wjpmr, 2025, 11(5), 165-173

SJIF Impact Factor: 6.842

WORLD JOURNAL OF PHARMACEUTICAL AND MEDICAL RESEARCH

www.wjpmr.com

Review Article

ISSN 2455-3301

WJPMR

MOLINSPIRATION IS INSPIRATION TO MOLECULE BY SOFTWARE IN DRUG DISCOVERY

[1*]Dr. Dhrubo Jyoti Sen, [2]Dr. Pruthviraj K. Chaudhary, [2]Upasana D. Sharma, [2]Manthankumar V. Oza, [3]Dhruvee H. Raval and [4]Dushyant P. Chaudhary

[1]School of Pharmacy, Techno India University, Salt Lake City, Sector-V, EM: 4/1, Kolkata-700091, West Bengal, India.
[2]Shri Sarvajanik Pharmacy College, Gujarat Technological University, Arvind Baug, Mehasana-384001, Gujarat, India.
[3]Sal Institute of Pharmacy, 19-Sola Kalol Road, Village: Bhadaj, 20, Opp. Science City, Sola Road, Ahmedabad-380060, Gujarat, India.
[4]The University of Texas at Arlington, 701 S Nedderman Drive, Arlington, Texas-76019, USA.

***Corresponding Author: Prof. (Dr.) Dhrubo Jyoti Sen**

School of Pharmacy, Techno India University, Salt Lake City, Sector-V, EM: 4/1, Kolkata-700091, West Bengal, India.

Article Received on 16/03/2025 **Article Revised on 06/04/2025** **Article Published on 26/04/2025**

ABSTRACT

Molinspiration is a widely utilized cheminformatics platform designed to assist in the prediction of molecular properties and biological activities of chemical compounds. This article provides a brief overview of the software, its features, and its relevance in pharmaceutical research. The inference and conclusion sections highlight its significance in early drug discovery and its practical applications for researchers. Molinspiration is a cheminformatics software company that provides tools for drug discovery and development, particularly in the areas of molecular property prediction, bioactivity prediction, and virtual screening. Their software helps researchers analyze and predict the properties of molecules, aiding in the identification of potential drug candidates. Molinspiration offers both software tools and free online services for various cheminformatics tasks. Molinspiration offers a molecular processing and property calculation toolkit written in Java. The toolkit may be used in a batch mode to process large number of molecules (processing speed is about 10,000 molecules/minute), or accessed through web interface directly on your intranet.

KEYWORDS: Lipinski's rule of five, Smiles notation, QSAR, Drug target, Cheminformatics, Lead molecule.

INTRODUCTION

The application of computational tools in drug discovery has become increasingly critical due to their efficiency in screening and evaluating large libraries of chemical compounds. Molinspiration is one such tool that provides researchers with the ability to perform rapid molecular property calculations and bioactivity predictions. This paper aims to present a concise examination of Molinspiration and its academic relevance, particularly for emerging researchers. Molinspiration offers broad range of cheminformatics software tools supporting molecule manipulation and processing, including SMILES and SDfile conversion, normalization of molecules, generation of tautomers, molecule fragmentation, calculation of various molecular properties needed in QSAR, molecular modelling and drug design, high quality molecule depiction, molecular database tools supporting substructure and similarity searches. An SD file, often referred to as an SDF file, is a file format used to store chemical structures and associated data. It utilizes the MOL connection table format, which describes the structure using text that lists atoms, bonds, connectivity, and coordinates. Chemical software can interpret this text to generate an image of the structure and display the associated data in a table. Our products support also fragment-based virtual screening, bioactivity prediction and data visualization. Molinspiration tools are written in Java, therefore can be used practically on any computer platform. SMILES notation is relatively easy to learn: "C" means carbon, "H" means hydrogen, "O" means oxygen, and so on, as defined in the periodic table.[1-3]

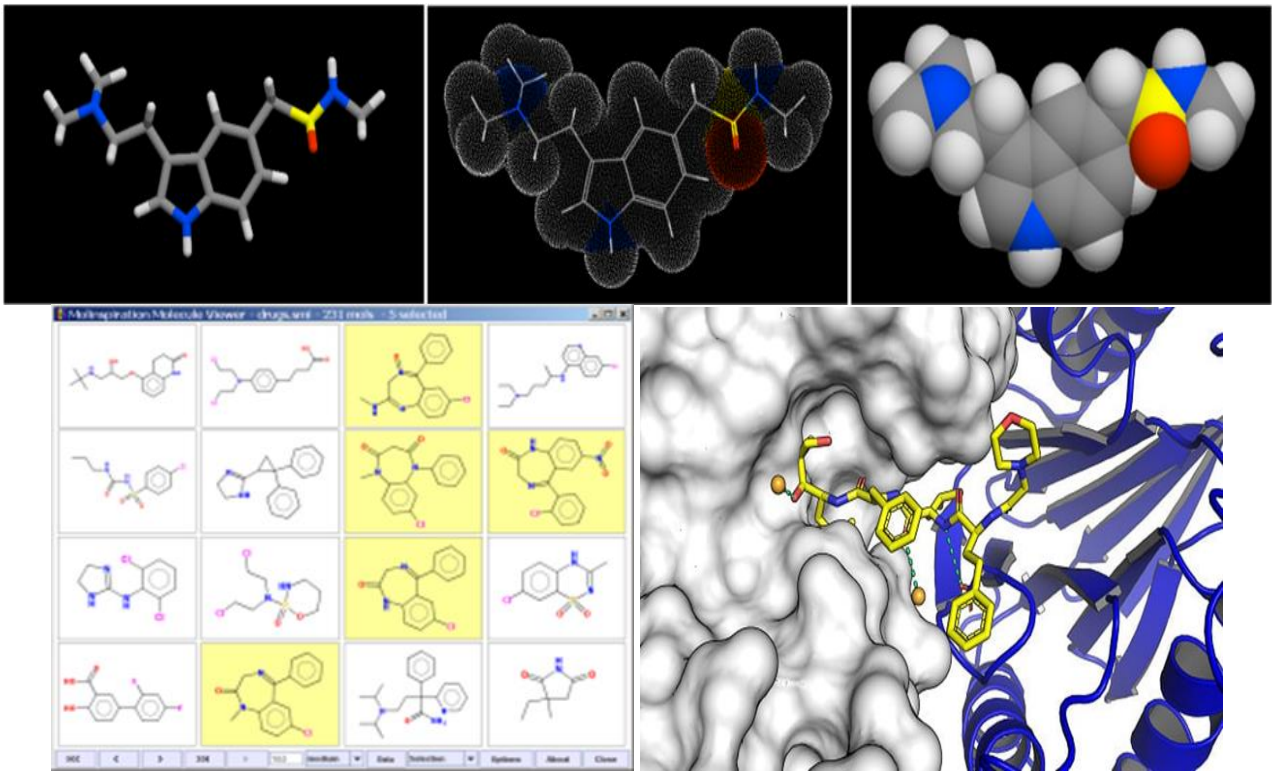


Figure 1: Chemical structure by software.

Single bonds are implied (common in condensed chemical formulas), double bonds are represented by "=", and triple bonds are represented by "#". Thus, CO2 is "O=C=O".

1. Molecular weight (MW) <500 Da
2. Number of hydrogen bond acceptors <10
3. Number of hydrogen bond donors <5
4. Calculated n-octanol-water partition coefficient (Clog P) <5
5. Rotational bond <10

Overview of Molinspiration: Molinspiration offers a user-friendly web interface that allows for the calculation of various molecular descriptors. These include LogP (octanol-water partition coefficient), topological polar surface area (TPSA), molecular weight, number of hydrogen bond donors and acceptors, and the number of rotatable bonds. Additionally, the software evaluates drug-likeness based on Lipinski's Rule of Five, a widely accepted criterion for oral bioavailability.

The platform also predicts bioactivity scores for key pharmacological targets, such as G-protein coupled receptors (GPCRs), ion channel modulators, kinase inhibitors, nuclear receptor ligands, and general enzyme inhibitors. These predictions are based on fragment-based models developed using large data sets of biologically active molecules. Cheminformatics enables the comparison of multiple compound structures, highlighting structural similarities and differences. This helps identify common motifs associated with specific bioactivities. SAR analysis often involves integrating chemical data (structure) with biological data (activity).[4-6]

Inference: The utility of Molinspiration lies in its ability to generate meaningful inferences regarding the biological potential of compounds. For instance, a compound with high predicted activity against GPCRs and favorable physicochemical properties may be considered a promising lead candidate. These predictions allow researchers to prioritize compounds for synthesis and in vitro testing, thereby optimizing time and resources. In Molinspiration, a bioactivity score greater than 0.00 suggests considerable biological activity, while scores between -0.50 and 0.00 indicate moderate activity, and scores less than -0.50 suggest inactivity. Bioactivity Score > 0.00: Indicates the molecule is likely to exhibit considerable biological activity.

Bioactivity Score between -0.50 and 0.00: Suggests moderate biological activity.

Bioactivity Score < -0.50: Indicates the molecule is likely to be inactive.

Molinspiration's Role: Molinspiration is an online software used for predicting physicochemical properties and bioactivity scores of molecules.

How it works: Molinspiration calculates the bioactivity score as a sum of activity contributions from fragments within the molecule.

Molinspiration's tools: Molinspiration offers free online services for calculating molecular properties and predicting bioactivity scores for drug targets.

Molinspiration Software Products: Molinspiration specializes in the development of cheminformatics

software in Java. Molinspiration tools are therefore platform independent and may be run on any PC, Mac, UNIX or LINUX machine. The software is distributed in a form of engines, which may be used as stand-alone computational engines, used to power web-based tools, or easily incorporated into larger in-house Java applications.

The following software is currently available

Mib engine: - calculation of important molecular properties, molecular processing (SMILES canonicalisation, normalization of charges), conversion between SMILES and SDfiles, SMILES depiction, generation of molecular images powered by the mib engine).

mib batch molecule processing v2024.01

Molinspiration mib engine allows batch processing of molecules encoded as SMILES or SDfiles. The engine supports broad range of cheminformatics functionalities, for example file conversion, structure normalization, generation of tautomers, calculation of molecular physicochemical properties and many others. The mib program is able to process large molecule files. For example, as a part of our research activities 33 million molecules from a PubChem database was converted from SDfile format to SMILES, normalised and properties for the molecules were calculated. mib is also used to standardize molecules and calculate properties by the ZINC virtual screening database.[7-9]

The program is written in Java, therefore is platform independent and runs on any Windows PC, Mac or LINUX server where Java runtime (version 11 or better) is available.

Running the program
The program is started by the following code:
java -jar mib.jar input_option [processing_options]

Input options
Molecules stored in the Daylight SMILES format or MDL SDfile format may be processed. Molecules from a file may be read by using the option
-f file_name
where the file_name is a file containing set of SMILESes, or SDfile. SDfile will be automatically recognized by an extension ".sdf", ".sd" or ".mol". All other files are assumed to contain SMILES. In this case SMILES must be a first item in a line. The line may contain also other items (molecule name, other data), tab separated.

Compressed files with extension .gz, gzip, or zip may be processed without necessity to unpack them.

Data from the SDfile may be retrieved by using the -keep parameter. For example:
java -jar mib.jar -f mdpi.smi -keep "MolName,Amount"
retrieves also parameters named MolName and Amount from the SDfile.
If you want to retrieve all parameters use the parameter -keepall
Processing of a single SMILES is possible by using a -smi input parameter (in this case SMILES string must be in quotes).
java -jar mib.jar -smi 'molecule_smiles'
Output options: When no output options are provided, a file with canonised SMILES is generated and sent to the standard output.
When a SDfile should be generated, the parameters -out sdf is required.
Processing options: When no processing options are given, canonical SMILESes of inputted molecules are generated and sent to the standard output. This may be redirected to a file by the > redirection operator

Molecule normalization: Various parameters allow modification and processing of molecules.
-nostereo stereo information in molecules will not be considerer
-normalizeCharges atomic charges will be normalized when possible
-singlePart only the main (largest) part of a multipart molecule will be processed
-standardize is a shortcut for all three previous options together
-normalizeIsotopes removes all isotope labels from atoms
-isostandardize is a shortcut for -standardize plus -normaliseIsotopes

The mib package performs strict valence checking and discards molecules violating organic valence rules (when skipping molecules with errors, respective error messages are issued). They keyword:
-kmwve (mnemonic for "keep molecules with valence errors") allows processing also of molecules with non-standard valencies

Calculation of molecular properties

- Molecular properties for molecules on input are calculated when using the keyword -properties
- The following properties are available on the output (in this order); items are tab separated:
- logP octanol-water partition coefficient
- PSA polar surface area
- Number of nonhydrogen atoms
- Molecular weight
- Number of hydrogen-bond acceptors (O and N atoms)
- Number of hydrogen-bond donors (OH and NH groups)
- Number of Rule of 5 violations
- Number of rotatable bonds
- Molecular volume

When using the keyword -header in the SMILES output

mode, the first line of output is a header with property names.

The mib property calculation engine is used in numerous instances by our industry customers and powers also our free online property calculation tool.[10-12]

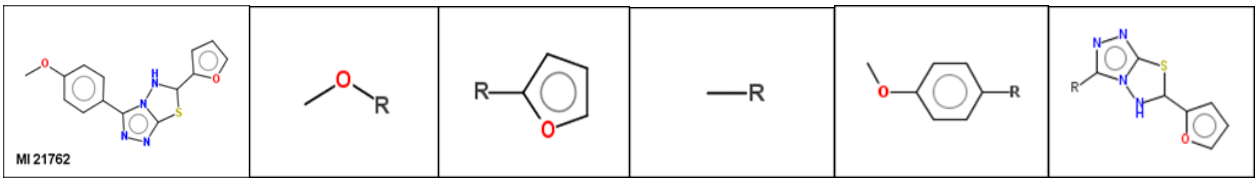


Figure 2: Molecular fragmentation.

Molecule formula: When using the keyword -formula the molecule formula is part of the output. This keyword may be used together with the -properties keyword.

Molecule fragmentation: mib allows fragmentation of molecules into various types of fragments. Below examples of various fragmentation options are given.

The parent molecule used for the fragmentation is the structure shown above.
-r1 - substituents (Rgroups); all "breakable" nonring single bonds are broken to generate substituent
-r2 - spacers (groups with 2 attachment points)

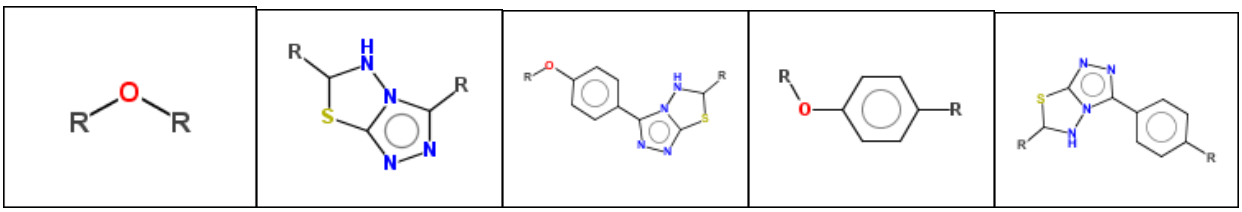


Figure 3: Ring orientation.

- **ringsystems -** ring systems is a collection of fused or spiro rings

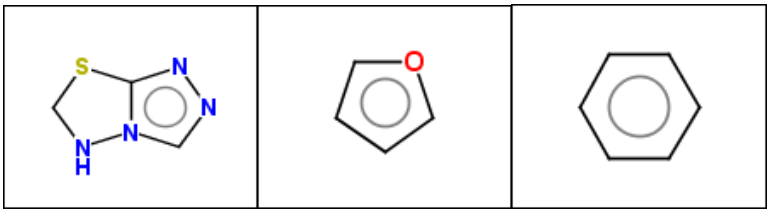


Figure 4: Ring systems.

-simple Rings - simple rings which this molecule contains. Simple ring does not need to be a valid molecule (in example below, in the sulfur ring only 2 atoms are aromatic) therefore results are provided as fragment SMILES (note that aromatic bonds in fragments are displayed as dashed lines on images below)
C1Sc:nN1
c:1:n:n:c:n:1
c:1:c:c:c:c:c:1
o:1:c:c:c:c:1

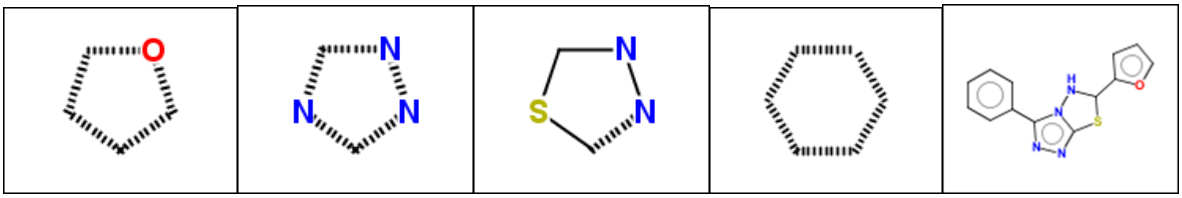


Figure 5: Ring scaffolds.

-scaffold - is ring part of a molecule (rings systems and their connections) without aliphatic substituents

-hose - generates so called HOSE fragments (atoms with environment). A HOSE fragment consists of a central atom (first atom in HOSE SMILES) and several levels of surrounding atoms.

HOSE fragments may be used as structural descriptors by QSAR studies or fragment-based property prediction applications.

Fragmentation parameters.[13-15]

By default, the size of the r1 and r2 fragments is limited to 15 atoms. This may be changed by a parameter -maxsize n (this parameter does not affect other types of fragments).
Generated fragments are written in the output line after input SMILES (in a canonized form) and any other parameters from the input. All items are tab separated.

Parameter- List allows to perform fragmentation statistics for large collections of molecules. On the output a list of fragments is provided, together with the number of molecules containing these fragments.

The following command provides list of substituents up to 8 atoms, which are most common in GPCR ligands.
java -jar mib.jar -f gpcr.smi -standardize -r1 -max 8 -list > gpcr.r1

The first lines of the output file are

[R]C	539
[R]c1ccccc1	213
[R]O	204
[R]OC	193
[R]N	191
[R]Cl	172
[R]F	133
[R]CC	83
[R]CCC	71
[R]C(O)=O	67

When using parameter -count also the number of fragments of particular type will be provided, in the form fragment1 count1 fragment2 count2 (tab separated)

For example command
Java -jar mib.jar -smi 'c1ncccc1' -hose -maxSize 1

Provides output
c1ccncc1 [n] [cH]

While when using also the parameters -count the output includes also the number of respective fragments in the molecule

c1ccncc1 [n] 1 [cH] 5

When using the parameter -count together with the parameter -list, the number on output provides the total number of fragments of this type in the molecule set (and not just the number of molecules with this fragments as by -list alone).

-maxsize sets the maximum size of generated fragments. This is ignored when generating rings and scaffolds, and makes sense only by -r1 and -r2 fragments and HOSE fragments (in this case -maxsize is the number of surrounding levels, 1 - just central atom, 2 - single level of neighbors, 3 - 2 levels of neighbors, etc).

Fragmentation is applied only to the main part of multipart molecules (as the keyword -singlepart would be used). [This may be modified in later release of the toolkit].

Generation of tautomers: Tautomers of processed molecules may be generated by using the option -tautomer. In the output line canonized SMILES of the original molecule, followed by eventual data contained in the input line are provided, followed by a number giving the number of generated tautomers and SMILES codes of these tautomers. All data in line are tab separated.

The command java mib -smi 'n1c(O)cccc1' -tautomers provides the following output
Oc1ccccn1 2 O=c1cccc[nH]1 Oc1ccccn1

To get tautomers of a single molecule one tautomers SMILES per line (this output may be displayed for example by the Molinspiration molecule viewer) use the -list option.

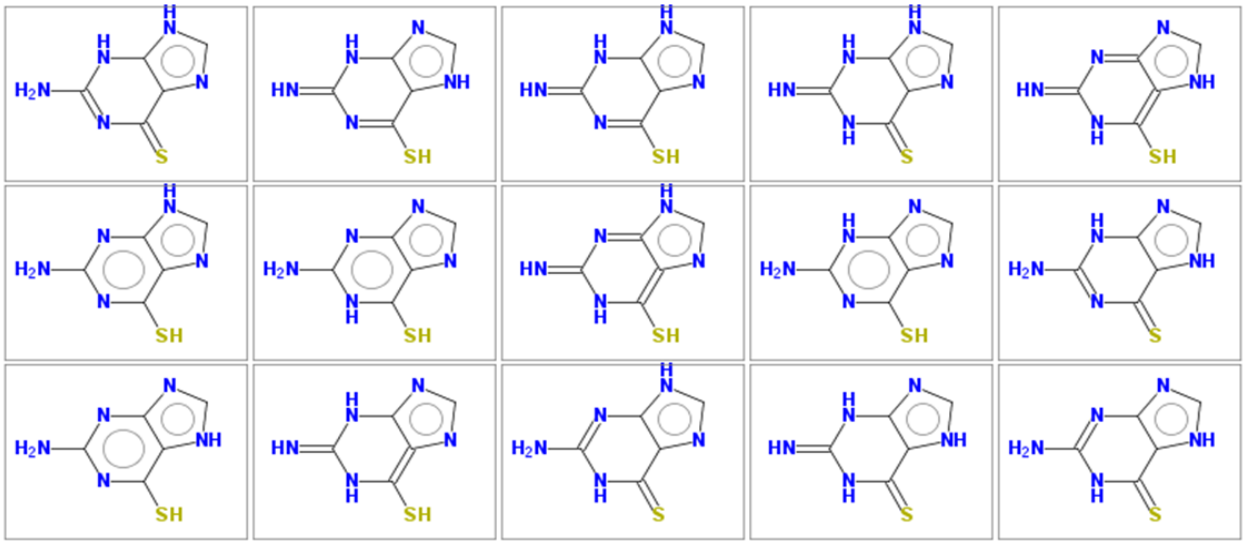


Figure 6: Tautomers.

The command

java -jar mib.jar -smi 'Nc2nc1nc[nH]c1c(=S)[nH]2' -tautomers -list > tautomers.smi saves the following output to the tautomers.smi file (the source SMILES in this example is thioguanine)

Nc2nc(=S)c1nc[nH]c1[nH]2	1
Sc1nc(=N)[nH]c2nc[nH]c12	1
Sc1nc(=N)[nH]c2[nH]cnc12	1
N=c2[nH]c(=S)c1nc[nH]c1[nH]2	1
Sc1[nH]c(=N)nc2nc[nH]c12	1
Nc2nc(S)c1nc[nH]c1n2	1
Nc2nc1ncnc1c(S)[nH]2	1
Sc1[nH]c(=N)nc2[nH]cnc12	1
Nc2nc(S)c1ncnc1[nH]2	1
Nc2nc(=S)c1[nH]cnc1[nH]2	1
Nc2nc(S)c1[nH]cnc1n2	1
Sc1[nH]c(=N)[nH]c2ncnc12	1
Nc2nc1[nH]cnc1c(=S)[nH]2	1
N=c2[nH]c(=S)c1[nH]cnc1[nH]2	1
Nc2nc1nc[nH]c1c(=S)[nH]2	1

The 15 tautomers generated are shown below

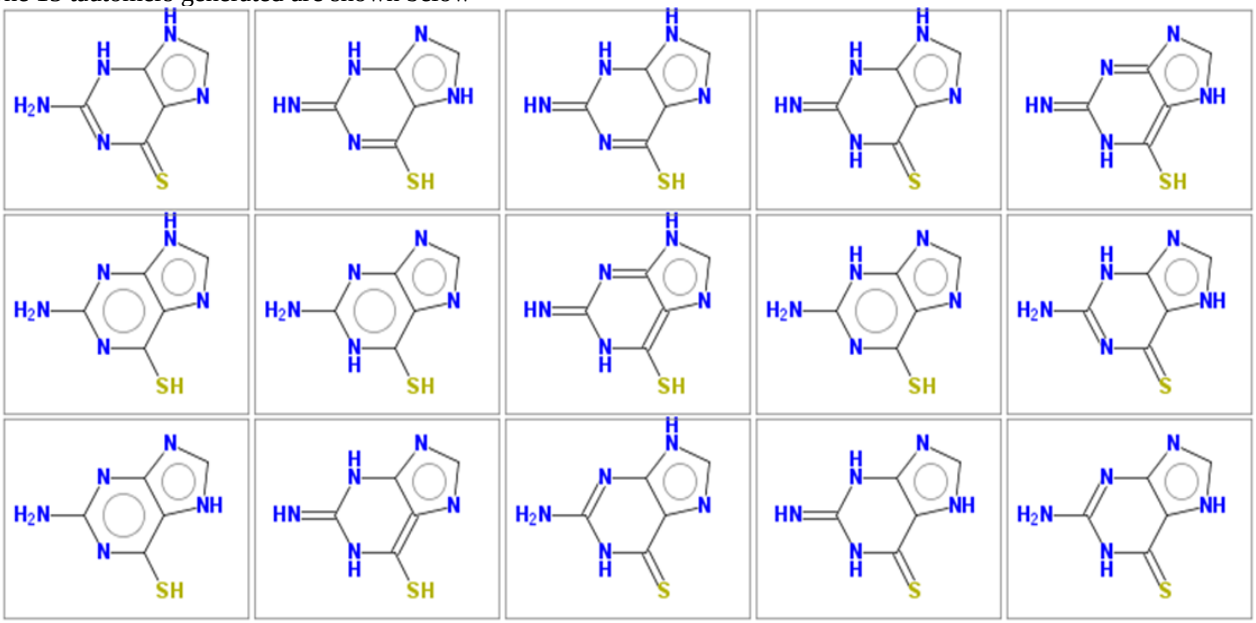


Figure 7: Molecular Tautomers.

Some molecules may have very large number of tautomers (several hundreds), to keep computational time reasonable, the default number of generated tautomers is limited to 50. This limit may be increased by parameter -maxtautomers n. Tautomers are listed on the output in alphabetic order.

EZ stereochemistry on tautomeric bonds is not preserved during tautomer enumeration.

Contact us please at info[at]molinspiration.com to arrange an evaluation license of mib.

Misearch engine:- Flexible engine supporting substructure, similarity and pharmacophore similarity searches.

Miscreen engine- virtual screening engine enabling development of pharmacophore models, validation and screening of large molecular libraries [Predict Bioactivity]).

Galaxy:- 3D structure generator. Generates 3D structures from SMILES. Currently in beta.

Galaxy Visualizer is a web tools that allows easy creation of 3D molecular structures from SMILES by using Molinspiration Galaxy 3D generator. Created molecules may be interactively examined in various display modes, including visualization of various surface properties, such as molecular lipophilicity potential (MLP) and polar surface area (PSA). MDL Molfiles of generated structures may be downloaded for use by in-house programs. Molecules may be visualized as wire-frame models, tube models, dotted molecular surfaces and space-filling CPK models.

Galaxy Visualizer allows to visualize molecular lipophilicity potential (MLP) on the molecular surface to see which parts of the surface are hydrophobic (encoded

by violet and blue colors) and which hydrophilic (orange and red). MLP is calculated from atomic hydrophobicity contributions, the same that are used to calculate the octanol-water partition coefficient (logP) by our miLogP method. MLP is useful property to rationalize various molecular ADME characteristics (like membrane penetration or plasma-protein binding). Analysis of 3-dimensional distribution of hydrophobicity on molecular surface is particularly helpful when explaining differences in observed ADME properties of molecules with the same logP, since, of course, 3D parameter contains much more information then logP expressed by just a single value.[16-18]

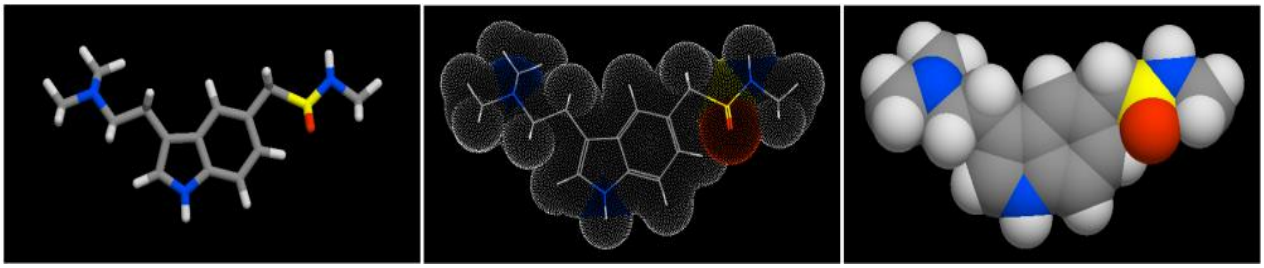


Figure 8: 3D structures.

Several common drugs having the same logP (about 2.5) but exhibiting very different 3D hydrophobicity distribution.

Molinspration Property Calculator: - easy interactive calculation of molecular properties, generation of QSAR tables.

Calculation of molecular physicochemical properties relevant to drug design and QSAR, including logP, molecular polar surface area (PSA), and the Rule of 5 descriptors. More information about the calculated parameters; see also the property calculation FAQ. Calculation of bioactivity score and drug-likeness for GPCR ligands, ion channel modulators, kinase inhibitors and nuclear receptor ligands (interactive virtual screening), choose the [Predict Bioactivity] option.

More information about calculation of bioactivity scores and virtual screening. Generation of 3D molecular geometry from molecular connectivity information (SMILES) by a Molinspiration 3D structure generator Galaxy (currently in beta). Substructure and similarity search to illustrate the Molinspiration web-based structure search technology.

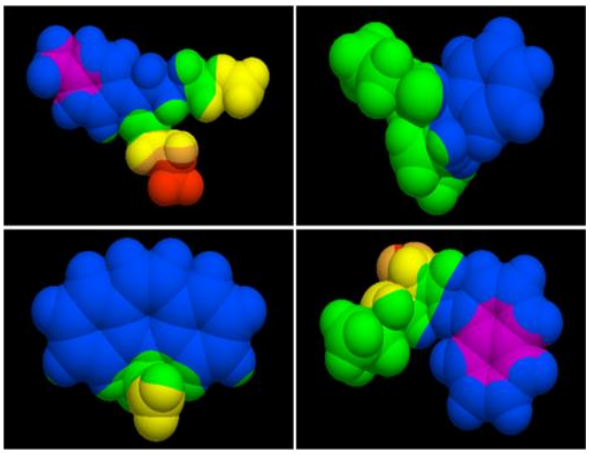


Figure 9: 3D structures by chem sketch.

More information about the structure search engine. The future of free Molinspiration interactive services depends also on you! Let us know which other services would you find useful in your work. Any comments and suggestions are welcome!
Molinspiration Molecule Viewer:- Visualization of large sets molecules.
Molinspiration Data Viewer:- Visualization of QSAR datasets with interactive molecule display.

Molinspiration DataViewer midv supports visualization of molecules and related numerical data and easy data mining. Additionally, the midv allows generation of graphs in publication quality. Even very large collections of molecules (100'000 structures) can be interactively visualized. Viewer is written in Java, therefore is platform independent and may be used on any computer where the Java runtime (version 1.4 or better) is installed.[19]

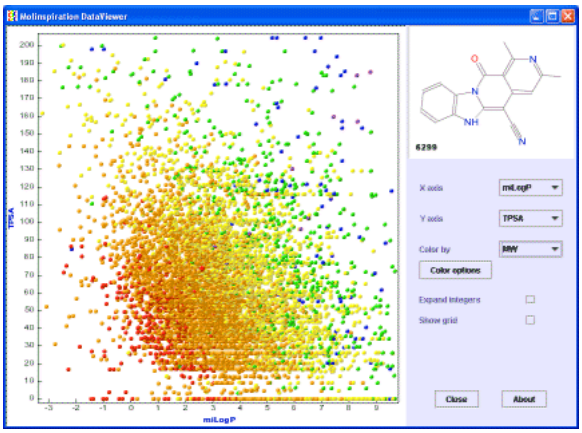


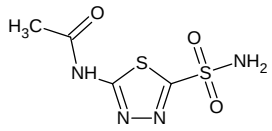
Figure 10: Electronic cloud.

Molinspiration Depiction:- High quality depiction of molecules encoded as SMILES of MDL Molfile. Molinspiration Depiction software allows generation of high-quality molecule images in png format from a Daylight SMILES string or MDL Molfile. The program may be used either from a command line as described

below, or be incorporated into a cgi script or a servlet to generate depictions of molecules in various interactive cheminformatics web services. You may see the Molinspiration Depiction in action by entering SMILES to depict into this interface. The program is started by a command:
Java -jar depiction.jar -smi 'smiles' | -f file [-options] > image.png
Where the 'file' is a MDL Molfile or a file containing single SMILES string

Options are used to set-up various image parameter
-x imageWidth -y imageHeight determine size of the image
-bw black-and-white image will be generated
-blackbg image with black background will be generated
-border a border around image will be rendered
-text 'infoText' text information will be added to the image
-cg common functional groups will be collapsed (useful when rendering large complex molecules)

Acetazolamide



O=S(N)(=O)c1nnc(NC(C)=O)s1

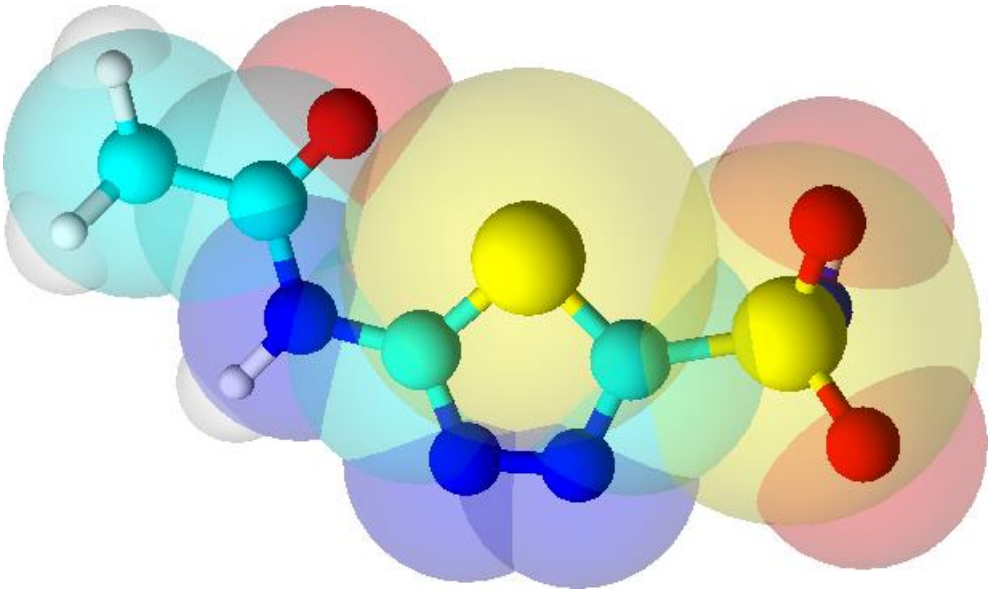


Figure-11: Drug structure, smiles, 3D view with electron cloud.

-new when rendering molecule from Molfile new geometry will be generated from connectivity (otherwise 2D coordinates from the source Molfile are used)
-transp generates molecule image with transparent backgrund, allowing to change background programatically with JavaScript
-aab changes the default depiction of aromatic rings with inner "cicles" to display with alternating single and double bonds.

Also highlighting of various parts of the molecule (atoms, bonds, rings) is possible. This feature is still in beta, so if you are interested, please contact us for details.

Database of Bioactive Substituents and Linkers: - database of 21 thousand substituents and 49 thousand linkers extracted from bioactive molecules including also calculated properties.

Collection of Substituents and Spacers Extracted from Bioactive Molecules.

Molinspiration offers a database of substituents and spacers (linkers) obtained by substructure analysis of a collection of current drugs, development drugs and other molecules with biological activity containing about 17000 entries. The database is provided in SMILES or SDfile format and includes also calculated physicochemical properties (the same properties as offered by our interactive property calculation service). This dataset contains about 21 thousand substituents and 49 thousand linkers (66% of those beeing ring systems) having up to 15 nonhydrogen atoms.

Possible application area of the database includes virtual combinatorial chemistry, generation of bioactive molecules with desired properties by combining spacers and substituents, or bioisosteric design by replacing selected substructures in target molecules by their analogs identified by property similarity search. Molinspiration can offer help in implementing these or similar applications.[20]

Example data
20 most common substituents in SMILES format

20 most common substituents in SDfile format
20 most common spacers in SMILES format
20 most common spacers in SDfile format

CONCLUSION

Molinspiration serves as an essential tool in computational chemistry and drug design. Its predictive capabilities provide valuable insights that support decision-making in the early stages of pharmaceutical research. For researchers tools such as Molinspiration not only facilitate a deeper understanding of molecular behavior but also play a critical role in translating theoretical knowledge into practical applications in drug development. Molinspiration supports internet chemistry community by offering free on-line services for calculation of important molecular properties (logP, polar surface area, number of hydrogen bond donors and acceptors and others). Number of molecules processed per month exceeds 100,000! Molinspiration is a privately owned company specializing in cheminformatics software and tools. They provide a range of software and web-based services for molecular manipulation, property calculation, and bioactivity prediction, particularly in drug discovery and related fields. Their tools are used by researchers in academia and industry for tasks like QSAR (Quantitative Structure-Activity Relationship) analysis, molecular modeling, and virtual screening.

REFERENCES

1. Lipinski, C. A. Lead- and drug-like compounds: the rule-of-five revolution. Drug Discovery Today: Technologies, 2004; 1(4): 337–341.
2. Moreira, I.S.; Fernandes, P.A.; Ramos, M.J. Protein-protein docking dealing with the unknown. J. Comput. Chem., 2010; 31: 317–342.
3. Dominguez, C.; Boelens, R.; Bonvin, A.M. HADDOCK: A protein-protein docking approach based on biochemical or biophysical information. J. Am. Chem. Soc., 2003; 125: 1731–1737.
4. Lyne, P.D. Structure-based virtual screening an overview. Drug Discov. Today, 2002; 7: 649–657.
5. Stahura, F.L.; Bajorath, J. Virtual screening methods that complement HTS. Comb. Chem. High Throughput Screen, 2004; 7: 259–269.
6. Kodadek, T. The rise, fall and reinvention of combinatorial chemistry. Chem. Commun, 2011; 47: 9757–9763.
7. Oprea, T.I.; Matter, H. Integrating virtual screening in lead discovery. Curr. Opin. Chem. Biol., 2004; 8: 349–358.
8. Geppert, H.; Vogt, M.; Bajorath, J. Current trends in ligand-based virtual screening: Molecular representations, data mining methods, new application areas, and performance evaluation. J. Chem. Inf. Model, 2010; 50: 205–216.
9. Ripphausen, P.; Nisius, B.; Bajorath, J. State-of-the-art in ligand-based virtual screening. Drug Discov. Today, 2011; 16: 372–376.
10. Sliwoski, G.; Kothiwale, S.; Meiler, J.; Lowe, E.W., Jr. Computational methods in drug discovery. Pharmacol. Rev., 2013; 66: 334–395.
11. Inglese, J.; Auld, D.S.; Jadhav, A.; Johnson, R.L.; Simeonov, A.; Yasgar, A.; Zheng, W.; Austin, C.P. Quantitative high-throughput screening: A titration-based approach that efficiently identifies biological activities in large chemical libraries. Proc. Natl. Acad. Sci. USA, 2006; 103: 11473–11478.
12. Jarrahpour, A.; Fathi, J.; Mimouni, M.; Hadda, T.B.; Sheikh, J.; Chohan, Z.; Parvez, A. Petra, Osiris and Molinspiration (POM) together as a successful support in drug design: Antibacterial activity and biopharmaceutical characterization of some azo Schiff bases. Med. Chem. Res., 2012; 21: 1984–1990.
13. Milletti, F.; Storchi, L.; Sforna, G.; Cruciani, G. New and original pKa prediction method using grid molecular interaction fields. J. Chem. Inf. Model, 2007; 47: 2172–2181.
14. Spitzer, G.M.; Heiss, M.; Mangold, M.; Markt, P.; Kirchmair, J.; Wolber, G.; Liedl, K.R. One concept, three implementations of 3D pharmacophore-based virtual screening: Distinct coverage of chemical search space. J. Chem. Inf. Model, 2010; 50: 1241–1247.
15. Wolber, G.; Seidel, T.; Bendix, F.; Langer, T. Molecule-pharmacophore superpositioning and pattern matching in computational drug design. Drug Discov. Today, 2008; 13: 23–29.
16. Jones, G.; Willett, P.; Glen, R.C. A genetic algorithm for flexible molecular overlay and pharmacophore elucidation. J. Comput. Aided Mol. Des., 1995; 9: 532–549.
17. Martin, Y.C.; Bures, M.G.; Danaher, E.A.; DeLazzer, J.; Lico, I.; Pavlik, P.A. A fast new approach to pharmacophore mapping and its application to dopaminergic and benzodiazepine agonists. J. Comput. Aided. Mol. Des., 1993; 7: 83–102.
18. Richmond, N.J.; Abrams, C.A.; Wolohan, P.R.N.; Abrahamian, E.; Willett, P.; Clark, R.D. Galahad: 1. Pharmacophore identification by hypermolecular alignment of ligands in 3D. J. Comput. Aided Mol. Des., 2006; 20: 567–587.
19. Sen, D.J.; Nandi, K.; and Saha, D.; Rule of five: the five men army to cross the blood brain barrier for therapeutically potent: World Journal of Advance Healthcare Research, 2021; 5(3): 206–211.
20. Sen, D.J.; Information technique in biosystem by cheminformatics & bioinformatics: a unique tool in drug discovery: European Journal of Biomedical and Pharmaceutical Sciences, 2024; 11(3): 339-351.