DATE: 06/09/22

WEBLEM: 2

BIOVIA Draw Software & Open Babel Tool

AIM:

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

INTRODUCTION:

CHEMICAL STRUCTURE:

The chemical structure of a drug determines its physicochemical properties, further determines its ADME/Tox properties, and ultimately affects its pharmacological activity. Medicinal chemists can regulate the pharmacological activity of drug molecules by modifying their structure. Ring systems and functional groups are important components of a drug. The proportion of non-hydrocarbon atoms among non-hydrogen atoms reflects the heavy atoms proportion of a drug. The three factors have considerable potential for the assessment of the drug-like properties of organic molecules. However, to the best of our knowledge, there have been no studies to systematically analyze the simultaneous effects of the number of aromatic and non-aromatic rings, the number of some special functional groups and the proportion of heavy atoms on the drug-like properties of an organic molecule. To this end, the numbers of aromatic and non-aromatic rings, the numbers of some special functional groups and the heavy atoms proportion of 6891 global approved small drugs have been comprehensively analyzed.

I. 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, color and a variety of arrow styles.

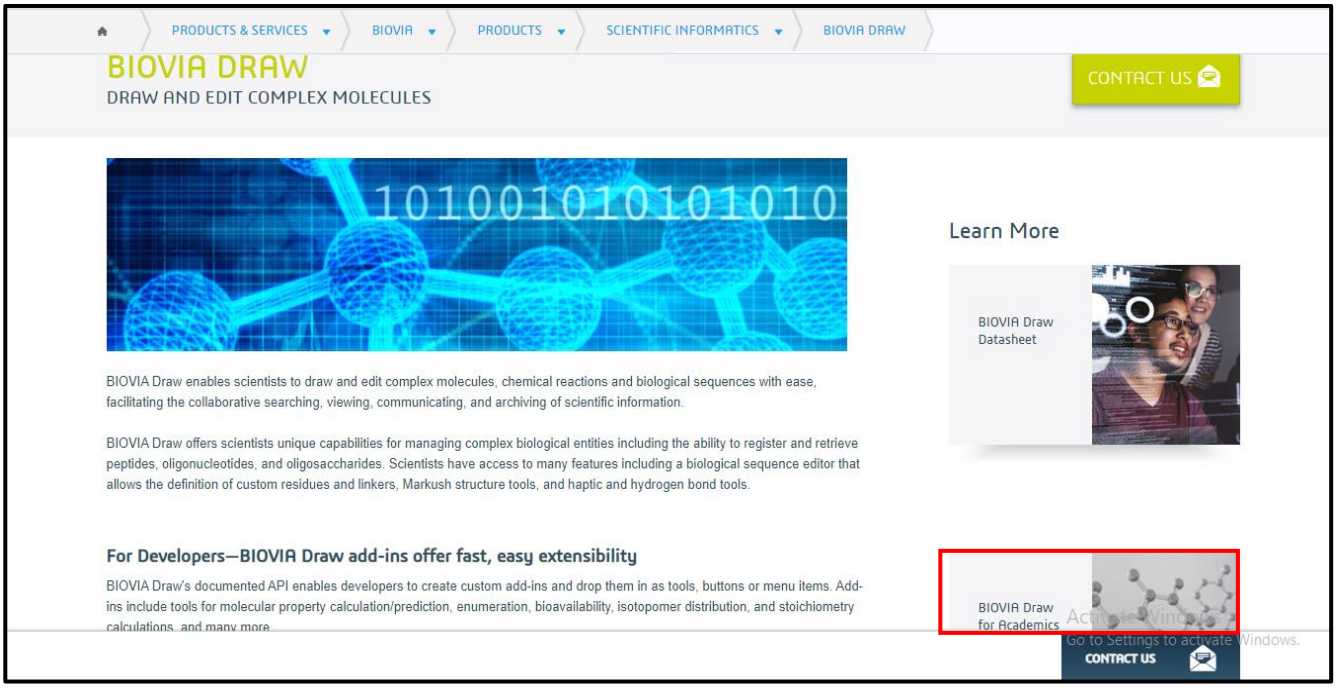
- Easily create publication-quality structures for inclusion in Microsoft Office documents and presentations.

APPLICATIONS:

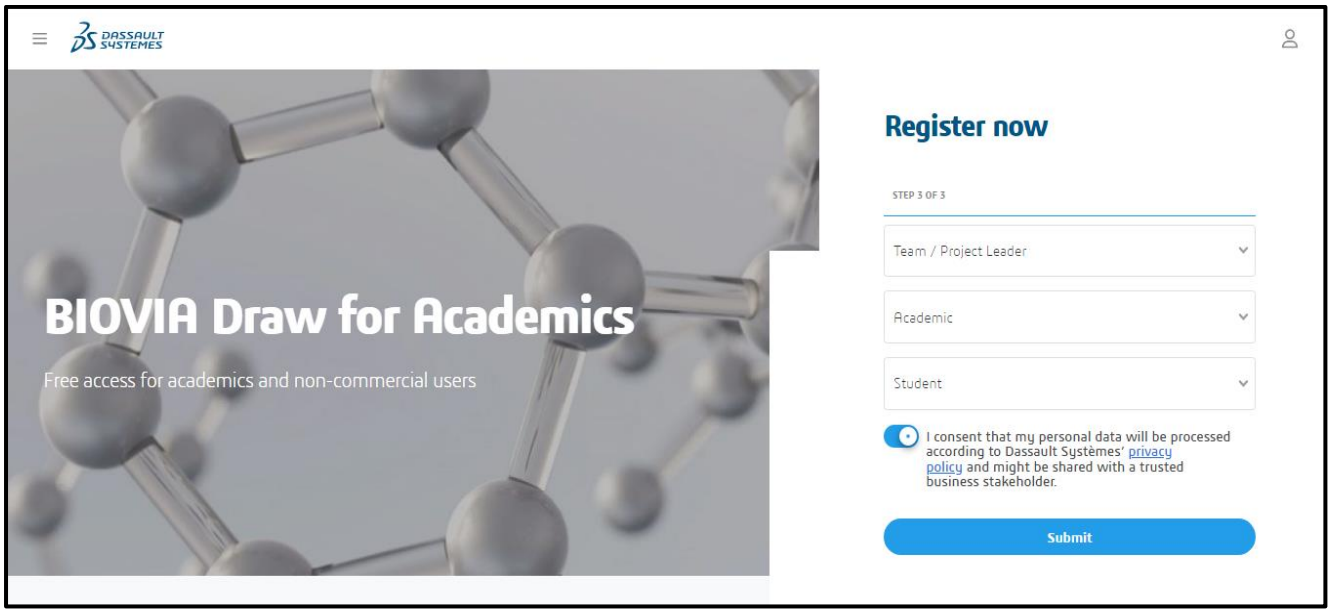
Simulate, visualize and analyze chemical and biological systems; and to communicate the results to other scientists.

INSTALLATION STEPS:

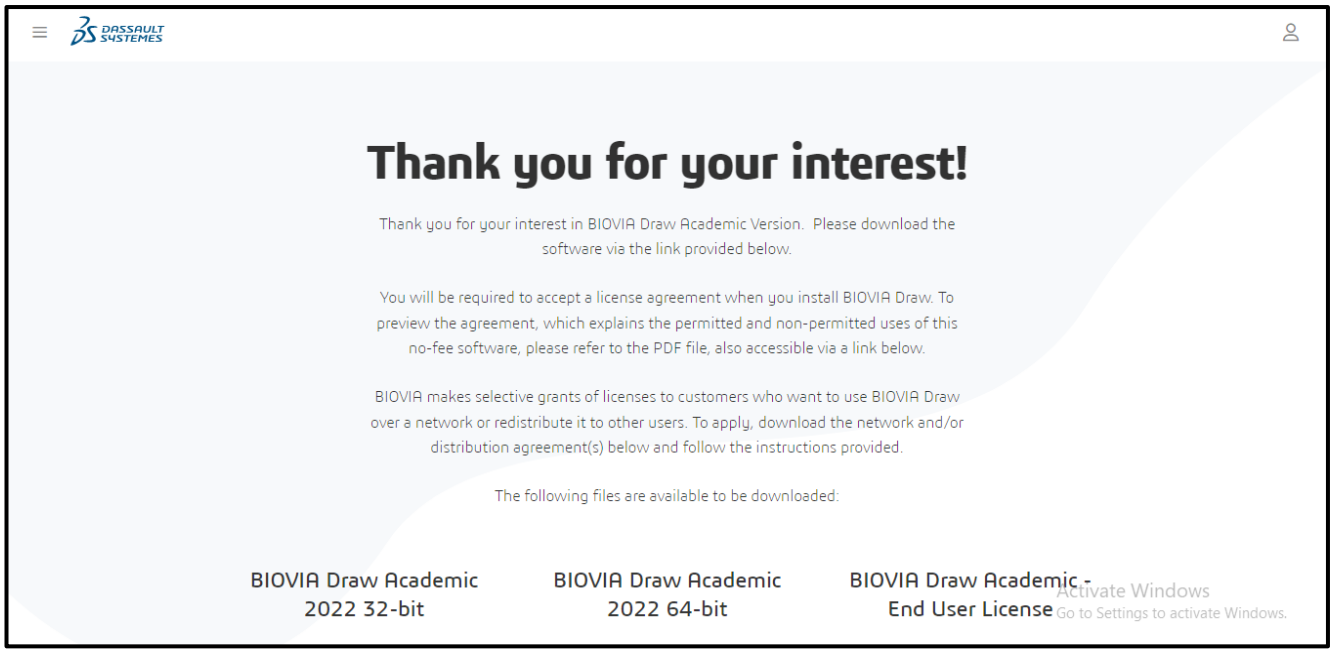
1) Open Homepage of BIOVIA DRAW software website and then click on BIOVIA Draw for Academics (**URL:** https://www.3ds.com/products-services/biovia/products/scientific-informatics/biovia-draw/).



2) Fill the registration details and click on Submit.

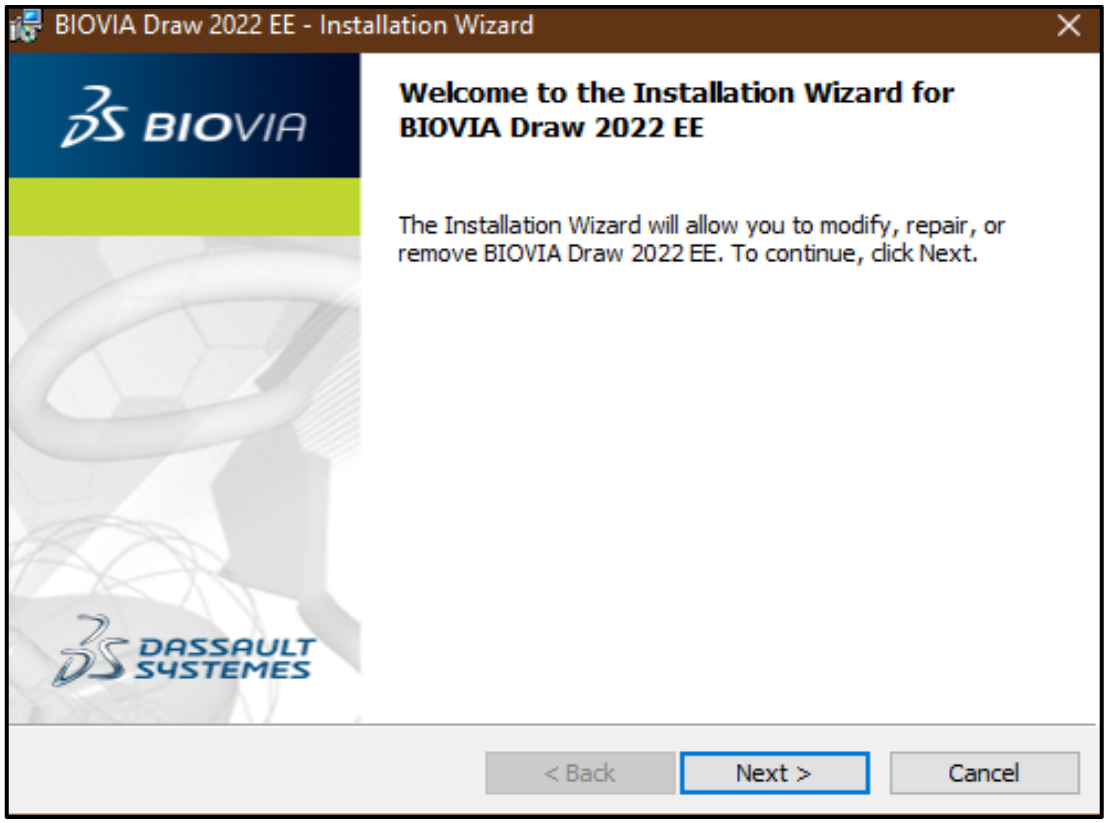


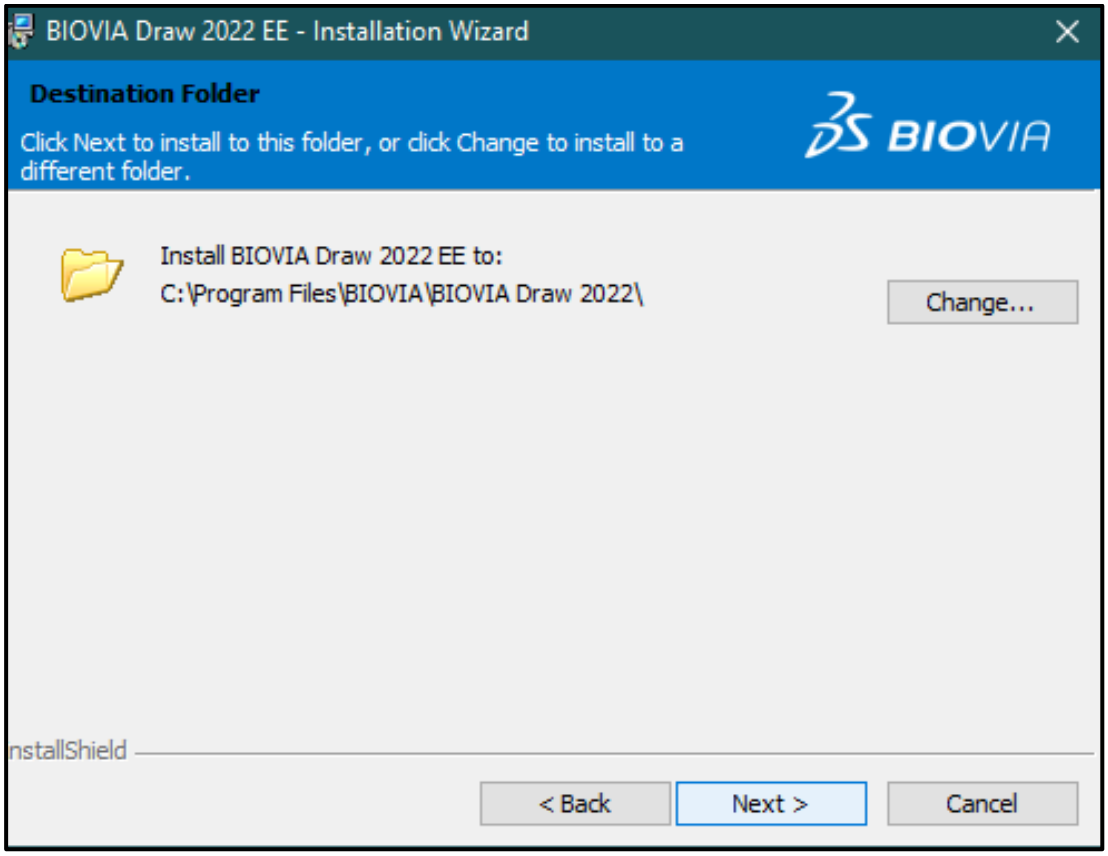
3) Download BIOVIA DRAW Academic 2022.

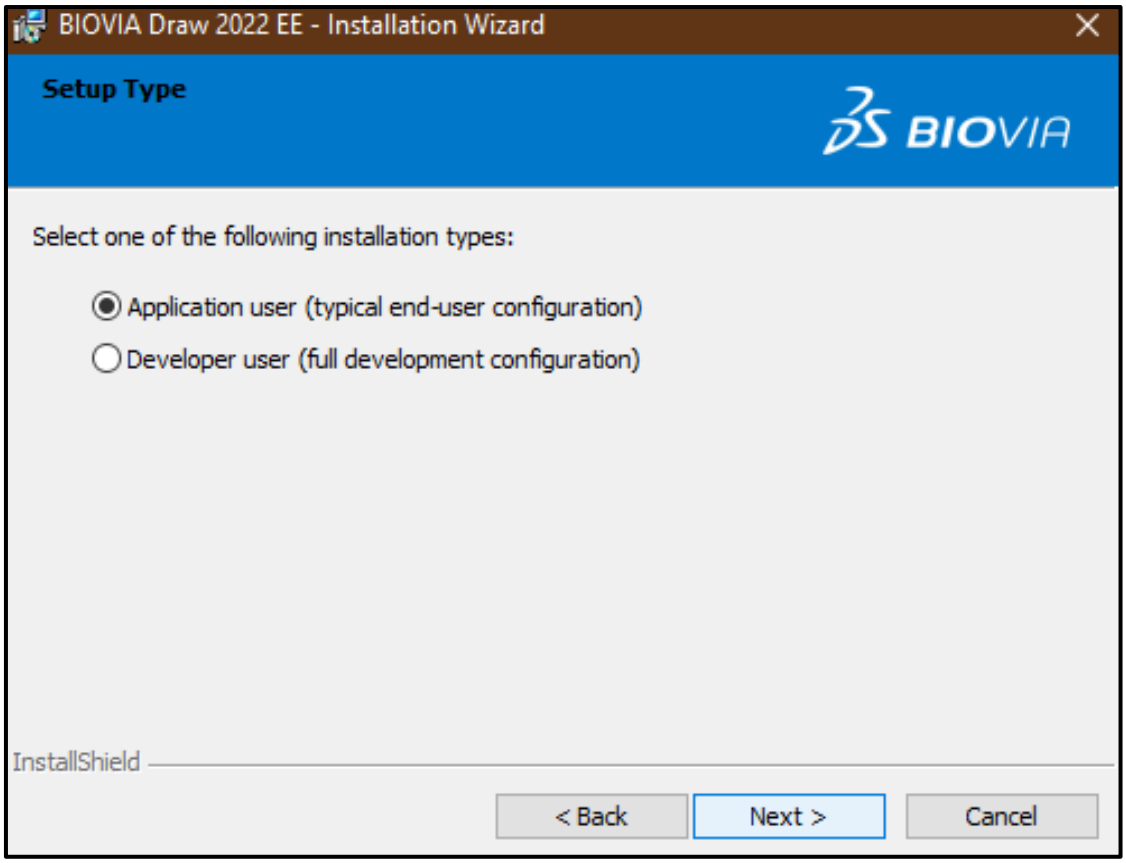


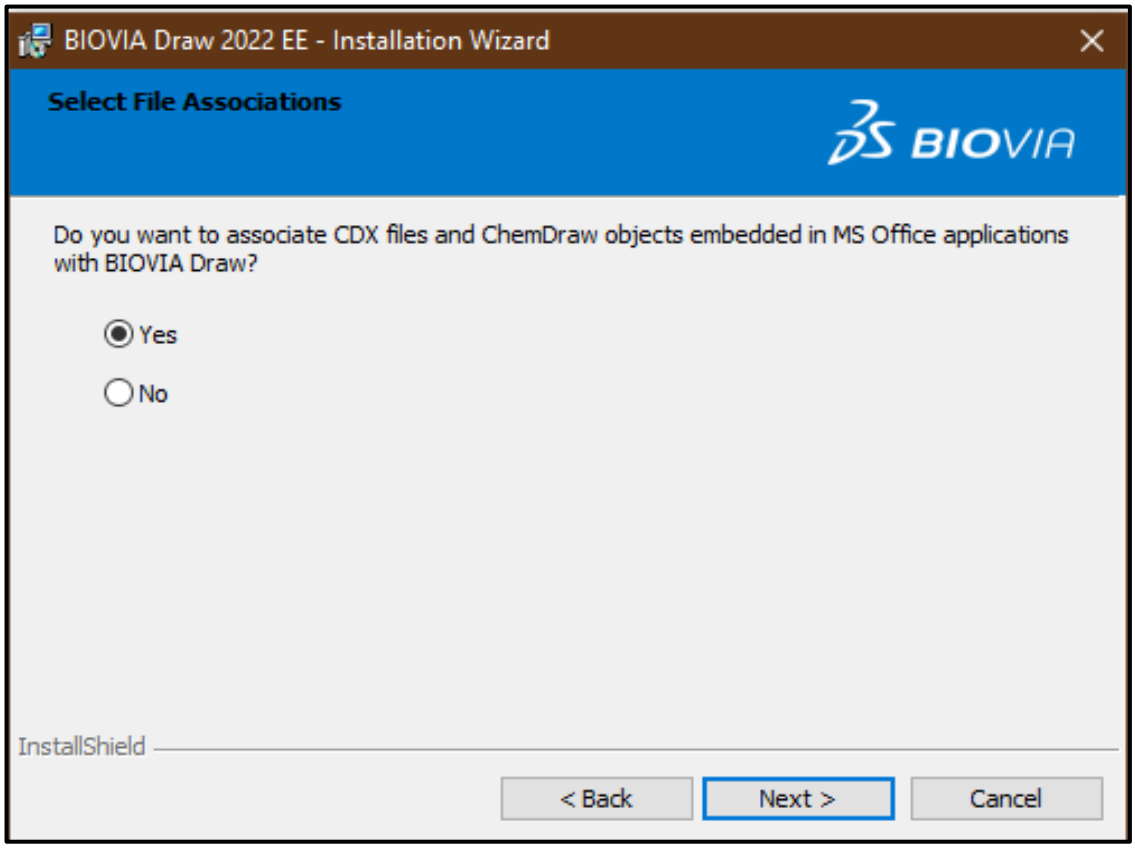
4) After Downloading, open it in your PC or Laptop.

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

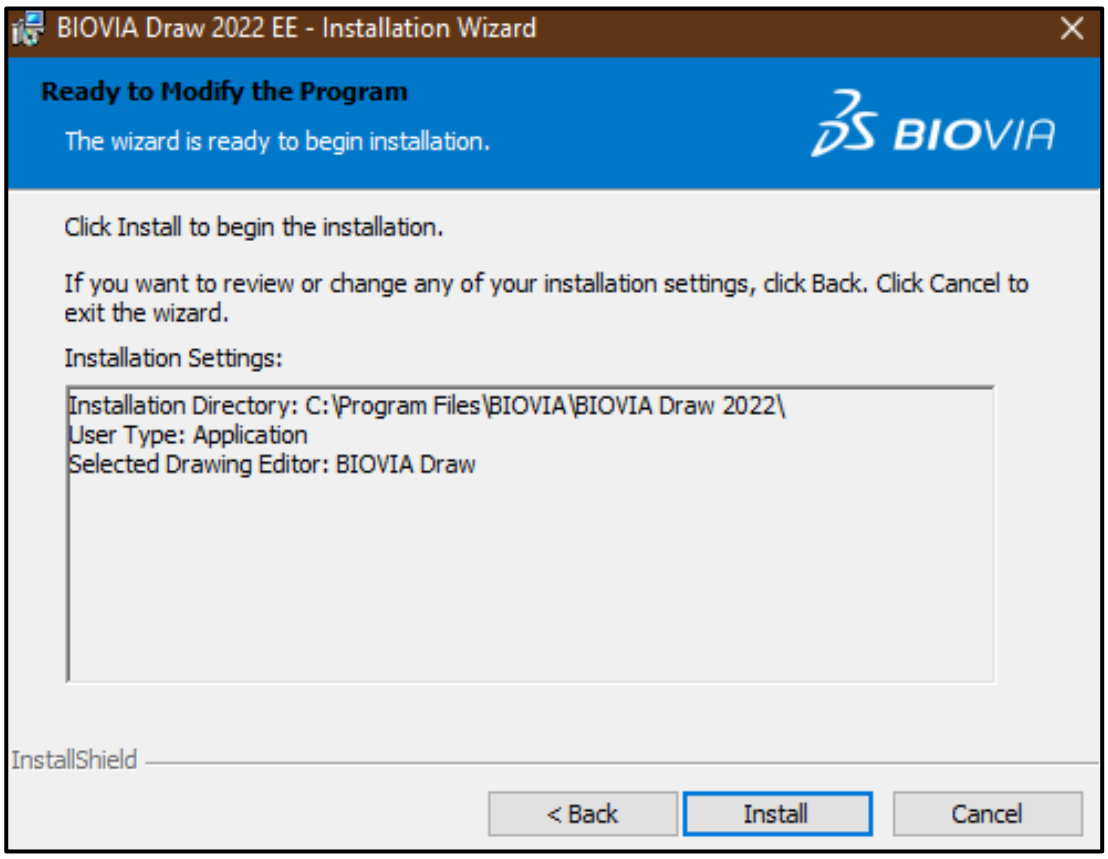

BIOVIA Draw 2022 EE - Installation Wizard
BIOVIA
Welcome to the Installation Wizard for BIOVIA Draw 2022 EE
The Installation Wizard will allow you to modify, repair, or remove BIOVIA Draw 2022 EE. To continue, click Next.
DASSAULT SYSTEMES
< Back
Next >
Cancel


BIOVIA Draw 2022 EE - Installation Wizard
Destination Folder
Click Next to install to this folder, or click Change to install to a different folder.
BIOVIA
Install BIOVIA Draw 2022 EE to:
C:\Program Files\BIOVIA\BIOVIA Draw 2022\
Change...
nstallShield
< Back
Next >
Cancel

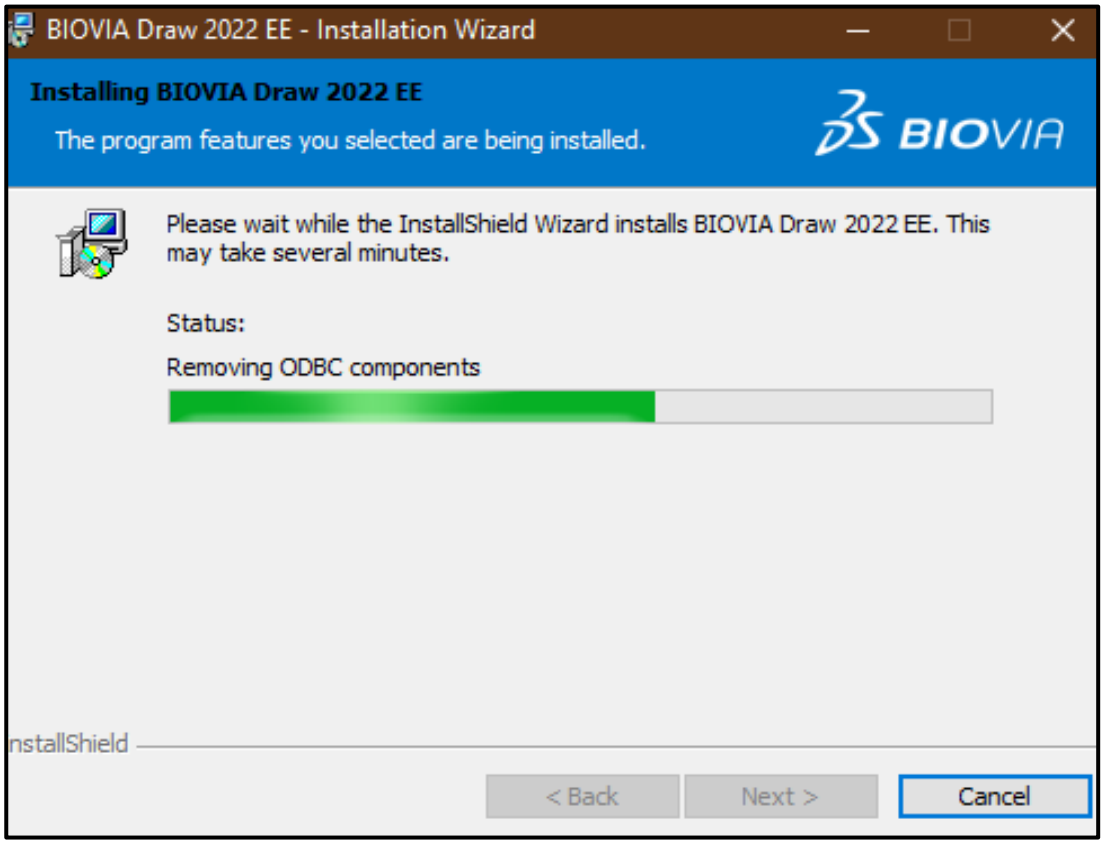

BIOVIA Draw 2022 EE - Installation Wizard
Setup Type
BIOVIA
Select one of the following installation types:
Application user (typical end-user configuration)
Developer user (full development configuration)
InstallShield
< Back
Next >
Cancel


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

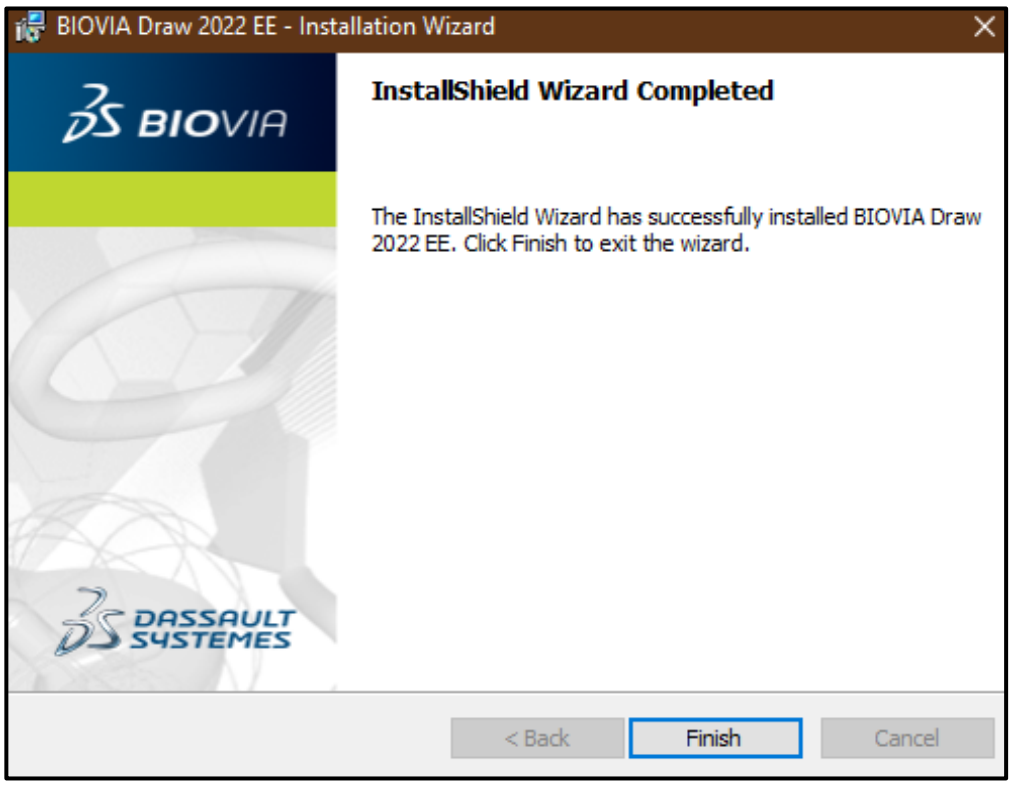
6) Click on Install to begin the installation.



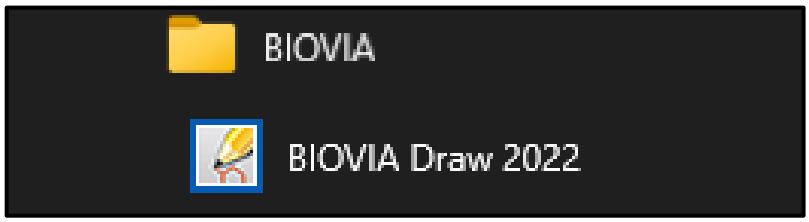
7) Setup has started installing BIOVIA Draw 2022.



8) The InstallShield Wizard has successfully installed BIOVIA Draw 2022. Click Finish to exit the wizard.



9) Icon of BIOVIA Draw software 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,

canonical numbering of molecular structures and fragments, molecular mechanics force fields, and the extensible interfaces provided by the software library to enable further chemistry software development.

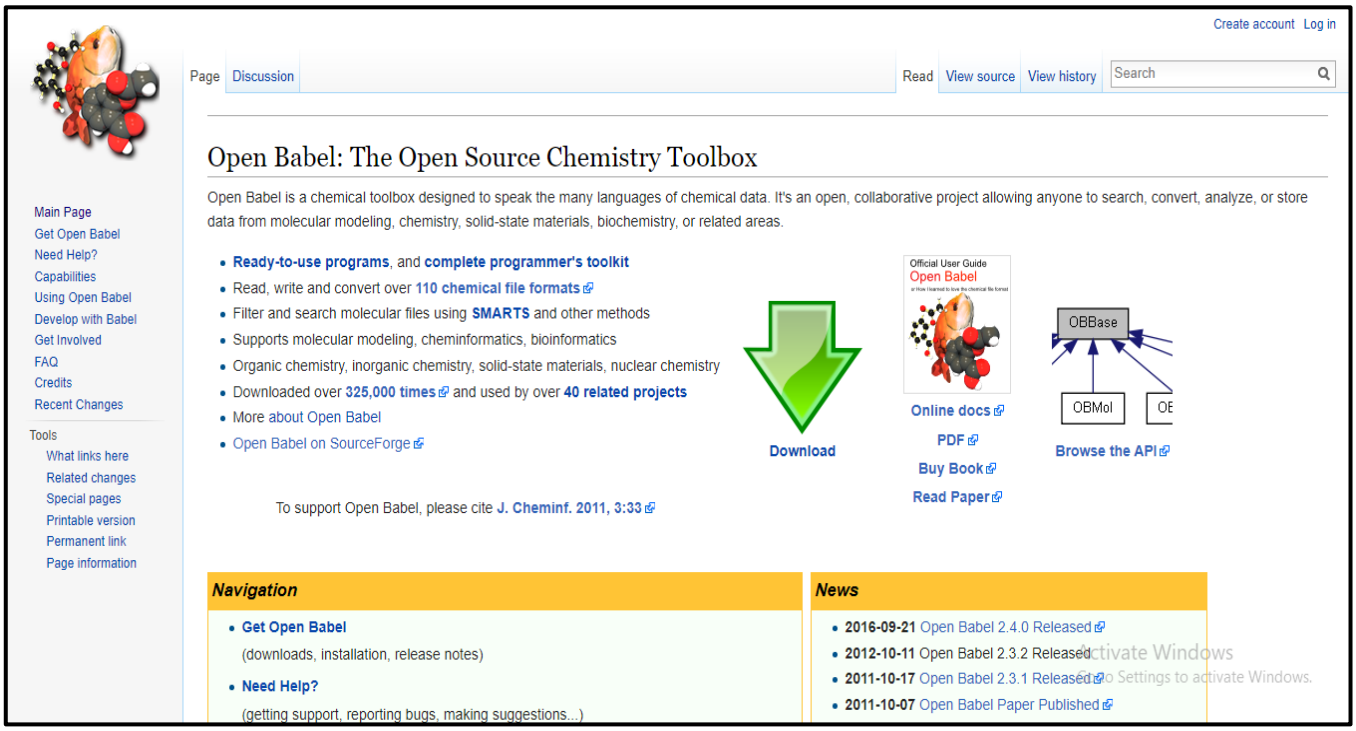
Open Babel has its origin in a version of OELib released as open-source software by OpenEye Scientific under the GPL (GNU Public License). In 2001, OpenEye decided to rewrite OELib in-house as the proprietary OEChem library, so the existing code from OELib was spun out into the new Open Babel project. 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:

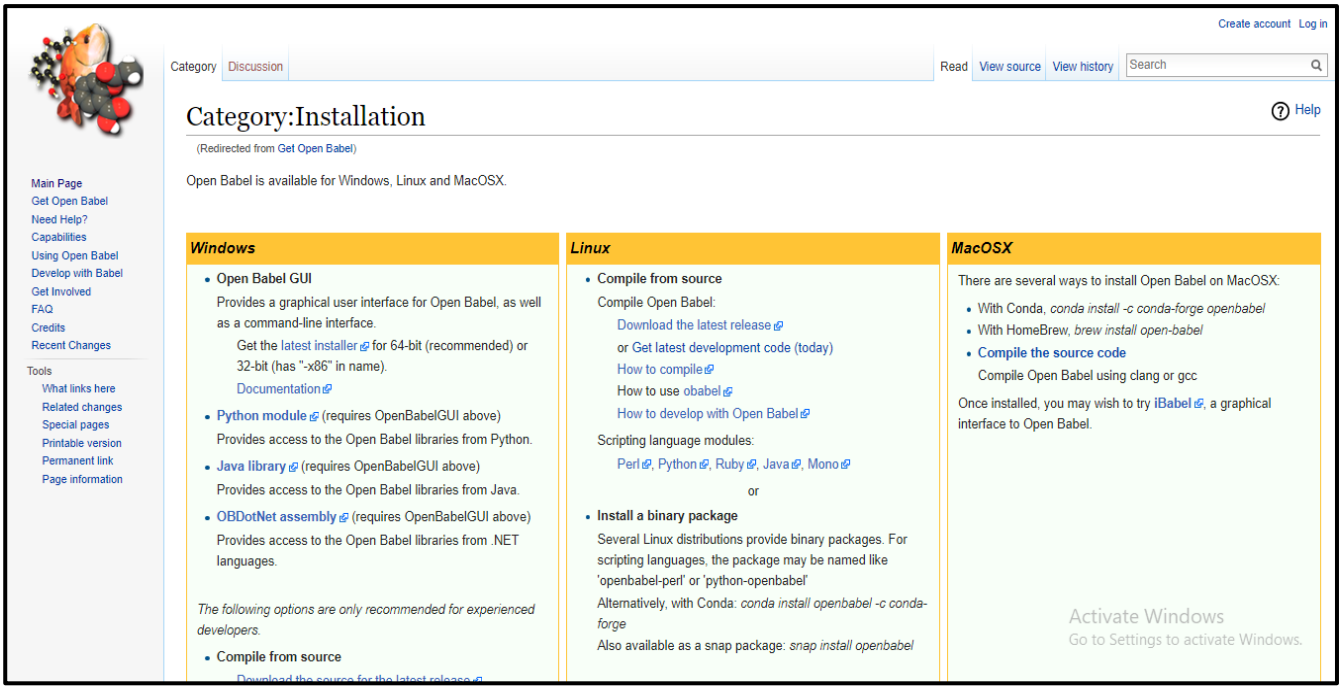
1) File Format Support.
2) Fingerprints and Fast Searching.
3) Bond Perception and Atom Typing.
4) Canonical Representation of Molecules.
5) Coordinate Generation in 2D and 3D.

INSTALLATION STEPS:

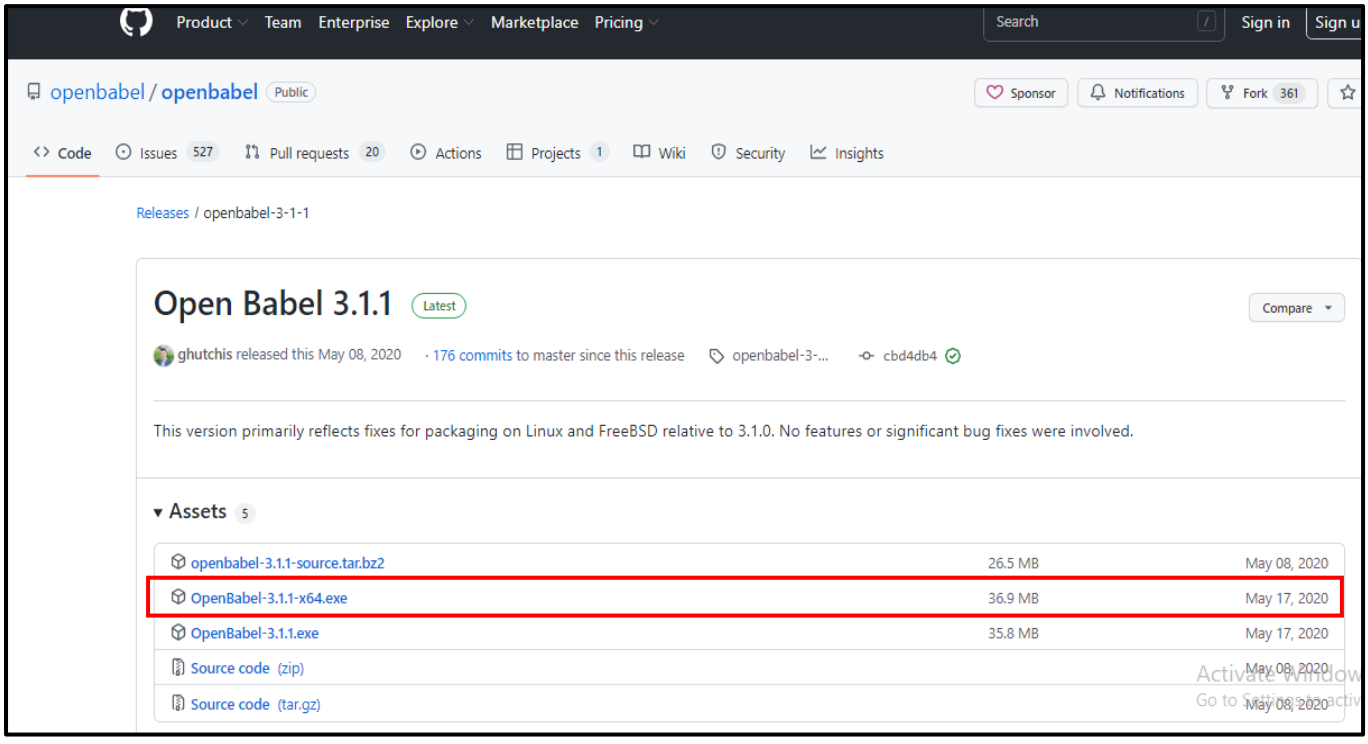
1) Open Homepage of Open Babel website and then click on download.
   (**URL:** http://openbabel.org/wiki/Main_Page).



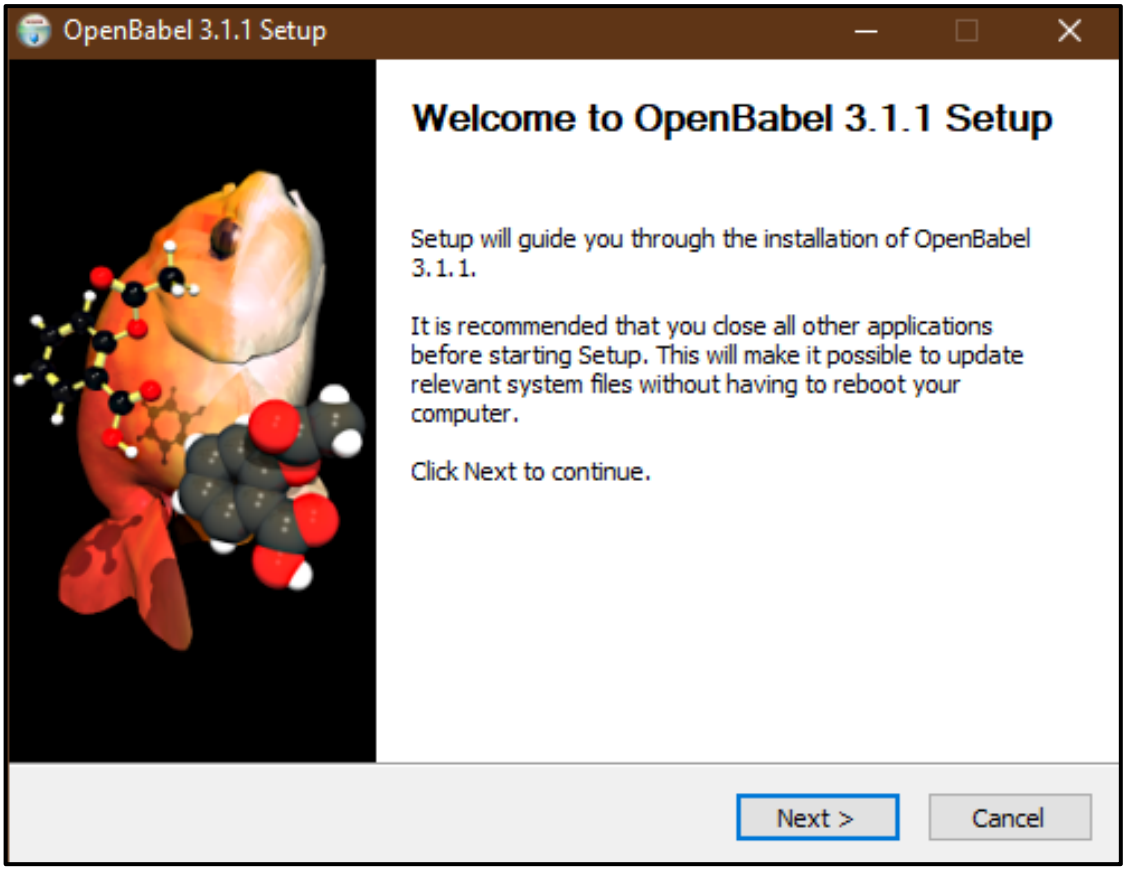
2) Open Babel is available for window, Linux, Mac version. For windows install the 64 bit.



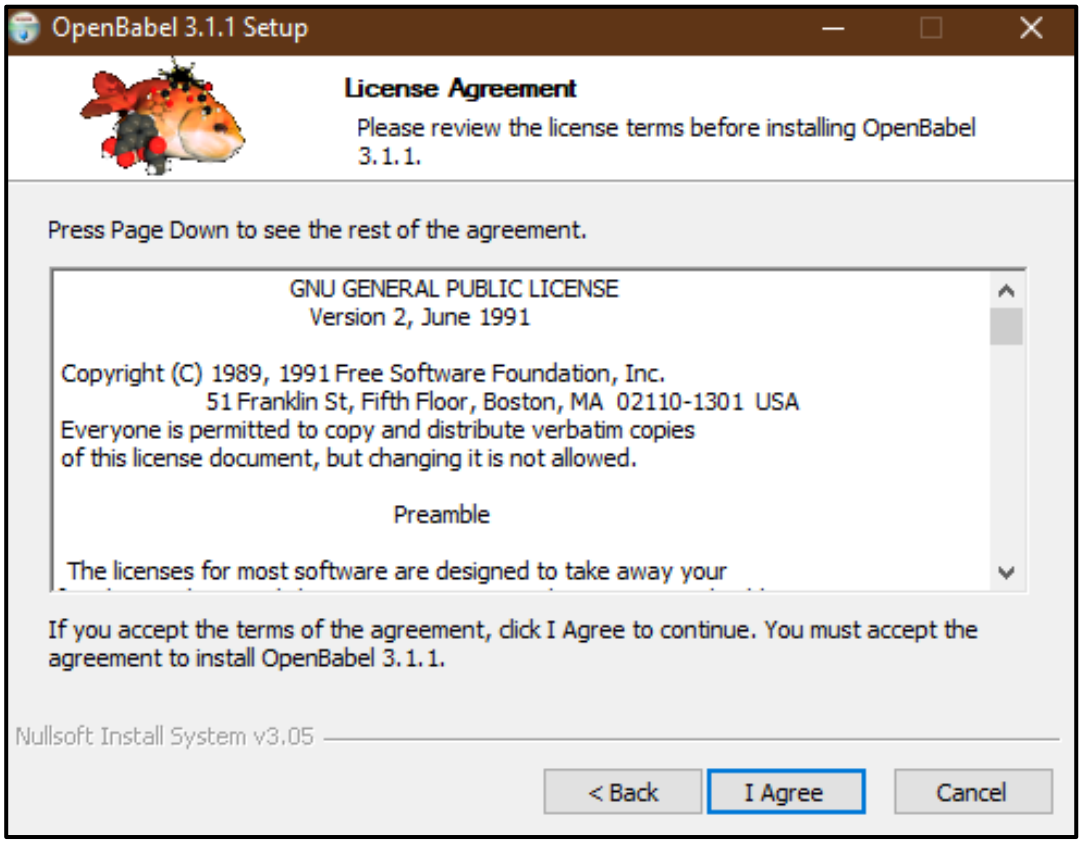
3) Click on OpenBabel-3.1.1-64.exe file.



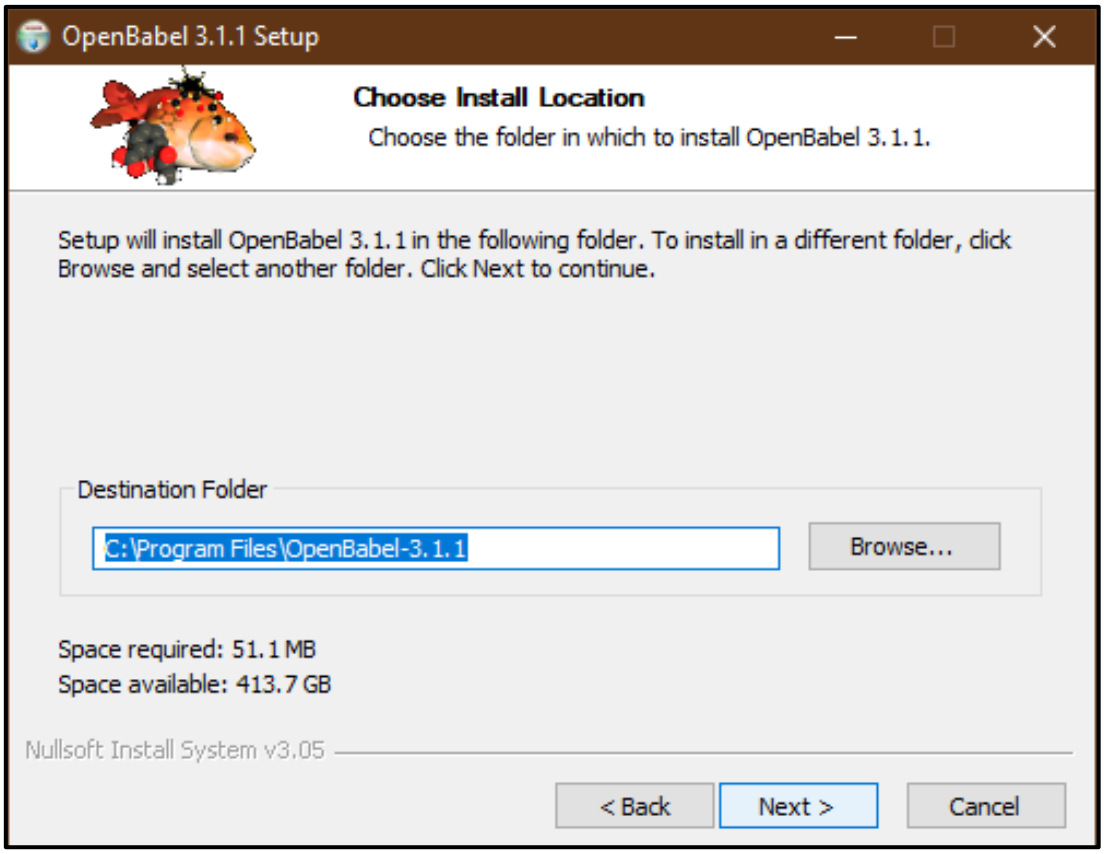
4) Click on ‘Next’.



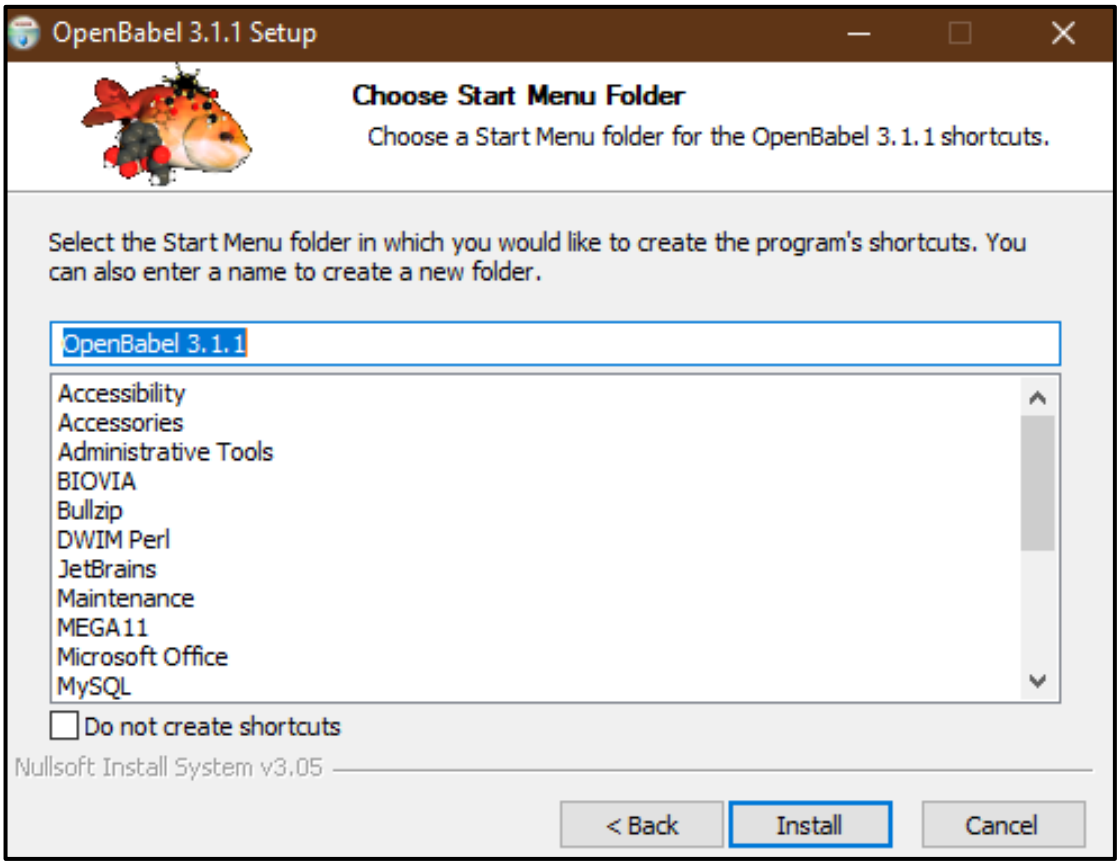
5) Review the license terms before installing OpenBabel 3.1.1. , and then click on ‘I Agree’ to accept the agreement.



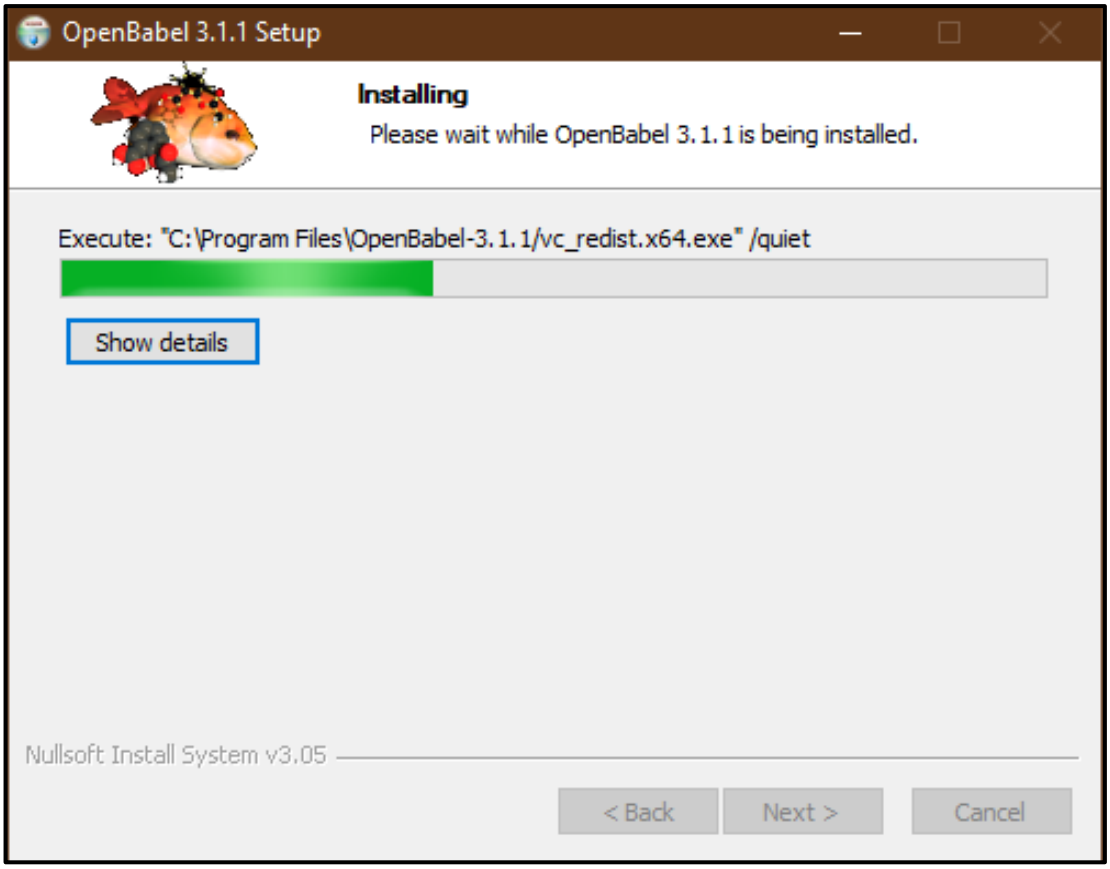
6) Choose the folder destination in which the setup will install OpenBabel 3.1.1 in the following folder and then click on ‘Next’.



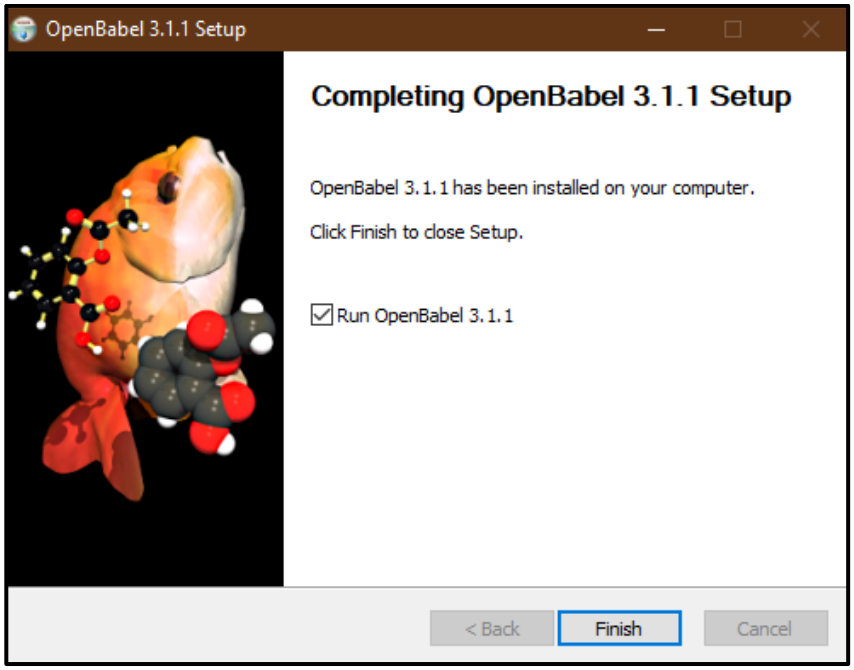
7) Select the start menu folder for creating OpenBabel 3.1.1 shortcut or else enter a name to create a new folder, and then click on ‘Install’.



8) Setup has started installing OpenBabel.



9) OpenBabel has been installed successfully. Click Finish to close the setup.



10) Icon of Open Babel Toolbox 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.

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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 "Thalidomide" using BIOVIA DRAW software.

INTRODUCTION:

Thalidomide, sold under the brand names Contergan, Thalomid among others, is a medication used to treat a number of cancers (including multiple myeloma), graft-versus-host disease, and a number of skin conditions including complications of leprosy. While it has been used in a number of HIV-associated conditions, such use is associated with increased levels of the virus. It is administered orally.

Common side effects include sleepiness, rash, and dizziness. Severe side effects include tumor lysis syndrome, blood clots, and peripheral neuropathy. Use in pregnancy may harm the fetus, including resulting in malformation of the limbs. In males who are taking the medication, contraception is essential if a partner could become pregnant. It is an immunomodulatory medication and works by a number of mechanisms, including stimulating T cells and decreasing TNF-α production.

Thalidomide is racemic; while S-thalidomide is the bioactive form of the molecule, the individual enantiomers can racemize to each other due to the acidic hydrogen at the chiral centre, which is the carbon of the glutarimide ring bonded to the phthalimide substituent. The racemization process can occur in vivo. The process of conversion of one enantiomer to its mirror-image version with no other change in the molecule is called chiral inversion.

BIOVIA Draw enables scientists to draw and edit complex molecules, chemical reactions and biological sequences with ease, facilitating the collaborative searching, viewing, communicating, & archiving of scientific information.

BIOVIA Draw offers scientists unique capabilities for managing complex biological entities including the ability to register and retrieve peptides, oligonucleotides, and oligosaccharides. Scientists have access to many features including a biological sequence editor that allows the definition of custom residues and linkers, Markush structure tools, and haptic and hydrogen bond tools.

BIOVIA Draw's documented API enables developers to create custom add-ins and drop them in as tools, buttons or menu items. Add-ins includes tools for molecular property calculation/prediction, enumeration, bioavailability, isotopomer distribution, and stoichiometry calculations, and many more.

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:

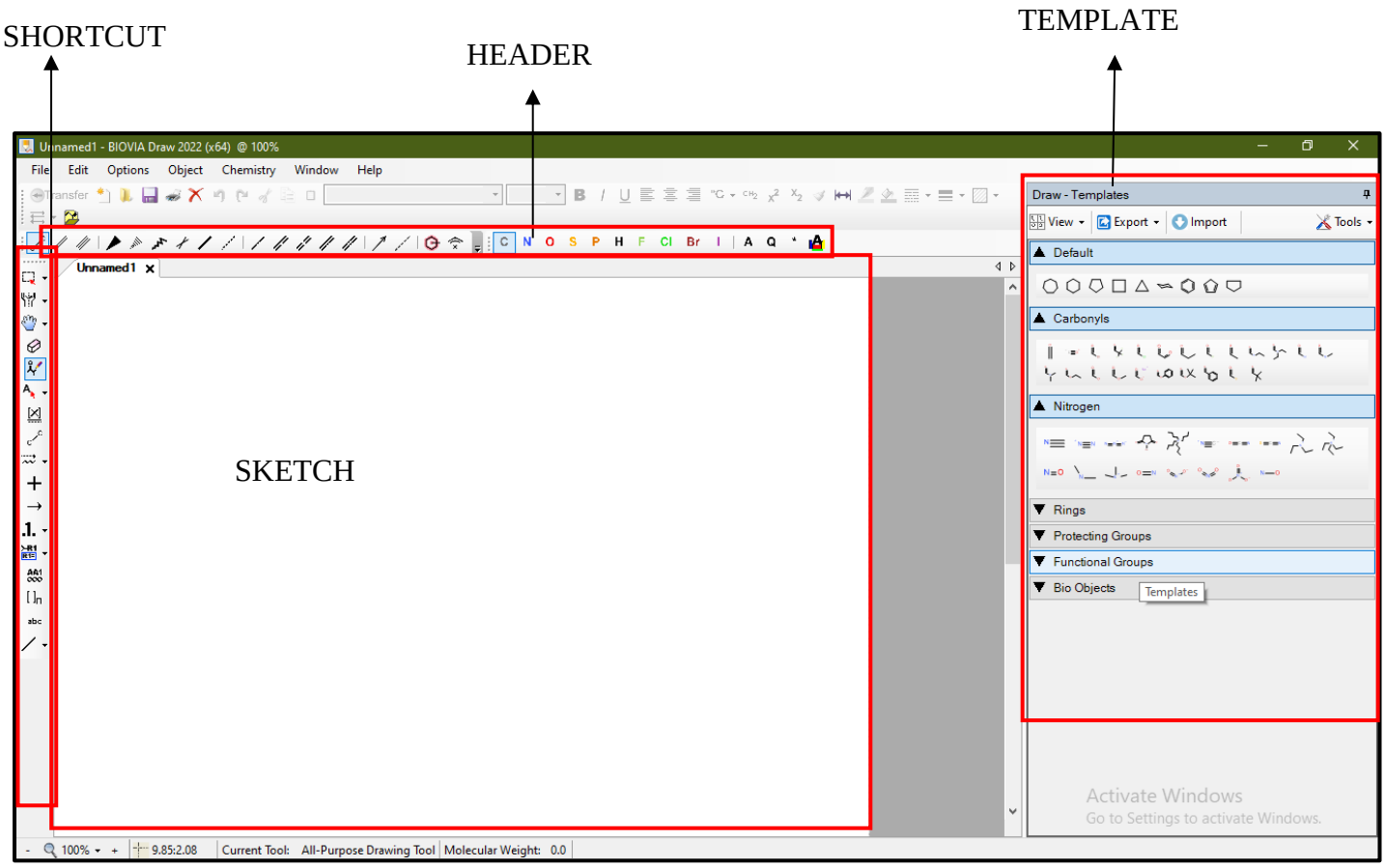

FIG1: Homepage of BIOVIA DRAW SOFTWARE

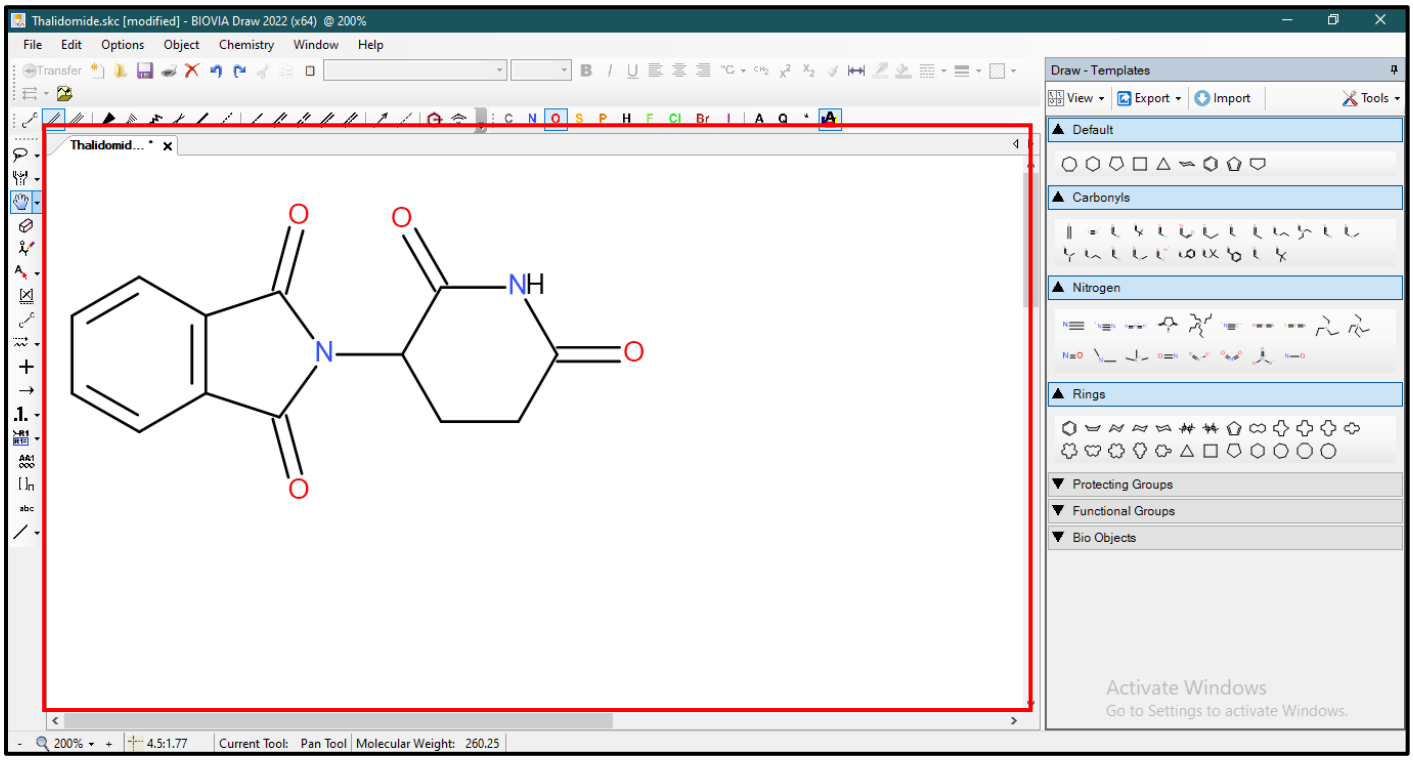

FIG2: Structure of Thalidomide chemical compound

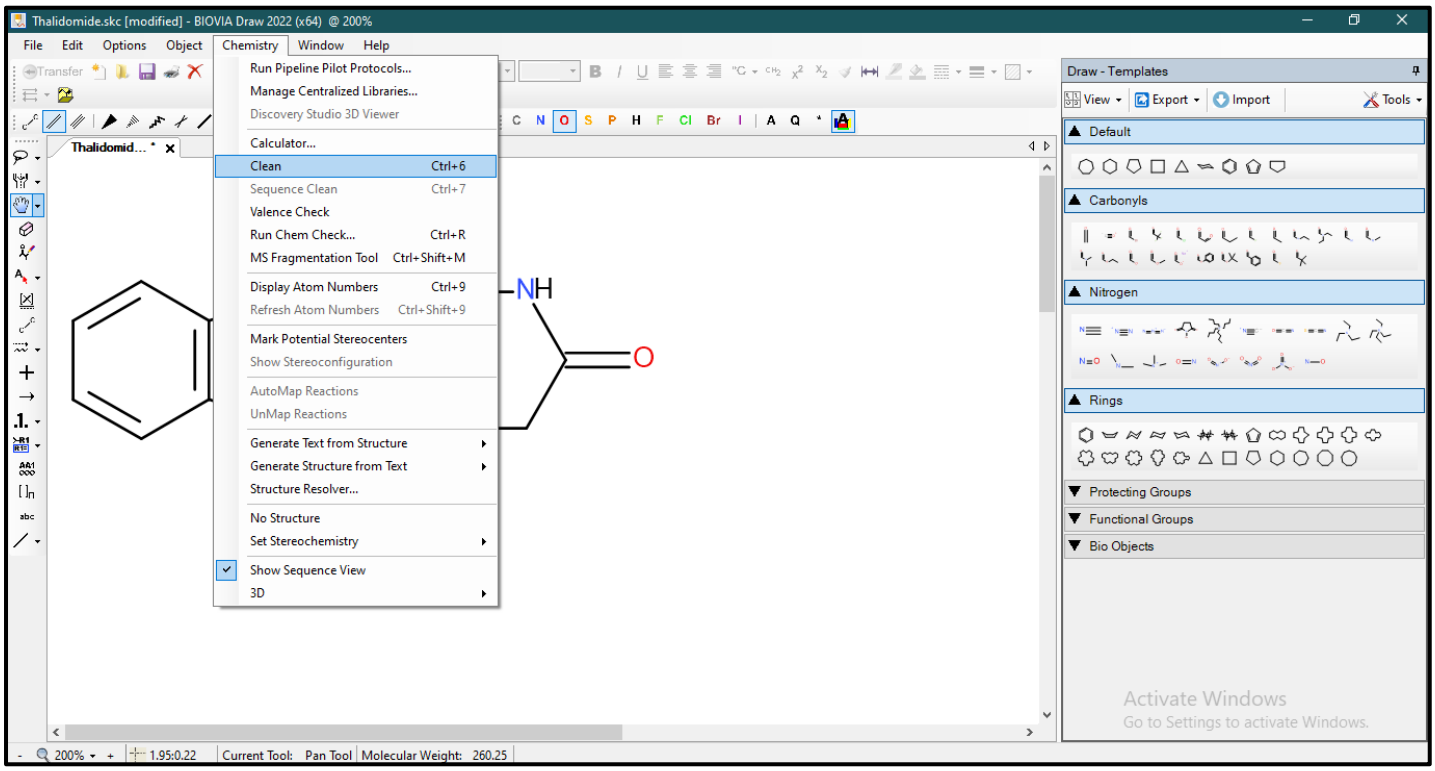

FIG3: Option applied:"Clean Structure"

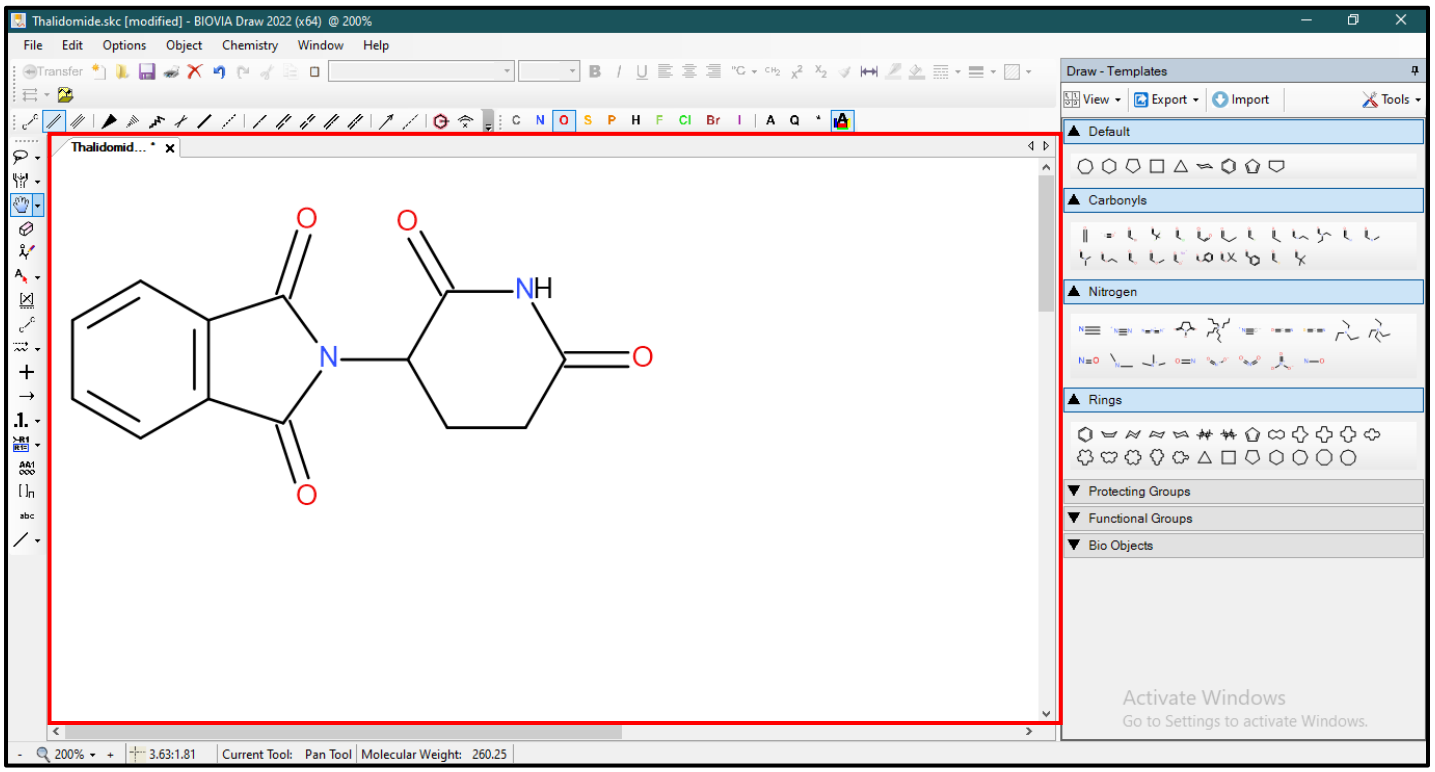

FIG4: Clean structure of Thalidomide

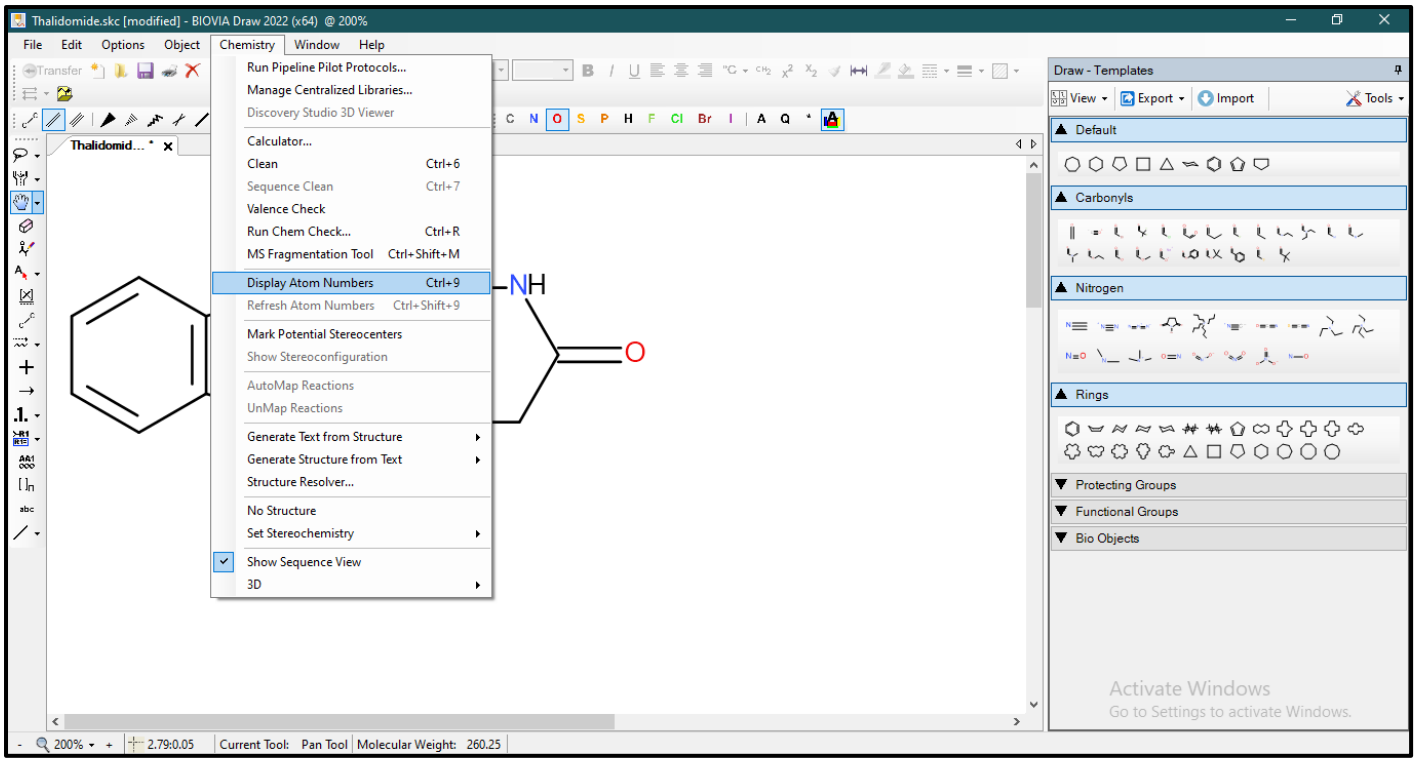

FIG5: Option applied: “Display Atom Numbers”

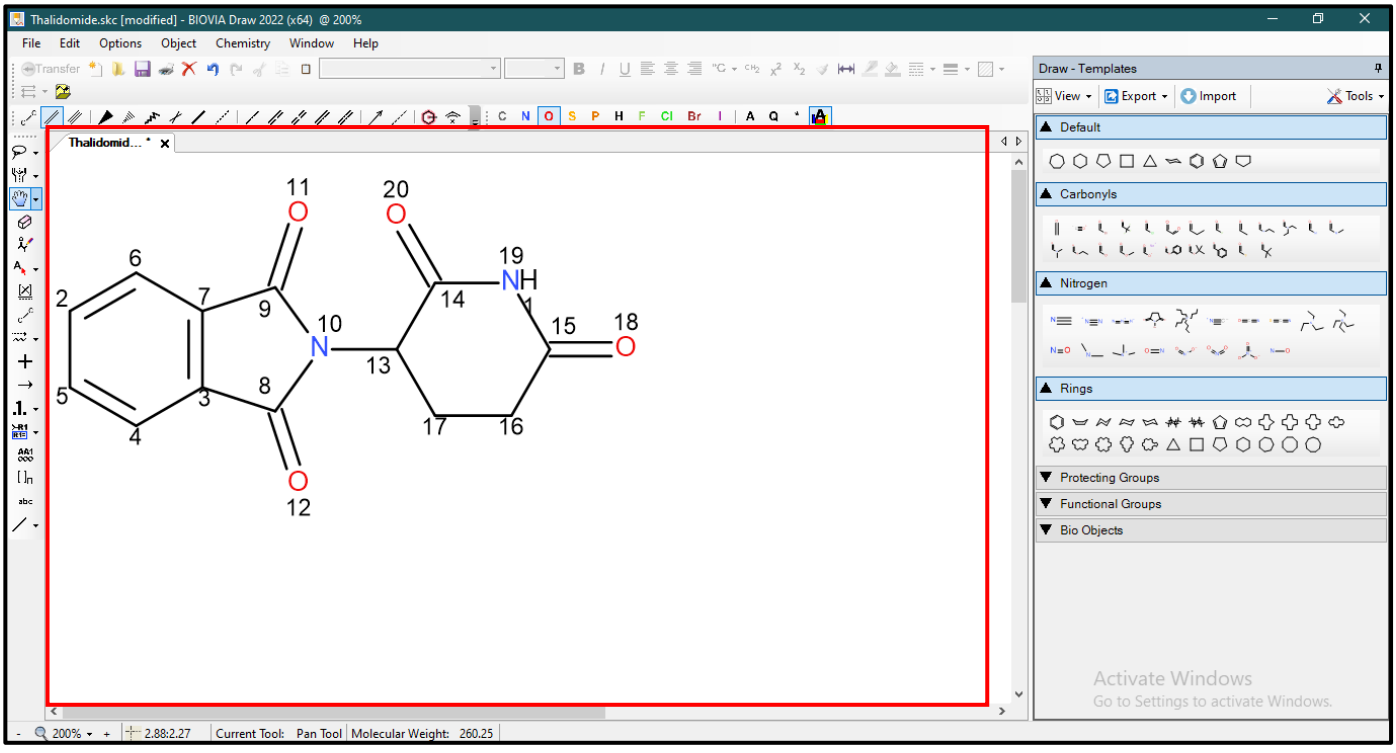

FIG6: Atom numbering of Thalidomide structure

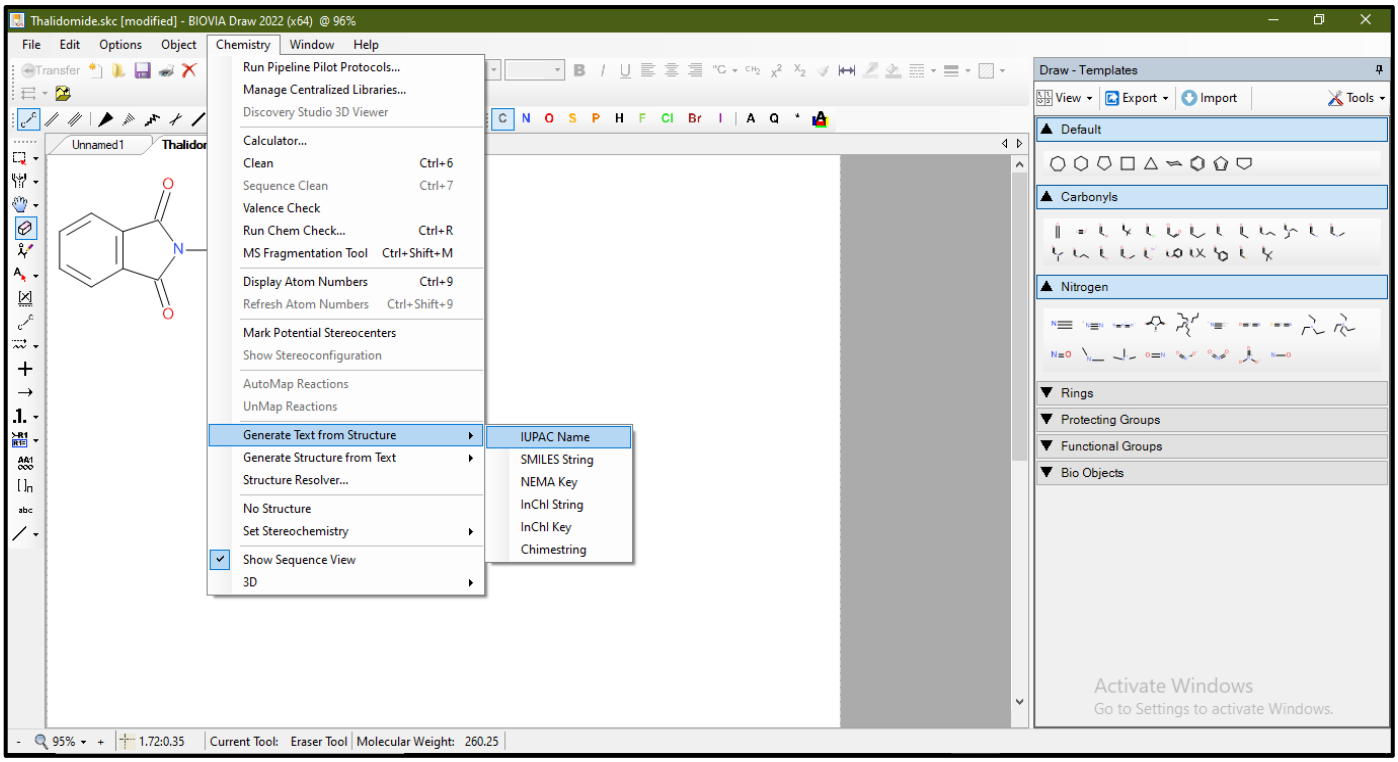

FIG7: Option applied:To generate IUPAC name

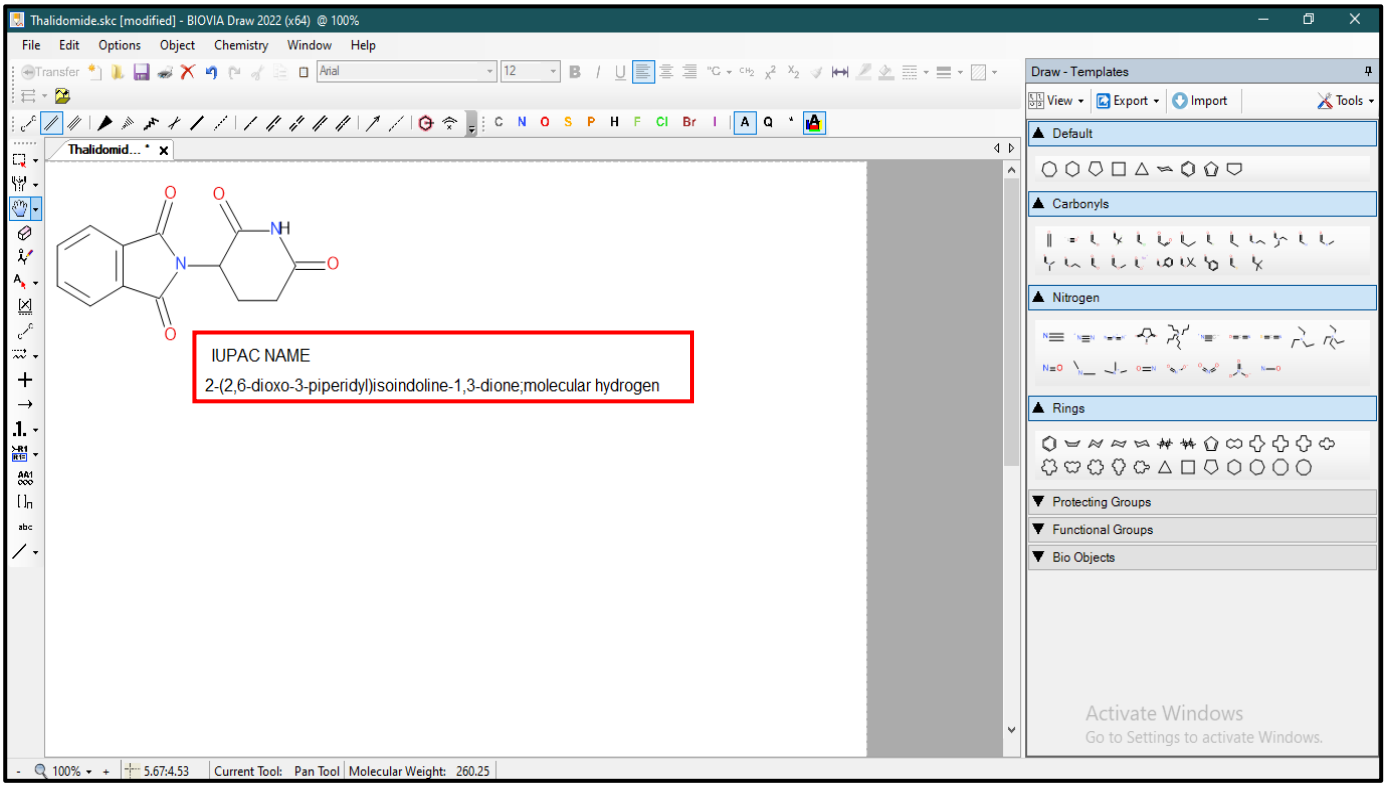

FIG8: IUPAC name of Thalidomide

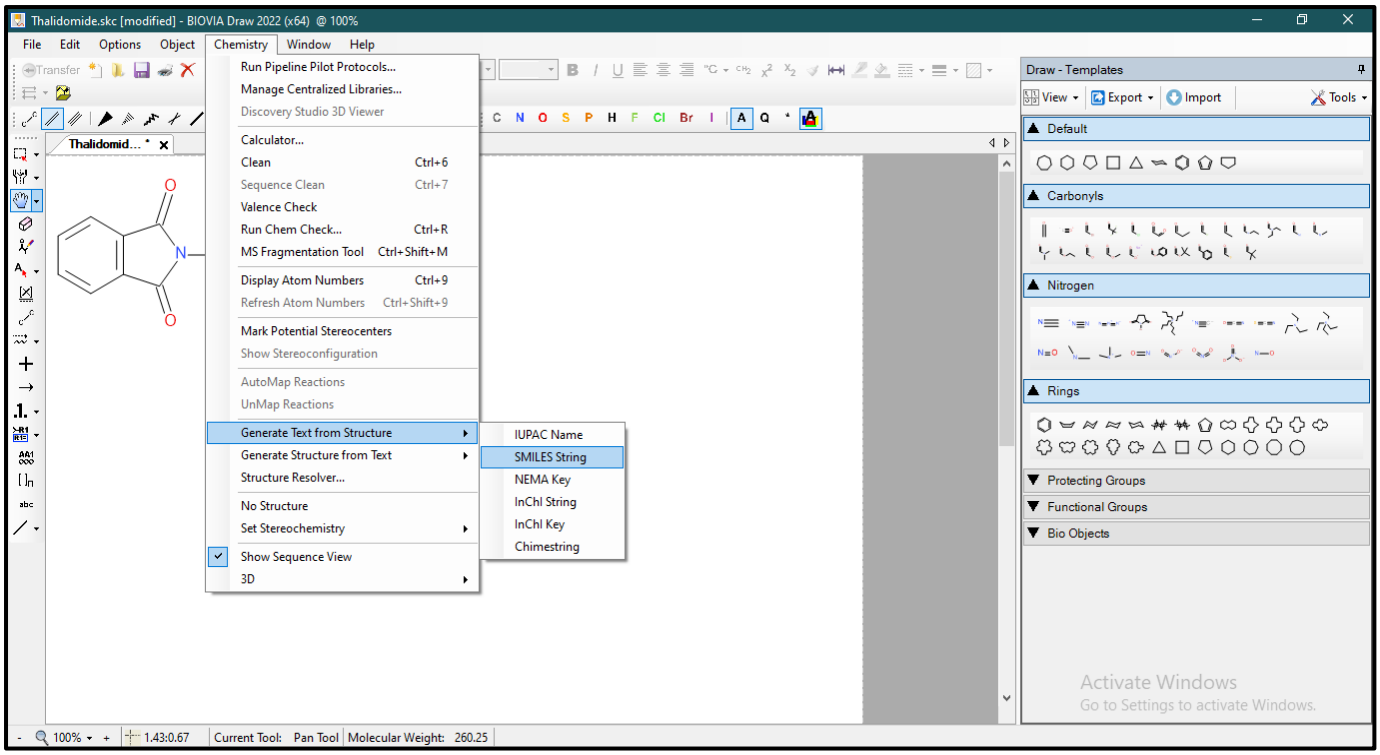

FIG9: Option applied: To generate SMILES String

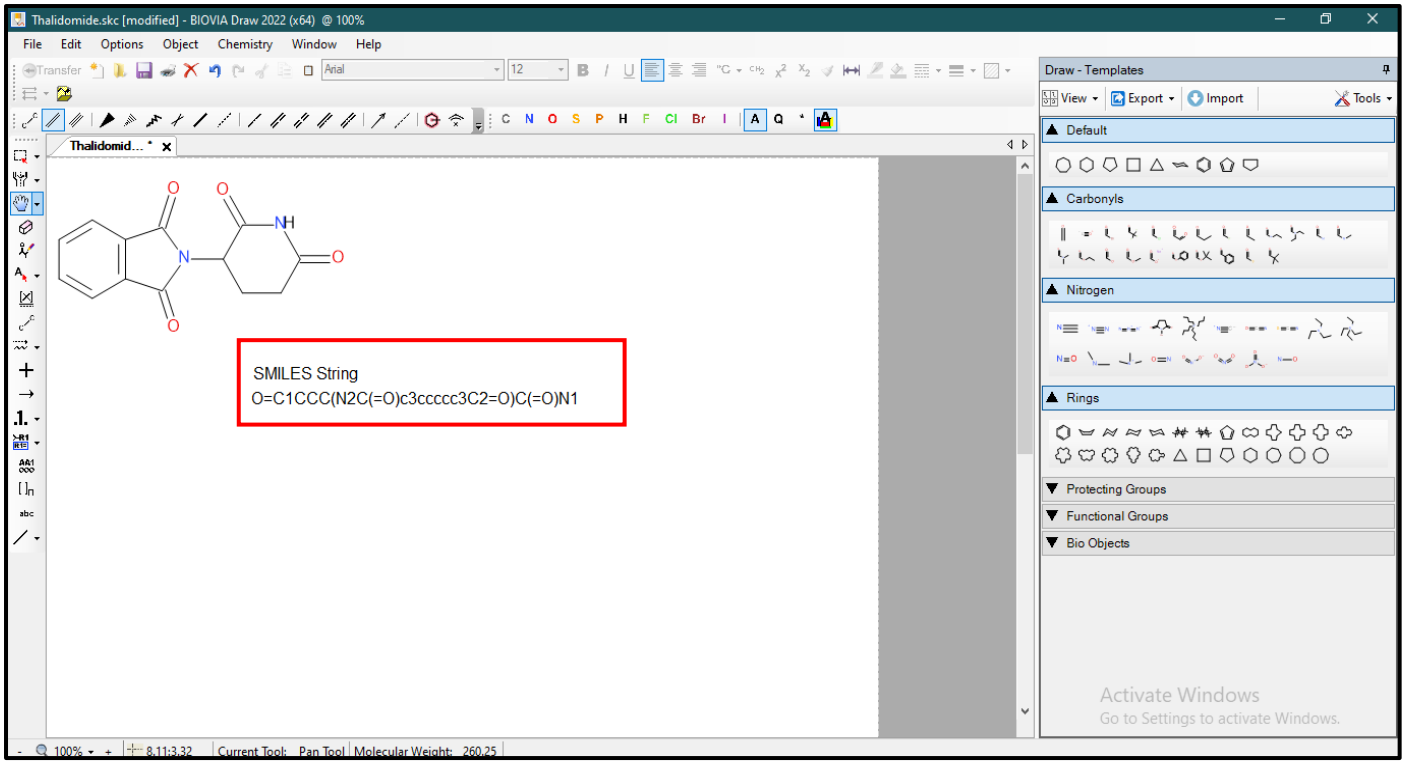

FIG10: SMILES String of Thalidomide

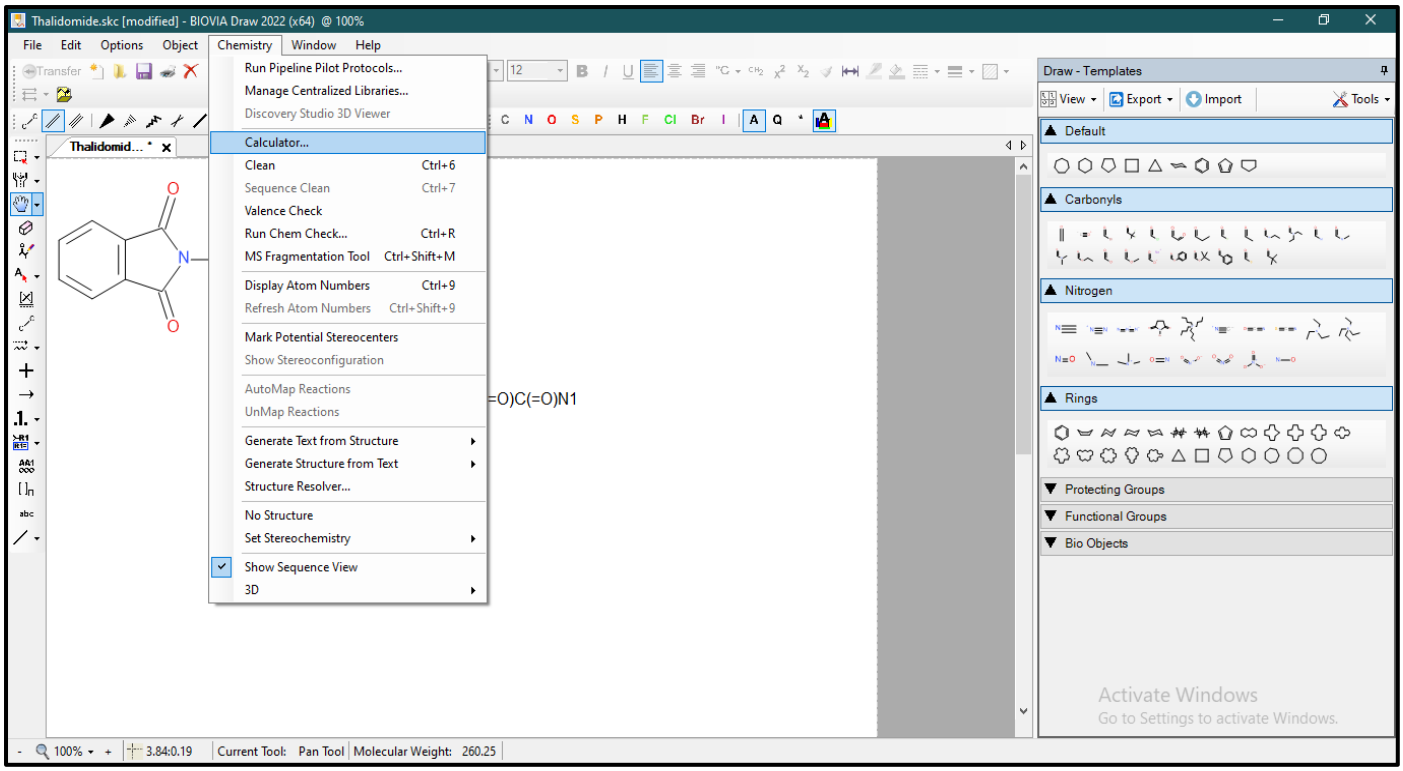

FIG11: Option applied:To calculate Physicochemical properties of Thalidomide

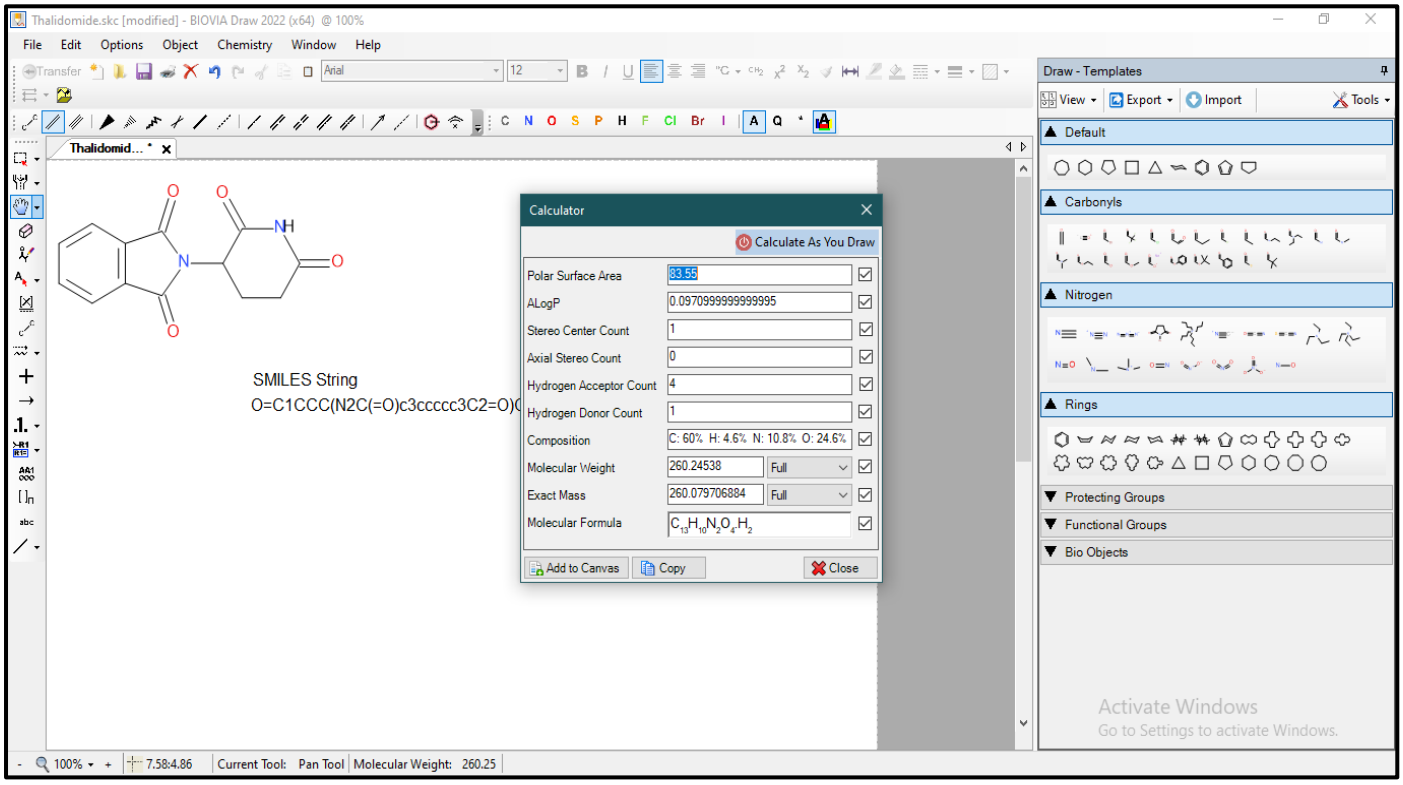

FIG12: Different physicochemical properties available for Thalidomide

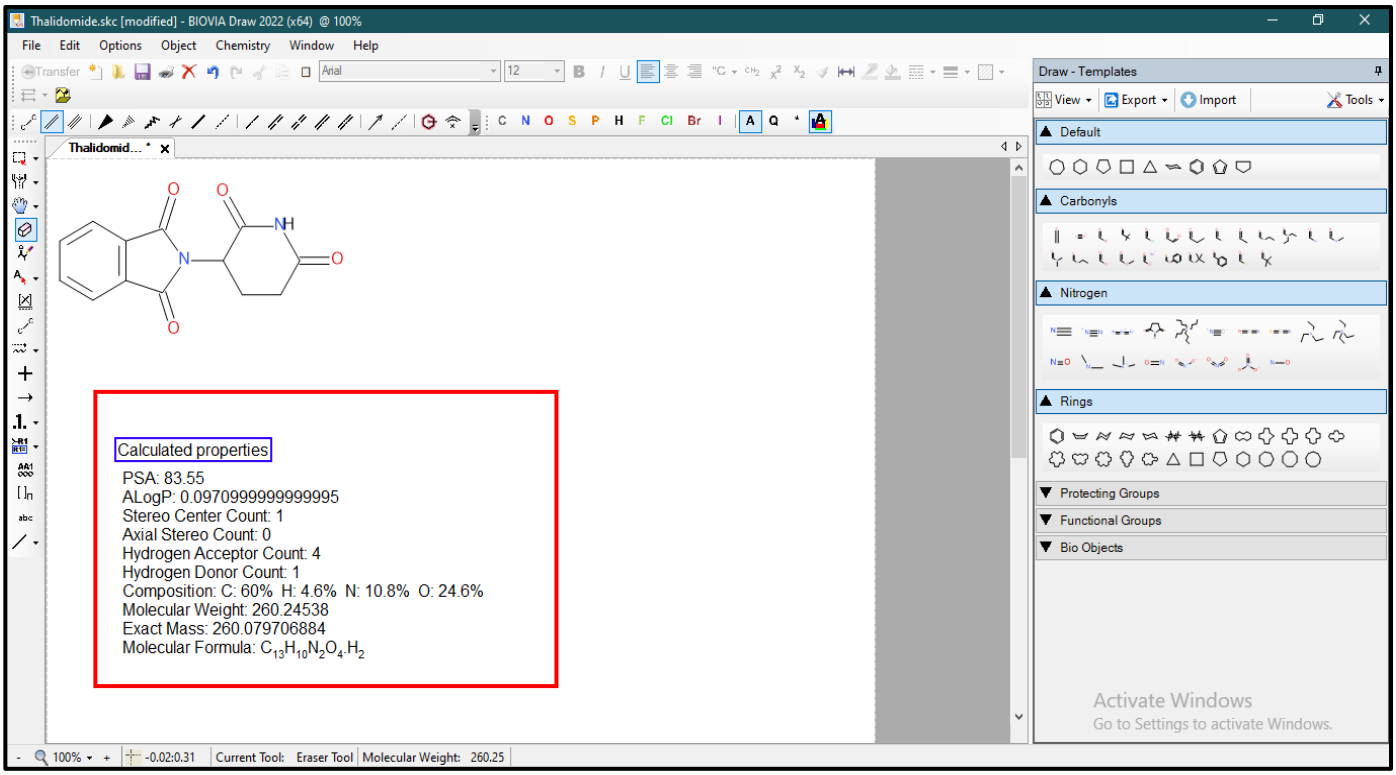

FIG13: Calculated Physicochemical properties of Thalidomide

RESULTS:

The structure of Thalidomide was drawn using the BIOVIA Draw Software. Following are the information retrieved for the structure using software in tabulated format.

SR.NO.	NAME OF OPTION	RESULTS
1.	**Physicochemical properties:**	PSA : 83.55 AlogP: 0.0970999999999995 Stereo Center Count: 1 Axial Stereo Count: 0 Hydrogen Acceptor Count: 4 Hydrogen Donor Count: 1 Composition: C: 60% H: 4.6% N: 10.8% O: 24.6% Molecular Weight: 260.24538 Exact Mass: 260.079706884 Molecular Formula: C13H10N2O4.H2
2.	**IUPAC Name:**	2-(2,6-dioxopiperidin-3-yl)isoindole-1,3-dione
3.	**SMILES String:**	O=C1CCC(N2C(=O)c3ccccc3C2=O)C(=O)N1

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.

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DATE: 06/09/22

WEBLEM: 2B

Open Babel Tool

AIM:

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

INTRODUCTION:

Aspirin is an orally administered non-steroidal anti-inflammatory agent. Acetylsalicylic acid binds to and acetylates serine residues in cyclooxygenases, resulting in decreased synthesis of prostaglandin, platelet aggregation, and inflammation. This agent exhibits analgesic, antipyretic, and anticoagulant properties. Aspirin or acetylsalicylic acid is perhaps the most commonly used analgesic and antipyretic medication worldwide, having been in clinical use for over 100 years. Aspirin can cause several forms of liver injury: in high doses, aspirin can cause moderate to marked serum aminotransferase elevations occasionally with jaundice or signs of liver dysfunction, and in lower doses in susceptible children with a febrile illness aspirin can lead to Reye syndrome.

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. (URL: https://pubchem.ncbi.nlm.nih.gov/).
2. Search for compound "Aspirin".
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 formats into the various structural file formats.
6. Observe the Aspirin structure in different file formats and interpret the result.

OBSERVATIONS:

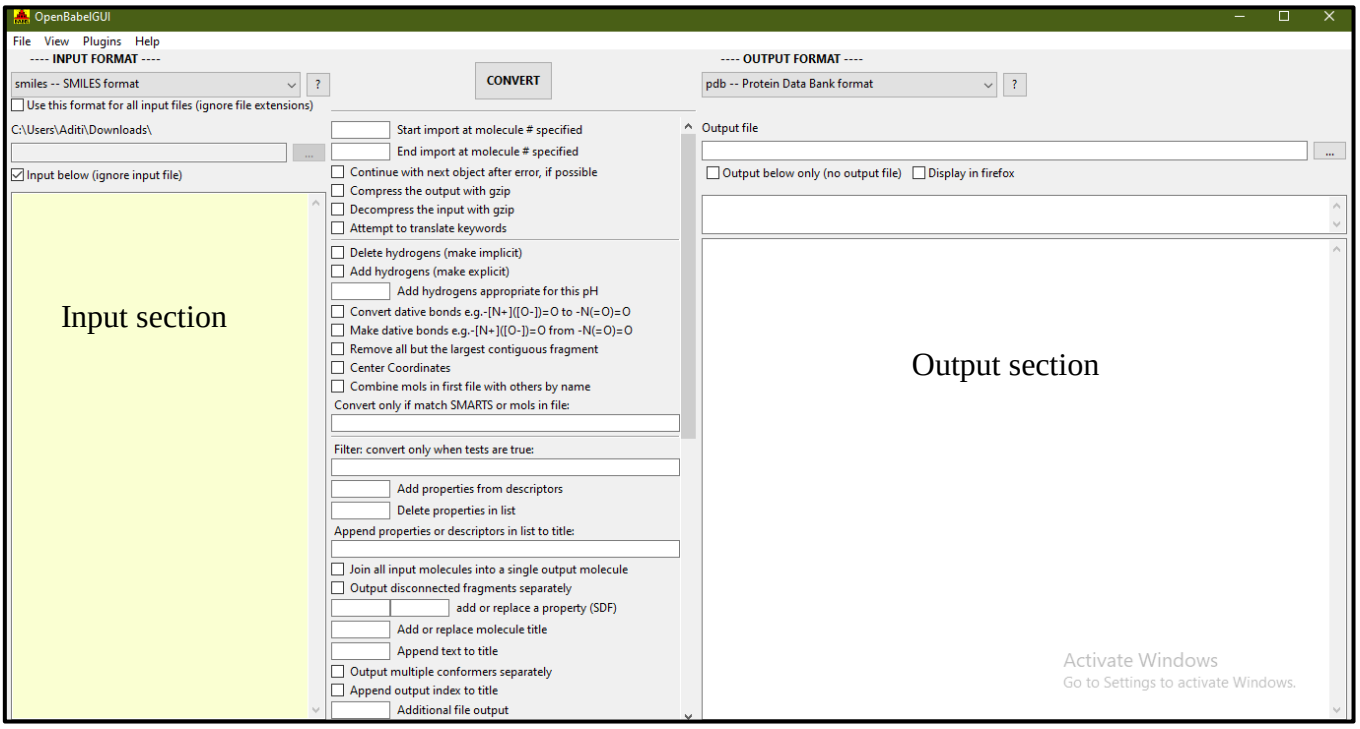

FIG 1: Homepage of OpenBabel Tool

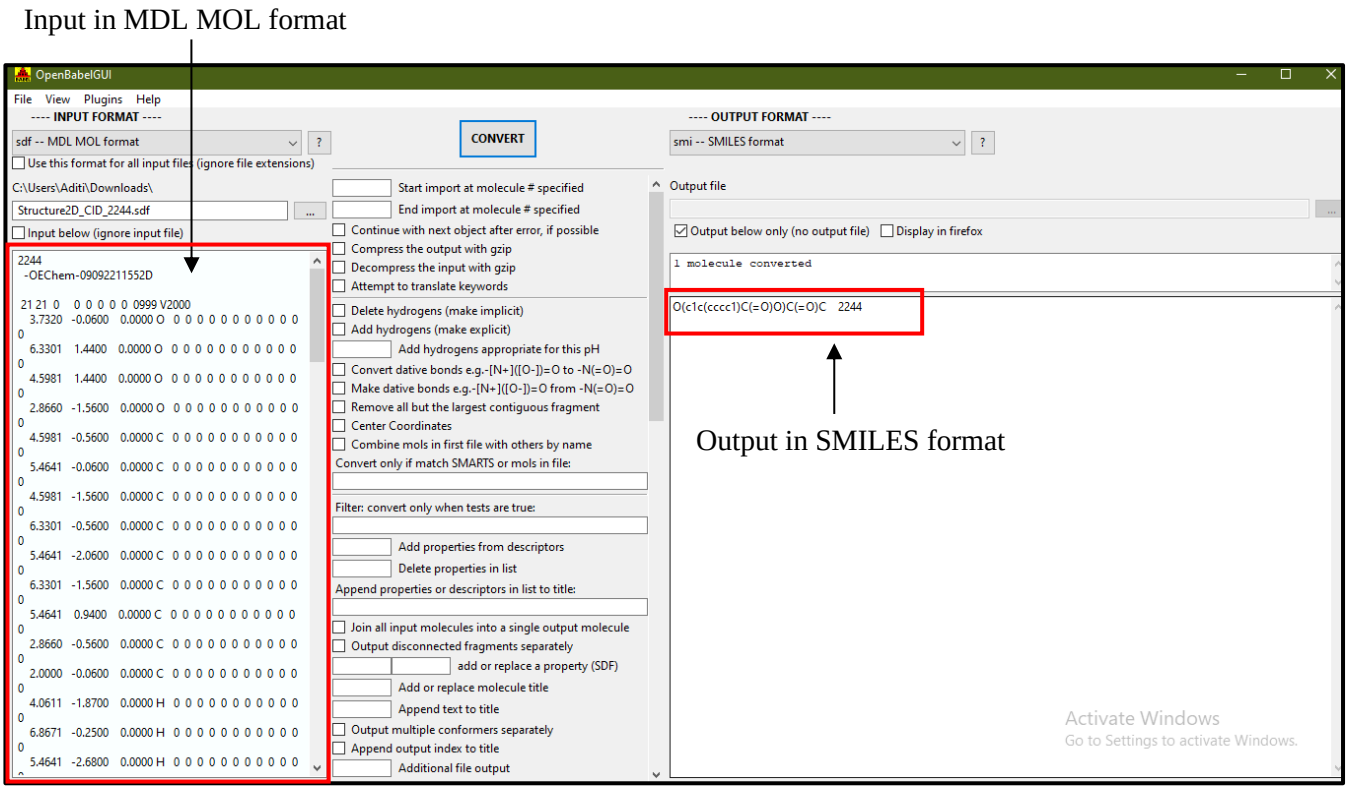

FIG 2: Convert sdf file into smiles file for Aspirin

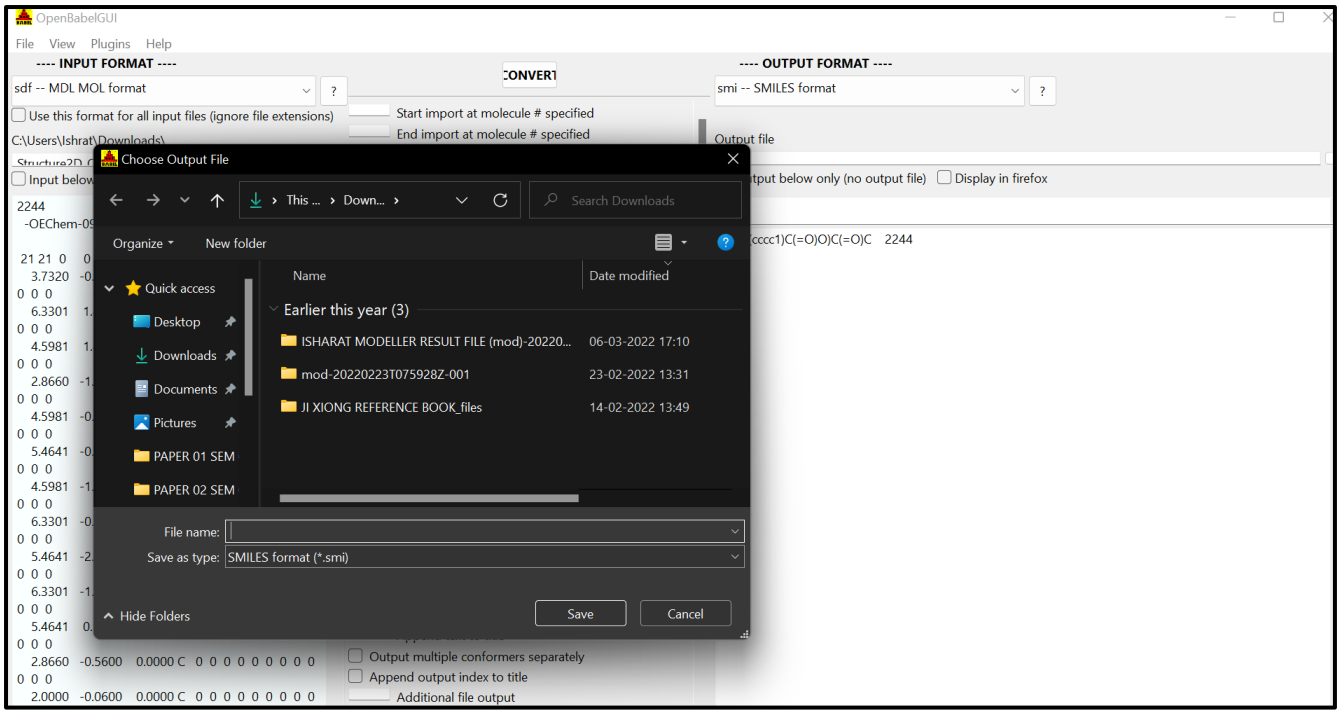

FIG 3: Storage Option for SMILES under Open Babel

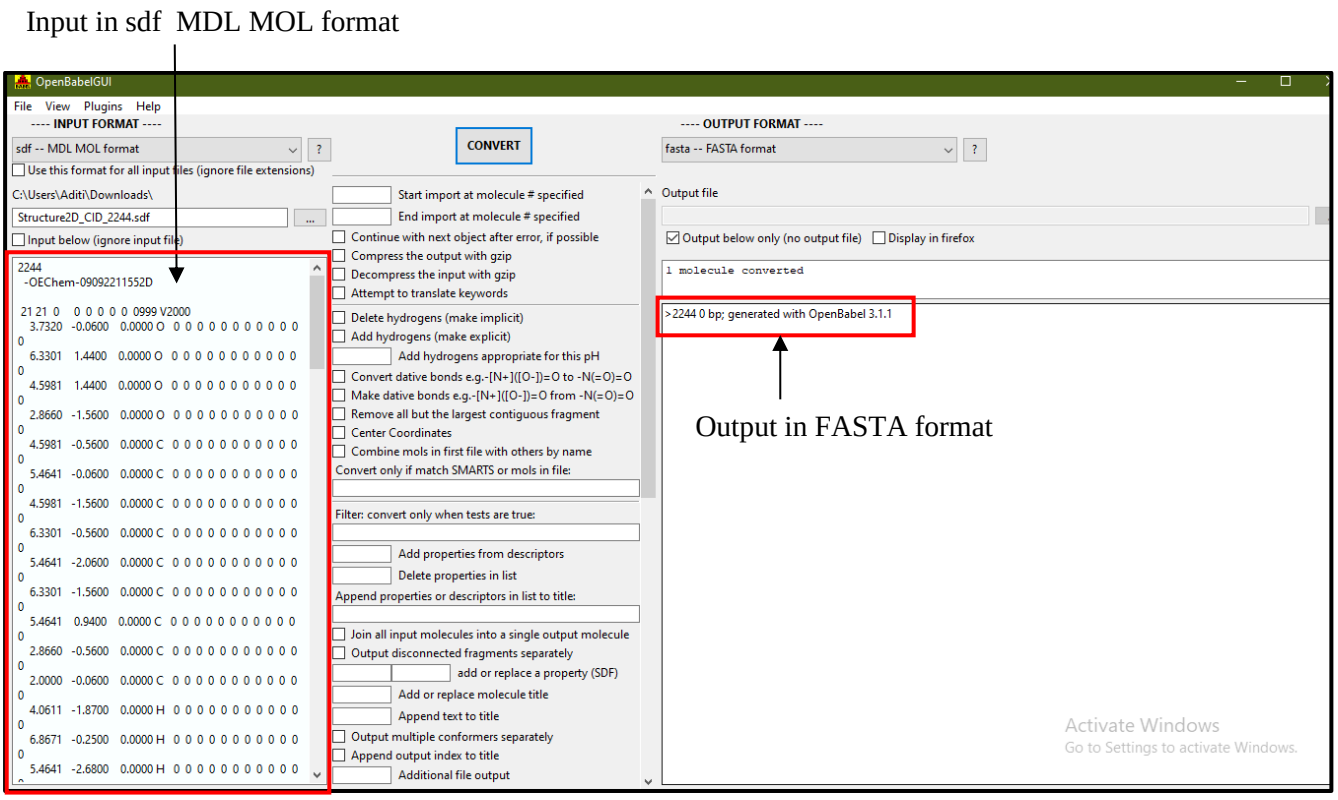

FIG 4: Convert sdf file into fasta file for Aspirin

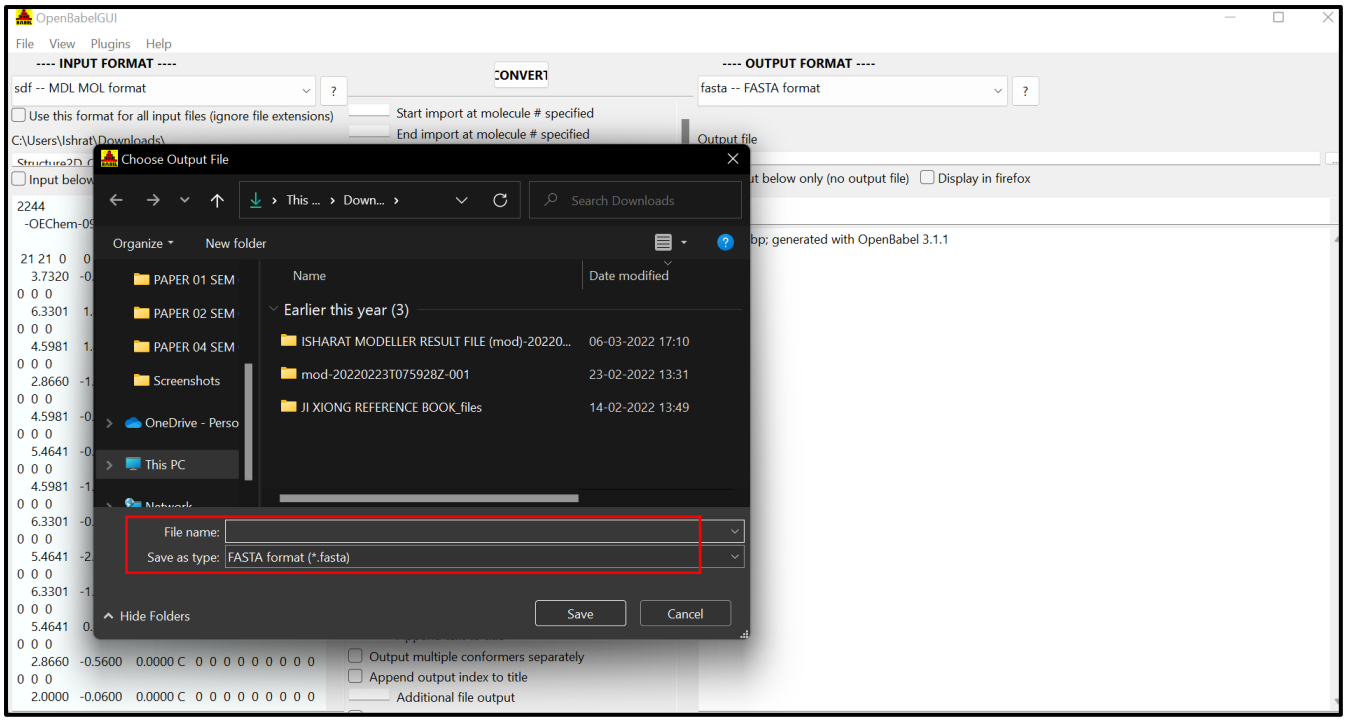

FIG 5: Storage Option for fasta under Open Babel

Input in SMILES format

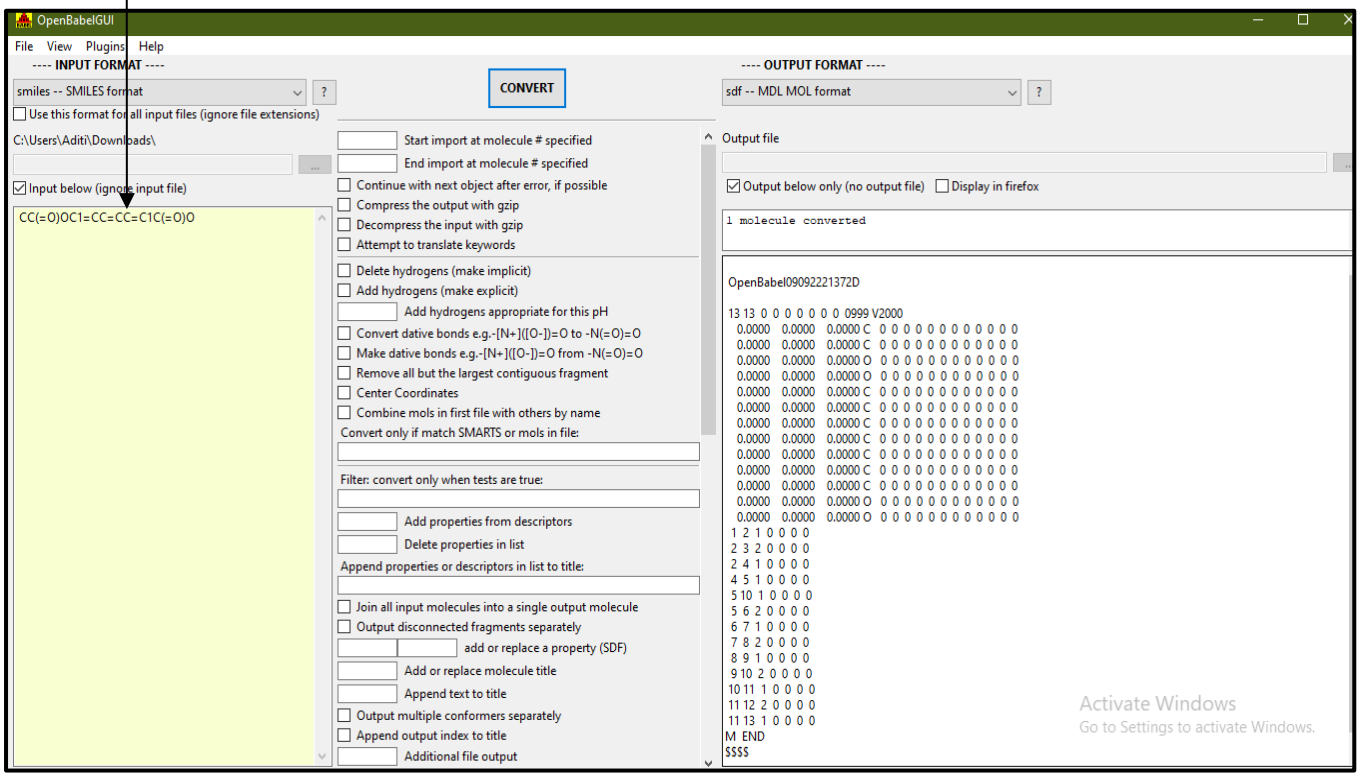

FIG 6: Convert smiles file into sdf file for Aspirin

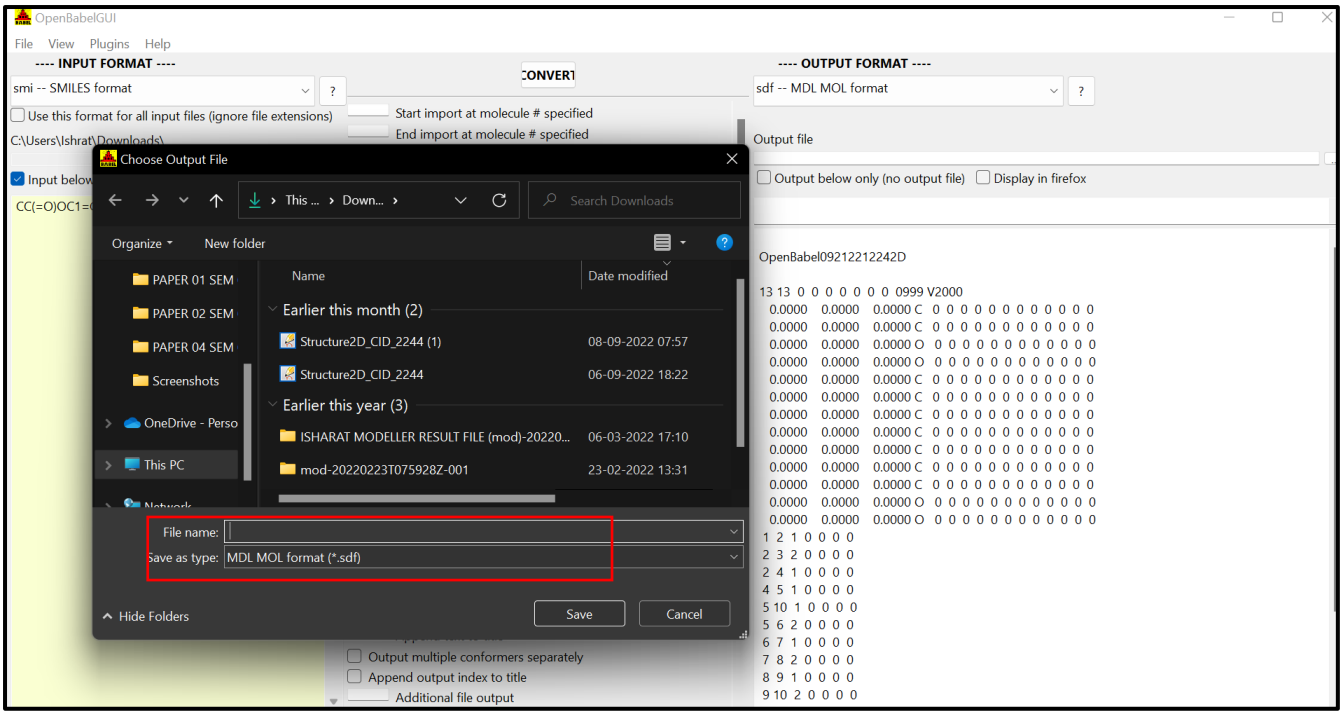

FIG 7: Storage Option for sdf under Open Babel

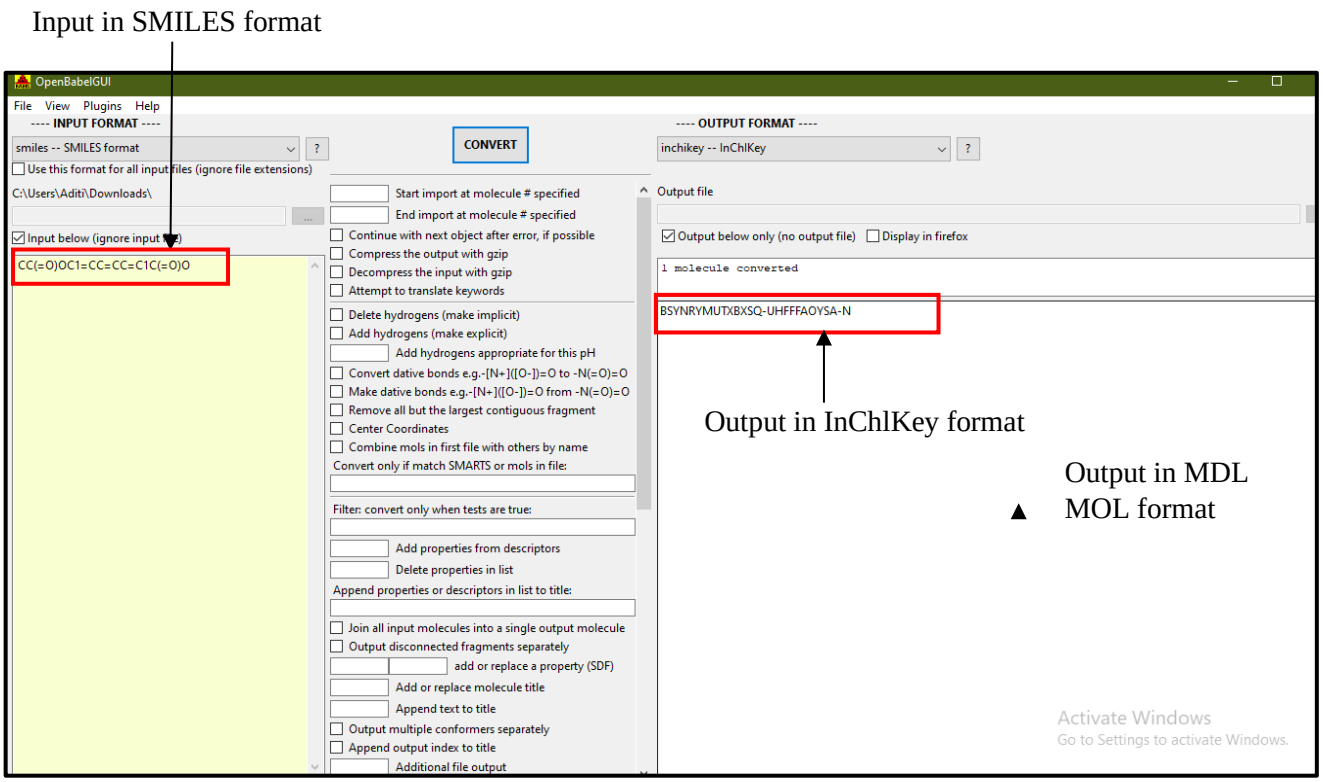

FIG 8: Convert smiles file into InChIKey file for Aspirin

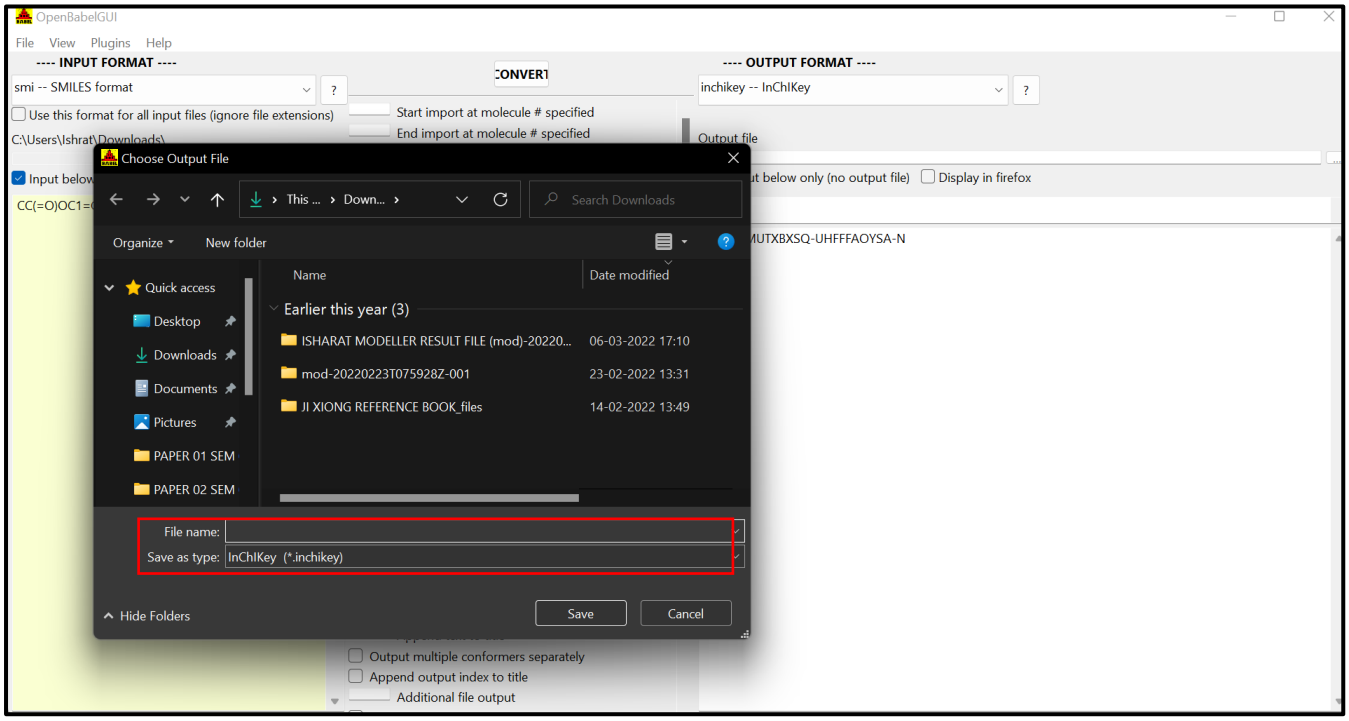

FIG 9: Storage Option for InChKey under Open Babel

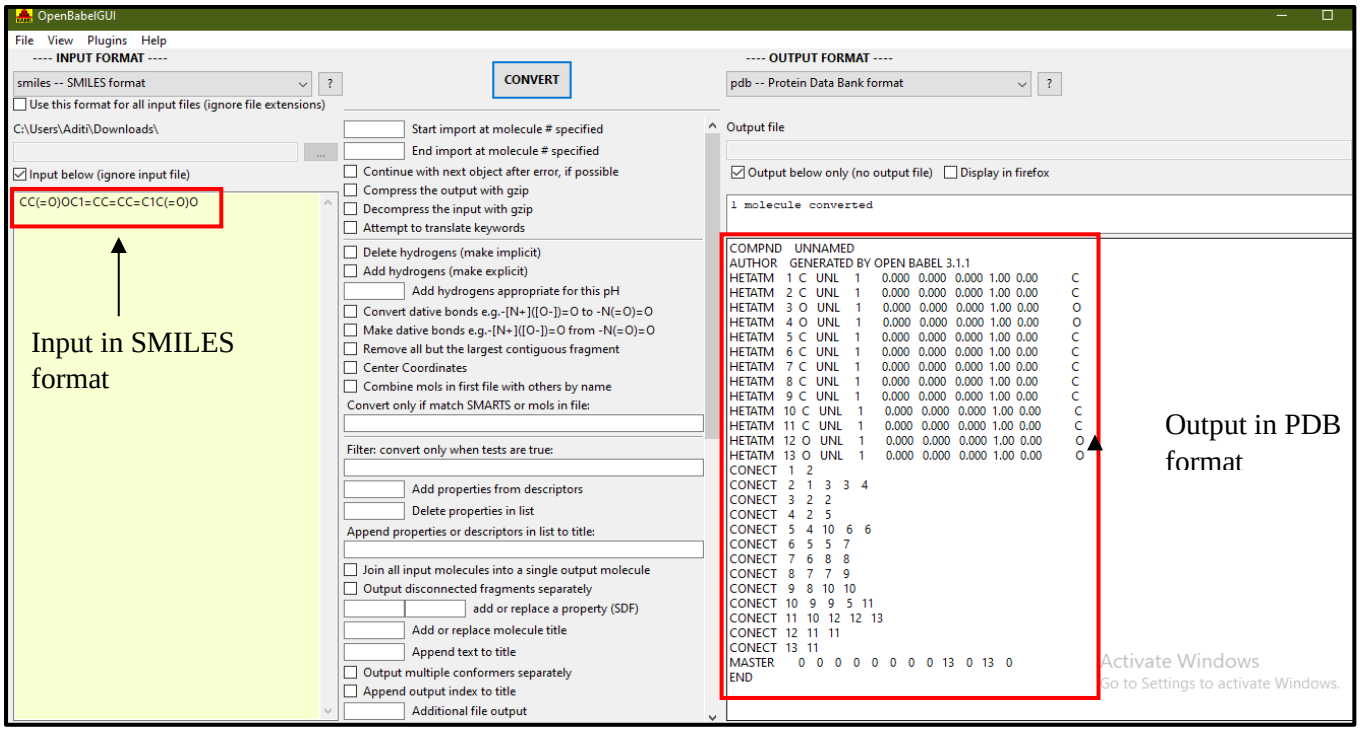

FIG 10: Convert smiles file into pdf file for Aspirin

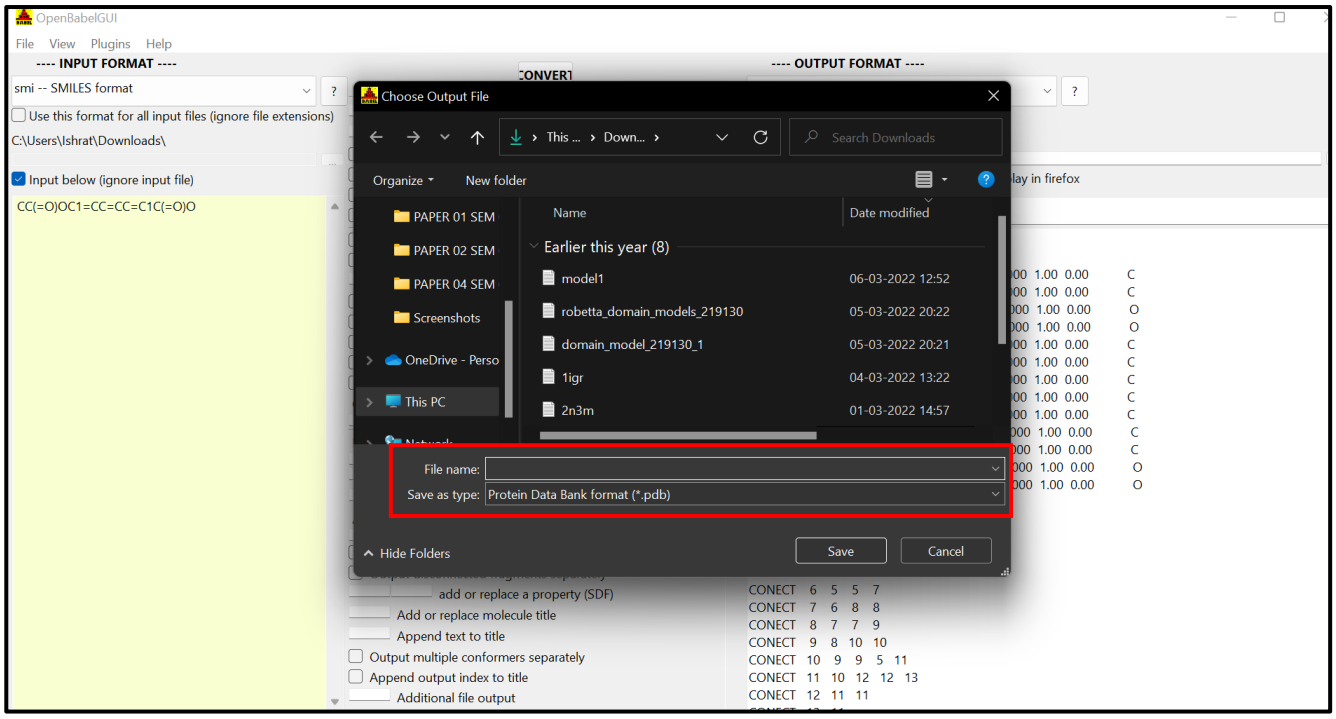

FIG 11: Storage Option for pdb under Open Babel

RESULTS:

The structure for Aspirin 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 “Aspirin” 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.

REFERENCES:

1. Tawfeek, N., Mahmoud, MF., Hamdan, DI., Sobeh, M., Farrag, N., Wink, M., El-Shazly, AM. (2021). Phytochemistry, Pharmacology and Medicinal Uses of Plants of the Genus *Salix*: An Updated Review. *Front Pharmacol*, *12(593856)*.

2. 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.