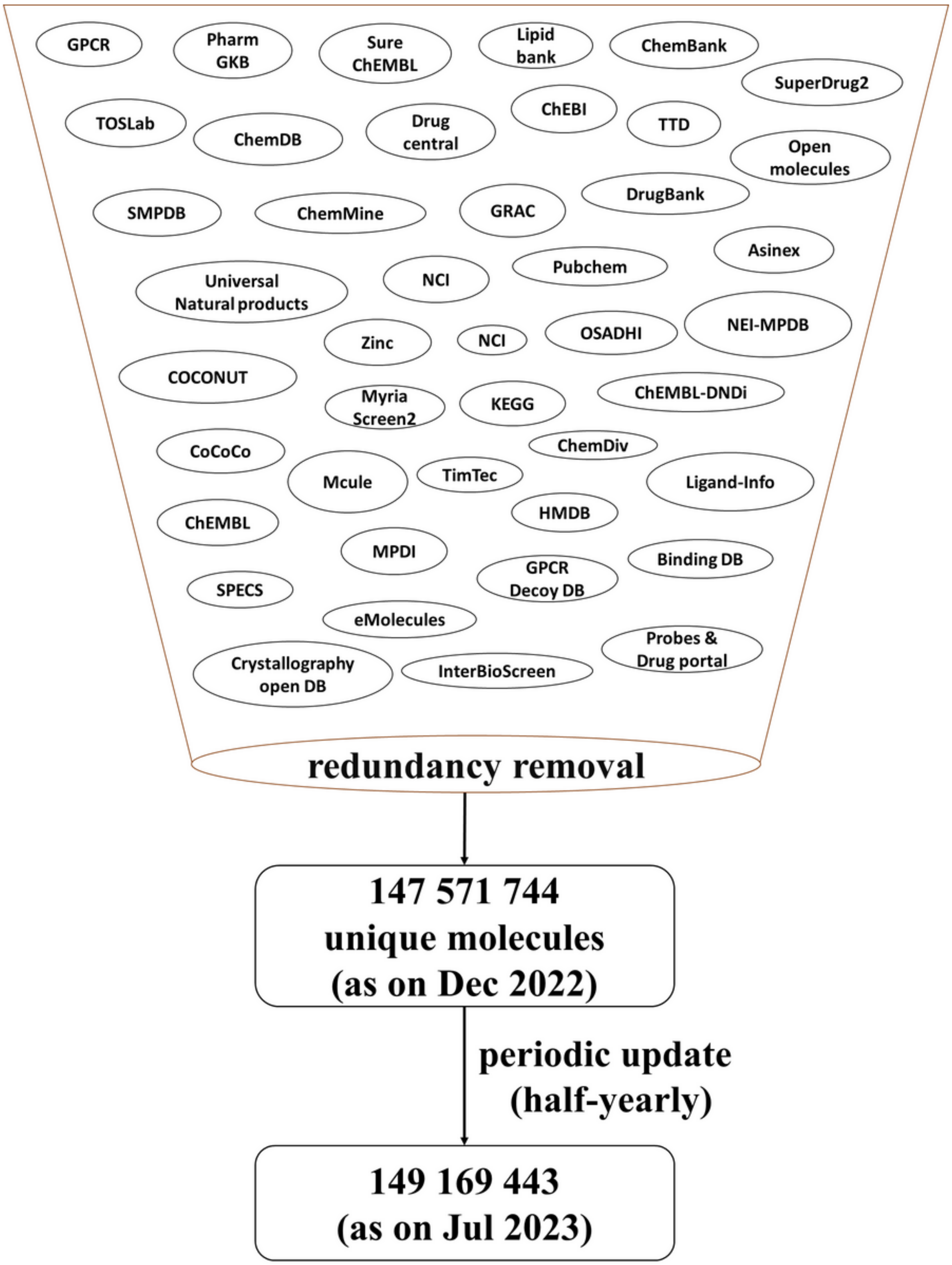


Figure 2

An overview of the development of the MPDS-CL, from the molecules downloaded from 42 databases. MPDS-CL had 147 571 744 molecules in December 2022. While the initial set of non-redundant molecules were obtained by employing the scripts in portions, the half-yearly updates use an entirely different approach to add molecules directly to the classes and clusters. Thus, the updates as on July 2023 is 149 169 443 number of unique molecules.

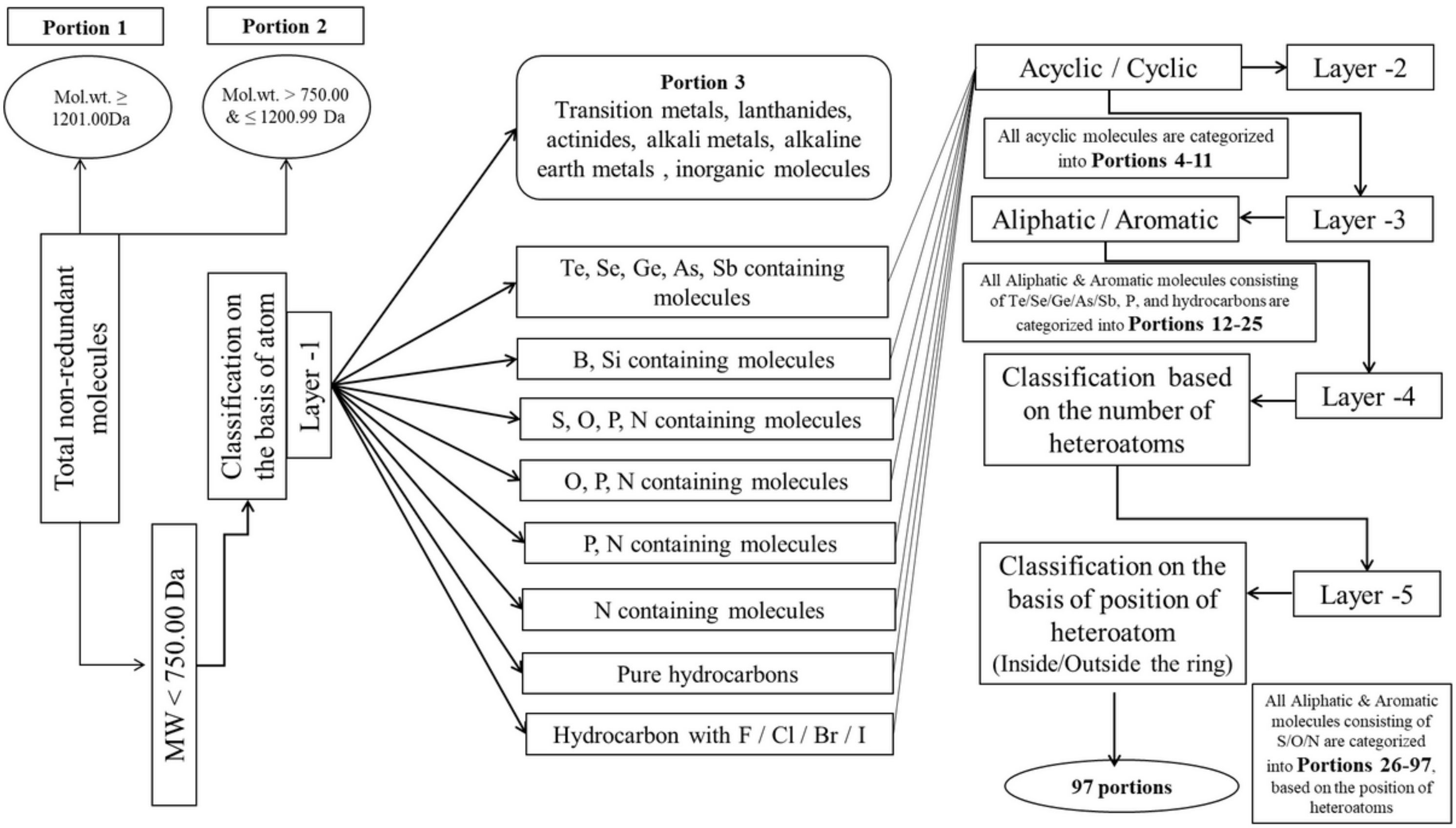


Figure 3

Diagrammatic representation of the scheme employed to obtain the atom-based division of molecules into 97 portions.

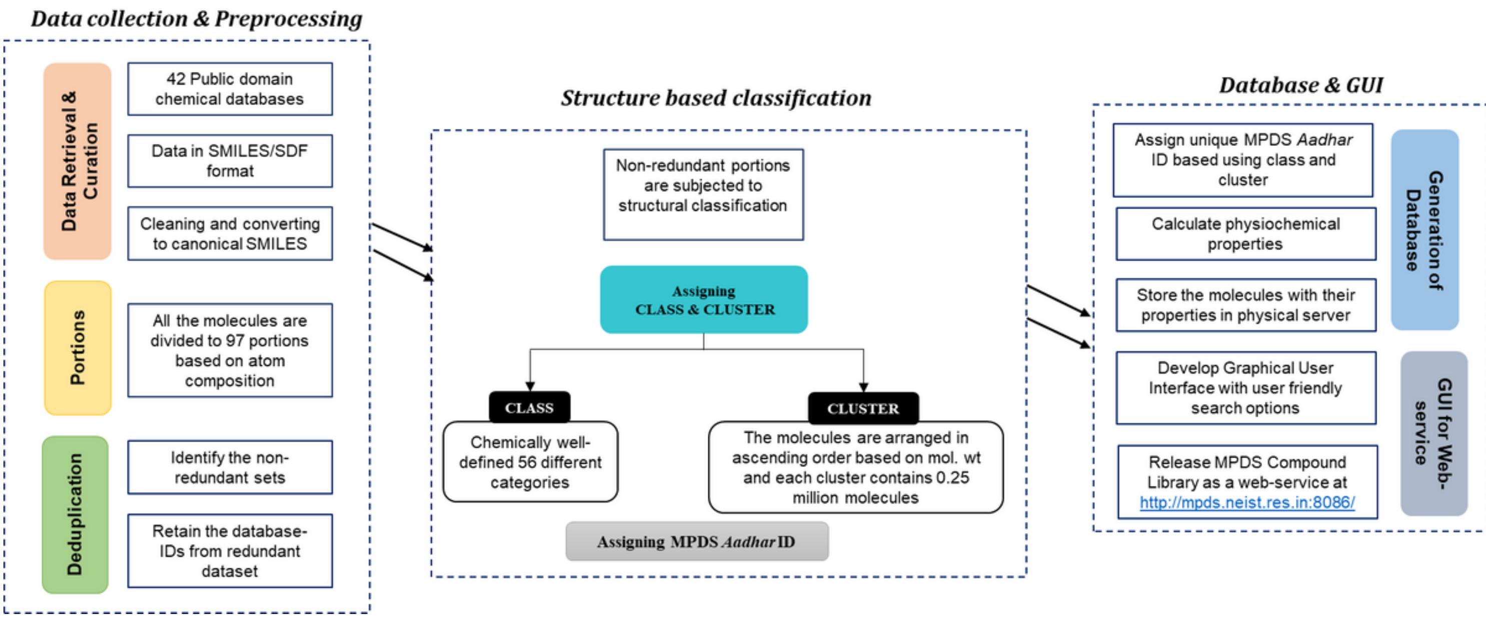


Figure 4

An illustration depicting the step-by-step protocol employed for developing the MPDS-CL.

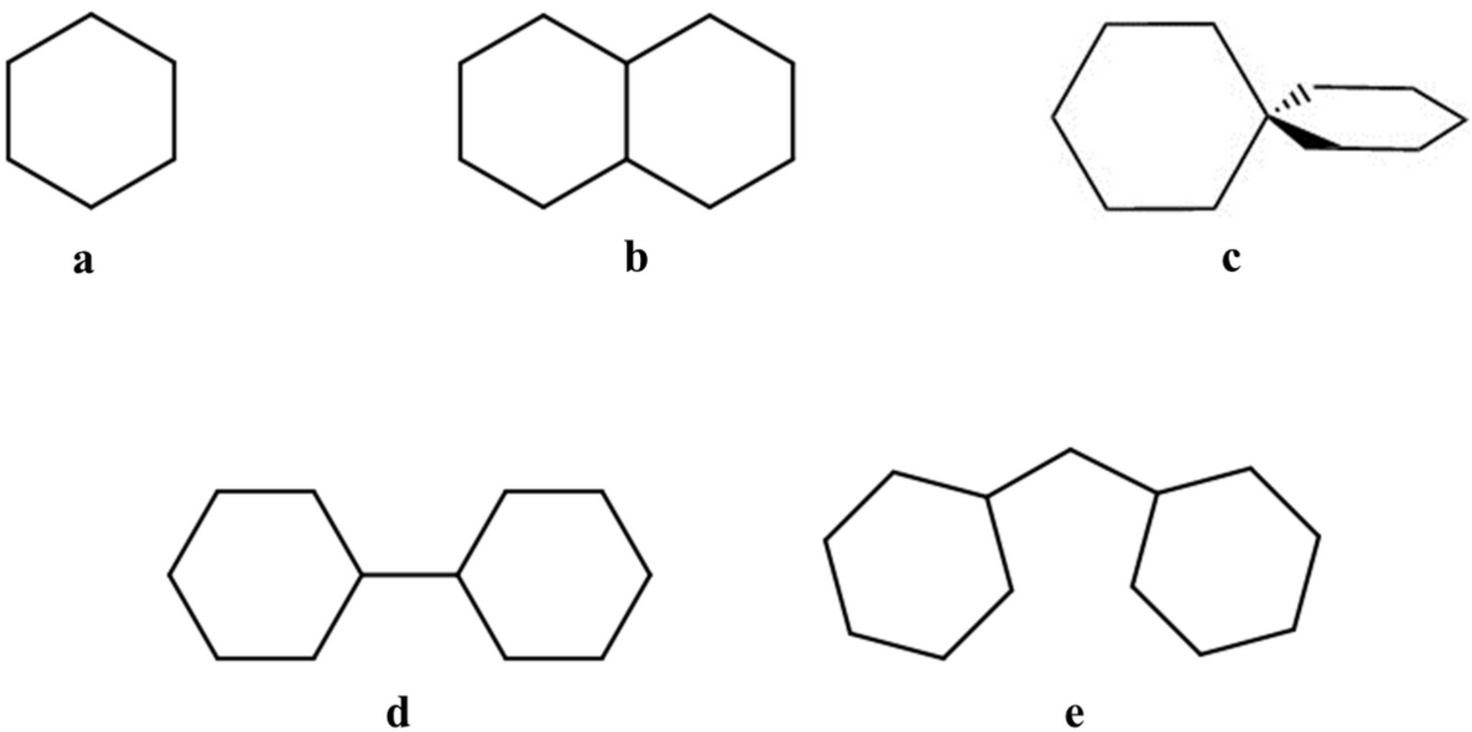


Figure 5

A schematic representation of a) unattached; b) fused; c) spiro; d) connected; e) disjointed ring systems. The first four scaffolds represent unique features and therefore can correspond to a unique class. However, in case of e) when a linker is involved, such an arrangement leads to a combination of more than one feature. This leads to the presence of more than one unique feature (correspond to a specific class) in a given molecule.

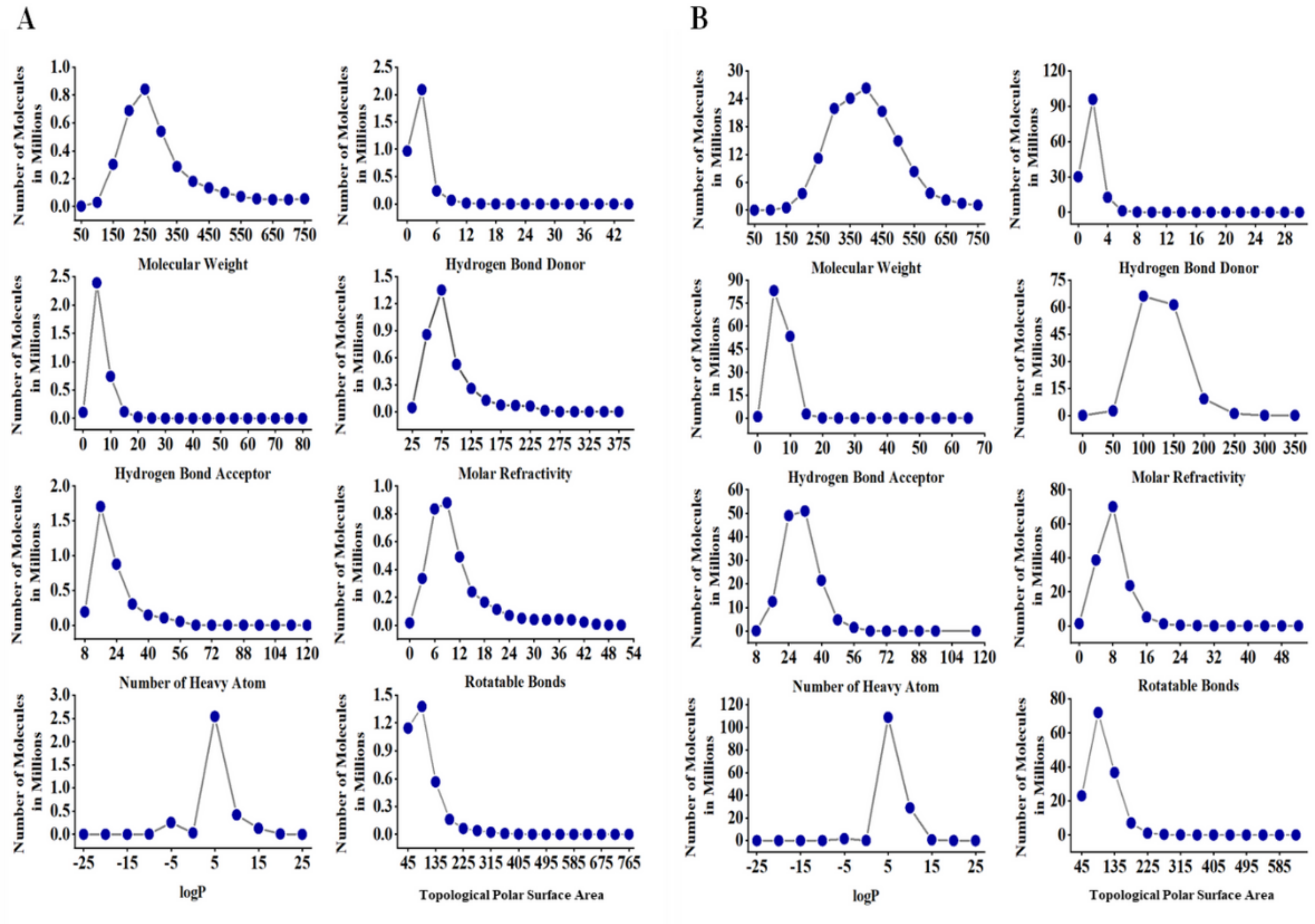


Figure 6

Figure displaying the population based distribution of selected molecular properties (for (A) acyclic and (B) cyclic molecules); a) molecular weight, b) hydrogen bond donor, c) hydrogen bond acceptor, c) molar refractivity, d) number of heavy atoms, e) rotatable bonds f) logP and g) topological polar surface area.

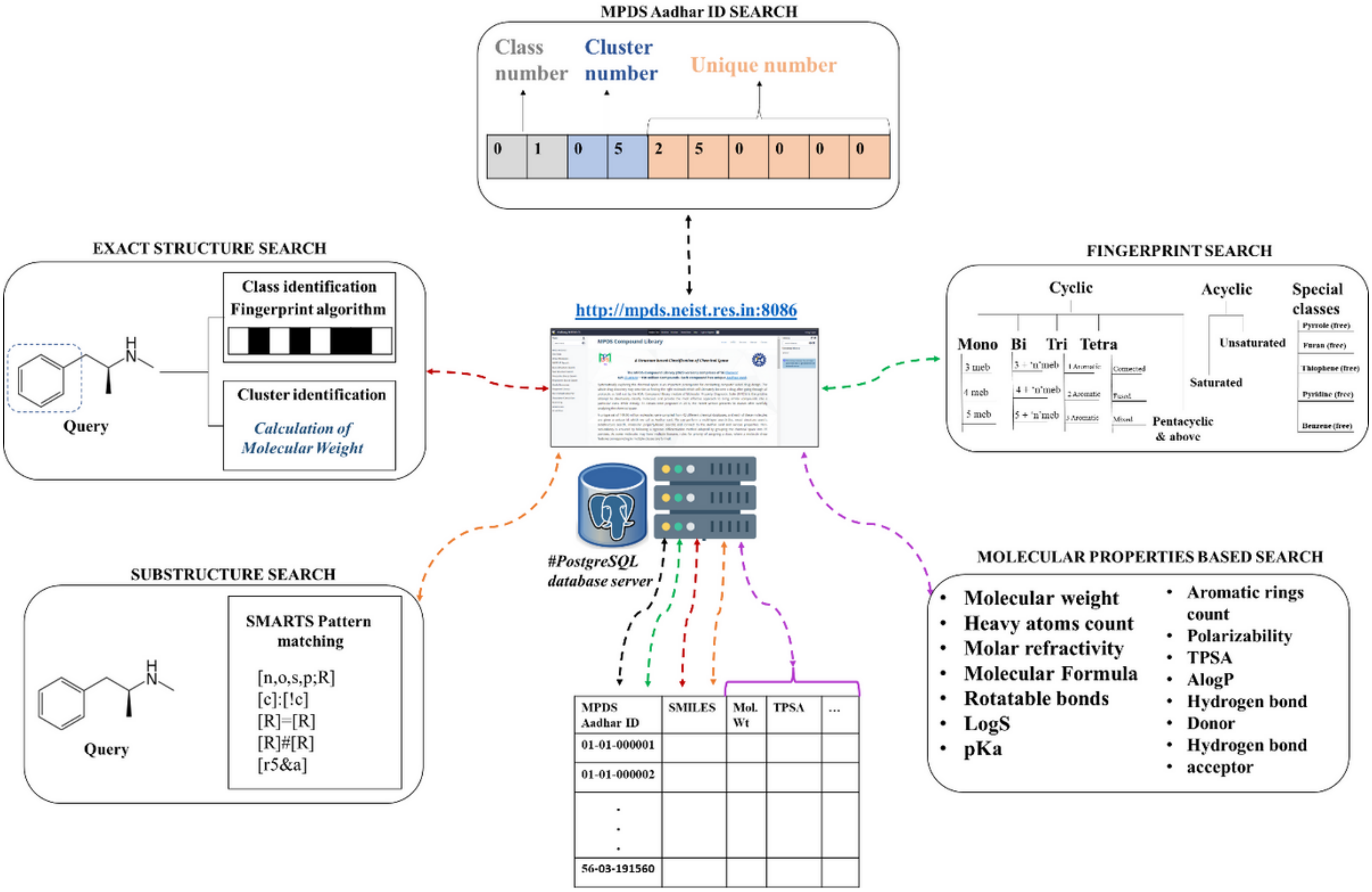


Figure 7

A schematic diagram explaining different search methods available in MPDS-CL. The database information is connected with the PostgreSQL server. The query via MPDS-CL is connected to the database via Galaxy and fetches the information from the server.

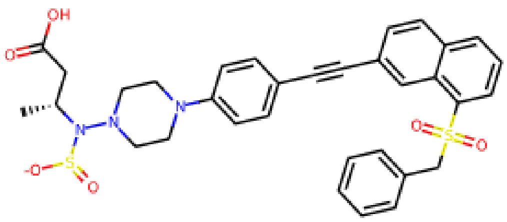
MPDS Aadhar ID: 32-19-122605			
		**Molecular Formula:** $C_{33}H_{32}N_3O_6S_2$ **IUPAC Name:** N-[(2R)-1-carboxypropan-2-yl]-4-{4-[2-(8-phenylmethanesulfonylnaphthalen-2-yl)ethynyl]phenyl}-N-sulfinatopiperazin-1-amine	
Canonical SMILES: S(=O)([O-])N(N1CCN(CC1)c1ccc(cc1)C#Cc1cc2c(S(=O)(=O)Cc3ccccc3)cccc2cc1)[C@@H](CC(=O)O)C		**InChIKey:** UIEDIXWMFRQARL-RUZDIDTESA-M	
Fingerprint: 00000000000010110001100000000001000000000000000000000000			
Molecular Properties:			
Mol. Wt.	630.754	LogP	3.25
HBD	1	LogS	-6.9
HBA	8	pKa	pKa1: 1.95; pKa2: 5.09; pKa3: 3.01; pKa4: -5.48
Molar refractivity	165.3	Polar surface area	121.29
Heavy atoms count	3,43,8,5	Aromatic Rings count	4
Rotatable bonds	10	Polarizability	67.17

Figure 8

The first page of MPDS *Aadhar card* generated from MPDS-ID search option of MPDS Compound Library. It depicts minimal critical information, which connects the unique *Aadhar card* number with: a) canonical SMILES, b) InChI Key, c) molecular formula, d) 2D structure, e) 56-bit fingerprint, f) IUPAC name, and g) molecular properties.

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- GA.png
- MPDSCLSupportingInformation.docx