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Drawing Software in Chemistry: Free/Open Source (Foss), Freeware- A Short Review

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ABSTRACT: COVID-19 pandemic made online education in vogue. It has become mandatory for chemistry community to know about various tools, which are available for their disposal. This short review lists various software, which can be used for drawing structures, writing equations etc. These software include Free/Open Source (FOSS) and freeware that can be easily downloaded from internet free of cost for academic purposes.

KEYWORDS: Software, Drawing, FOSS, Freeware

I. INTRODUCTION

The World Health Organization (WHO) declared the COVID-19 outbreak as a pandemic on 11 March 2020 [1]. Most of the governments all around the world temporarily closed down all educational institutions to prevent the spreading of virus. According to Wikipedia, by the end of July 2020, around 1.7 billion learners were affected by this lockdown [2]. Most of the schools, colleges and universities were forced to switch over to “online mode” of synchronous and asynchronous teaching and learning. UNESCO recommended the use of distance learning programs and open educational applications and platforms for students and teacher for better teaching learning experience [2].

Software is a general term used to describe an organized collection of data and instructions that directs the computer hardware to perform a specific function. Based on the degree of freedom given to the users software can be divided into – Proprietary and Free/Open source software (FOSS). Proprietary software is a software with restrictions on use/private modification/copying or publishing of modified or unmodified versions. These restrictions are placed on it by one of its proprietors (owners) [3]. Examples: Microsoft Windows, RealPlayer, MATLAB, Adobe Photoshop. Free/Open source software (FOSS), as the name implies, is a software which is liberally licensed to grant the right of users to study, change and improve its design through the availability of its source code [4]. Examples: Apache, Firefox, GNOME, OpenOffice.org and Thunderbird.

FOSS should not be confused with freeware. Freeware is computer software that is available for use at no monetary cost, which may have restrictions such as redistribution prohibited, and for which source code may not be available [5]. Traditionally, chemistry has been one subject which use a lot of board writing for drawing molecular structures, equations etc. This unprecedented crisis, however made chemistry enthusiasts to tread on unfamiliar territory of recording videos, annotating on slides and even thinking of a virtual chemistry laboratory. A good tablet or a digital pen may serve purpose for a synchronous session, however for preparing notes, manuscripts and presentations one has to know with the resources at their disposal. This review is aimed for chemistry fraternity to familiarize with various free and open source tools, freeware and resources which are available in the internet. Website url is also given so that desired webpage can be accessed.

II. STRUCTURE DRAWING SOFTWARE IN CHEMISTRY

A few decades ago, chemistry professionals used ink-pen, chemical stencil sets, free-hand chemical drawings for journals and presentations. Quite often, these drawings appear grotesque even in the case of simple molecular drawings. But increasing availability of “chemistry drawing software” have made the matter much simpler. Both proprietary and free/open software are available for chemistry drawing purposes. Every software available has its own unique features, advantages and disadvantages. Interestingly many of the software available are coupled with additional features such as three-dimensional visualization of the molecule in space and spectral simulation.

TABLE I: List of Proprietary and Free/Open Source drawing (2D) software.

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Proprietary

Open Source

Freeware/Free for Academics

GPL

ACDChemsSketch,
Draw,

Symyx

BK Chem, Molsketch,
Xdrawchem, SketchEl

Marvin sketch, Chemwindow

III. LIST OF DRAWING SOFTWARE IN CHEMISTRY

Some software packages are stand-alone applications while others form a part of integrated suites. Certain proprietary software like Chemoffice, ChemDoodle, Chem 4D etc do not offer free download for academic purposes but offer free trial. These are very expensive too. For example latest version of Chemistry 4-D Draw Office costs \$ 699 and \$399 for industries and academics respectively. Students are repelled by this price tag and go for alternate sources. Now let us discuss some freely downloadable chemistry software.

1. ACD/CHEMSKETCH

1. ACD/ChemSketch is perhaps the most popular free drawing software. ChemsSketch can be downloaded freely for academic purposes. It also includes features such as calculation of molecular properties (e.g., molecular weight, density etc.), 2D and 3D structure viewing etc. The download URL is given below.

URL: <https://www.acdlabs.com/resources/freeware/chemsSketch/>

A simple drawing by using ACD/ChemsSketch is given below (Fig 1).

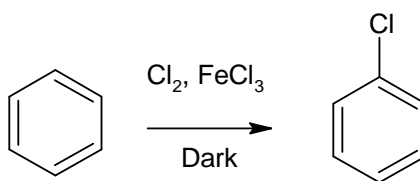


Fig 1. A simple drawing using ACD/ChemsSketch

2. BIOVIA DRAW

Biovia draw can be used to draw and edit complex molecules, chemical reactions etc. It can be downloaded freely for academic purposes. The download URL is given below.

URL: <https://discover.3ds.com/biovia-draw-academic>

3. MARVINSKETCH

Marvinsketch is a Java based chemical editor for drawing structures, reactions etc for web application.

URL: <https://revamp.chemaxon.com/products/marvin>

4. AVOGRADO

Avogadro is a molecule editing and visualizing software with many other features. It is free and open source.

URL: <https://sourceforge.net/projects/avogadro/files/latest/download>

5. MOLVIEW

MolView is an open source web based application to draw simple molecules.

URL: <https://molview.org/>

6. MOLSKETCH

Molsketch is a 2D molecular drawing and editing tool.

URL: <http://molsketch.sourceforge.net/>

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7. BKCHEM

BKChem is an opensource chemical structure drawing and editing program. It was conceived and written by Beda Kosata, hence the name BK Chem. This is largely platform-independent.

8. XDRAWCHEM

XDrawChem is a two-dimensional molecule drawing program. In addition to drawing, it can predict proton and ¹³C NMR shifts.

URL: <http://xdrawchem.sourceforge.net/>

9. WINPLT

WINPLT is a program for drawing chemical structures and creating hard copy on printers and other Windows-supported output devices.

URL: <http://www.chem.wisc.edu/areas/reich/plt/winplt.htm>

10. SKETCHEL

SketchEl is an interactive molecular drawing tool which can be used for drawing small molecular structures.

URL: <http://sketchel.sourceforge.net/>

A simple drawing by using BKChem is given below (Fig 2).

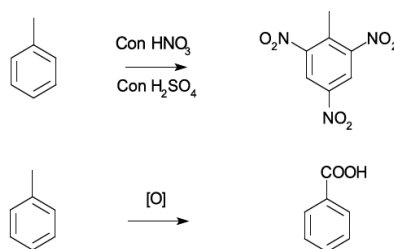


Fig 2. A simple drawing using BKChem

URL: <http://bkchem.zirael.org/index.html>

IV. CONCLUSION

This short review mentions the various chemistry structure drawing software that can be freely downloaded and used. These freeware are of immense help to chemistry community who cannot afford to buy expensive proprietary software.

REFERENCES

- [1] https://en.wikipedia.org/wiki/COVID-19_pandemic
- [2] https://en.wikipedia.org/wiki/Impact_of_the_COVID-19_pandemic_on_education
- [3] https://en.wikipedia.org/wiki/Proprietary_software
- [4] https://en.wikipedia.org/wiki/Free_and_open-source_software
- [5] <https://en.wikipedia.org/wiki/Freeware>