

KAHM Unity Women's College, Manjeri
Post Graduate Department of Chemistry

CERTIFICATE COURSE ON CHEMISTRY THROUGH THE LENS OF SOFTWARES

SYLLABUS

Module 1 (4 hrs)

Chemical Databases:- Pubchem, Search chemicals by name, molecular formula, structure, and other identifiers. Find chemical and physical properties, biological activities, safety and toxicity information, literature citations and more.

Module 2 (5 hrs)

Searching and downloading research papers using keywords in Scopus, Science direct, google scholar, and Sci-hub, Introduction to End Note and its applications

Module 3 (7 hrs)

Origin:- Introduction, download and installation process, basic features like Scientific graphing, drawing various 2D & 3D plots, Data analysis, signal processing, curve fitting, peak analysis, error bar, conversion of graph to various file format like JPEG, GIF, PNG etc

Module 4 (8 hrs)

ChemDraw Ultra:- Introduction, download and installation process, Drawing various simple and complex chemical structures, nomenclature generation, conversion of name into molecular structure, calculation of physical properties such as density, molecular weight, molecular formula, refractive index from structural formula. ^1H , ^{13}C NMR prediction from molecular structure, Drawing structure of bigger molecules such as proteins, carbohydrates, and RNA/DNA, bio arts, use of templates.

Module 5 (6 hrs)

ACD ChemSketch:- Introduction, download and installation process, Drawing various simple and complex chemical structures, conversion of name of molecule into its structure and vice versa, calculation of physical properties such as molecular weight, molecular formula, density, refractive index from structural formula, bond angles, bond lengths, dihedral angles.

REFERENCES

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2. K. I. Ramachandran, G Deepa and K Namboori, "Computational Chemistry and Molecular Modeling – Principles and Applications", Springer-Verlag, Berlin, Heidelberg, 2008, ISBN-13 978-3-540-77302-3.
3. Donald W Rogers, "Computational Chemistry Using PC", Wiley, (2003).
4. Prof. Dr. Stefan Bienz, "Short Manual to the Chemical Drawing Program ChemDraw"
5. Taylor Cornell and Geoffrey Hutchison, "Avogadro: Molecular Editor and Visualization
6. Phillip M. Edwards Origin 7.0: Scientific Graphing and Data Analysis Software
7. Sunghwan Kim, Paul A. Thiessen, Evan E. Bolton* , Jie Chen, Gang Fu, Asta Gindulyte, Lianyi Han, Jane He, Siqian He, Benjamin A. Shoemaker, Jiyao Wang, Bo Yu, Jian Zhang and Stephen H. Bryant, "PubChem Substance and Compound databases"
8. Amy Butros and Sally Taylor, "managing information: evaluating and selecting citation management software, a look at endnote, refworks, mendeley and zotero"
9. Baraa Rayan and Anwar Rayan, "Avogadro Program for Chemistry Education: To What Extent can Molecular Visualization and Three-dimensional Simulations Enhance Meaningful Chemistry Learning?"
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