DATE: 06-09-22

WEBLEM 2

BIOVIA Draw software & Open Babel Tool

Aim:

Introduction to Chemical Strucutre (1D, 2D and 3D), Drawing using BIOVIA DRAW Software and File conversion using Open Babel Tool

Introduction:

Chemical Structure:

A drug's chemical composition impacts its physicochemical characteristics, which in turn influence its ADME/Tox characteristics, which in turn influence its pharmacological action. By changing the shape of drug molecules, medicinal chemists can control the pharmacological activity of a given substance. A drug's ring systems and functional groups are crucial parts. The percentage of heavy atoms in a medicine is determined by the ratio of non-hydrogen to non-hydrocarbon atoms. The three variables have a lot of potential for determining whether organic compounds have drug-like characteristics. To the best of our knowledge, however, no studies have been done to systematically examine the simultaneous impacts of the quantity of aromatic and non-aromatic rings, the quantity of specific functional groups, and the fraction of heavy atoms on the drug-like qualities of an organic molecule.

1. BIOVIA Draw Software:

History:

Accelrys was formed in 2001 as a wholly owned subsidiary of Pharmacopeia, Inc. from the fusion of five companies: Molecular Simulations Inc., Synopsys Scientific Systems, Oxford Molecular, the Genetics Computer Group (GCG), and Synomics Ltd. MSI, itself a result of the combination of Biodesign, Cambridge Molecular Design, Polygen and, later, Biocad and BiosymTechnologies.

Introduction:

BIOVIA is a software company headquartered in the United States, with representation in Europe and Asia. It provides software for chemical, materials and bioscience research for the pharmaceutical, biotechnology, consumer packaged goods, aerospace, energy and chemical industries. Previously named Accelrys, it is a wholly owned subsidiary of Dassault Systèmes after an April 2014 acquisition and has been renamed BIOVIA.

BIOVIA Draw has the same look-and-feel as ISIS/ Draw, but brings additional speed and efficiency to chemical structure drawing:

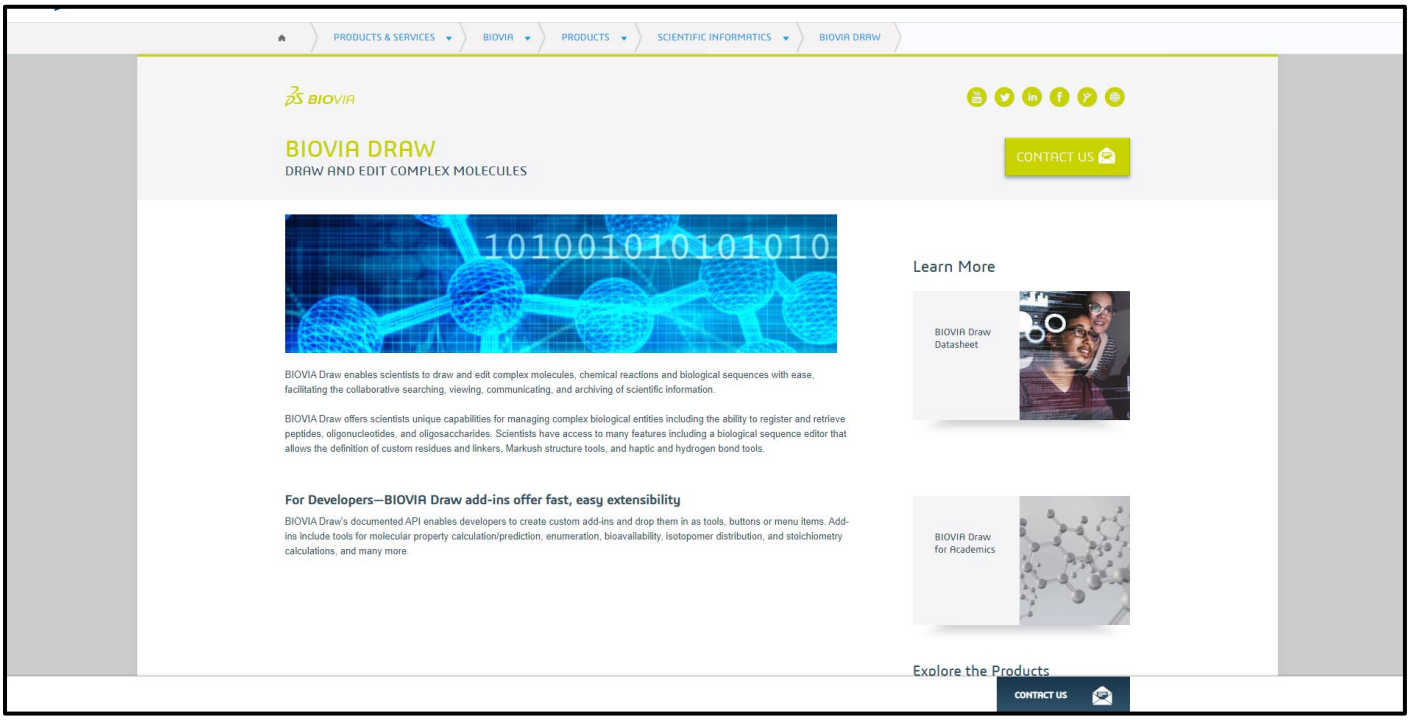
- Continuously draw bonds, pull out rings and add atoms using all-purpose drawing tool
- Drag-and-drop commonly-used structures and chemical abbreviations onto the toolbar for reuse
- Right-click for atom, bond, fragment properties and query options
- Hover over atoms and edit them without right-click
- Quickly retrace steps using Multiple Undo/Redo
- Easily create structures with R groups for queries or enumerations
- Annotate reaction schemes with text, colour and a variety of arrow styles
- Easily create publication quality structures for inclusion in Microsoft Office Documents and presentations.

Applications:

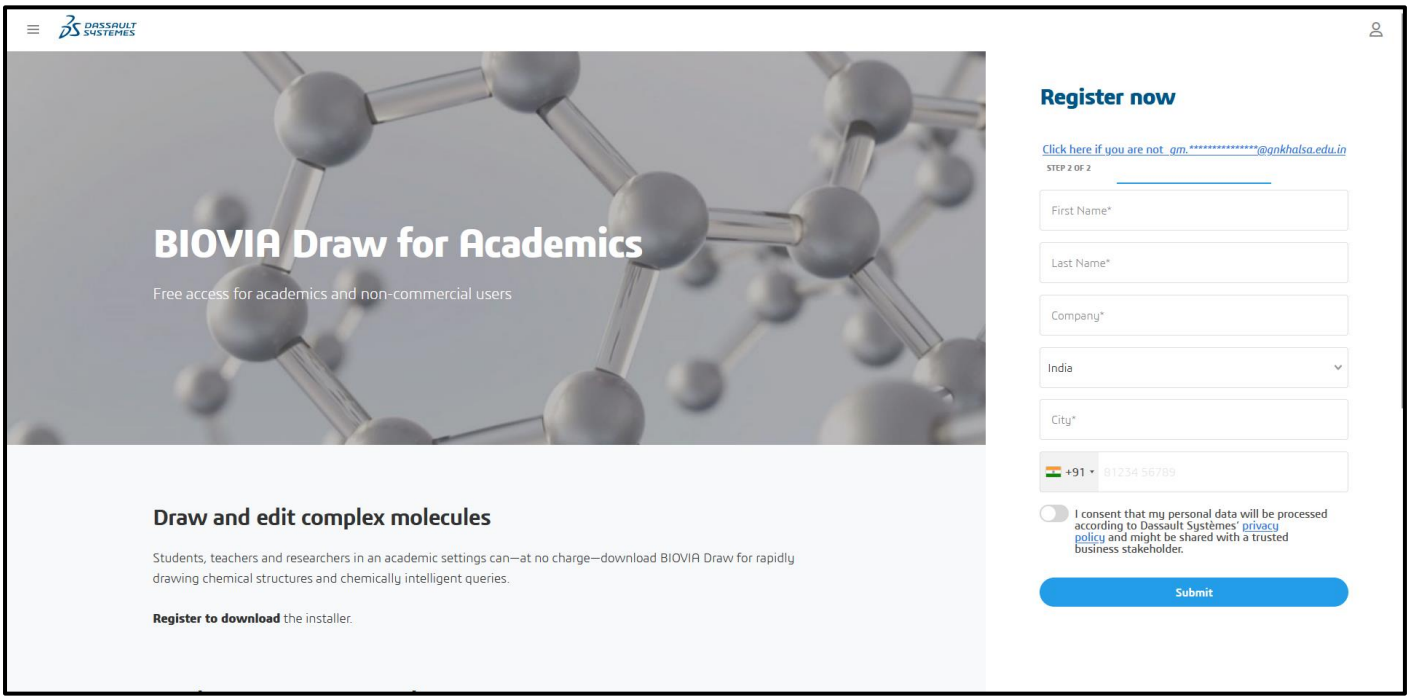
Simulate, visualize and analyse chemical and biological systems and to communicate the results to other scientists.

Installation Steps:

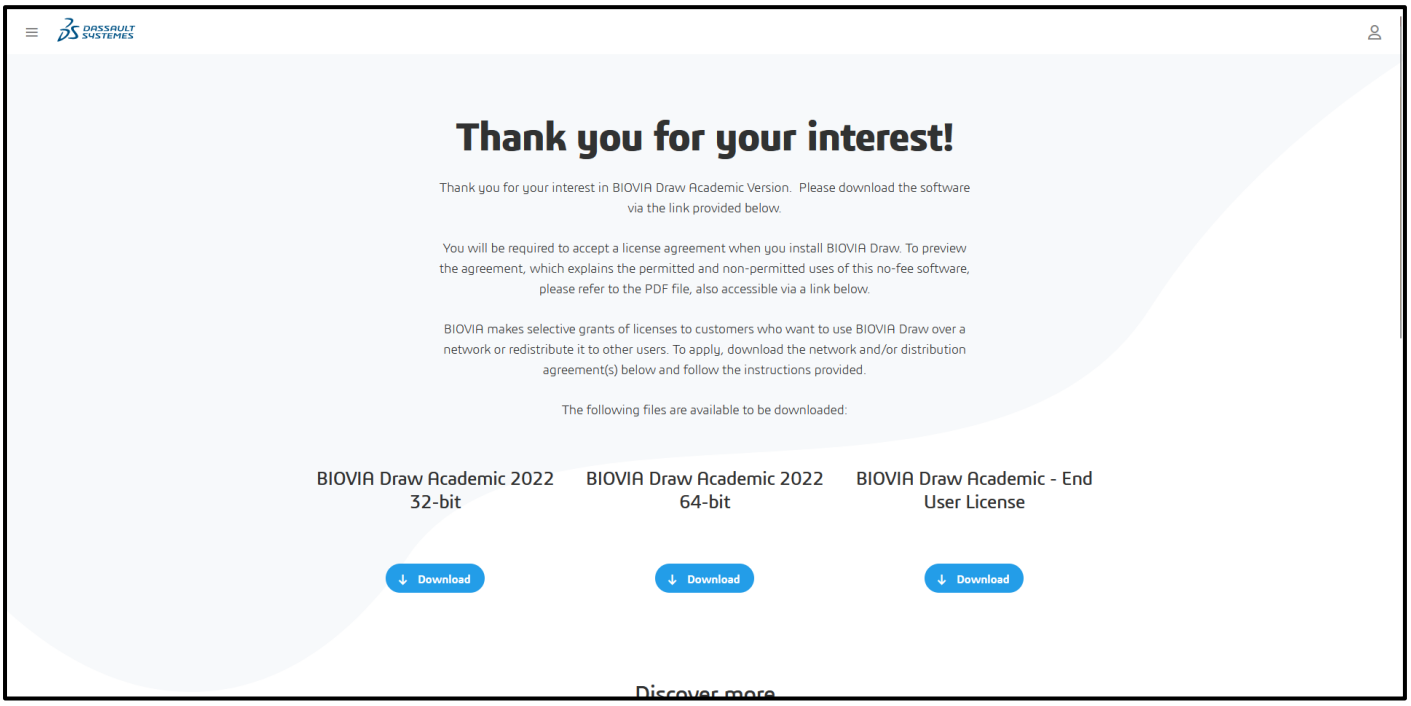
1. Open Homepage of BIOVIA DRAW software website and then click on BIOVIA Draw for Academics (URL: https://www.3ds.com/products-services/biovia/products/scientific-informatics/biovia-draw/).



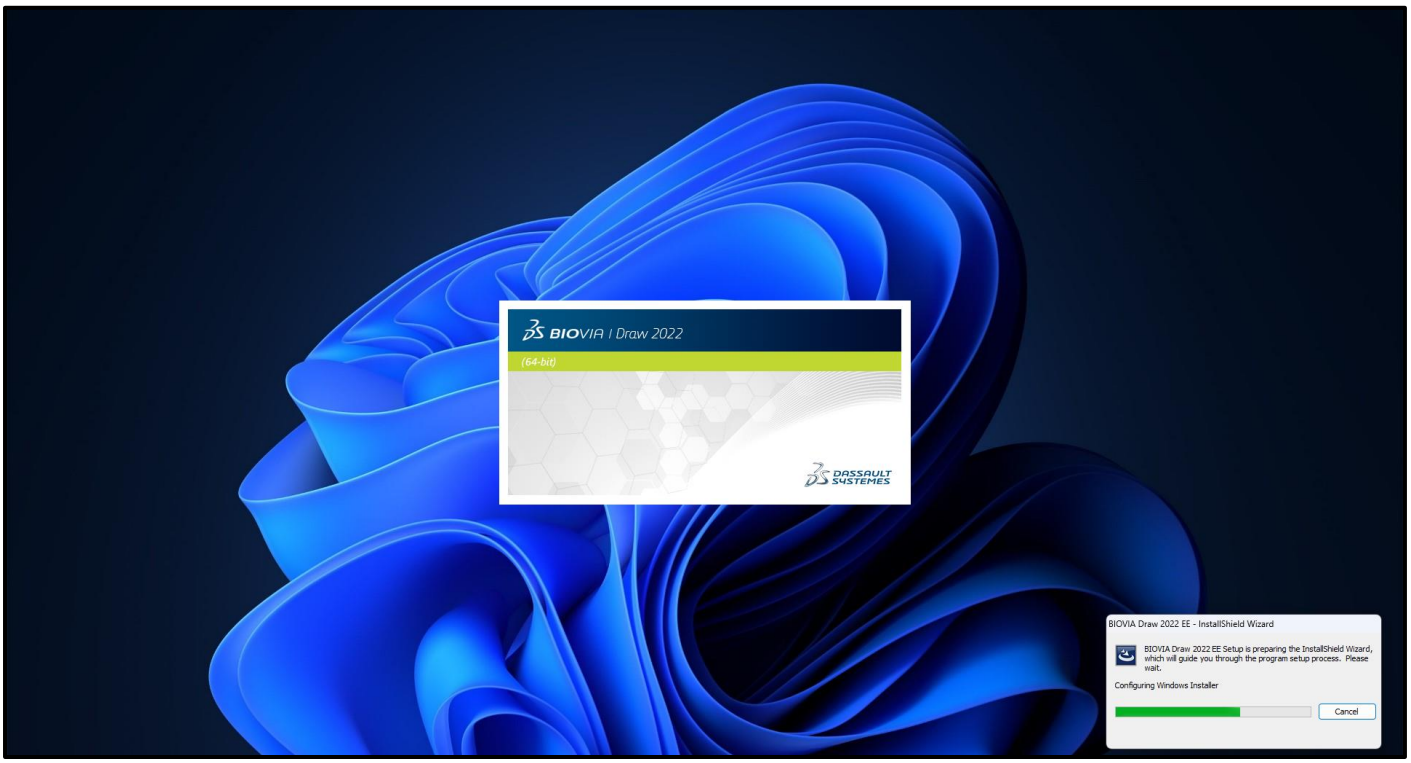
2. Fille the registration details and click on submit



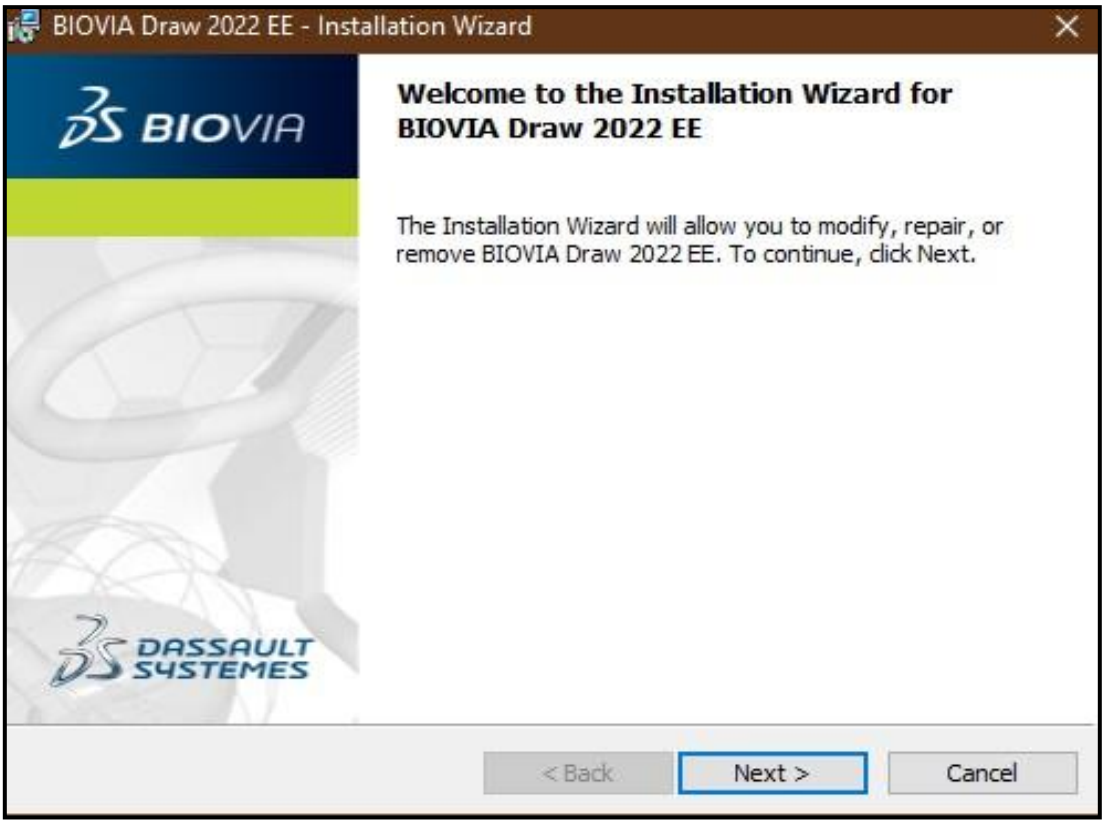
3. Download BIOVIA DRAW Academic 2022

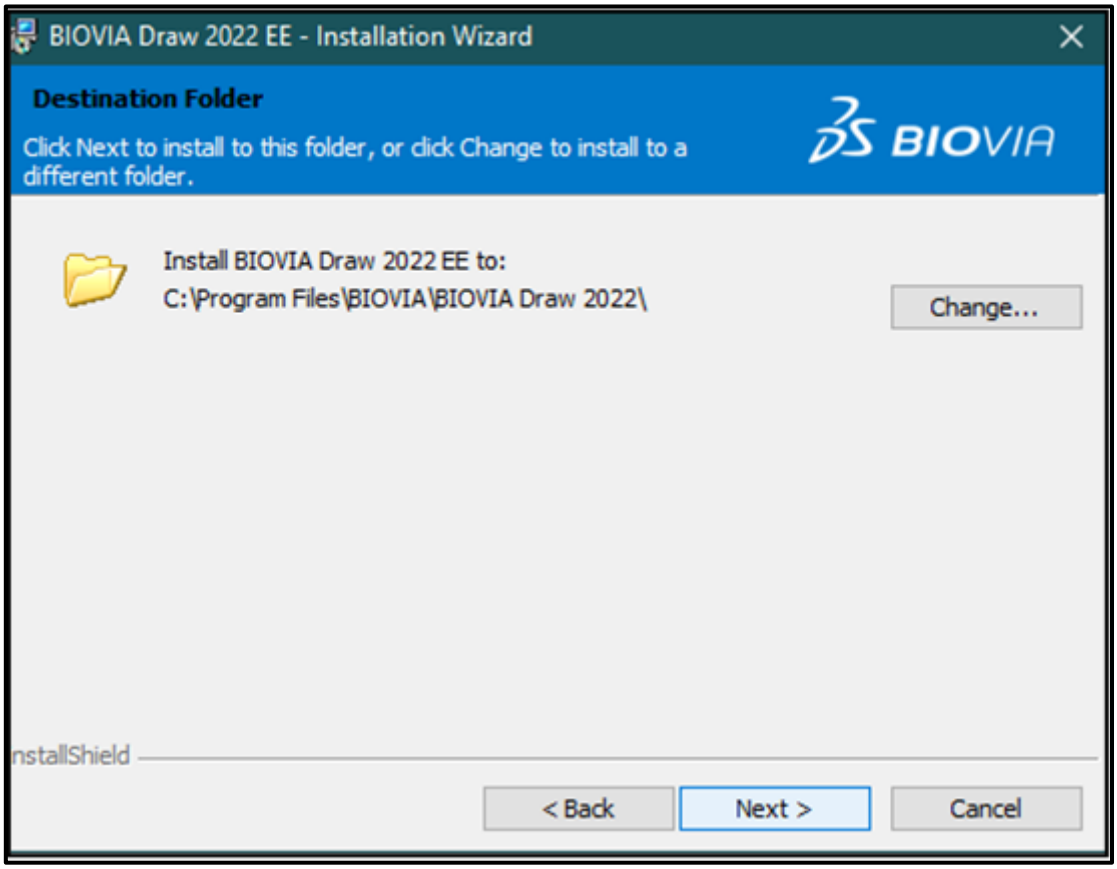


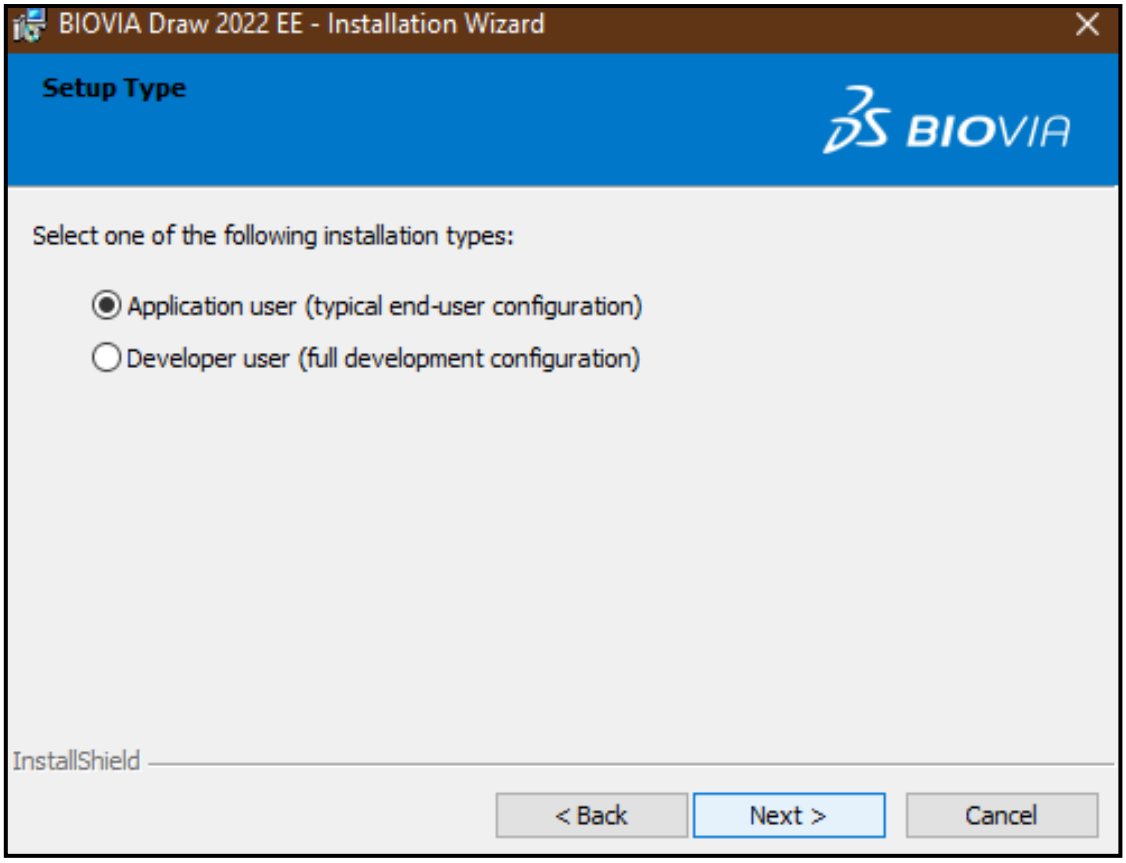
4. After Downloading, open it on your PC or Laptop

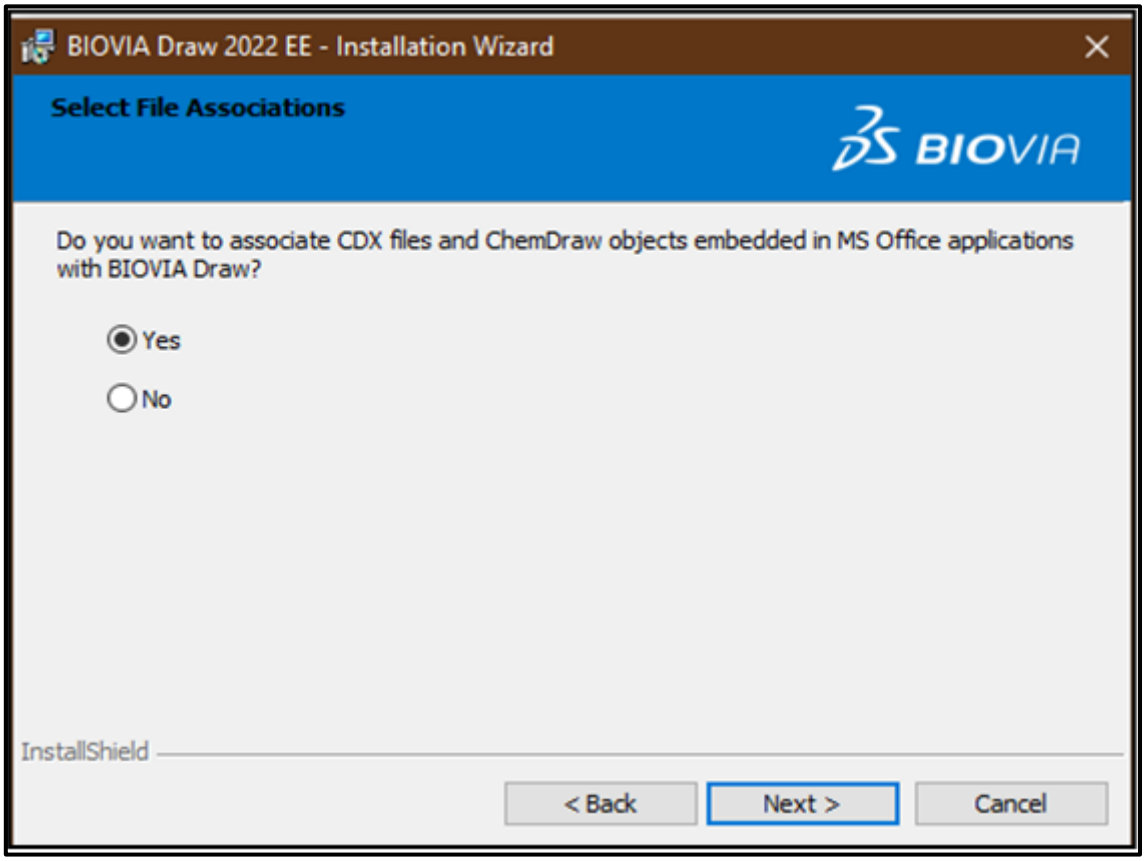


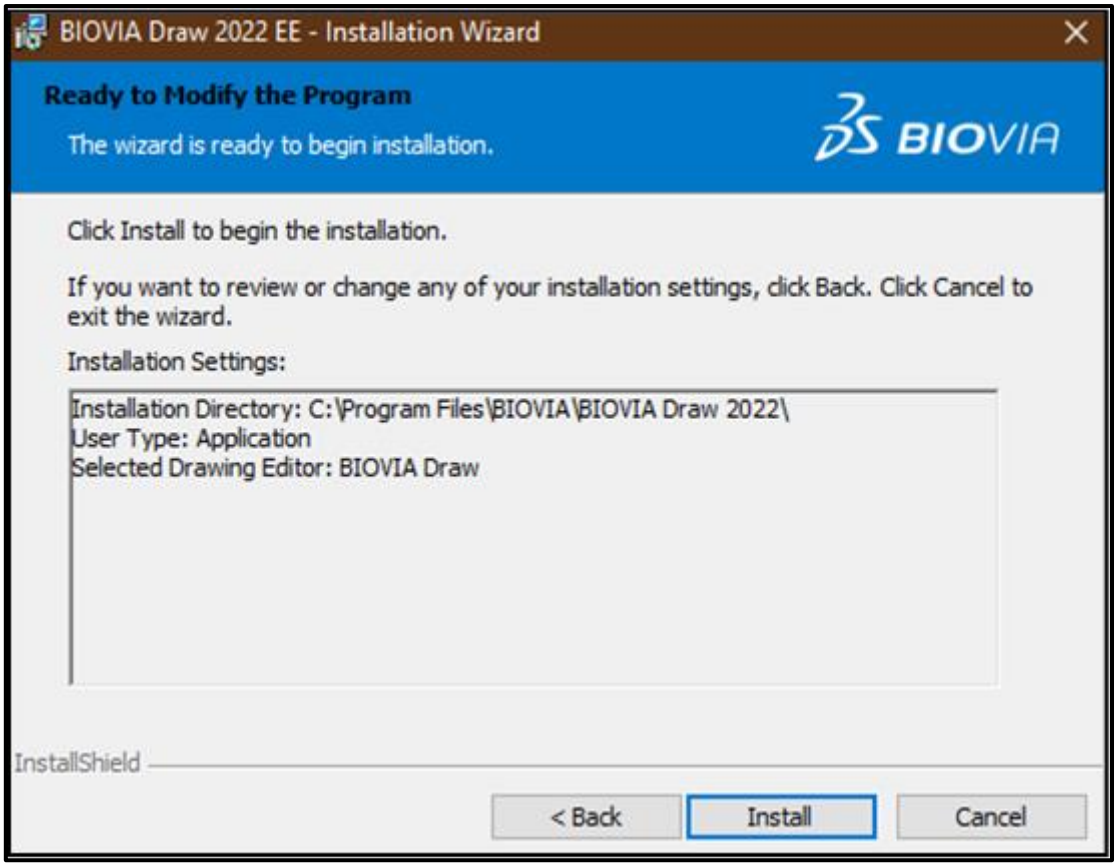
5. Check and select the optional components, and then click on ‘Next’

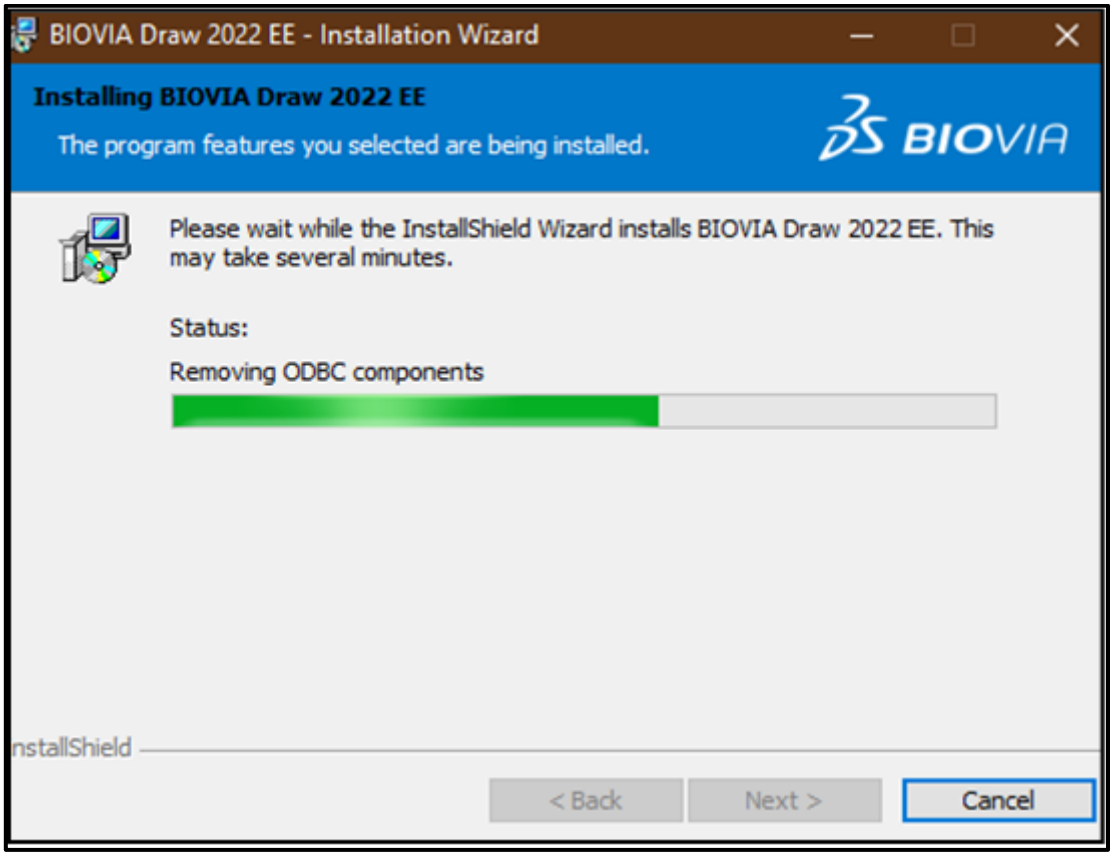




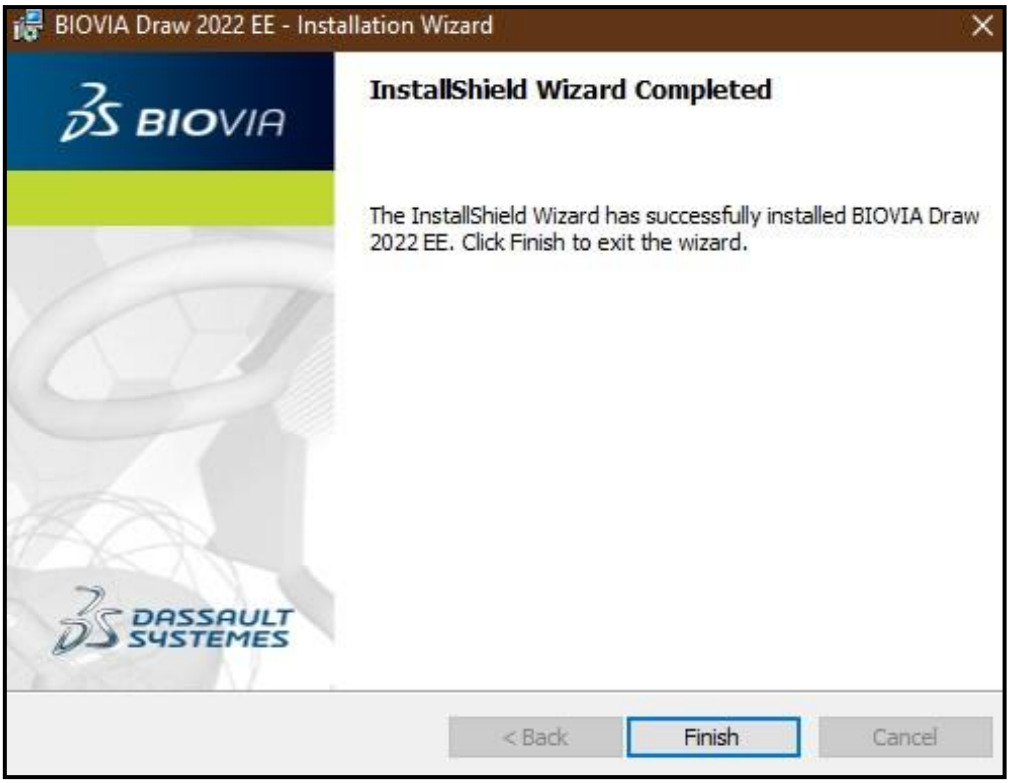

BIOVIA Draw 2022 EE - Installation Wizard
Setup Type
BIOVIA
Select one of the following installation types:
Application user (typical end-user configuration)
Developer user (full development configuration)
InstallShield
< Back
Next >
Cancel


BIOVIA Draw 2022 EE - Installation Wizard
Select File Associations
BIOVIA
Do you want to associate CDX files and ChemDraw objects embedded in MS Office applications with BIOVIA Draw?
Yes
No
InstallShield
< Back
Next >
Cancel

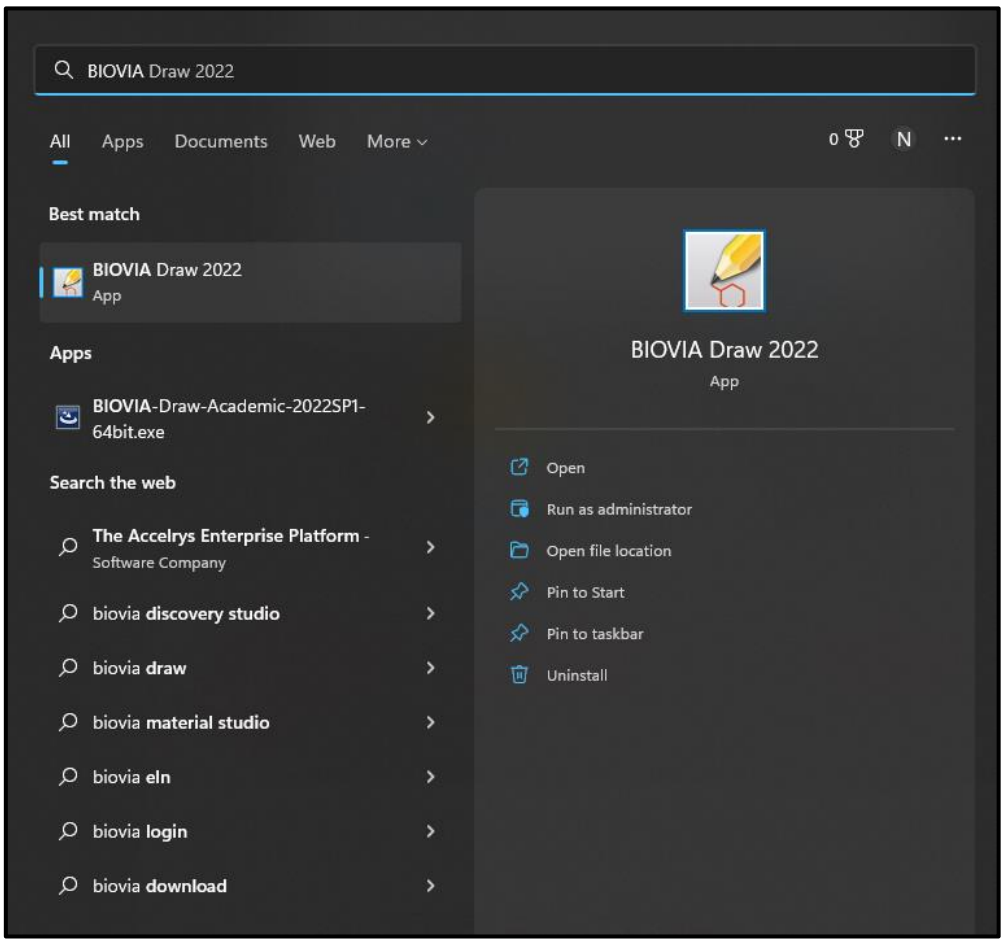

BIOVIA Draw 2022 EE - Installation Wizard
Ready to Modify the Program
The wizard is ready to begin installation.
BIOVIA
Click Install to begin the installation.
If you want to review or change any of your installation settings, click Back. Click Cancel to exit the wizard.
Installation Settings:
Installation Directory: C:\Program Files\BIOVIA\BIOVIA Draw 2022\
User Type: Application
Selected Drawing Editor: BIOVIA Draw
InstallShield
< Back
Install
Cancel


BIOVIA Draw 2022 EE - Installation Wizard
Installing BIOVIA Draw 2022 EE
The program features you selected are being installed.
BIOVIA
Please wait while the InstallShield Wizard installs BIOVIA Draw 2022 EE. This may take several minutes.
Status:
Removing ODBC components
nstallShield
< Back
Next >
Cancel

6. The Installation is completed. Click finish to exit the wizard



7. BIOVIA after installation



II. OPEN BABEL Tool

HISTORY:

Open Babel and JOELib were derived from the OELib cheminformatics library. In turn, OELib was based on ideas in the original chemistry program Babel and an unreleased object-oriented programming library called OBabel.

INTRODUCTION:

The development and use of the Open Babel project, a full-featured open chemical toolbox, designed to "speak" the many different representations of chemical data. It allows anyone to search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas. It provides both ready-to-use programs as well as a complete, extensible programmer's toolkit for developing cheminformatics software. It can handle reading, writing, and interconverting over 110 chemical file formats, supports filtering and searching molecule files using Daylight SMARTS pattern matching and other methods, and provides extensible fingerprinting and molecular mechanics frameworks. We will discuss the frameworks for file format interconversion, fingerprinting, fast molecular searching, bond perception and atom typing.

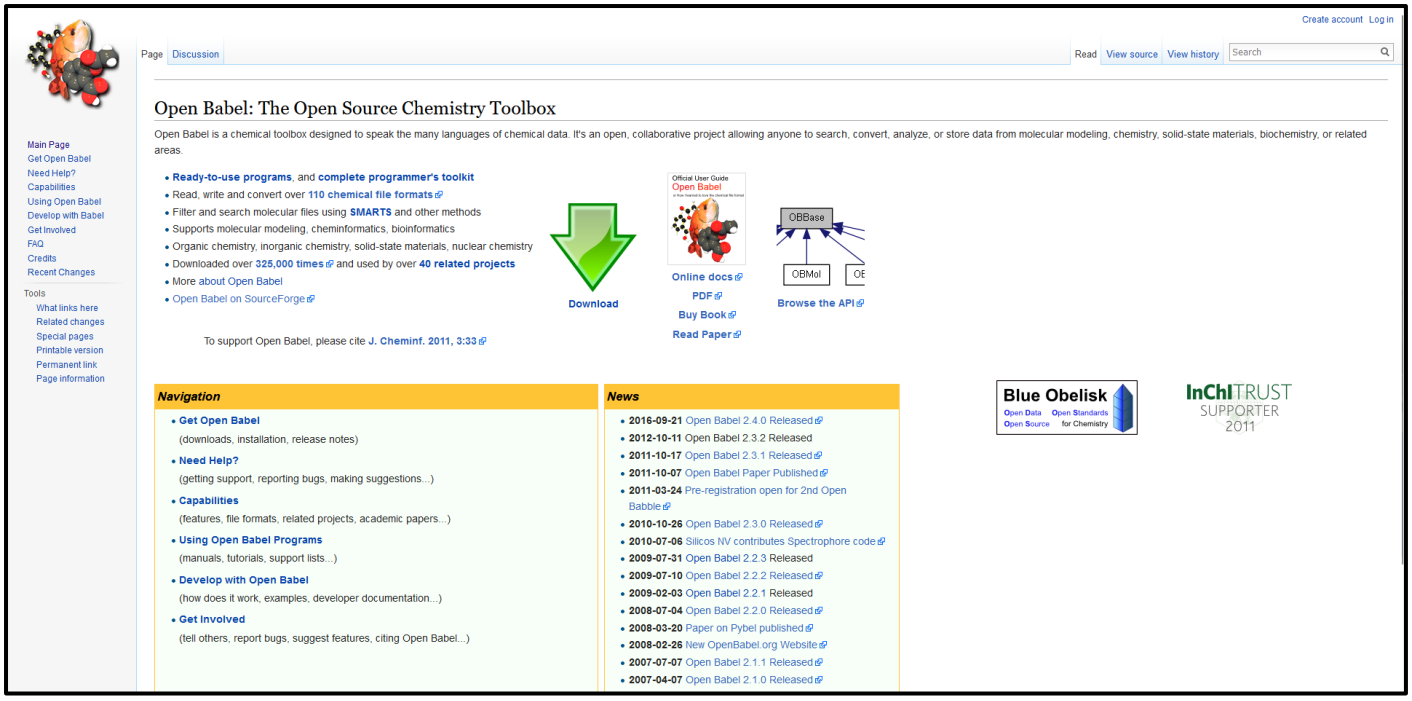
Open Babel has its origin in a version of OELib released as open-source software by OpenEye Scientific under the GPL (GNU Public License). In 2001, OpenEye decided to rewrite OELib in-house as the proprietary OEChem library, so the existing code from OELib was spun out into the new Open Babel project. Since 2001, Open Babel has been developed and substantially extended as an international collaborative project using an open-source development model. It has over 160,000 downloads, over 400 citations, is used by over 40 software projects, and is freely available from the Open Babel website.

FEATURES:

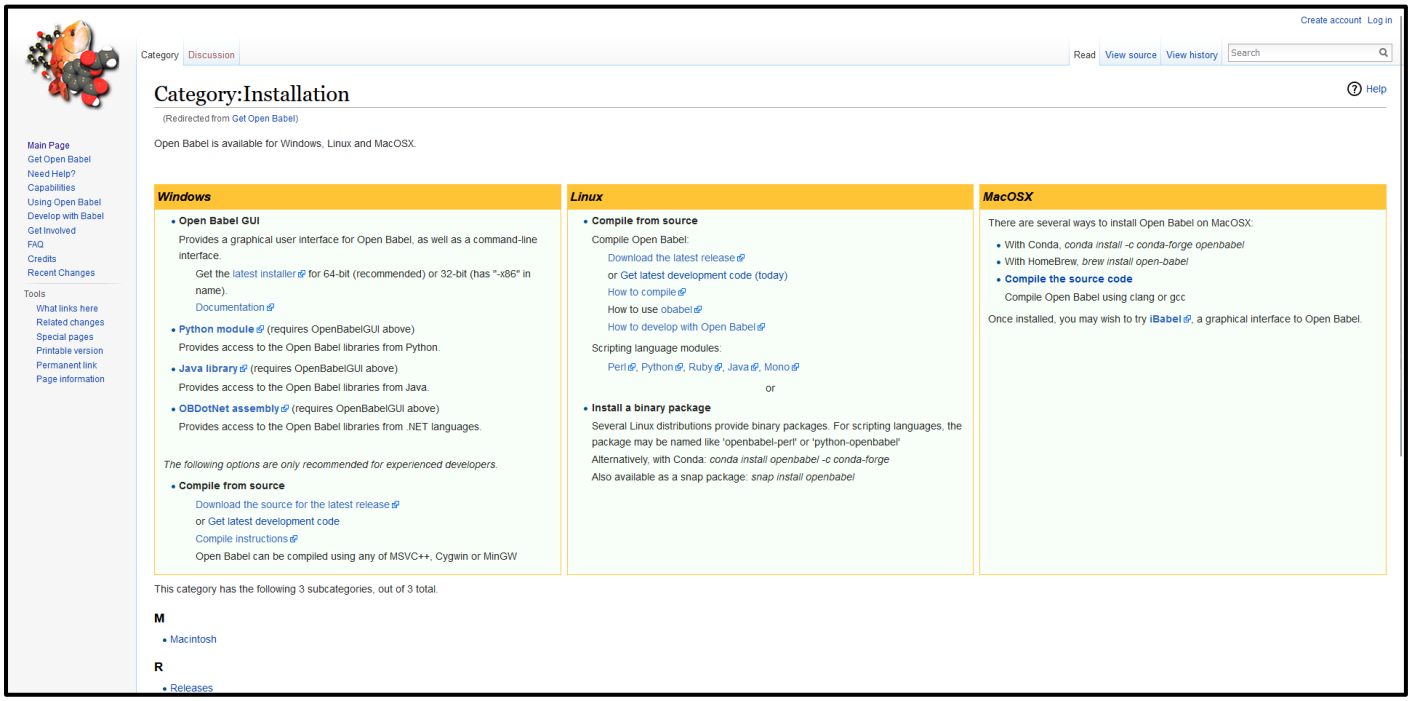
1) File Format Support.
2) Fingerprints and Fast Searching.
3) Bond Perception and Atom Typing.
4) Canonical Representation of Molecules.
5) Coordinate Generation in 2D and 3D.

Installation Steps:

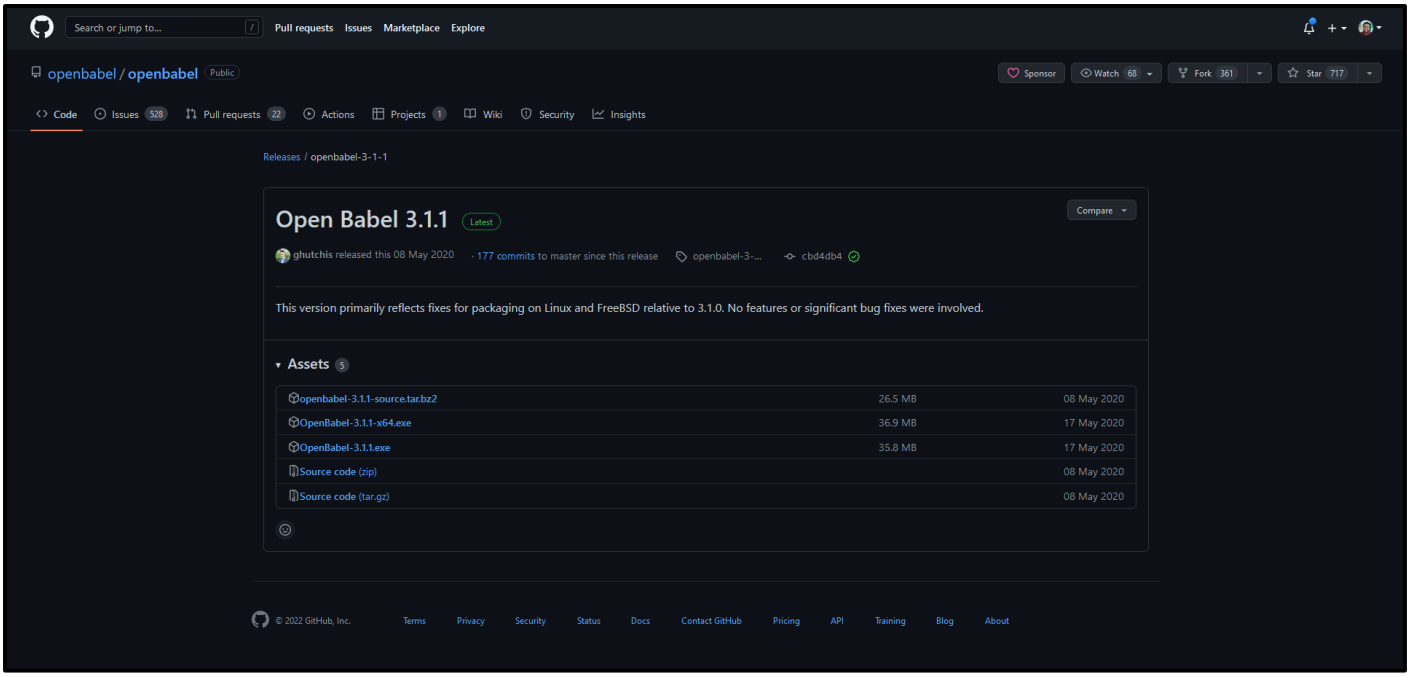
1. Open Homepage of Open Babel website and then click on download (URL: http://openbabel.org/wiki/Main_Page).



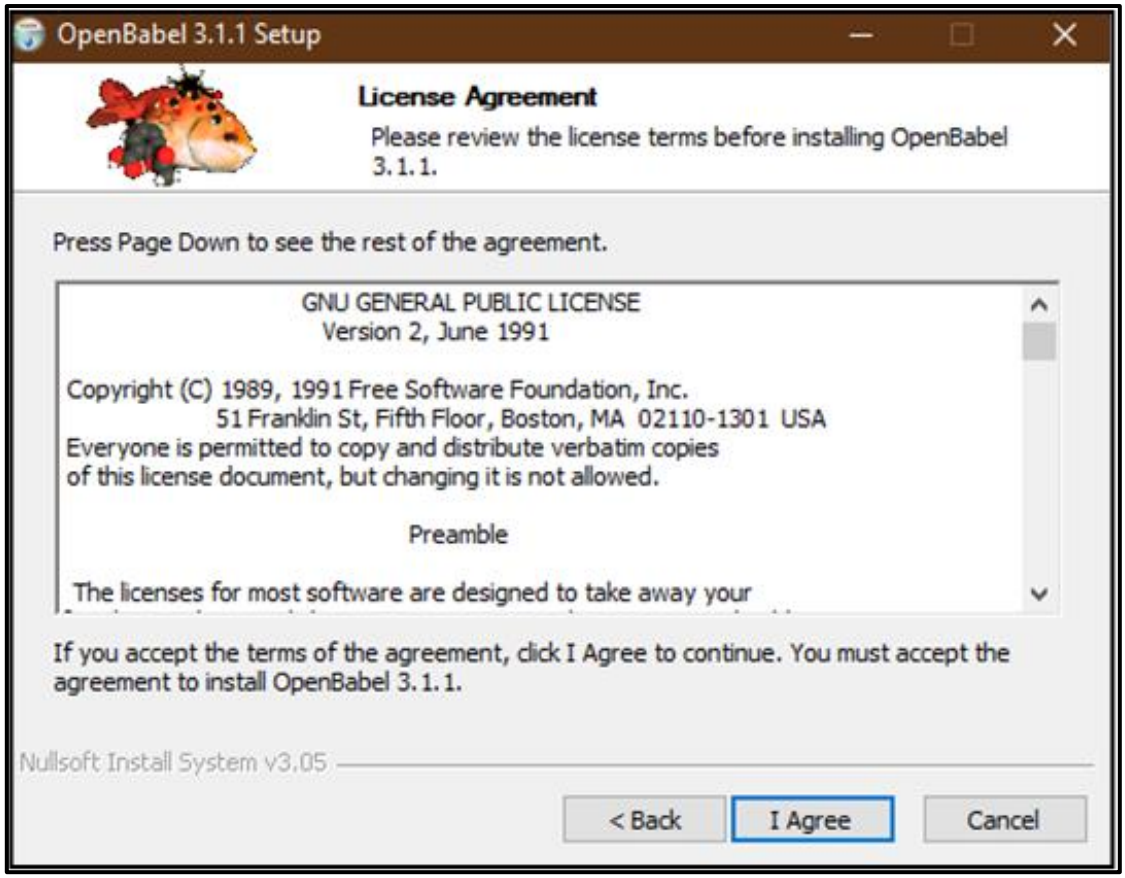
2. Open Babel is available on Windows, Linux and Mac. For Windows install the 64bit version.

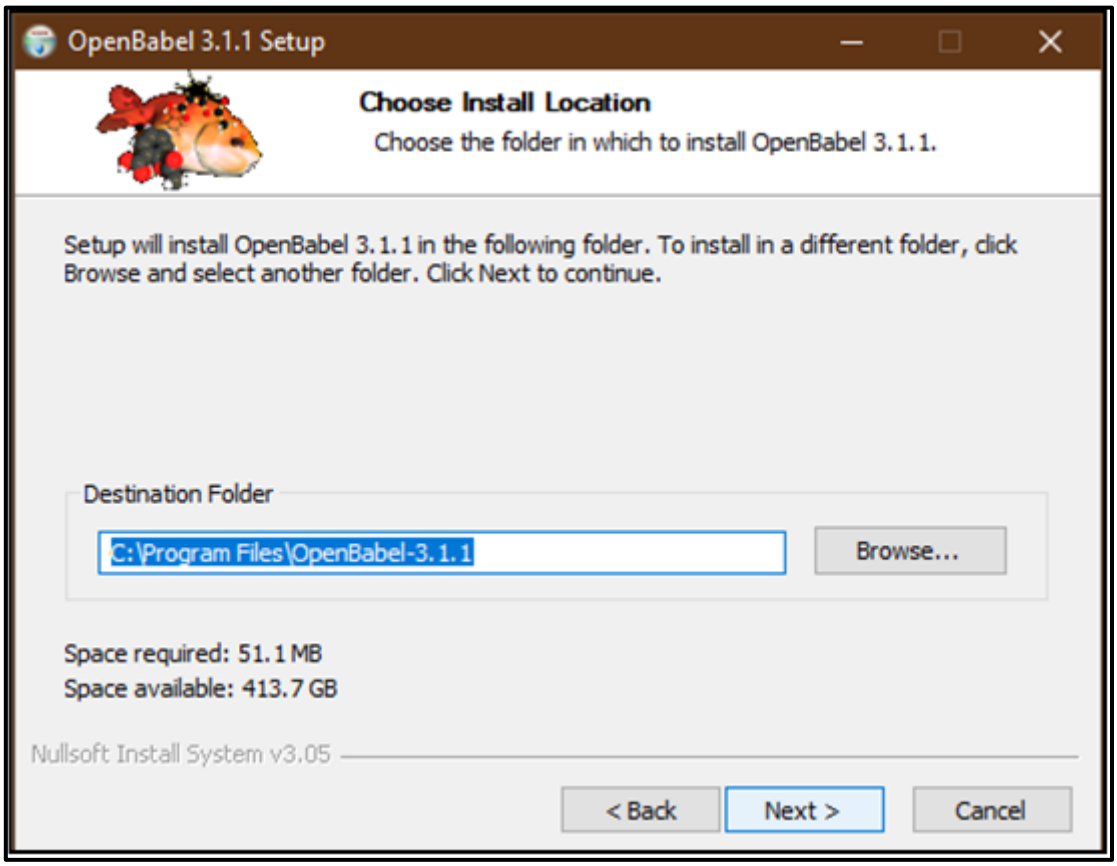


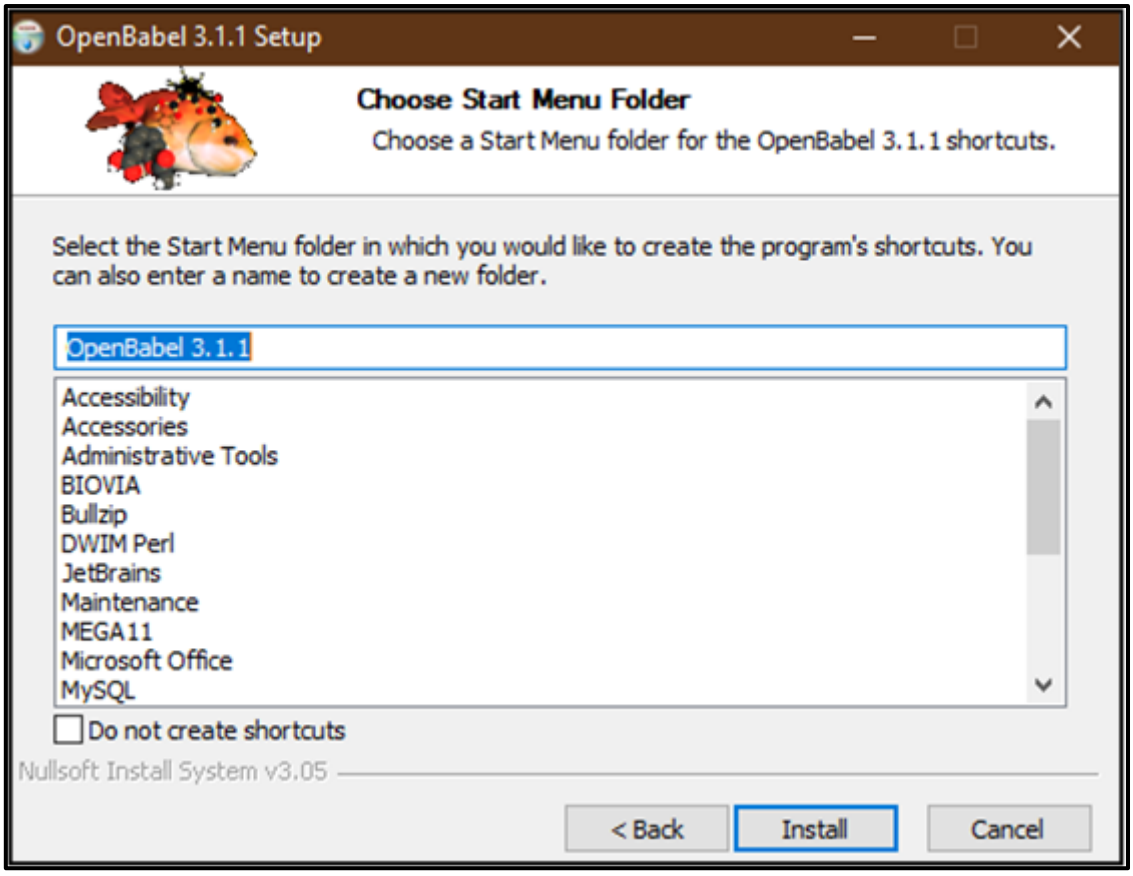
3. Click on OpenBabel-3.1.1.-64.exe

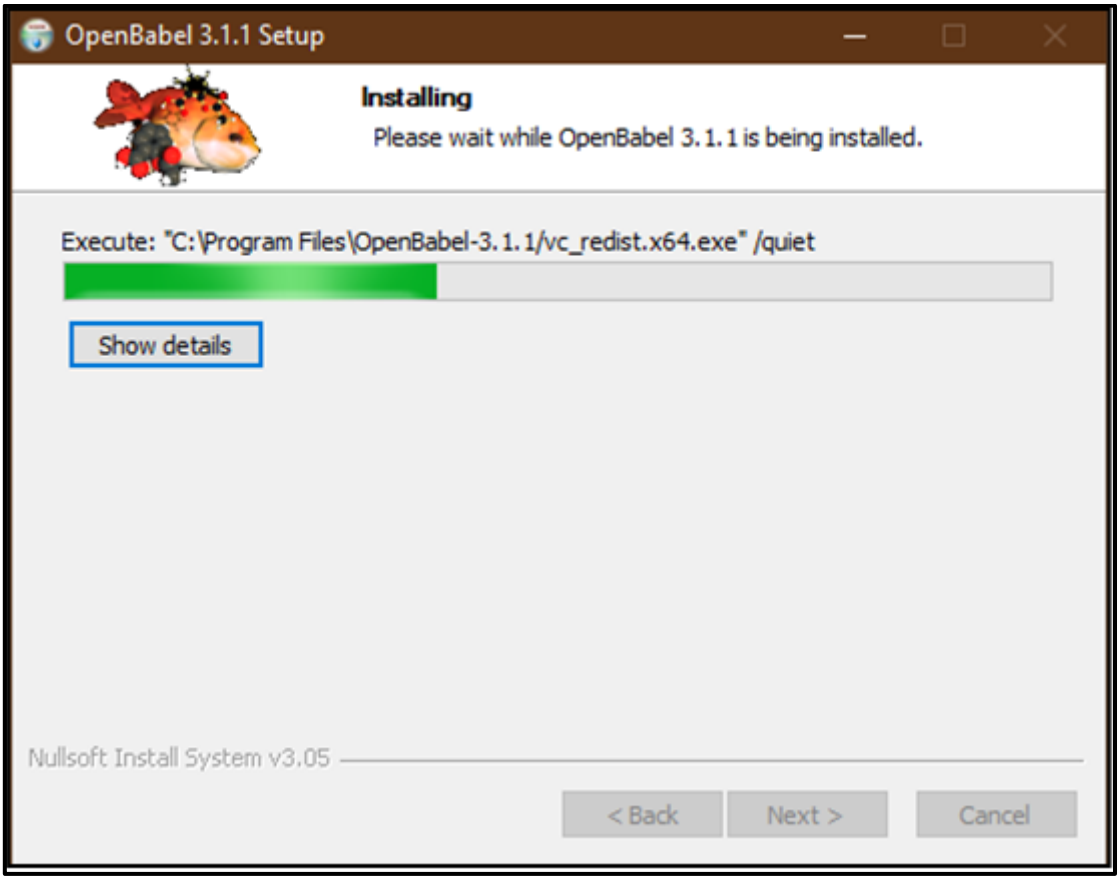


4. GO through the installation procedure

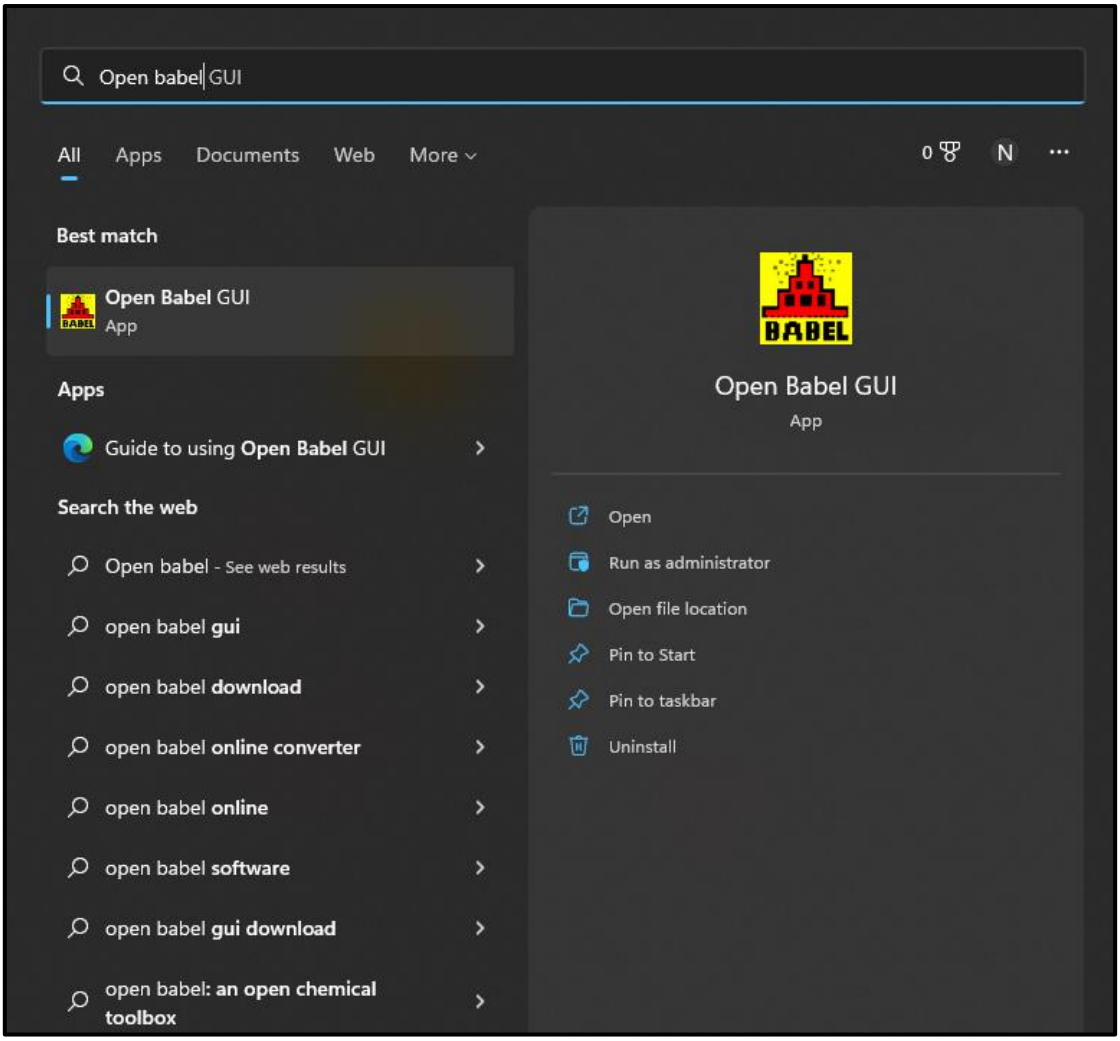

OpenBabel 3.1.1 Setup
License Agreement
Please review the license terms before installing OpenBabel 3.1.1.
Press Page Down to see the rest of the agreement.
GNU GENERAL PUBLIC LICENSE
Version 2, June 1991
Copyright (C) 1989, 1991 Free Software Foundation, Inc.
51 Franklin St, Fifth Floor, Boston, MA 02110-1301 USA
Everyone is permitted to copy and distribute verbatim copies
of this license document, but changing it is not allowed.
Preamble
The licenses for most software are designed to take away your
If you accept the terms of the agreement, click I Agree to continue. You must accept the agreement to install OpenBabel 3.1.1.
Nullsoft Install System v3.05
< Back
I Agree
Cancel


OpenBabel 3.1.1 Setup
Choose Install Location
Choose the folder in which to install OpenBabel 3.1.1.
Setup will install OpenBabel 3.1.1 in the following folder. To install in a different folder, click Browse and select another folder. Click Next to continue.
Destination Folder
C:\Program Files\OpenBabel-3.1.1
Browse...
Space required: 51.1 MB
Space available: 413.7 GB
Nullsoft Install System v3.05
< Back
Next >
Cancel


OpenBabel 3.1.1 Setup
Choose Start Menu Folder
Choose a Start Menu folder for the OpenBabel 3.1.1 shortcuts.
Select the Start Menu folder in which you would like to create the program's shortcuts. You can also enter a name to create a new folder.
OpenBabel 3.1.1
Accessibility
Accessories
Administrative Tools
BIOVIA
Bullzip
DWIM Perl
JetBrains
Maintenance
MEGA11
Microsoft Office
MySQL
Do not create shortcuts
Nullsoft Install System v3.05
< Back
Install
Cancel


OpenBabel 3.1.1 Setup
Installing
Please wait while OpenBabel 3.1.1 is being installed.
Execute: "C:\Program Files\OpenBabel-3.1.1/vc_redist.x64.exe" /quiet
Show details
Nullsoft Install System v3.05
< Back
Next >
Cancel

5. Icon of Open Babel GUI after installation



References:

1. Biovia draw. (n.d.). BIOVIA Draw. Retrieved September 7, 2022, from https://lib.cnu.edu.tw/3_2_eresource/doc/biovia-draw.pdf
2. Price Waterhouse Coopers (PWC) From Vision to Decision. Pharma 2020 Report. PWC; London, UK: 2012. [(accessed on 16 November 2015)].
3. Weininger, D. (1988). SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules. J Chem Inf Comput Sci. 28, 31-36.

DATE: 06-09-22

WEBLEM: 2A

BIOVIA DRAW SOFTWARE

(URL:https://www.3ds.com/products-services/biovia/products/scientific-informatics/biovia-draw/).

Aim:

To perform drawing, editing & manipulation of 2D & 3D structures for query "Penicillin" using BIOVIA DRAW software.

Introduction:

Penicillin V is a member of the penicillin family exhibiting broad-spectrum antibiotic property. Penicillin V binds to penicillin binding proteins (PBP), the enzymes that catalyze the synthesis of peptidoglycan, which is a critical component of the bacterial cell wall. This leads to the interruption of cell wall synthesis, consequently leading to bacterial cell growth inhibition and cell lysis.

Phenoxymethylpenicillin is a narrow spectrum antibiotic also commonly referred to as Penicillin V or Penicillin VK. It is a phenoxymethyl analog of Penicillin G, or [benzylpenicillin]. An orally active naturally penicillin, phenoxymethylpenicillin is used to treat mild to moderate infections in the respiratory tract, skin, and soft tissues caused by penicillin G--sensitive microorganisms. Phenoxymethylpenicillin has also be used in some cases as prophylaxis against susceptible organisms. While there have been no controlled clinical efficacy studies that were conducted, phenoxymethylpenicillin has been suggested by the American Heart Association and the American Dental Association for use as an oral regimen for prophylaxis against bacterial endocarditis in patients with congenital heart disease or rheumatic or other acquired valvular heart disease when they undergo dental procedures and surgical procedures of the upper respiratory tract, except for those who are at an elevated risk for endocarditis.

With the use of BIOVIA Draw, scientists can quickly and easily sketch and edit complex compounds, chemical reactions, and biological sequences, easing group searches, viewing, sharing, and archiving of scientific data. With the ability to save and retrieve peptides, oligonucleotides, and oligosaccharides, among other complicated biological things, BIOVIA Draw provides scientists with specialised management skills. A biological sequence editor that enables the definition of unique residues and linkers, Markush structure tools, and haptic and hydrogen bond tools are just a few of the features available to scientists. Developers can build unique add-ins and drop them in as tools, buttons, or menu items using BIOVIA Draw's published API. Tools for enumeration, bioavailability, isotopomer distribution, stoichiometry calculations, and many other tasks are available as add-ins.

Methodology:

1. Open BIOVIA Draw software.
2. Draw the Chemical Structure using various tools.
3. In the chemistry option use Clean the Structure.
4. Apply different filter options such as Calculator, Atom Number, Generate Text from Structure (IUPAC, SMILE), Show sequence view, etc.
5. Observe and save the results.

Observations:

Shortcut **Header** **Template**

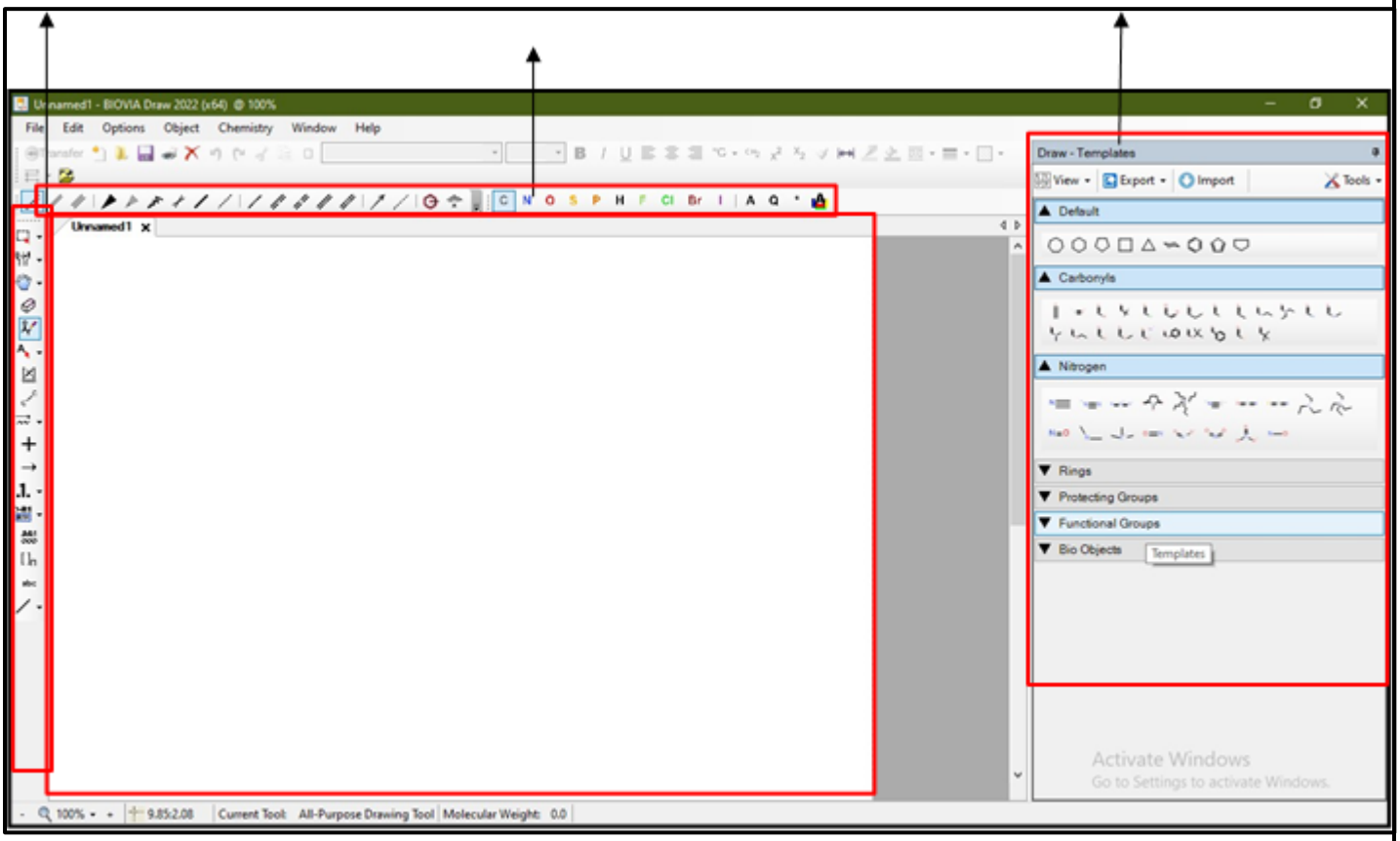


Fig 1. Homepage of BIOVIA DRAW SOFTWARE

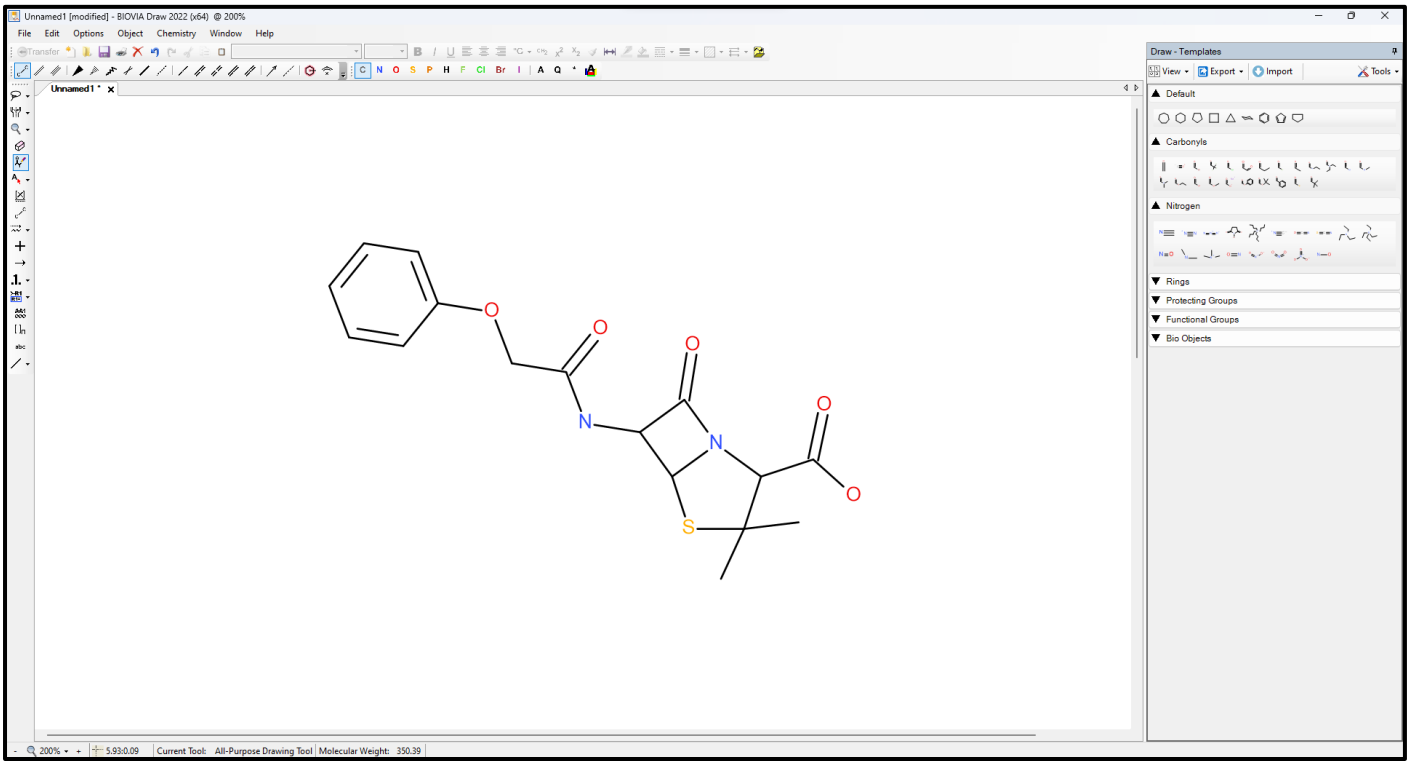


Fig 2. Structure of Penicillin chemical compound

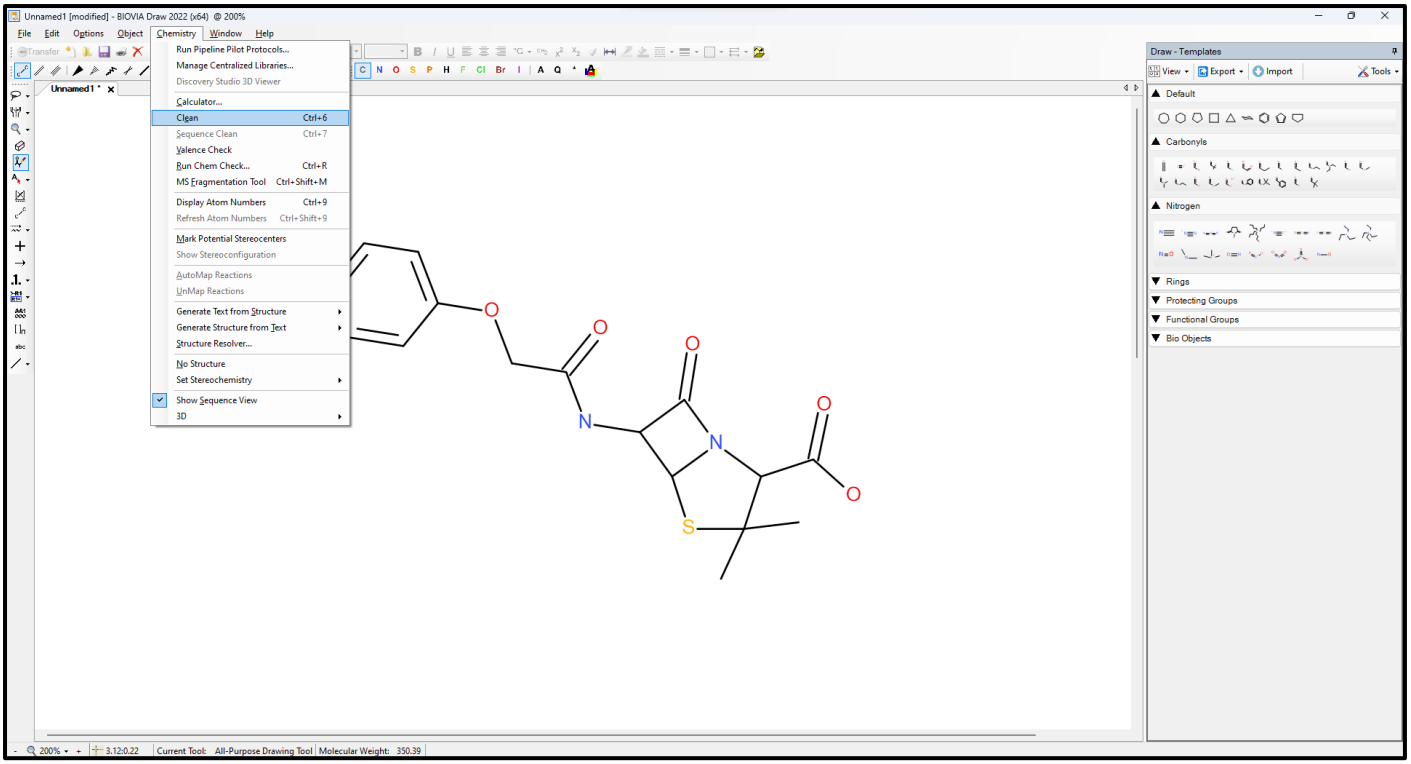


Fig 3. Option applied “Clean structure”

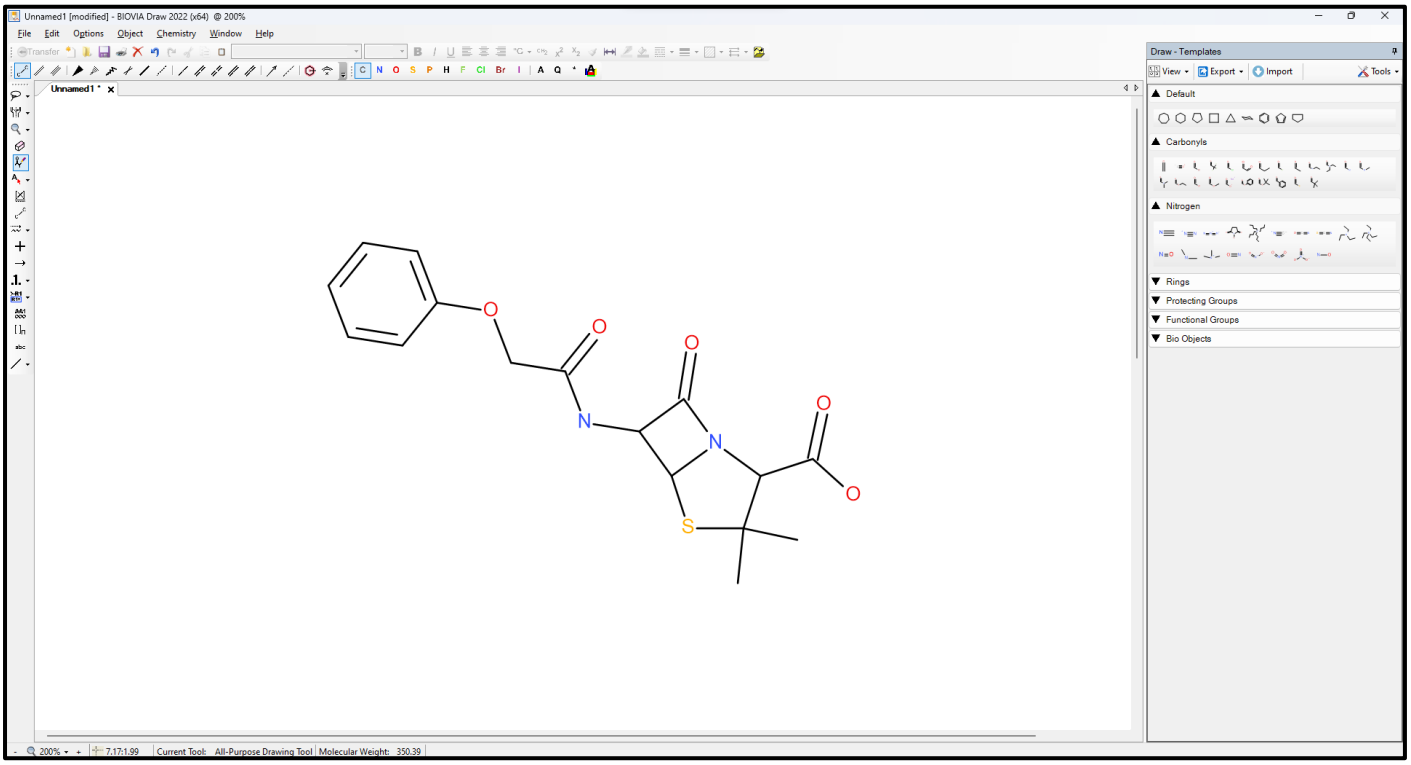


Fig 4. Clean structure of Penicillin

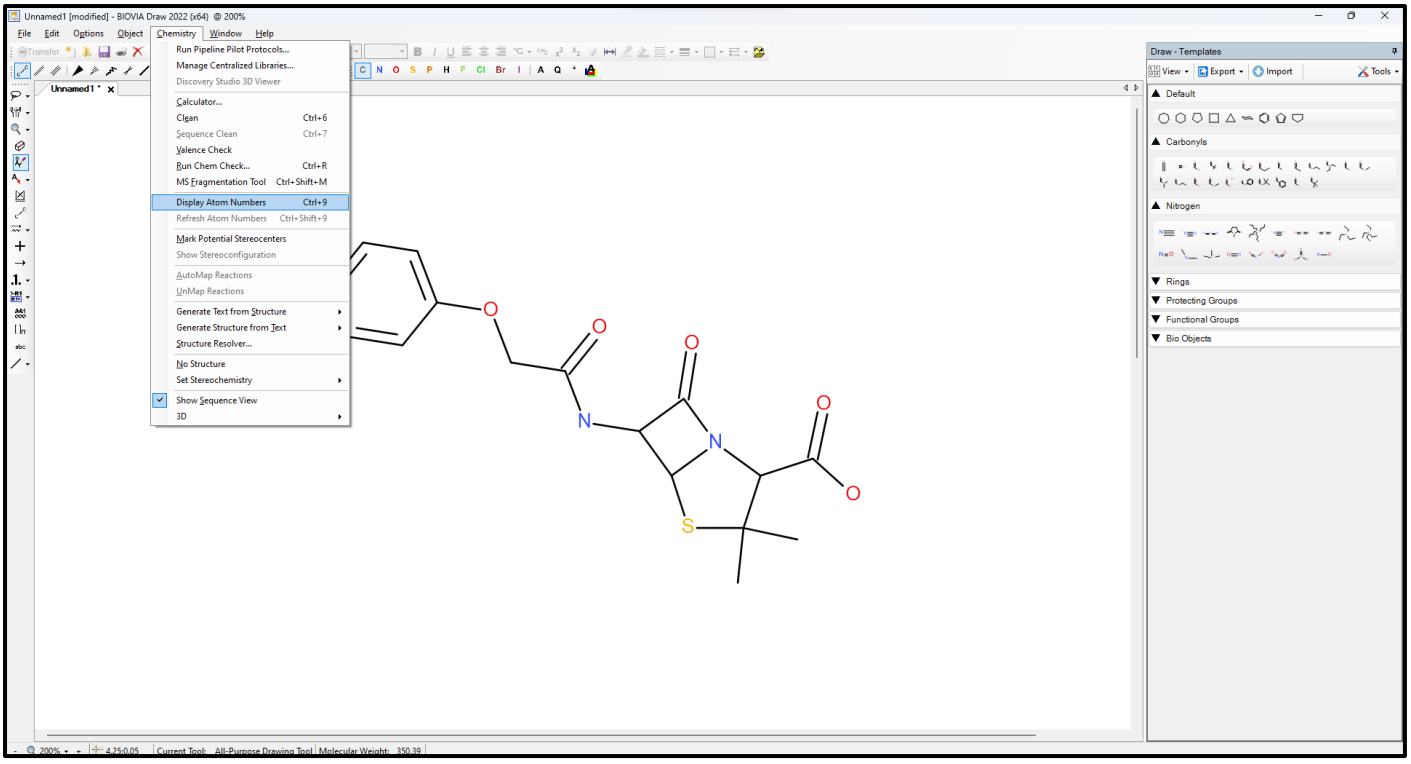


Fig 5. Option applied "Display Atom Numbers"

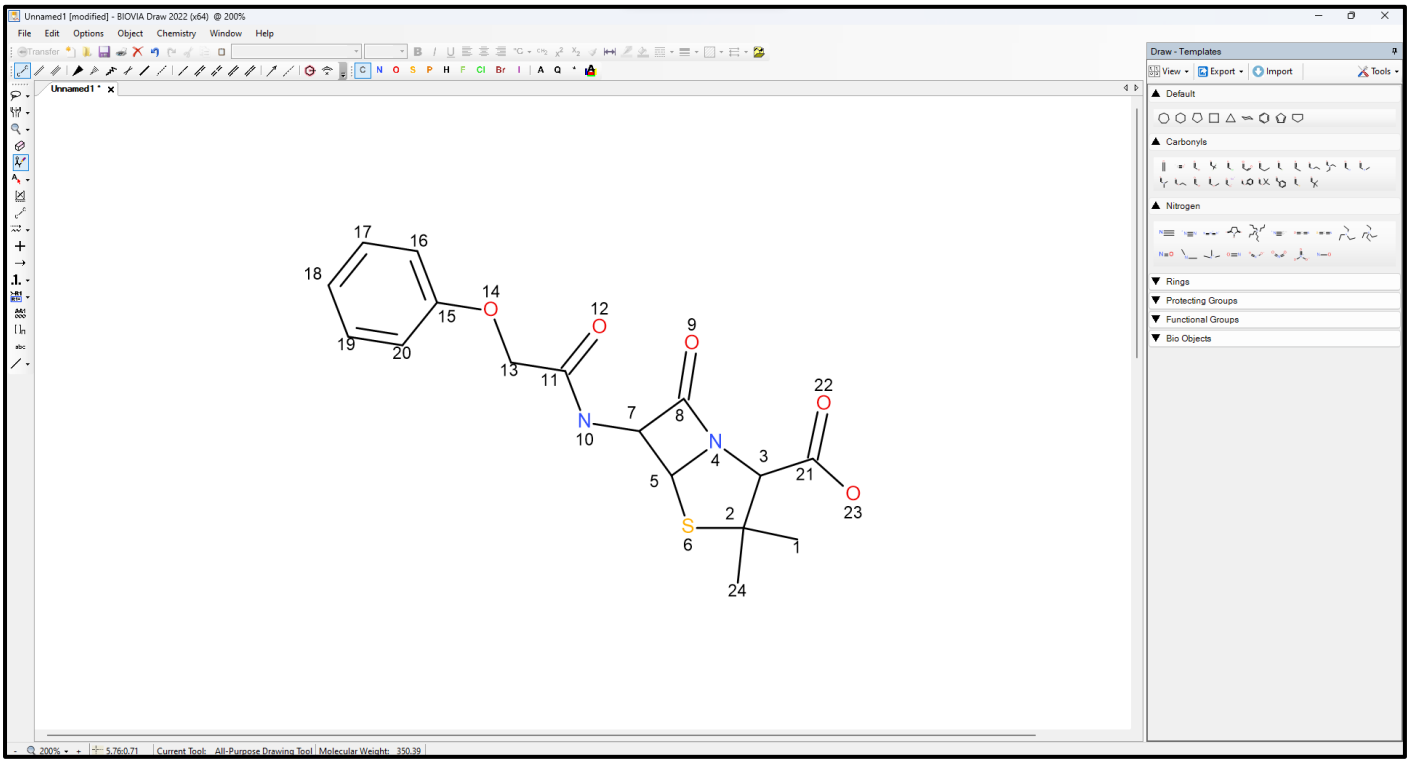


Fig 6. Atom numbering of Penicillin structure

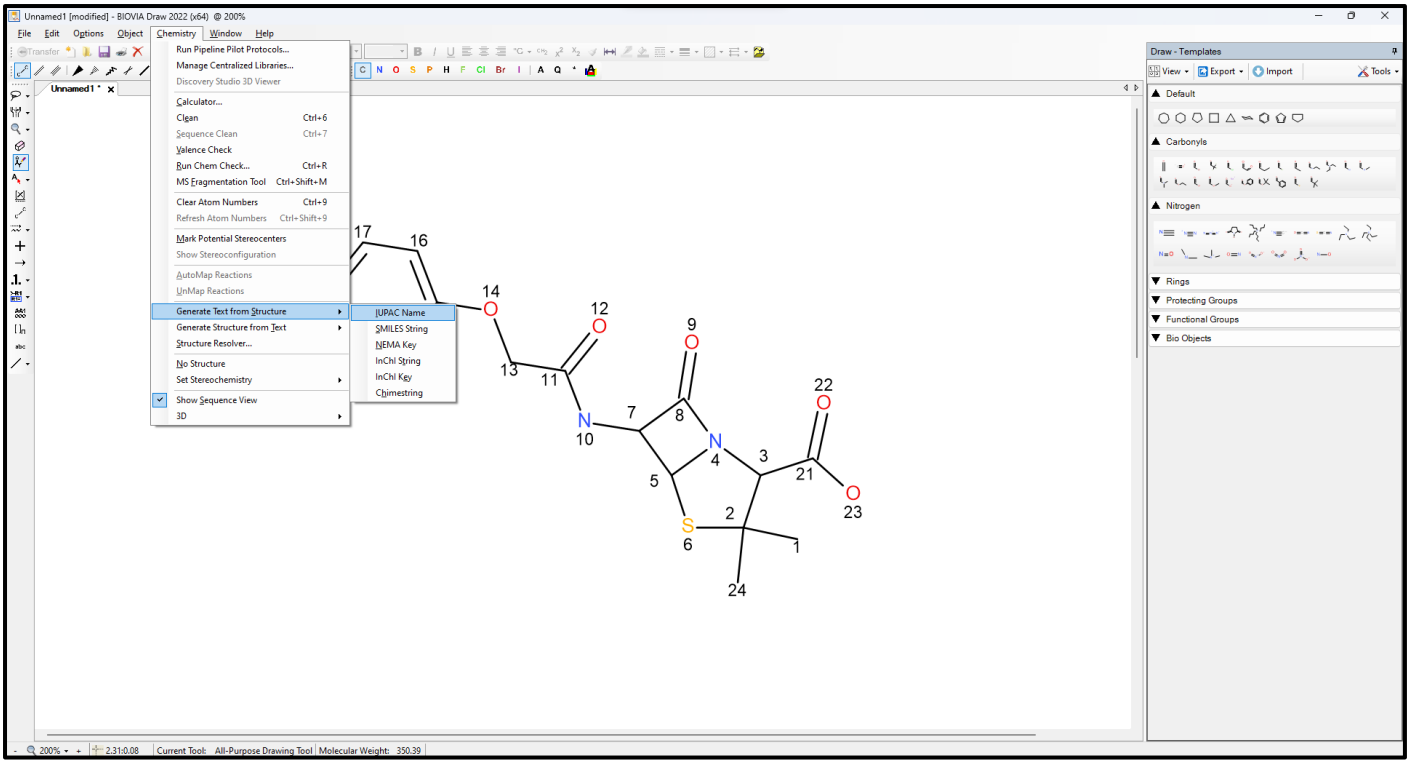


Fig 7. Option applied: To generate IUPAC name

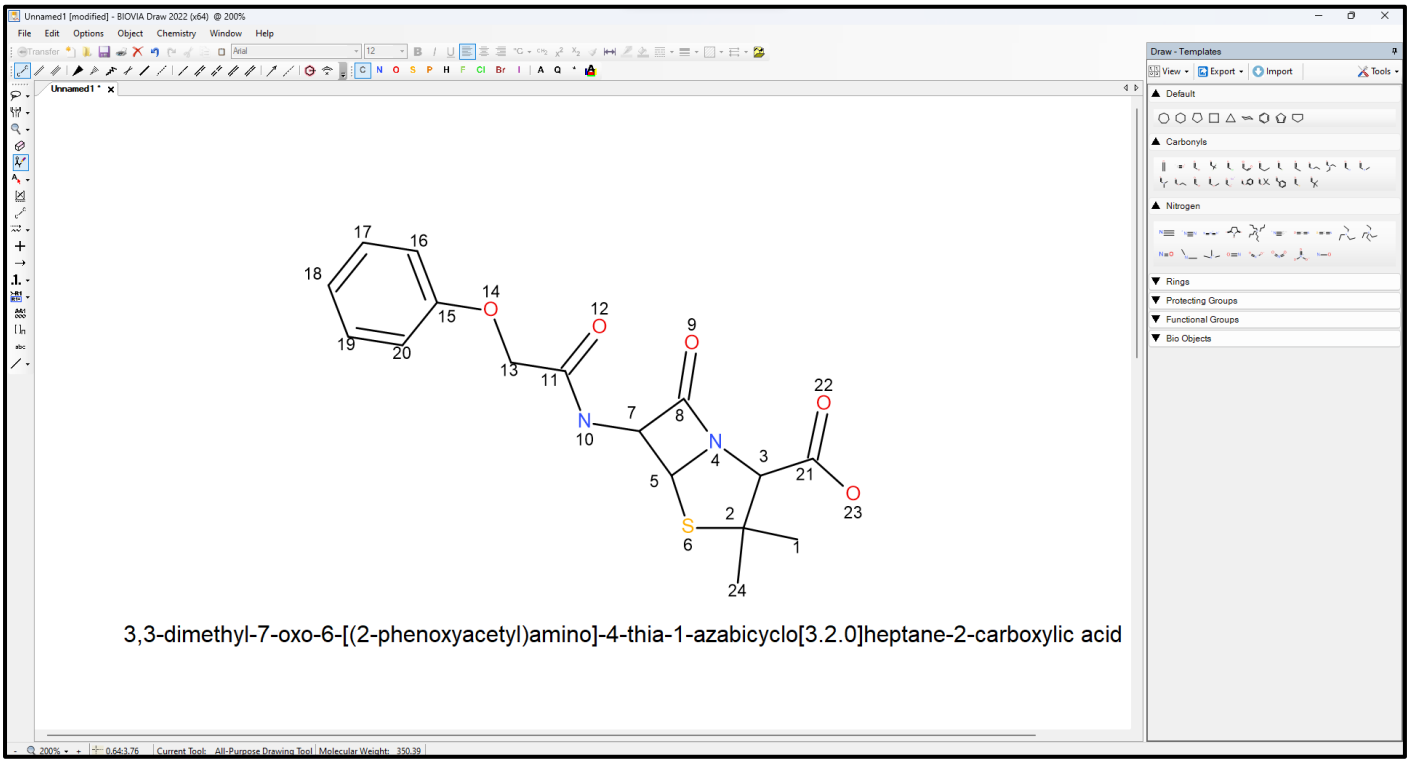


Fig 8. IUPAC name of Penicillin

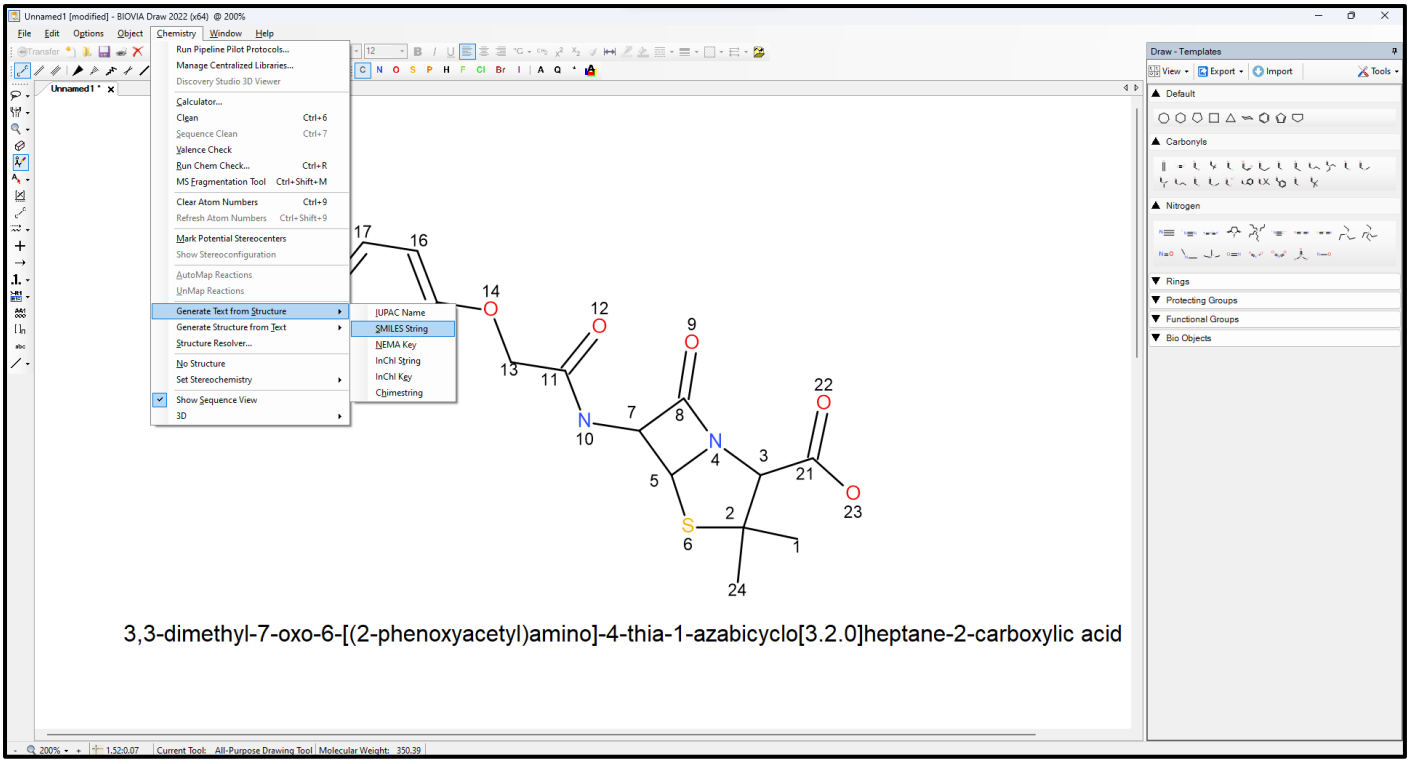


Fig 9. Option applied: To generate SMILES string

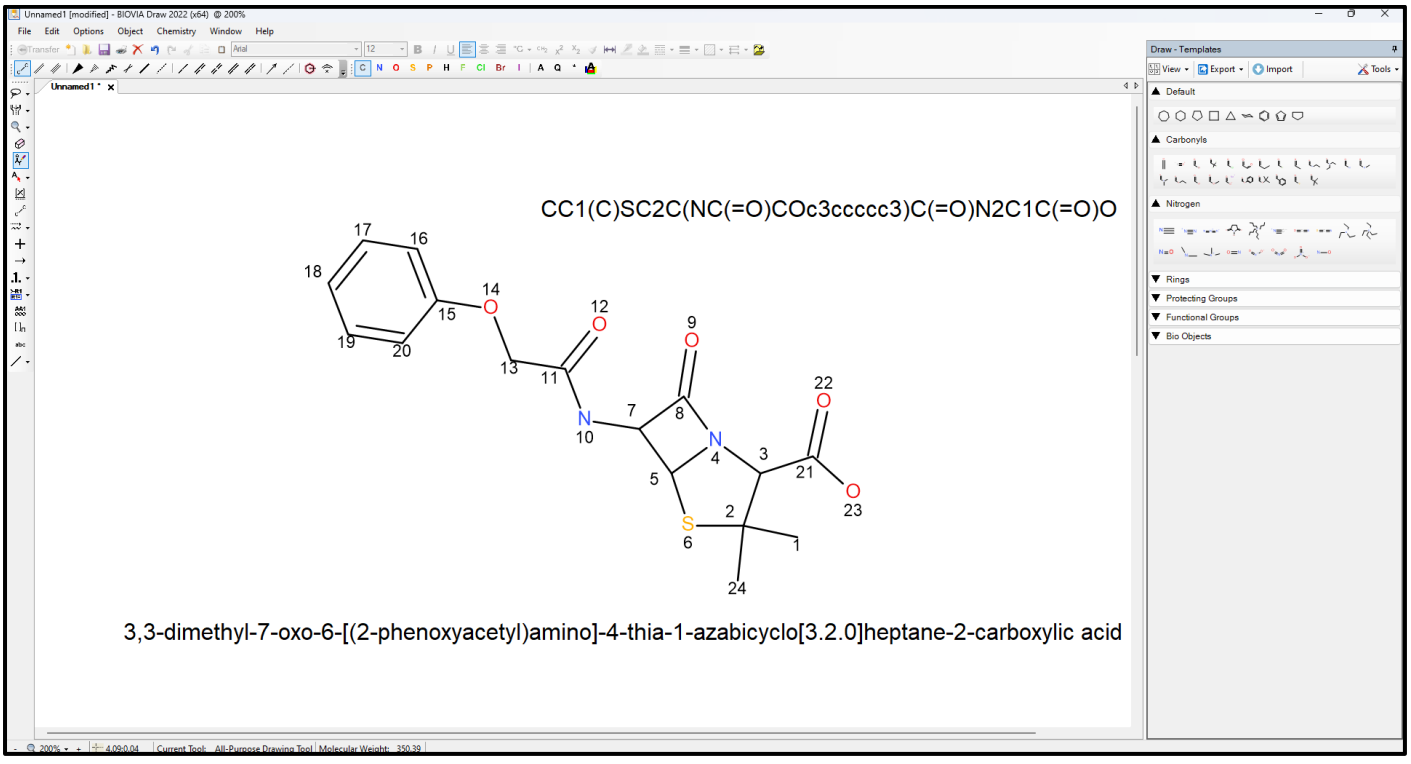


Fig 10. SMILES string of Penicillin

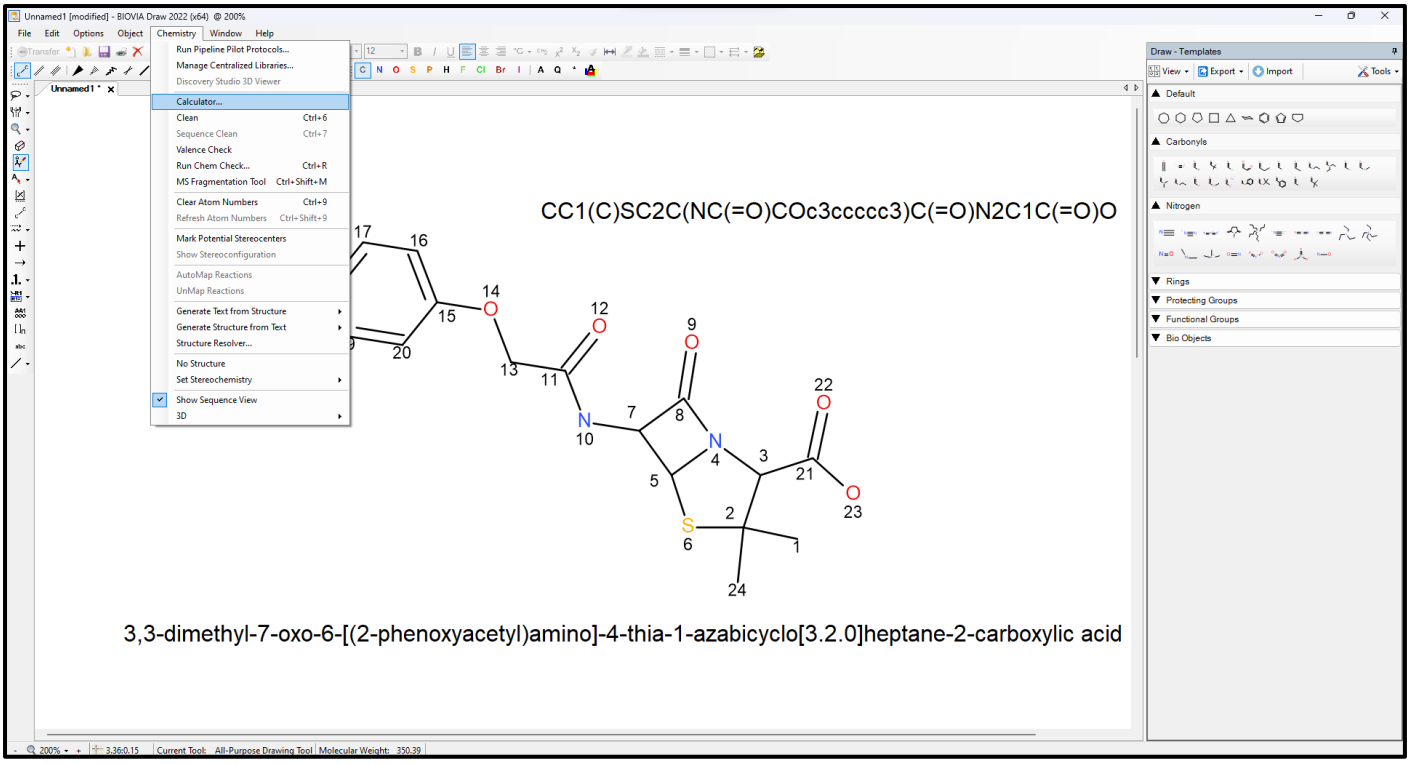


Fig 11. Option applied: To calculate Physicochemical properties of Penicillin

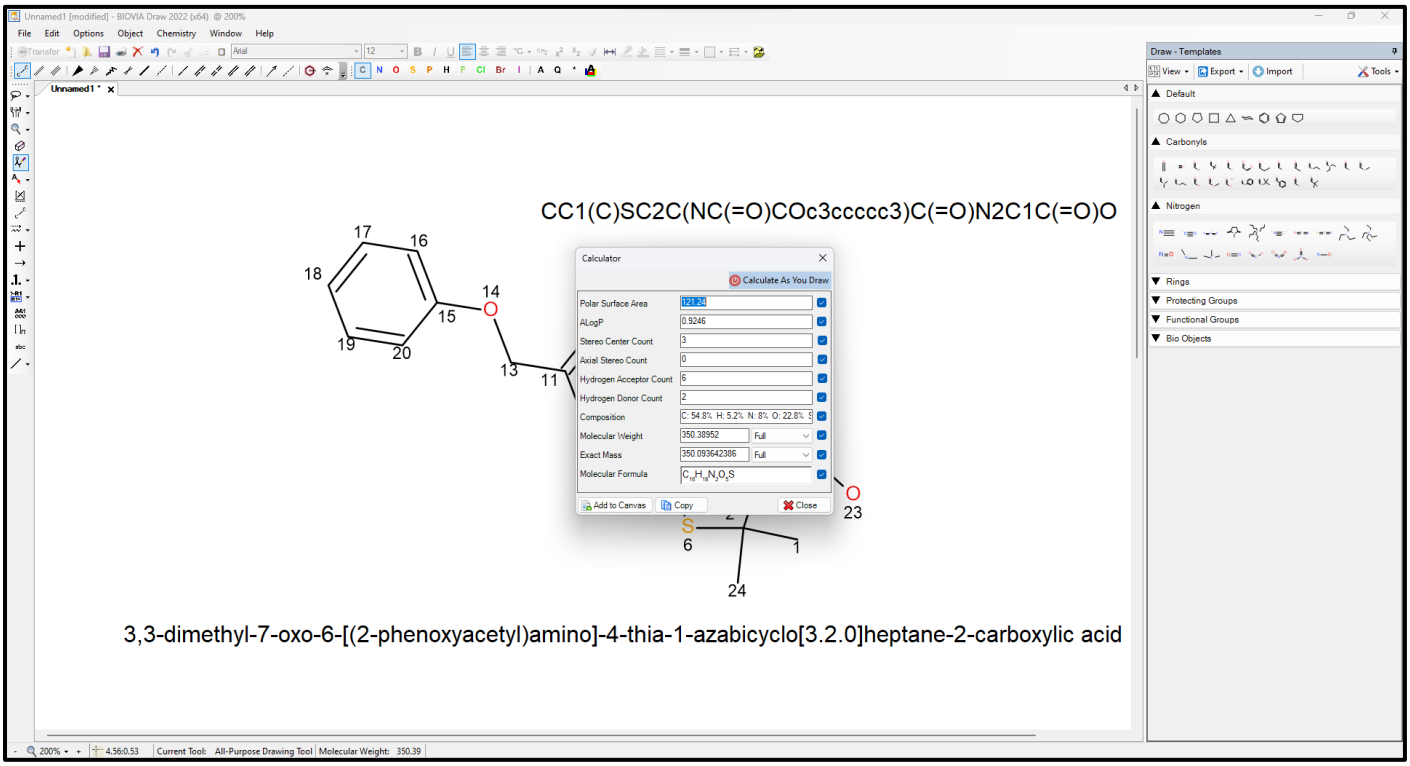


Fig 12. Different Physicochemical properties available for Penicillin

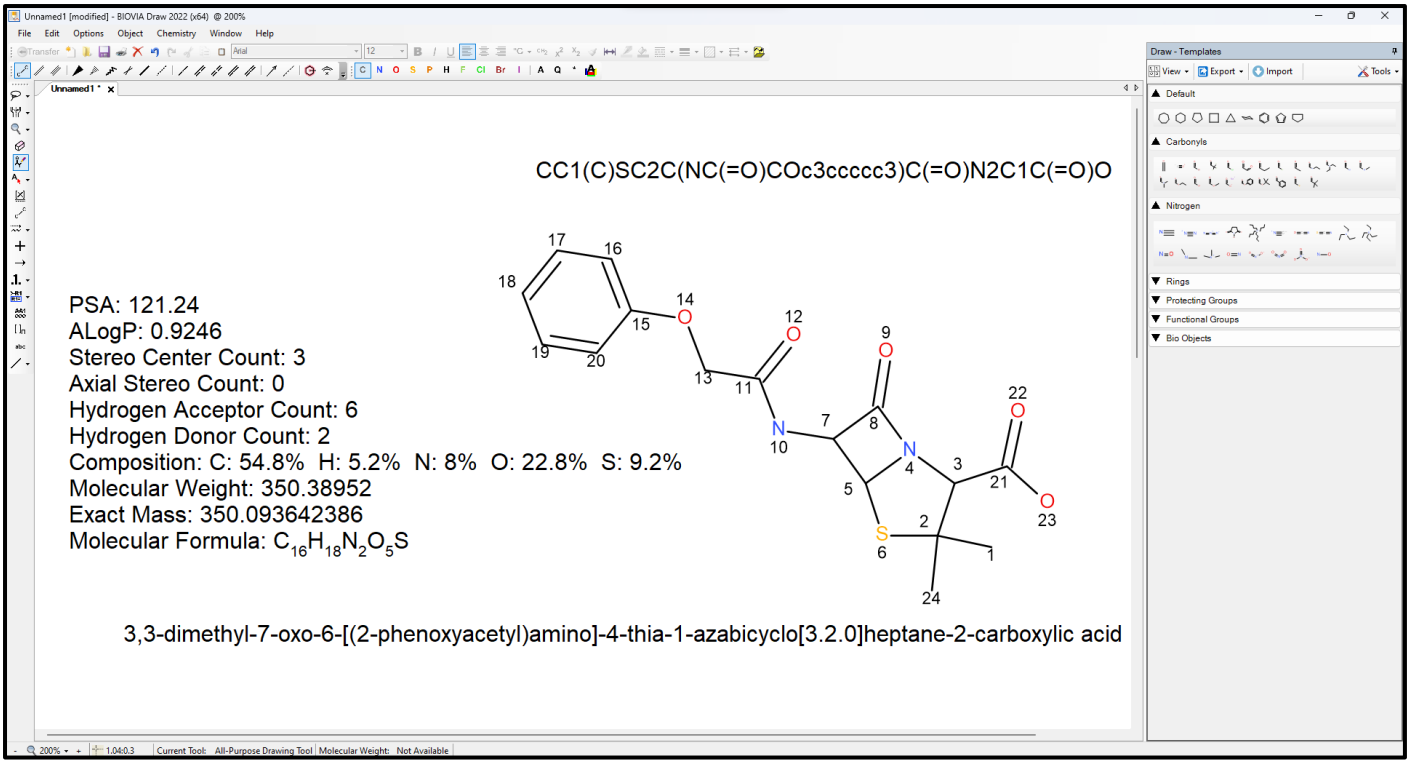


Fig 13. Calculated Physicochemical properties of Penicillin

Results:

The structure of Penicillin was drawn using the BIOVIA DRAW structure. Following are the information retrieved for the structure using software in tabulation format

SR NO	Name of Option	Results
1.	Physicochemical Properties	PSA: 121.24 ALogP: 0.9246 Stereo Center Count: 3 Axial Stereo Count: 0 Hydrogen Acceptor Count: 6 Hydrogen Donor Count: 2 Composition: C: 54.8% H: 5.2% N: 8% O: 22.8% S: 9.2% Molecular Weight: 350.38952 Exact Mass: 350.093642386 Molecular Formula: C16H18N2O5S
2.	IUPAC name	3,3-dimethyl-7-oxo-6-[(2-phenoxyacetyl)amino]-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid
3.	SMILES string	CC1(C(N2C(S1)C(C2=O)NC(=O)COC3=CC=CC=C3)C(=O)O)C

Conclusion:

BIOVIA Draw enables the drawing and editing of complex biologics, molecules and chemical reactions. It provides structure and query drawing, allows registering, searching and reporting on chemically modified peptide or nucleotide sequences and to add structure drawing and display to user's applications, and customizing according to their organizational workflows. The software can facilitate the collaborative searching, viewing, communicating and archiving of scientific information as well.

References:

1. Klein, F., Mouquet, H., Dosenovic, P., Scheid, JF., Scharf, L., Nussenzweig, MC. (2013). Antibodies in HIV-1 vaccine development and therapy. Science,341(6151), 1199-204. doi: 10.1126/science.1241144
2. Pirard, D., Vereecken, P., Mélot, C., Heenen, M. (2005). Three percent Thalidomide in 2.5% hyaluronan gel in the treatment of actinic keratoses: a meta-analysis of the recent studies. Arch DermatolRes, 297(5), 185-9.

DATE: 06-09-22

WEBLEM 2B

Open Babel Tool

Aim:

To retrieve, convert & store structure for "Penicillin" query and study various file formats using Open Babel Tool

Introduction:

Penicillin V is a member of the penicillin family exhibiting broad-spectrum antibiotic property. Penicillin V binds to penicillin binding proteins (PBP), the enzymes that catalyze the synthesis of peptidoglycan, which is a critical component of the bacterial cell wall. This leads to the interruption of cell wall synthesis, consequently leading to bacterial cell growth inhibition and cell lysis.

Phenoxymethylpenicillin is a narrow spectrum antibiotic also commonly referred to as Penicillin V or Penicillin VK. It is a phenoxymethyl analog of Penicillin G, or [benzylpenicillin]. An orally active naturally penicillin, phenoxymethylpenicillin is used to treat mild to moderate infections in the respiratory tract, skin, and soft tissues caused by penicillin G--sensitive microorganisms. Phenoxymethylpenicillin has also be used in some cases as prophylaxis against susceptible organisms. While there have been no controlled clinical efficacy studies that were conducted, phenoxymethylpenicillin has been suggested by the American Heart Association and the American Dental Association for use as an oral regimen for prophylaxis against bacterial endocarditis in patients with congenital heart disease or rheumatic or other acquired valvular heart disease when they undergo dental procedures and surgical procedures of the upper respiratory tract, except for those who are at an elevated risk for endocarditis.

Open Babel is a free, open-source version of the Babel chemistry file translation program. Open Babel is a project designed to pick up where Babel left off, as a cross-platform program and library designed to interconvert between many file formats used in molecular modeling, computational chemistry, and many related areas. Open Babel includes two components, a command-line utility and a C++ library. The command-line utility is intended to be used as a replacement for the original babel program, to translate between various chemical file formats. The C++ library includes all of the file-translation code as well as a wide variety of utilities to foster development of other open source scientific software.

Methodology:

1. Open homepage for Pubchem database
2. Search for compound "Penicillin"
3. Download the compound in various file formats such as SMILES, sdf and mol file formats
4. Open the OPEN BABEL Tool and upload the structure file derived from pubchem
5. Convert the file format into the various structural file formats
6. Observe the penicillin in different file formas and interpret the results

Observations:

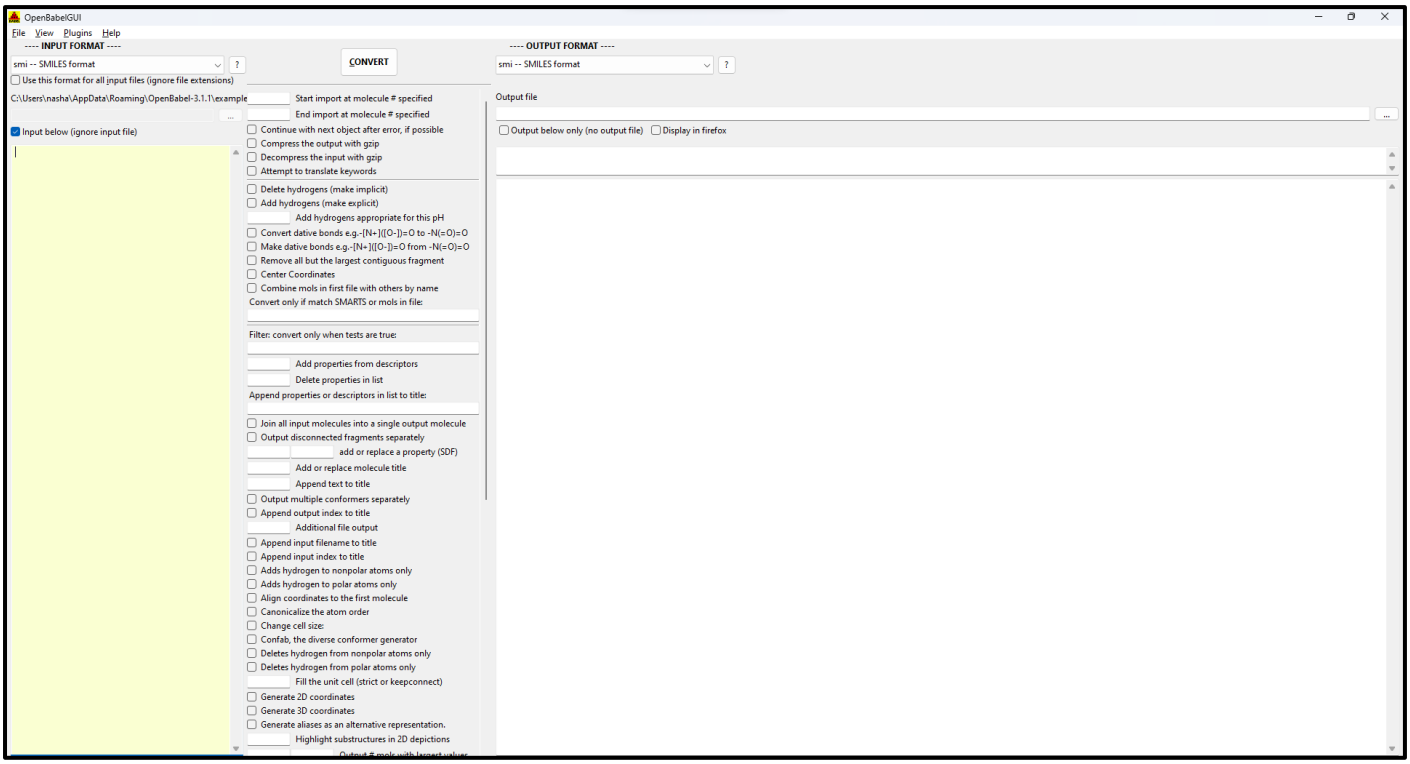


Fig 1. Homepage of OpenBabel tool

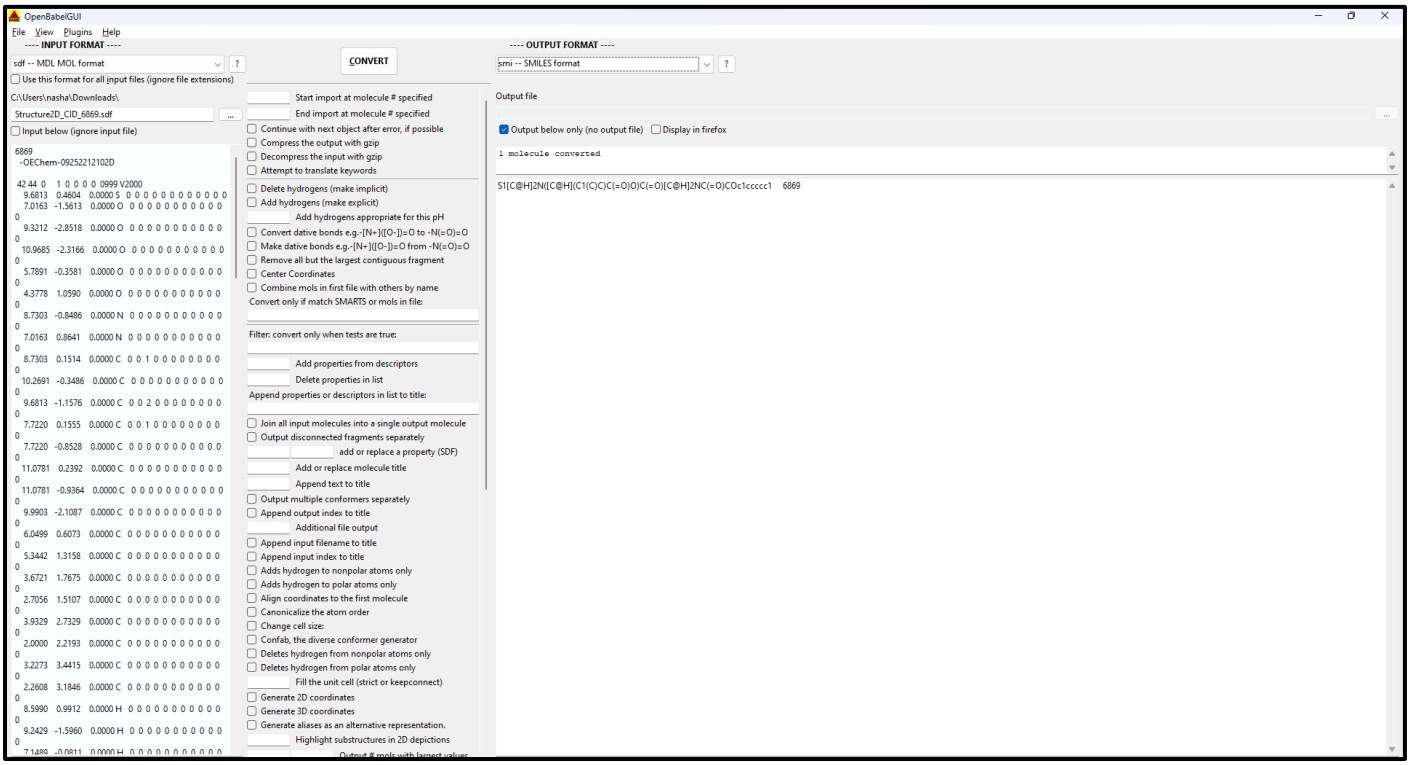


Fig 2. Convert sdf file into smiles for Penicillin

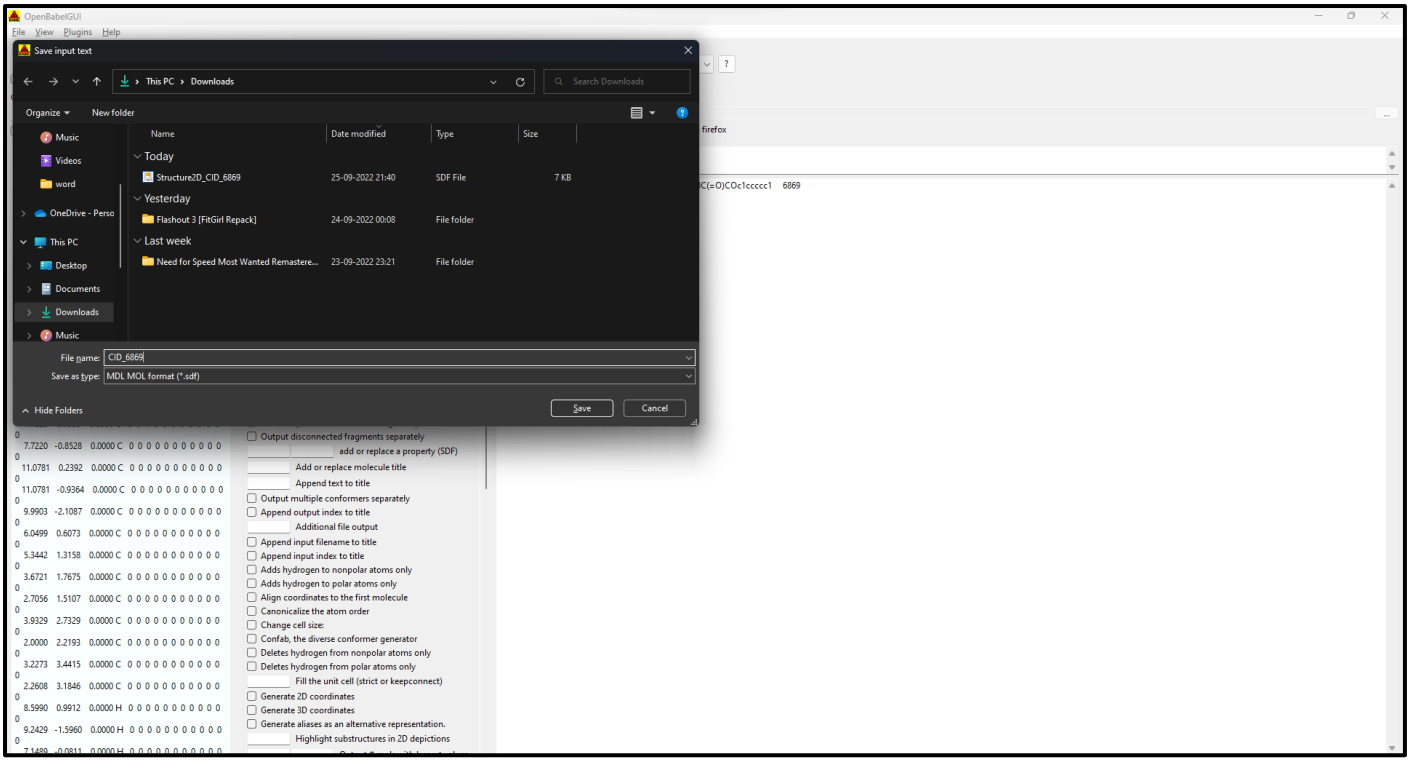


Fig 3. Storage Option for SMILES under Open Babel

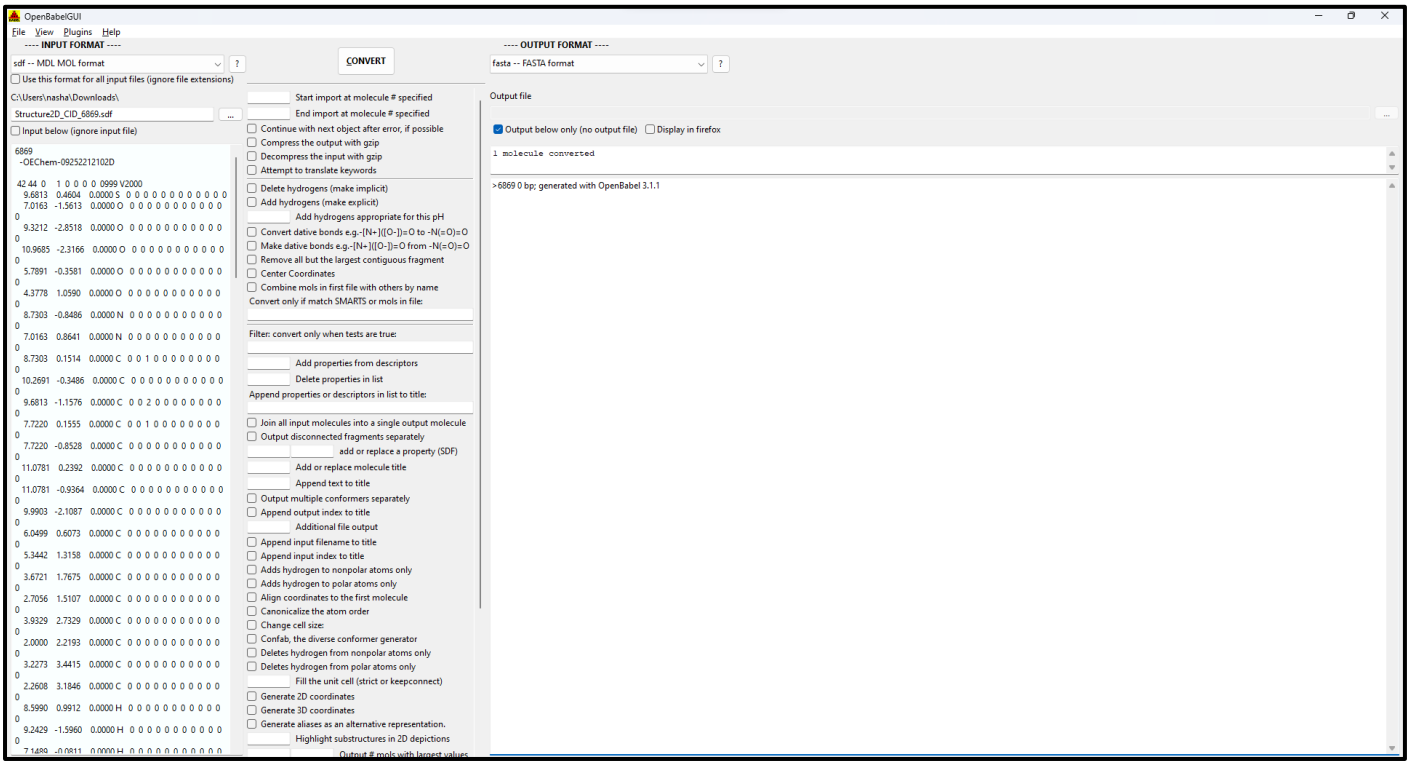


Fig 4. Convert sdf file into fasta file for Penicillin

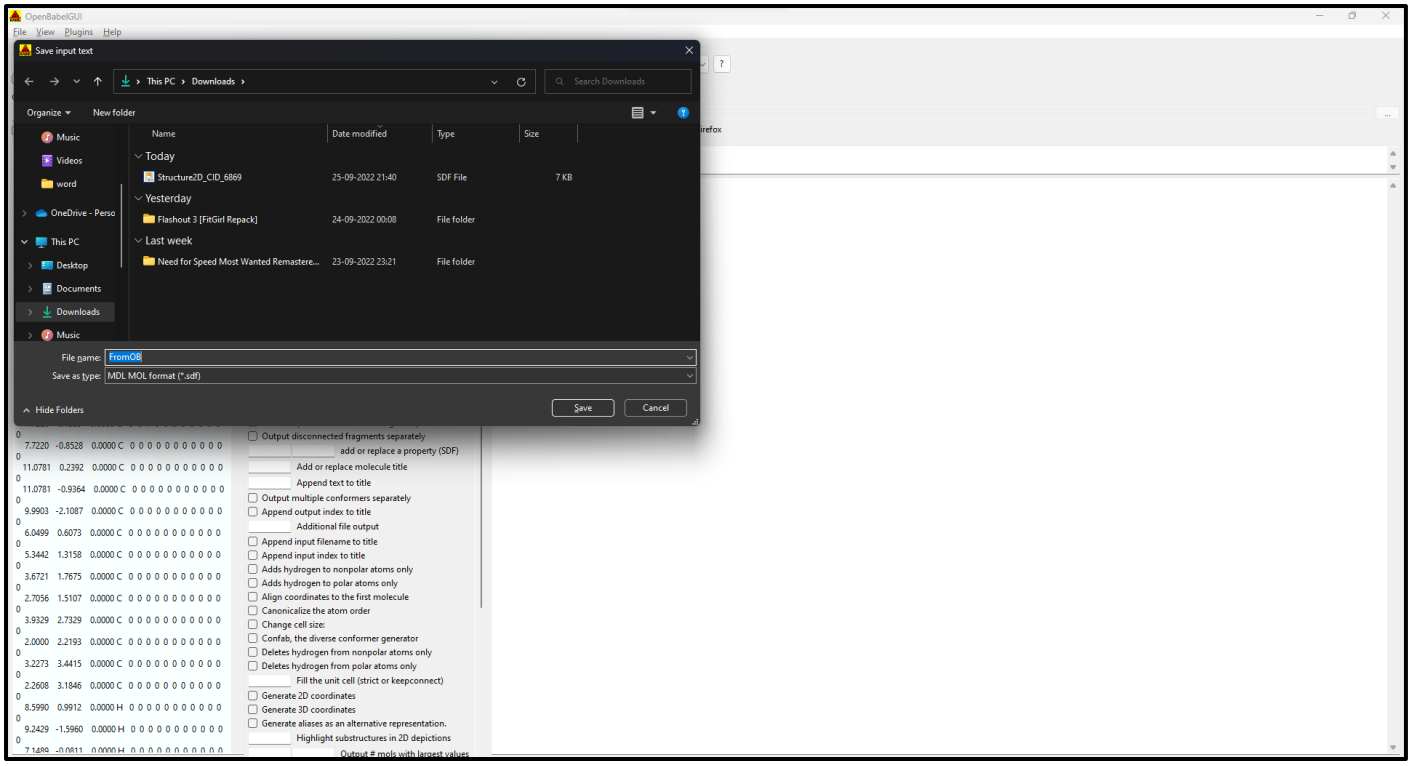


Fig 5. Storage option for fasta under Open Babel

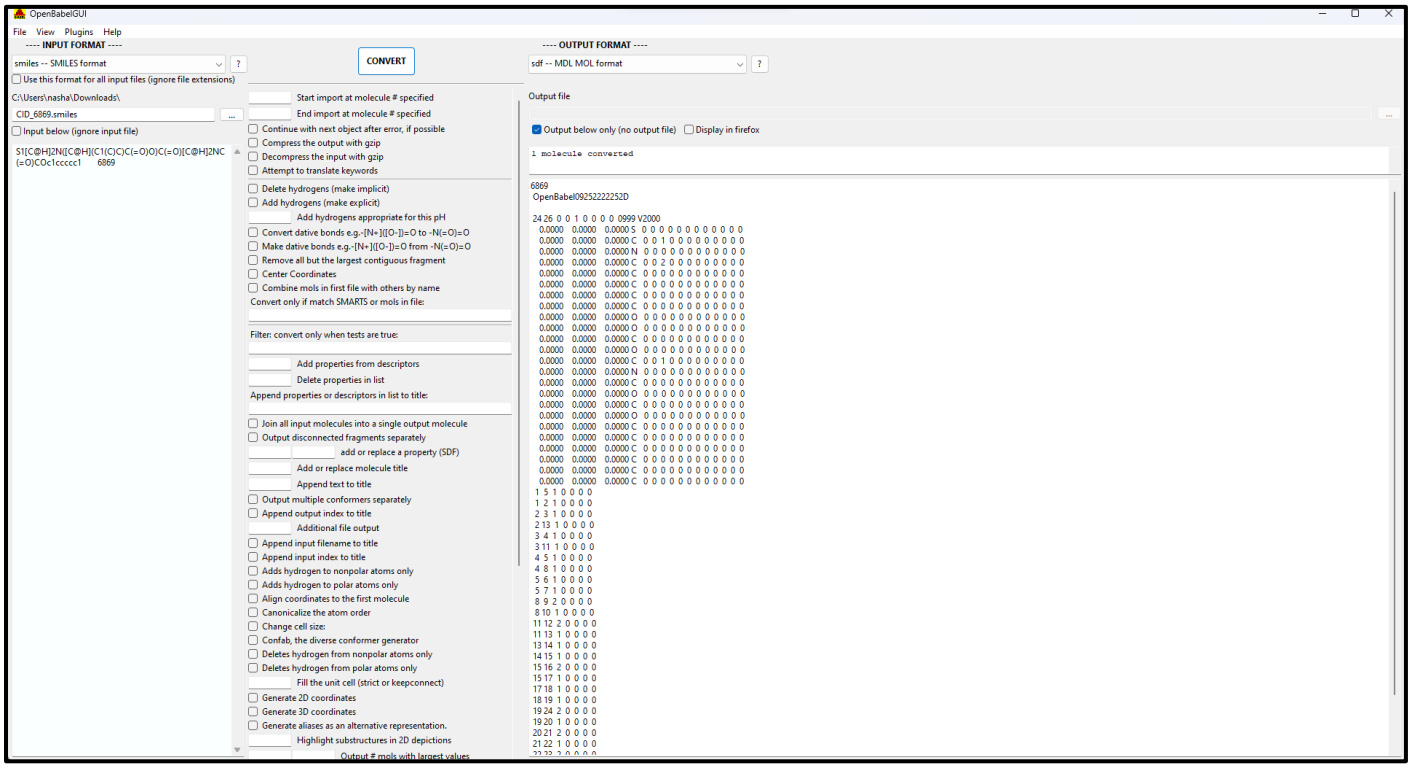


Fig 6. Convert smiles file into SDF file for Penicillin

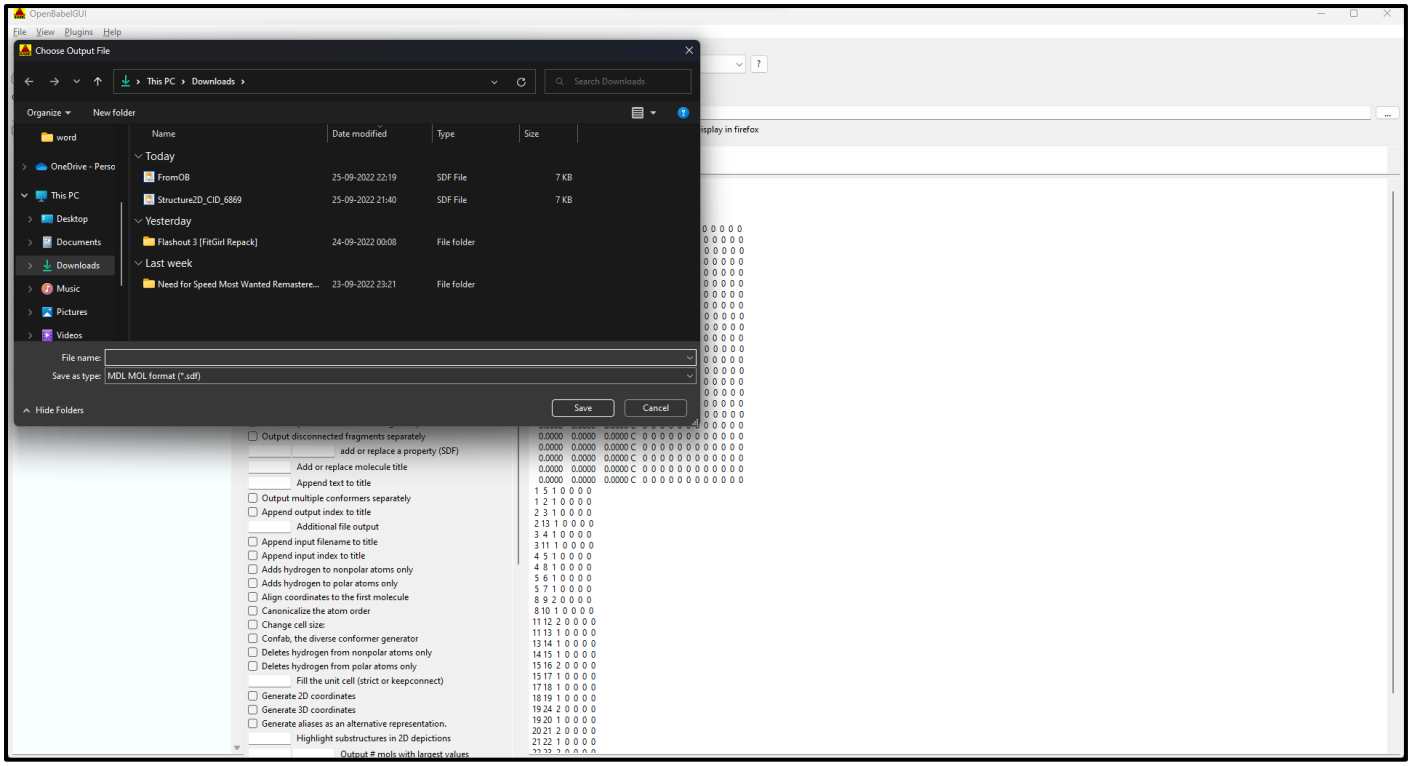


Fig 7. Storage options for sdf under Open Babel

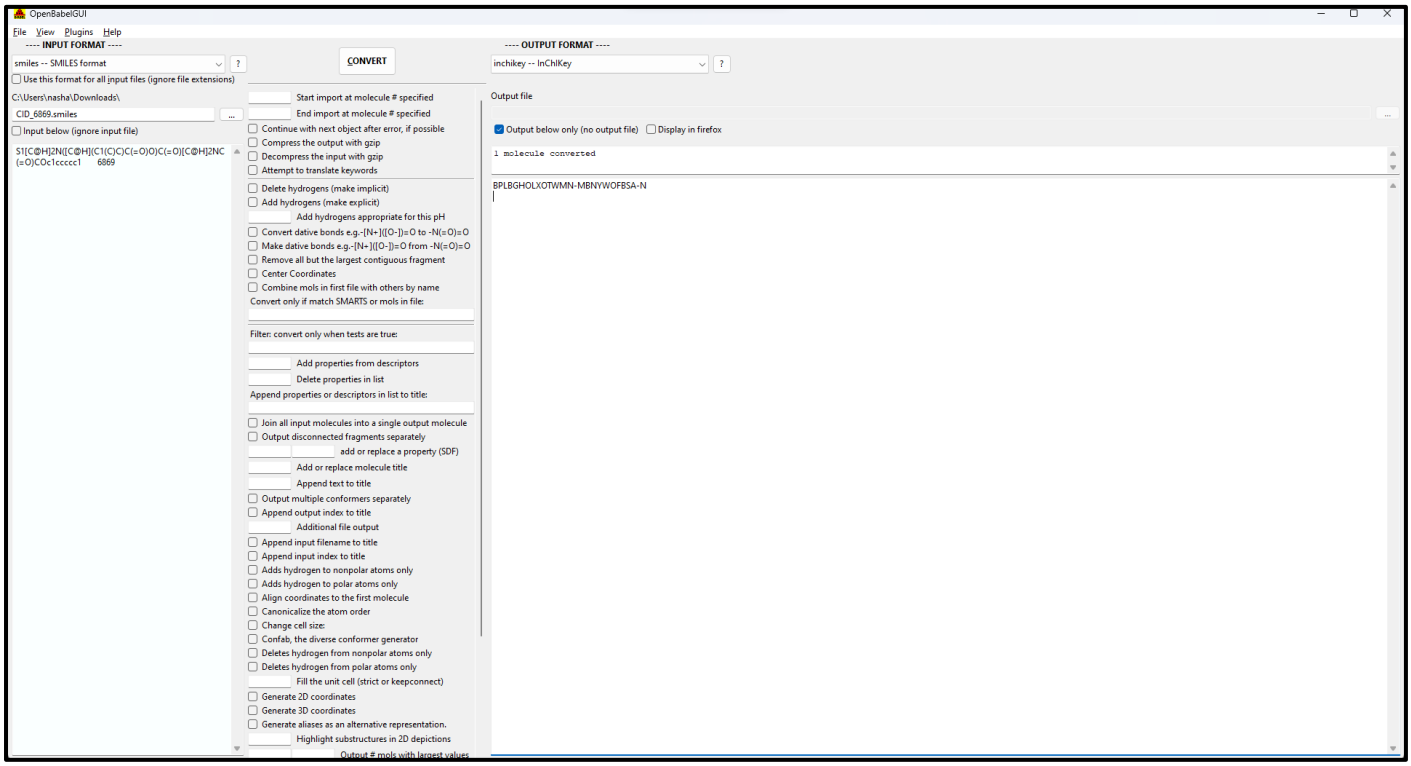


Fig 8. Convert smiles file into InChIKey file for penicillin

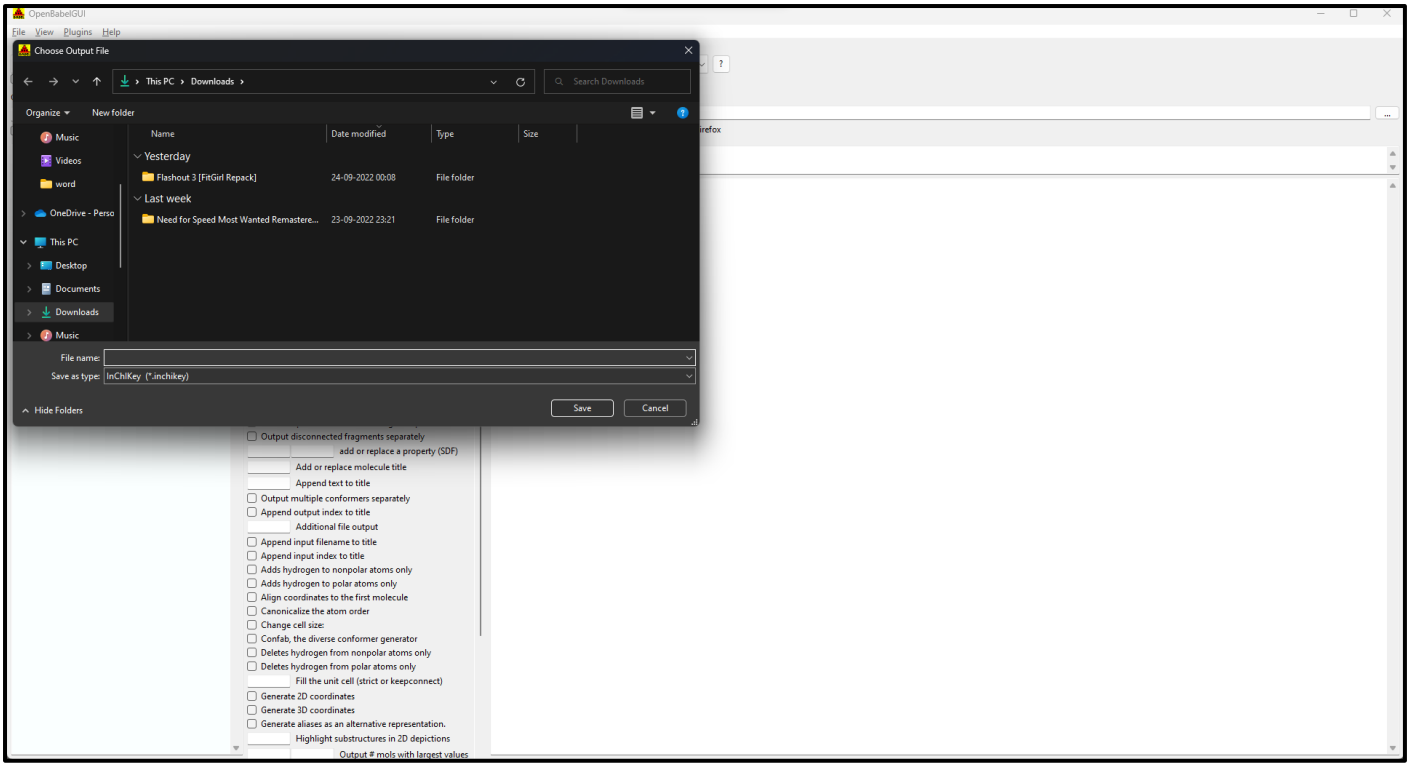


Fig 9. Storage options for InChIKey under open babel

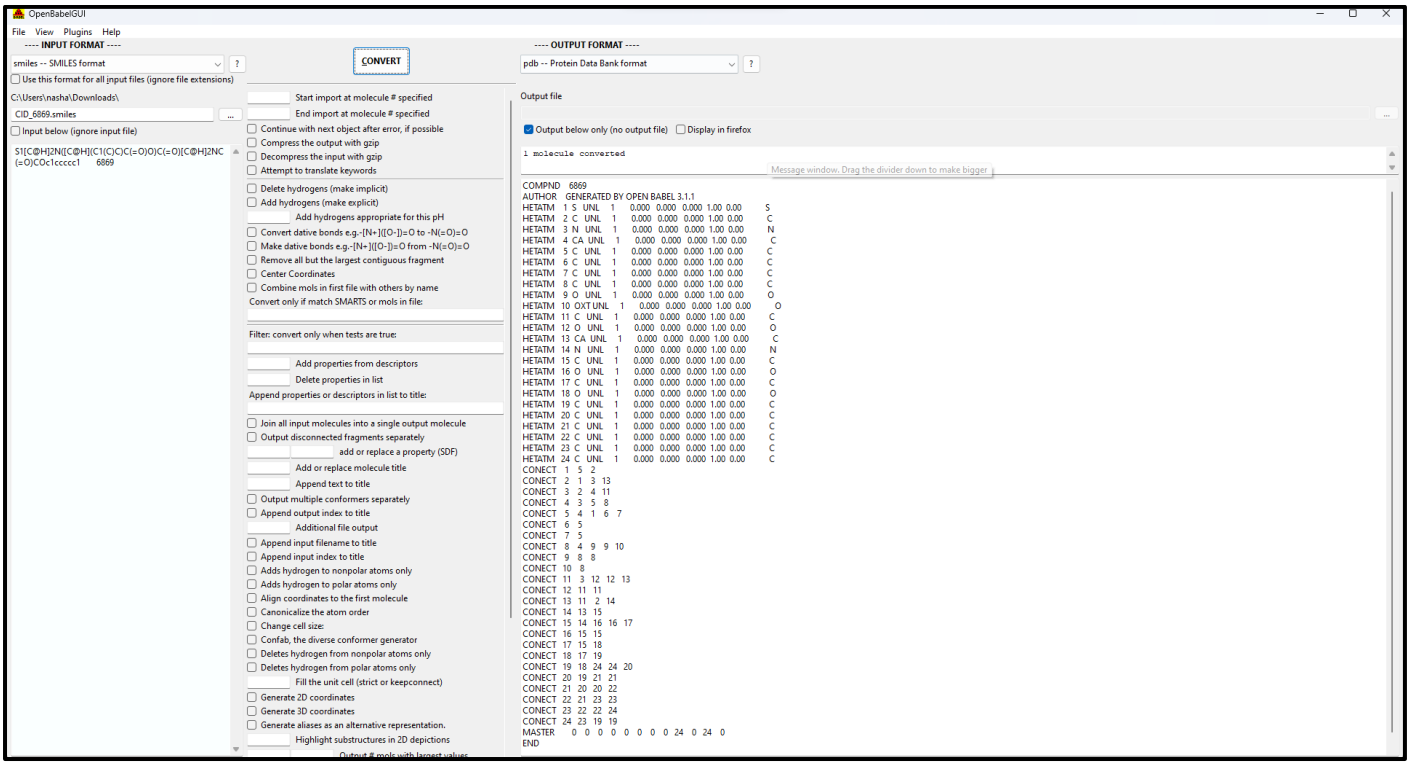


Fig 10. Convert smiles file into pdb file for penicillin

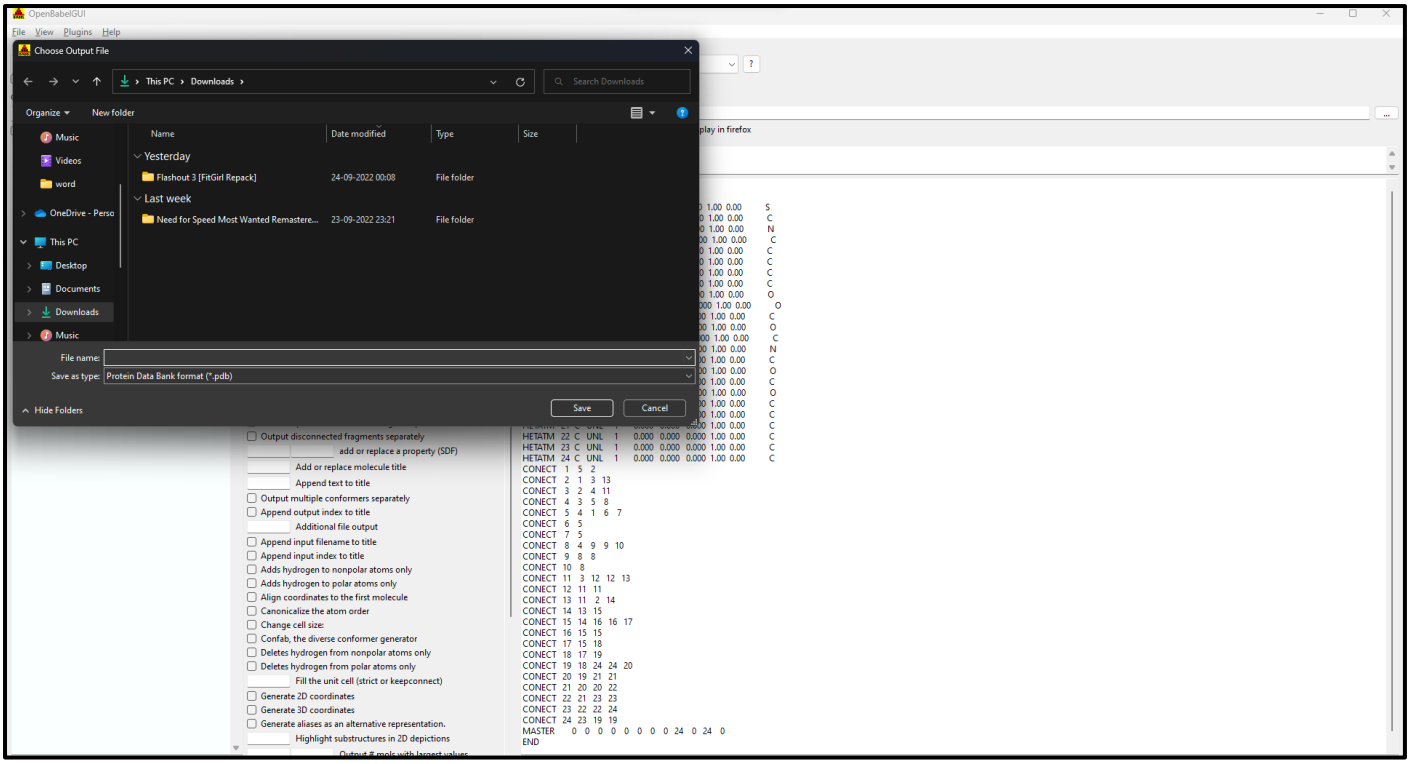


Fig 11. Storage Option for pdb under Open babel

Results:

The structure for Penicillin was retrieved from PUBCHEM in sdf file format. By using Open Babel tool, it was possible to convert various structural file formats into various other formats such as SMILES, MDL MOL, fasta, pdb, InChl key and the output is saved in the desired format for further studies

Conclusion:

The data of the chemical compound “Penicillin” was studied using different file formats. Therefore, the Open Babel tool presents a solution to the increase of multiple chemical file formats. It gains by way of its users, contributors, developers, related projects, and the general chemical community. It allows searching, converting, analyzing, or storing data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas. It provides both ready-to-use programs as well as a complete, extensible programmer's toolkit for developing cheminformatics software.

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1. Tawfeek, N., Mahmoud, MF., Hamdan, DI., Sobeh, M., Farrag, N., Wink, M., El-Shazly, AM. (2021).
2. Phytochemistry, Pharmacology and Medicinal Uses of Plants of the Genus Salix: An Updated Review. Front Pharmacol, 12(593856).
3. Weininger, D. (1988). SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules. J Chem Inf Comput Sci. 28, 31-36.