FEASIBILITY OF DOING INSIGHTFUL FINAL YEAR PROJECTS IN CHEMICAL SCIENCES AT HOME

Concepts, Themes, Outcomes, Challenges, Resources, Journals

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ABSTRACT

Complete and partial restriction in the access to the laboratories in many countries has imposed a long-term lockdown to safeguard the citizens from the corona virus/omicron pandemic. Hence, e-teaching is in force effectively to teach theoretical as well as experimental courses. Unfortunately, undergraduate and postgraduate students of doing chemical sciences are missing their one-time opportunity for doing project during their course work. In this report, we discuss the *feasibility of doing final year projects in chemical sciences at home*. We suggest some themes, and concepts on which the students can take-up and carryout with the supervision of their professors. The resources and tools that is available online for executing the final year project is identified and explained. The practical approaches, directions for fruitful outcomes are discussed with the understanding on the limitations of such projects. This report would serve the chemical science students and teachers as one point reference material to identify a suitable theme for completing the final year project. *[African Journal of Chemical Education—AJCE 13(1), January 2023]*

INTRODUCTION

Purpose of Final Year Projects in a Chemical Science Course Curriculum

Purpose of final year projects in the curriculum of any chemical science program is to provide the students an opportunity to practice the theoretical knowledge that they have gained through core courses. Learning by doing is the ultimate objective of the final year projects. Students at the end of the course learn to define the problem for the projects, approach of investigation of the problem and methods to be adopted for investigating problem through the regular interaction with the teachers/ supervisors. Final year project is a platform for the students to understand their laboratory skills and competence. Apart from the scientific objectives demonstrated above the final year projects help the students to develop interpersonal skills, problem solving skills and being creative in solving any problem in general.

The Pandemic Impact

Lockdown imposed throughout the world due to covid and omicron pandemic since December 2019 has become a great barrier for knowledge transfer process. Students are unable to access the laboratories for carrying out experiments, project work and research work till now. The situation has not developed instead the context has worsen than earlier. Covid cases and death due to pandemic are increasing day by day unexpectedly. Although the partial knowledge transfer

process is happening through online platforms, students are facing difficulties and losing their learning experience that they are supposed to gain through project work.

Identifying the feasibility of doing project at home using online resources is an essential task now. Hence, this article investigates the feasibilities of completing an insightful undergraduate and postgraduate final year project with the help of online resources. In this review, some of the concepts, themes, outcomes, challenges, resources, and journals useful for completing the final project are proposed.

A perfect literature review precisely narrates and communicates by connecting the chronological advancement with respect to the scientific fundamentals [1]. Writing literature review on a selected topic is one of the highly prioritized, feasible and meaningful ways of doing research at home. Writing a literature review on a specific theme involves certain set of process. The student has to select a topic for literature review, carryout extensive online search for identifying suitable articles, reading the collected reprints, developing the scheme of the review work, and scripting the review manuscript. Conducting a literature survey and scripting the findings based on the development in the field chronologically helps to understand the advancement stages that help to build our knowledge. In addition to that, literature survey and writing a review helps to narrow down the topic of further research or could be able to suggest specific research problems to be explored.

Although, carrying out a literature survey has become easier than earlier with the evolution of internet and ICT tools, writing an impressive literature review article is a time-consuming

complex process. Selecting a topic for literature survey is a great challenge for the beginners (students) and hence the meticulous guidance by the supervisor is required. Otherwise, the students would be wasting most of the time and get frustrated due to the lack of ability and confidence to decide. Students find difficult to understand the research papers. In general, students of graduate programs and even doctoral research scholars used to compose all the data, information and details obtained through Google search in a review report. And most of the literature review compilations by the students are lacking connectivity and continuity. Supervisors always identify the deviation of discussion / narration developed by the scholars/students in a literature review report. Research supervisors generally observe the lack of *connective description of scientific findings with chronological advancement* in the review reports drafted by the scholars and graduate students. But such defects can be rectified through the frequent short virtual/offline discussion and meticulous guidance by the supervisors for beginners. Attempting to write *narrative reviews* are suitable for graduate students rather than *systematic review* [2].

Themes: Generally, doctoral students would have many defined topics for writing a literature review. But, suggesting / finding a topic for writing a literature review for a graduate student, the supervisor has to do some preliminary searches. Usually, university professors used to suggest a topic for literature survey relevant to the supervisor's current research interests. Literature reviews based on (i) performance comparison of application materials/molecules, (ii) current / emerging areas, (iii)

discoveries and breakthrough advancements, (iv) scope for further advancements, are some of common themes.

Outcomes: The student gain (i) insights on the current status of the research theme discussed in the review article and, (ii) recommendations and suggestions for further research.

Challenges: A *systematic review* is focused on finding answer for a specific question and hence excludes holistic compilation of literature whereas the *narrative review* article is highly scattered in manner due the random selection of literature data.

Resources: Google Scholar [3], Web of Science [4], Scopus [5], SciFinder [6], PubMed [7], and Reaxys [8] are the major electronic resources for retrieving relevant literature data.

Journals: Nature Chemistry (*Nature*), Chemical Reviews (*ACS*), Chemical Society Reviews (*RSC*), Coordination Chemistry Reviews (*Elsevier*), Reviews and Advances in Chemistry (*Springer*), Comments on Inorganic Chemistry (*T&F*).

Concept: Theoretical Chemistry; Predicting the molecular function

Theoretical chemistry demonstrates the properties and structure of molecules. Theoretical chemistry is the branch of chemistry which develops theoretical generalizations that are part of the theoretical arsenal of modern chemistry: for example, the concepts of chemical bonding, chemical reaction, valence, the surface of potential energy, molecular orbitals, orbital interactions, and molecule activation. Computational chemistry, molecular modelling, molecular dynamics, molecular mechanics, mathematical chemistry, cheminformatics and theoretical chemical kinetics are some of

the main branches of theoretical chemistry. Understanding the molecular physics, atomic physics, and chemical physics are also related to theoretical chemistry discipline. In general, laboratory experiments and experimental chemistry research are the outcome of theoretical concepts. Experimental results are demonstrated using the theoretical principles and the theoretical chemistry insights evolves to set experimental hypothesis [9]. Hence, experimental research in chemical sciences and the theoretical chemistry insights are inseparable. However, deriving new concepts, principles, equations, theorems, tools, and resources for understanding the functions of atoms and molecules are the main purpose of theoretical chemical research.

Themes: Although, many non-experimental branches of research are possible in theoretical chemistry. Feasibility of doing undergraduate and postgraduate final year project in molecular mechanics, molecular dynamics, and cheminformatics is very less. But, learning the computational tools for molecular modelling, docking, molecular energy minimization, molecular energy estimation using the online serves, tools and visualization tools would be easy.

Outcomes: Students could realize the connection between chemistry, physics, and mathematics and computer science by taking up a project on theoretical chemistry. Students understand the importance of developing models based on logical theories to corroborate with the results obtained though experiments.

Challenges: Generally, theoretical chemistry research needs collaboration with physics, mathematics and computer science researchers. And, graduate students may not be interested in taking up topics on core theoretical chemistry themes.

Resources: The self-guided introduction on theoretical chemistry for College Students and non-experts developed by Jack Simons, Professor of Chemistry at the University of Utah would be good starting point for the beginners [10].

Journals: Nature Chemistry (*Nature*), J.of Chemical Theory and Computation (*ACS*), Computational and Theoretical Chemistry (*Elsevier*), Theoretical Chemistry Accounts(*Springer*), Int. J. of Quantum Chemistry (Wiley), J. of Computational Biophysics and Chemistry(*World Scientific*).

Concept: Computational Chemistry; Insights on Molecules

Computational chemistry is a branch of theoretical chemistry that computes the behaviour of molecules in various materials like nanoparticles, catalysts, adsorbents, surfactant, proteins, polymers, drugs etc., Generally, researchers understand the functioning of the molecules/atoms / sub atomic particles by imagination and speculate. The instrumental techniques like microscopic and spectroscopic results are indirect methods to understand the behaviour and functioning of molecules in materials. Such, behaviours could be made available for visualization through computational chemistry tools. Computational parameters like energy, thermodynamic data, HOMO-LUMO, electrostatic maps, electron density, steric effect, binding energy, complementarity scores, docking

scores are used as complimentary data for the experimental results. In some research investigations like drug discovery, pharmacophore synthesis designare finalized based on the computational and simulation results [11,12].

Themes: Computational chemistry themes could be broadly classified in to two categories namely (i) structure of molecules, (ii) reactivity of molecules. Estimating the energy of a molecular structure is one of key aspect of computational chemistry. Computing bond angles, dihedral angles, bond lengths and electrostatic potential maps. Optimization of structure by minimizing the energy of molecules, prediction of possible isomers and understanding the spatial arrangement of atoms are some of the specific feasible themes that could be useful for the graduate students. Hence, computational chemistry is highly useful in understanding the chemistry of materials without doing much wet lab investigations.

Outcomes: In general, computational chemistry yields molecular, atomic and sub atomic level insights. In addition to the results obtained, visualizing the trajectories computed provides clarity on the changes due to reaction / interactions. Students would be able to gain knowledge on the molecular dynamics during and after the reaction. Insights on molecular/atomic structure, enthalpy of reactions, different types of interactions, interactions beyond molecules, electrostatic interactions, binding energies, and thermodynamic parameters, and vibrational frequencies, mechanical and electrical properties of molecules of different application materials can be derived.

*Challenges:*Students find difficulties in learning the computational tools. However, students can familiarize and improve proficiency by self-learning by using online tutorials with the guidance of project supervisors.

Resources: www.vcclab.org, www.computationalscience.org/ccceehttp, www.ccl.net, https://chemcompute.org– are few resources useful for the beginners.

Journals: J. of Chemical Information and Modelling (*ACS*),Applied Computational Chemistry (*RSC*), J. of Chemical Physics (*AIP*),J. of Computational Chemistry, (*Wiley*),J. of Molecular Structure, (Elsevier), J. of Computer-Aided Molecular Design, Structural Chemistry, J. of Molecular Modeling (Springer), Molecular Physics, Molecular Simulation (T & F).

Concept: Molecular docking; Molecule-Molecule binding

Molecular docking is an effective method to assess and interpret the binding of molecules on each other [13,14]. The crystallographic data (3D structural data) of molecules are used in docking software like Patchdock [15] and Autodock [16] for evaluating the binding ability of ligand on the target. Docking simulations yields different ligand-target complex with variable energies. The trajectory / conformation with lowest energy is identified as stable *ligand-target* complex.Molecular docking investigations with different ligands (drug) on a specific single target molecule would be useful in finalizing the most probable ligand with strong binding attributes. Such docking studies are helpful in finalizing the selection of ligand for further synthesis in the wet lab through experimental procedures. Docking investifations are useful to derive insights on, binding of drug molecules on

proteins, small molecules docking, supramolecular complex formation, and orientation preference of guest molecule into the host molecule, drug designing, and enzyme activation energy.

Themes: Binding site prediction, small molecule docking, molecular interactions, host-guest docking, reaction mechanism interpretation, lead optimization, predicting the energetically favourable orientation/conformation/binding, assessing the suitabilityof drug (ligand) molecule for the disease (target) molecule under investigation, protein-protein interaction.

Outcomes: Upon practicing molecular docking studies, students would get familiar about the docking and visualization tools. Students would be able to identify the binding sites in ligand and target, understand the atomic level interactions leading to the intermolecular forces, compare the binding strength of different drugs on the target, efficacy and toxicity of drugs.

Challenges: Beginners should familiarize the 3D structure generation tools and crystallographic data file handling before learning the docking technique. Understanding the 3D structure data takes much time for the undergraduate level students, however, it is possible to overcome by self-learning through online tutorials and with the help of project supervisors.

Resources: Click2Drug [17] is one of the comprehensive resource that consists of structural databases and relevant resources. Downloadable small molecule 3D structures can be obtained from, ACD (Available Chemical Directory) [18], CSD (Cambridge Structural Database) [19], MDDR (MDL Drug Data Report) [20], NCI (National Cancer Institute Database) [21].

Journals: J. of Chemical Information and Modelling (*ACS*),Applied Computational Chemistry (*RSC*), J. of Chemical Physics (*AIP*),J. of Computational Chemistry, (*Wiley*),J. of Molecular Structure, (Elsevier), J. of Computer-Aided Molecular Design, Structural Chemistry, J. of Molecular Modeling (Springer), Molecular Physics, Molecular Simulation (T & F).

Concept: Molecular Property Prediction;

Properties of molecules (drug) could be predicted using the molecular property predictor tools. Molecular attributes [22] like pKa, binding affinity, stability, solubility, weak interactions, electrostatic dynamics, H bonding, membrane permeability, transport, metabolic mechanism, pi electrons, sigma electrons, polarity, dipole moment, hetero atoms, aliphatic chains, aromatic cycles, rigid and rotatable bonds, receptor moieties, hetero cycles, rings, conjucation, accessible surface area, aliphatic rings, aromatic rings, hydrogen bond donor and acceptor, lipinski hydrogen bond donor, number of atoms, pKa, hetero cycles, molecular weight, topology, hydrophobicity, size, flexibility, rigidity, steric effect, molecular polar surface area, toxicology, efflux characteristics, Aqueous solubility calculation and electronic distribution could be calculated using the various molecular property tools.Drug-Target Binding Affinities (DTBA), Quantitative structure–activity relationship (QSAR) and quantitative structure–property relationships (QSPR), quantitative structure–chromatography relationships (QSCRs), quantitative structure–reactivity relationships (QSRRs), quantitative structure–toxicity relationships (QSTRs), quantitative structure–electrochemistry relationships (QSERs), quantitative structure–biodegradability relationships

(QSBRs), and absorption, distribution, metabolism, excretion, and toxicity (ADMET) studiesare essential in drug design and development.

Themes: Molecular property prediction, QSAR, QSPR, drug-likeness, physiochemical properties prediction, drug-target binding affinities.

Outcomes: Students could easily familiarize a set of online molecular property predictor. Efficiency of similar drug compounds could be estimated using the molecular property predictor.

Limitations: Prediction results and interpretations would be an outcome of the chosen molecular descriptors and molecules. However, project supervisor's guidance is a vital role in identification of the problem for the study.

Resources: MolGpKa (https://xundrug.cn/molgpka), Virtual Computational Chemistry Laboratory (http://www.vcclab.org/), mcule (https://mcule.com/apps/property-calculator/),QSAR, drug design, molecular modelling, similarity searches. (https://www.molinspiration.com/), Drug Likeness prediction (https://molsoft.com/mprop/),chemspider (https://www.chemspider.com/ACDLabs.aspx), chemical interference with a biological pathway (http://www.thegreentest.com/),ToxiM (http://metagenomics.iiserb.ac.in/ToxiM/), ADMET [23] analysis; BioTransformer (https://bitbucket.org/djoumbou/biotransformerjar/), SwissADME (http://www.swissadme.ch/), ADMETlab (https://admetmesh.scbdd.com/), vNN-ADMET (https://vnnadmet.bhsai.org/vnnadmet/login.xhtml).

Journals: Scientific Reports (nature), Journal of Chemical Information and Modeling (ACS), QSAR & Combinatorial Science, Molecular Informatics (Wiley), SAR and QSAR in Environmental Research, Expert Opinion on Drug Discovery(T & F), Molecules (mdpi).Journal of Cheminformatics (BMC),

Concept: In silico analysisof proteins; Predicting protein properties

The UniProt (www.uniprot.org) database consists of around 6 million protein sequences. The protein data available in UniProt database are highly curated by the experts. Protein sequence data can be easily downloaded from the database through a search interface (https://www.uniprot.org/uniprot/?query=reviewed:yes) by typing the protein of interest. The protein sequence retrieval process is similar to the google search. The physico-chemical and structural properties of the retrieved protein sequences could be analysed using various protein sequence analysis tools and servers. Most of the sequenced proteins lack a descriptive, documented physico-chemical and biochemical characterization. Because, experimental methods are trial and error-based and time consuming. Hence, computational approaches become especially significant. The tools and prediction servers available on the Internet, predict the various physico-chemical and biochemical properties and parameters required for designing the experiments for further protein analysis, thereby, minimizing the number of experimental trials and reduces the cost of experimental analysis. The whole process takes very little time and it provides not only faster but also accurate results.

Themes: physico-chemical parameters of protein sequences such as theoretical isoelectric point, molecular weight, total number of positive and negative residues, extinction coefficient, half-life, instability index, aliphatic index and grand average hydrophathycould be computed using the Expasy's ProtParam (http://us.expasy.org/tools/protparam.html) prediction server. The tools SOPM, SOPMA and SSCP servers could be used for predicting the secondary structure of proteins [24].

Outcomes: Students could familiarize the various bioinformatics tools and understand the role of molecular moieties / scaffold (functional groups) responsible for the characteristics of proteins.

Challenges: Understanding the protein sequence formats existing in the databases would be difficult for the beginners. Fixing the set of physico-chemical parameters for analysis and familiarizing the relevant tool would be difficult where project supervisor's guidance is mandatory. It could also be achieved through collaborating with researchers with suitable expertise.

Resources: The following list of online bioinformatics servers could be useful in predicting the physico-chemical properties of proteins (sequences). Tools for Sequence Analysis (http://www.expasy.ch/tools/),Compute pI/Mw tool (http://au.expasy.org/tools/pi_tool.html), ExPASy'sProtParam (http://us.expasy.org/tools/protparam.html), NetOGlyc (http://www.cbs.dtu.dk/services/NetOGlyc/), NetNGlyc (http://www.cbs.dtu.dk/services/NetNGlyc/), NetPhos(http://www.cbs.dtu.dk/services/NetPhos/), SignalP (http://www.cbs.dtu.dk/services/SignalP/),

SAPS (http://www.isrec.isb-sib.ch/software/SAPS-form.html),

SOPM (http://npsa-pbil.ibcp.fr/cgi-bin/npsa_automat.pl?page=npsa_sopm.html),

SOSUI (http://sosui.proteome.bio.tuat.ac.jp/cgi-bin/adv_sosui.cgi),

TMHMM (http://www.cbs.dtu.dk/services/TMHMM-2.0/).

Journals: Briefings in Bioinformatics (Oxford University Press), Computational Biology and Chemistry (Elsevier), Bioinformatics (BMC),Advances in Bioinformatics (hindawi), Austin Journal of Proteomics, Bioinformatics & Genomics (Austin Publishing Group),Bioinformation (Biomedical Informatics).

Concept: Homology modelling; shaping the structure of protein

Proteins function depends on its shape (i.e., three dimensional structure) and the shape of a protein depends on its primary structure (i.e., sequence of amino acids). Hence, the knowledge of proteins shape (3D structure) plays a vital role in understanding the functions of proteins. 3D structure of proteins provides a solid framework for planning experiments and for the interpretation of their results. Experimental structure determination methods are highly expensive, time consuming due to elaborate technical procedures. And the experimental methods are not always successful because many proteins fail to crystallize and cannot be dissolved in large quantities. Till data more than 10 million protein sequences are deposited by the scientists of different countries in the databases like Uniprot, International Protein Sequence Database, and Protein Research Foundation. But, the 3D structure of just 1.85 Lac proteins is estimated through experimental methods and deposited in

Protein Data Bank (https://www.rcsb.org/). It is obvious now that 3D structure of more than 10 million protein sequences is not estimated experimentally. Hence, computational method is preferred to build (model) the protein three-dimensional structure. Well established procedures with the help of online servers and tools highly quality 3D structure (of proteins) can be modelled from the primary structure (amino acid sequence) of a protein. Homology modelling is one of the simplest and fastest ways of constructing the 3D structure of a protein.

The major sequential steps in homology modelling are, (i) searching known 3D structures that are related to the target sequence, (ii) selecting the suitable 3D structures that will be used as templates, (iii) aligning the target sequence with the template structure, (iv) building the model for target sequence based on the alignment with the template, (v) evaluating the built model with the help of various tools. Alignment and model building is repeated until a quality 3D structure is achieved.

Themes: Homology modelling of protein [25, 26].

Outcomes: Students could familiarize the tools useful for homology modelling of proteins.

Challenges: Familiarizing the homology modelling tools and servers would be difficult task for the beginners. However, learning through online video tutorials would be helpful.

Resources: Protein similarity (3D structure) search tool; Blastp (https://blast.ncbi.nlm.nih.gov/Blast.cgi),

3D structure modeling servers; swissmodel (https://swissmodel.expasy.org/),ESyPred3D (https://www.unamur.be/sciences/biologie/urbm/bioinfo/esypred/),Protein 3D structure quality predictors; ProQ (https://proq.bioinfo.se/ProQ/ProQ.html), Ramachandran Plot Server(https://zlab.umassmed.edu/bu/rama/). The databases, ModBase (http://alto.compbio.ucsf.edu/modbase-cgi/index.cgi) and 3Dcrunch (http://www.expasy.org/swissmod/SM_3DCrunch.html) consist of protein structures obtained by homology modeling.

Journals: Journal, Briefings in Bioinformatics (Oxford University Press), Computational Biology and Chemistry, Computational and Structural Biotechnology (Elsevier), Bioinformatics (BMC), Advances in Bioinformatics (hindawi), Austin Journal of Proteomics, Bioinformatics & Genomics (Austin Publishing Group),Bioinformation (Biomedical Informatics), Journal of Biomolecular Structure and Dynamics (T & F).

CONCLUDING REMARKS, SUGGESTIONS AND RECOMMENDATIONS

Usually, students think about the selection of research problem for project work in the final semester. Considering the continuing pandemic situation since 2019, final year project work should be initiated in the lower semester itself. Various themes suggested in this report relevant to the

chemical science concepts such as literature review, theoretical chemistry, computational chemistry, molecular docking, molecular property prediction, in silico analysis of protein sequences, and homology modelling would be useful for carrying the project work at home using online tools.

However, the meticulous supervision through online teaching platform is required to make it as an insightful one. Learning the tools related to various themes (search engines, docking, online servers, etc.,) would be definitely a challenging aspect to the students. But project supervisors can suggest suitable online tutorials (preferably video) to learn the tools quickly. The relevant resources and journals suggested for the various concepts and themes would be the additional reference.

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