**KAHM UNITY WOMEN’S COLLEGE, MANJERI**

**DEPARTMENT OF CHEMISTRY**

**Certificate course in Molecular Visualization Softwares**

**(Programme Code: CHE05CC10)**

For

**UG & PG Students**

**Duration of course: 3 Months**

**Total hours: 30 Hours**

**SYLLABUS**

**Module 1**

**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.

**Module 2**

**Avogadro:-** Introduction, download and installation process, Drawing various simple and complex chemical structures, Sketch the molecule using avogadro and get the coordinates of the molecule, Single point energy calculation, Geometry optimization, Fundamental vibrational frequency analysis of different molecules, Conformational analysis of ethane and butane

**Module 3**

**PyMOL:-** **:-** Introduction, download and installation process, visualization of different kinds of molecules such as proteins, compounds, or molecules. export files into different formats. Perform various operations on structures such as removing atoms or residues, changing colors, labeling residues, and so on.

**REFERENCES**

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2. Donald W Rogers, “Computational Chemistry Using PC”, Wiley, (2003).
3. Taylor Cornell and Geoffrey Hutchison, “Avogadro: Molecular Editor and Visualization
4. Baraa Rayan and Anwar Rayan, “Avogadro Program for Chemistry Education: To What Extent can Molecular Visualization and Three-dimensional Simulations Enhance Meaningful Chemistry Learning?
5. Arvin Moser, “ACD/ChemSketch Quick Start Guide”, http://www.acdlabs.com/chemsketch/
6. Jamal Raiyn and Anwar Rayan, “How Chemicals’ Drawing and Modeling Improve Chemistry Teaching in Colleges of Education”, World Journal of Chemical Education, 2015, Vol. 3, No. 1, 1-4
7. DeLano, Warren L. "Pymol: An open-source molecular graphics tool." *CCP4 Newsl. Protein Crystallogr* 40.1 (2002): 82-92.
8. DeLano, W. L., & Bromberg, S. (2004). PyMOL user’s guide. *DeLano Scientific LLC*, *629*.
9. Seeliger, Daniel, and Bert L. de Groot. "Ligand docking and binding site analysis with PyMOL and Autodock/Vina." *Journal of computer-aided molecular design* 24.5 (2010): 417-422.
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