Implementation of Problem-Based Learning (PBL) Approach for Computer Aided Drug Designing (CADD) Course

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***Abstract*—Computer-aided drug design (CADD) is a course that provides a foundational understanding of the concepts and methods of computational drug design techniques that are used by the biggest biotech and pharmaceutical companies in the world today. PBL is an instructional methodology in where learners work in teams to find a solution for open-ended problems in order to gain information about specific topics. The aim of this study is to apply PBL model in the CADD course to analyze to what extent this encourages students to engage in group activities which fosters experiential learning and critical thinking and focuses on the course's foundations and applications. The students were asked to form teams and work to solve the problem statement "Pharmacoinformatics based screening of potential drug candidates from Indian medicinal plants against Cancer targets" provided. Mini-project, laboratory examination, manuscript submission, Monograph presentations were part of the course evaluation which were evaluated based on the framed rubrics. The evaluation scores, student outcomes, survey feedback and qualitative testimonies received from students, highlights the positive role of PBL model in knowledge and skill acquisition among students in this course. The exercises were helpful in addressing the following graduate attributes: the ability to identify and solve problems, determine appropriate tools, analyze and interpret data, communicate effectively, and work well in teams were the main outcomes of this course. Further implementations and future studies may bring in additional insights into this model of teaching-learning.**

***Keywords*—Bioinformatics, Education, Drug Design, PBL, Student outcome.**

***JEET Category*—Research**

I. INTRODUCTION

THE process of finding and developing new drugs is a rigorous, drawn-out, multidisciplinary undertaking. The process of discovering new drugs has been completely transformed by the contributions of computational approaches (Skjevik et al., 2009).

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It is a valuable tool for researching the connection between biological activity and molecular structure and is therefore crucial to the process of developing sensible medication designs. All researchers in this sector will have a unique platform to screen novel pharmacological entities thanks to this technique (Kapetanovic, 2008). Computational design techniques are used by the biggest biotech and pharmaceutical companies in the world today (Lin et al., 2020). The majority of students who enroll in a Bachelor of Technology in Biotechnology degree anticipate that employment as a research scientist is the pathway to a job in the pharmaceutical sector (Khan, 2018). Nowadays, the majority of biotechnology degree curriculum includes a strong emphasis on drug design and related technologies in order to meet student expectations and the skill needs for biotechnologists (Duelen et al., 2019). The course on computer-aided drug design provides a foundational understanding of the fundamental concepts and methods of drug discovery through the application of all major computational approaches.

Problem-Based Learning (PBL) is an approach to learning that is more inductive and student-led (Ansari et al., 2015). PBL refers to instructional strategies that are based on an inquiry process. In this method, which is student-centered, the instructor creates the assignment or tasks and encourages, supports, and guides the educational activities (Ali, 2019). Students are encouraged to assume greater accountability for their own learning process in this way. They must determine their own necessary learning demands and make use of already-existing knowledge (Ngereja et al., 2020). It has been demonstrated that PBL inspires students to actively search for and investigate fresh evidence. PBL is more successful than traditional teaching methods at fostering a critical thinking approach, analytical skills, process skills, and deep learning (Sukackė et al., 2022). PBL typically involves small-group collaboration, which adds the benefit of helping students develop their project management and teamwork abilities (Casquero-Modrego et al., 2022). Thus, PBL is an active, student-centered method of learning that is supported by several Accreditation Councils for Engineering Education. PBL allows for the use of any led by students instructional strategy meant to develop higher order cognitive and academic abilities (Moallem, 2019). PBL activities include research, fieldwork, case studies, both solo and team projects, and more.

PBL has the benefit of helping pupils learn far more than just the material (Vani et al., 2021). They gain knowledge on how to collaborate with others, troubleshoot issues, clearly communicate their ideas to an audience, and grow from their errors (Almulla, 2020).

II. CADD COURSE IN PBL MODE

Based on feedbacks and discussion with alumni who currently work in pharmaceutical field it was determined that the curriculum's drug design and development education needed to be updated and fine-tuned to meet the industry requirements. Up until now, courses on drug discovery, development, and its process have been scarce in undergraduate and even in post-graduate programs. Students frequently lack the knowledge and skills necessary to appreciate the job prospects available in the business as a result (Gross & Sohl, 2021). Importantly, understanding the drug discovery and development process is crucial for those who do intend to pursue a career in pharmaceutical research. It will make it easier to comprehend the chemical makeup, safety, and effectiveness of medications as well as the function of computational tools in drug creation (Romano & Tatonetti, 2019). This course's objective is to familiarize students with the concepts and methods of computational drug development.

Life science courses have traditionally emphasized teacher-led, deductive learning with information transfer from the instructor to the students (Hamilton, 2018). The passive transmission of information in this method results in surface learning and lowers student motivations, which are drawbacks (Howell, 2021). Developing self-directed learning skills is the aim of teaching reform using the PBL method, which aims to address the current issues in computer-aided drug design education.

III. METHODOLOGY

A. *Course Design*

The course 'Computer Aided Drug Design' is an elective course for third-year Bachelor of Technology students at Department of Biotechnology. The course is an Integrated Theory with Practical category course with 3-credits devoted to an introduction into computational drug discovery and development methods. The course is structured around the principles of PBL in order to inspire, challenge, and encourage students to learn deeply. We describe and assess a set of computer laboratory exercises designed to educate students the fundamentals of rational drug design. These experiments include everything from an overview of protein–ligand interactions to automated docking and quantum chemistry-based geometric optimization of possible therapeutic candidates.

Faculty research interests and teacher knowledge sharing are fundamental to research-led teaching approaches. Along with learning the necessary information, students who receive instruction in a more research-oriented manner also focus on the process of acquiring that knowledge (Afdal & Spernes, 2018). To promote deeper learning and critical thinking even more in the present course, it was decided to take it a step further and use a research-based design. Inquiry-based activities within a research-based design will encourage students to learn like researchers and reduce the gap between instructor and student (Marshall et al., 2017). Assistance in submitting their project work as a research paper to good quality Scopus indexed journal will be provided to participants.

TABLE I
DESIGN AND CONTENTS OF "COMPUTER AIDED DRUG DESIGN" COURSE

Module No.	Course Objectives	Learning Activities
1	Understand the basics of bioinformatics, chemo-informatics and its application for drug design and discovery process	• "Drug Design Workshop" - A web-based educational tool • Monograph presentations
2	Acquire the knowledge about protein structure prediction and visualization with their importance	• Mini-Workshop 1 on "Basics of CADD tools and its protocols"
3	Impart the knowledge on ligands to screen them using various databases and tools	• Lab Experiment sessions • Project Work
4	Perform and interpret the molecular docking and ADMET prediction studies	
5	Analyze the data acquired and prepare a report in form of manuscript	• Mini-Workshop 2 on "Basics of Research writing, usage of reference managers and article submission process" • Lab Experiment sessions • Project Work

Students in this innovative PBL-based course complete individual tasks in addition to working mostly in small groups on group projects. Lectures and workshops are among the supportive activities. Table 1 lists the course objectives together with the corresponding learning activities. The students were asked to form teams with a maximum group size of 3 members and work to solve the problem statement "Pharmacoinformatics based screening of potential drug candidates from Indian medicinal plants against Cancer targets" provided. The overview of the course design and the students' progress is highlighted in the Figure 1.

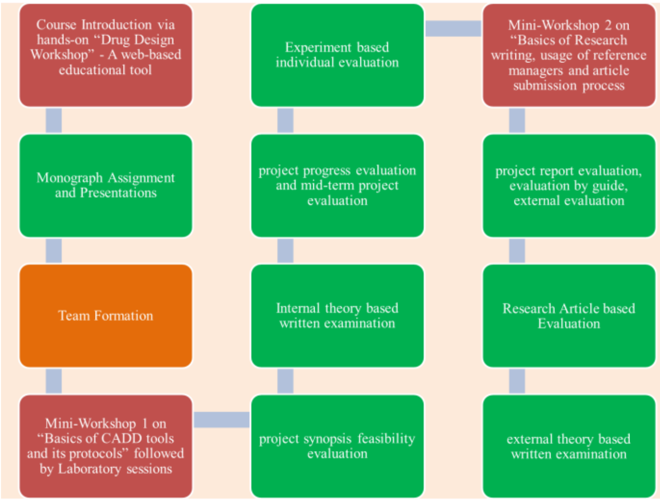

Fig. 1. Overview of the course design and the students' progress

B. *Pedagogy*

1) *Simulations & Workshops*

"Drug Design Workshop" - A web-based educational tool (http://www.drug-design-workshop.ch/) is a brand-new, publicly accessible web-based learning resource that explains the fundamentals of drug design and gives everyone access to basic computational techniques for conceptualizing and assessing compounds for possible therapeutic applications (Daina et al., 2017).

The students were provided with two mini-workshops to equip themselves with adequate knowledge to perform their mini-project. The initial workshop focused to train the students on various computer aided drug design tools and its protocols. The second workshop aimed to help the students understand the basics of manuscript writing, usage of reference managers and article submission process.

2) *Learning tools*

We took advantage of the opportunity presented by web technology and open-source resources available today to use as adaptable learning tools that are detailed in the below table 2 for this course. These tools aid the students in designing their project works in this course.

TABLE II
DETAILS OF VARIOUS OPEN-SOURCE RESOURCES AND TOOLS USED IN "COMPUTER AIDED DRUG DESIGN" COURSE

S. No.	Course Topics	Tools Used
1	Small molecule identification and retrieval	• Pubchem Database https://pubchem.ncbi.nlm.nih.gov/ • IMPPAT Database https://cb.imsc.res.in/imppat/
2	Protein Structure Identification and Retrieval	• Uniprot Database https://www.uniprot.org/ • RCSB PDB Database https://www.rcsb.org/ • Swiss model (Online Tool) https://swissmodel.expasy.org/
3	Literature search	• Pubmed Datbase https://pubmed.ncbi.nlm.nih.gov/ • Google Scholar https://scholar.google.com/
4	Target protein prediction	• TTD Database https://idrblab.net/ttd/ • KEGG Database https://www.genome.jp/kegg/pathway.html • Cytoscape (Software) https://cytoscape.org/
5	Protein structure visualization and optimization	• Swiss ODB Viewer (Software) https://spdbv.unil.ch/ • Biovia Discovery Studio (Software) https://discover.3ds.com/discovery-studio-visualizer-download • Pymol (Software) https://www.pymol.org/
6	Active site prediction	Prankweb (Online Tool) https://prankweb.cz/
7	Molecular docking and analysis	• PyRx (Software) https://pyrx.sourceforge.io/ • PLIP (Online Tool) https://plip-tool.biotec.tu-dresden.de/plip-web/plip/index
8	ADMET prediction	• Swiss ADME (Online Tool) http://www.swissadme.ch/ • PKCSM (Online Tool) https://biosig.lab.uq.edu.au/pkcsm/
9	Quantitative Structure Activity Relationship Prediction	Way2Drug Pass online (Online Tool) https://www.way2drug.com/passonline/
10	Manuscript preparation	Mendeley (Software) https://www.mendeley.com/

C. *Evaluation and Assessment*

The course was provided with autonomy for evaluation from the university. Thus, to meet the course needs the evaluation and assessment schemes were designed which consists of one internal theory based written examination, monograph individual assignment, experiment based individual evaluation, Project based team evaluation, research article based team evaluation and external theory based written examination. These exercises will be helpful in addressing the following graduate attributes: the ability to identify and solve problems, determine appropriate tools, analyze and interpret data, communicate effectively, and work well in teams were the main outcomes of this course. The list of evaluations and its respective weightage in this course is given in table 3.

TABLE III
DETAILS OF EVALUATION SCHEMES AND ITS RELEVANT WEIGHTAGE USED IN THE "COMPUTER AIDED DRUG DESIGN" COURSE

S. No.	Evaluation Scheme	Weightage in %
1	Internal theory based written examination	15
2	Monograph individual assignment (Written & Oral presentation)	10
3	Experiment based individual evaluation (Laboratory performance)	25
4	Project based team evaluation (Mini-Project)	25
5	Research article based team evaluation (Manuscript Preparation & Submission)	5
6	External theory based written examination	20

1) Internal and external theory based written examination

Testing theoretical knowledge traditionally is by a written examination. Essay-style responses work better on written exams in than multiple choice questions (Zeidner, 1987). While marking requires more effort overall, teachers are nevertheless satisfied that their students are honing a useful and applicable skill. The internal theory evaluation was conducted after sixth week of class to evaluate the theoretical knowledge of students towards the basic principles and knowledge acquired from initial class lectures and workshops. At the end of course, one external theory based written examination was conducted to assess the full course concepts and principles. This evaluation helps the facilitator to understand the knowledge level of students towards the basic concepts of the course.

2) Monograph Individual Assignment

The monograph assignment was evaluated based on written and oral presentations. Every student must prepare a two-page monograph on an FDA-approved medication. Selection of the drug is based on a first come, first served basis. Each written monograph had to be typed, and an indi vidual submission of five multiple-choice questions on the medication was required. The written monograph will be graded on its scientific accuracy, thoroughness, English grammar, punctuation, organization, and style of citation and references. It will be worth fifty points. The oral monograph presentation evaluation carries remaining fifty marks. It is imperative that the drug's key characteristics are briefly highlighted in both the written and spoken monographs. The entire class received a document that was generated and contained all of the monographs. Every student is required to develop a 10 to 12 minute PowerPoint presentation that highlights the key highlights of their medication. Following each lecture, the audience will have three minutes to ask questions. Every week, roughly fifteen students will give presentations. The following week will see the start of quizzes on the presentations from the previous week. This assignment was given to provide as a guide for understanding key drug features and conducting a critical assessment of drug information sources and also to obtain expertise in communicating scientific data.

3) Experiment based individual evaluation

The experiment based evaluation is conducted to assess individual student's practical skills. The students are asked to do an experiment that is then graded as per a set of rubrics. As CADD course involves handling various online and offline tools for drug design, the individual knowledge and skill of a student to use and apply these tools need to be tested. The students will be asked to perform individually an experiment and asked to record, analyze and interpret the results obtained from that experiment. The list of experiments performed by students and its relevant course objective under this course is given in table 4.

TABLE IV
LIST OF EXPERIMENT'S PERFORMED BY STUDENTS IN THE "COMPUTER AIDED DRUG DESIGN" COURSE

Experiment. No.	Title of the Experiment	Course Objectives covered
1	Accessing Biological Databases – Uniprot, PDB, TTD, Pubchem, IMPPAT	Impart the knowledge on ligands and target proteins to screen them using various databases and tools
2	Graph theoretical network analysis using Cytoscape software	
3	Retrieval, visualization and processing of protein structures – Swiss PDB viewer and Pymol softwares	Acquire the knowledge about protein structure prediction and visualization with their importance
4	Homology Modeling – Swiss Model Online tool	
5	Active site prediction – Prankweb Online tool	
6	Molecular docking – PyRx software	Perform and interpret the molecular docking and ADMET prediction studies
7	Protein – Ligand interaction analysis using PLIP, Pymol and Biovia Discovery Studio	
8	ADME Prediction using Swiss ADME Online tool	
9	Toxicity prediction using PKCSM Online tool	
10	QSAR prediction using PASS Online tool	
11	Citation and Referencing using Mendeley	Analyze the data acquired and prepare a report in form of manuscript

4) Project based team evaluation

The students as a team were asked to perform a mini-project as part of this course. The project work is the key feature of this course which is to solve the problem statement "Pharmacoinformatics based screening of potential drug candidates from Indian medicinal plants against Cancer targets" provided. To achieve this, the students use the knowledge they acquire during their initial lectures, workshops, simulations and laboratory modules. A Google Spreadsheet was used as a project tracker by the facilitator to monitor the progress of each student groups. The Google Spreadsheet was customized with dropdown options to get the status and overview of each individual teams on their work and its relevant progress periodically. The overview of the standard mini-project workflow to solve this problem statement is highlighted in the figure 2.

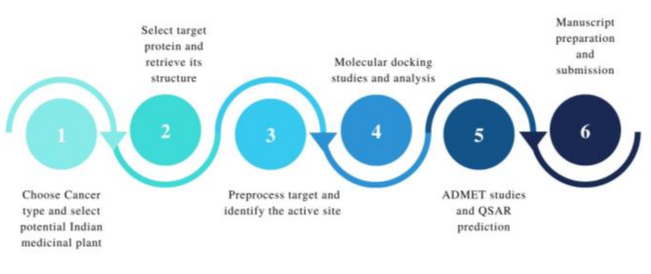

Fig. 2. Overview of the standard Mini-Project workflow followed by the students in this "Computer Aided Drug Design" Course

To evaluate student team's project through project-based evaluation a series of review assessments were framed periodically as depicted in Table 5.

TABLE V
LIST OF PERIODICAL REVIEWS PERFORMED UNDER PROJECT – BASED EVALUATION SCHEME TO ASSESS THE STUDENT TEAM'S MINI-PROJECT WORK IN THE "COMPUTER AIDED DRUG DESIGN" COURSE

Review #	Agenda of Review	Weightage in %
Review 1	Project Synopsis Feasibility Evaluation	9
Review 2	Project Progress Evaluation	9
Review 3	Mid-Term Project Evaluation	12
Review 4	Project Report Evaluation	12
Review 5	Evaluation by Guide	18
External Evaluation	Evaluation by external (End Semester Project evaluation)	40

The reason to have periodical evaluation is to give credit for their periodical progress instead of just a final outcome. This motivates the student to progress steadily throughout the course duration. In this course, we had five internal evaluations namely project synopsis feasibility evaluation, project progress evaluation, mid-term project evaluation, project report evaluation, evaluation by guide which carries 60% weightage and one external evaluation carrying 40% weightage. Rubrics were framed for each individual evaluation and were shared with students well in advance for them to ready for each evaluation.

5) *Research Article based Evaluation*

The student teams were asked to prepare a manuscript based on their project work and instructed to submit it in a suitable journal. A mini-workshop on manuscript preparation and submission held during the last phase of course assisted the students in accomplishing this task. As this task, is a bit complex for undergraduate students with limited course duration, a minimal weightage of 5% was given in overall grades. The objective of this evaluation is to encourage students to have understanding on scientific writing and publications.

D. *Feedback collection*

At the conclusion of course, a survey consisting of open-ended survey to be scored on a five-point Likert scale was done as part of the course. The results of the post-course survey are depicted in table 6.

TABLE VI
STUDENT'S RESPONSE[*] TO POST-COURSE SURVEY

Survey Items	Average of Response	Standard Deviation
I now have a clear understanding of how computational techniques are used in the development of novel medications due to this course	4.69	0.33
This was a challenging and interesting course	4.58	0.30
The learning exercises and tasks have just the right amount of diversity	4.42	0.25
The facilitator in this course was knowledgeable and very passionate	4.67	0.32
My interest towards Computational drug design and development has further developed as a result of taking this course	4.47	0.27
The course is well organized	4.42	0.25
The problem statement provided was clear and interesting to solve	4.36	0.24
The number of team discussion meetings with the course facilitator was sufficient	4.39	0.25
There was sufficient time planned for executing the course deliverables	4.50	0.27
Had useful learning experience from the lab-experiment sessions	4.44	0.26
Preparing a monograph presentation was useful learning experience	4.31	0.23
I have learned a lot from listening to other teams presentations throughout this course	4.33	0.24
Having periodical review is a good way to assess the progress of our mini-project	4.44	0.26
The writing of the research manuscript was instructive	4.39	0.25
I could use the skills and knowledge obtained in this group project in my future	4.56	0.28
Writing the research manuscript is a good way to finish this course	4.39	0.25

[*]Response based on a Likert scale on which 5 = strongly agree; 4 = agree; 3 = neutral; 2 = disagree; and 1 = strongly disagree; N = 36 students; No. of survey items = 16 questions

The data analysis of survey questions shows that majority of the respondents appeared to feel that the course "Computer Aided Drug Design" was highly effective in terms of knowledge and skill transfer. On a 5-point scale, the course received an overall rating of 4.46 which is calculated based on the weighted average value calculation (sum up mean values of each item and divide it by total number of items). The average weekly time spent by the students was reported to be

6.0 hours, which is more than the students reported for the other three credit courses in the Bachelor of Technology in Biotechnology program. Despite the fact that there is a time crunch on the students in this course, the evaluations showed encouraging results. The diversity of instruction and evaluation techniques is valued by the students. They found the coursework to be stimulating and demanding. Crucially, the student learners say that this course has provided them with a strong understanding of how computational methods are used in the discovery and development of new medications.

IV. DISCUSSION

Third-year undergraduate Biotechnology students have the opportunity to enroll in a new elective course called "Computer Aided Drug Design" in order to gain a deeper comprehension of the computer aided drug discovery and development processes. The goal of the course's design, which is centered on PBL principles, is to engage and inspire students through difficult tasks. The evaluation's findings are really encouraging.

As part of their course evaluation, the students individually and as a team performed well. The students actively participated in all activities related to the course like simulations, mini-workshops and seminars. The monograph assignment was submitted with all the individual students with good quality. Out of the 15 teams formed during this course 13 teams have successfully completed their mini-project work and achieved desirable results. Around 8 teams have prepared their manuscript as part of the research article based evaluation which is under correction with the course facilitator and soon will be ready for submission in Scopus indexed journals.

Because the many tasks greatly motivate and stimulate the student's, the PBL method of teaching is effective. In contrast to other courses, this one requires them to think critically and work as a team to solve challenges, and they spend a comparatively longer amount of time on it. The skills students attain in this course—collaboration and teamwork, time and project management, communication, critical thinking, and self-responsibility—have a lasting impact on their professional achievement and career readiness. Furthermore, it has been demonstrated that the evaluation techniques support deep learning and are consistent with the PBL style of instruction. The benefit of using a PBL approach, particularly for teaching staff, is one of PBL's purported strengths. Observing students' intense engagement is particularly motivating (Patil, 2016).

This course has certain shortcomings as well. There is a total of 36 students participated in this course with the maximum limit of 40. For the teachers, the laboratory portion in particular required a lot of work due to the limited availability of computers and supporting staffs in the department. This was managed with utilization of laptops available with few students and support rendered by research scholars. The course needs to be modified to accommodate larger groups of students because there are more and more students interested in it. To achieve this improvement in computer facility and supporting staffs to accommodate more student teams to facilitate practical session is essential. Also, the software's and tools used in this course were open-source software's and free tools which had certain limitations. To overcome this we have planned to purchase selected software's and to collaborate with industrial partners in future to get licensed tools to enhance the learning and exposure to full version of the tools.

Students feeling that their workload in PBL classes has increased are one of the other drawbacks of PBL. This is in fact also the case for this particular course. Students have expressed that they have been so engrossed in the course that they have occasionally neglected to pay attention to certain aspects of the other course that is offered at the same time. There is a need for closer observation of this area of focus. Additionally, it could be challenging for the students to cope with the group dynamics and acclimate to the method. While some students did require some time to acclimate to the high degree of autonomy and personal accountability in this course, they did so rather fast. Overall, students did not really struggle with group dynamics in this course. This is probably because many of the courses in the Bachelor of Technology program require students to work in diverse group compositions.

To summarize, the recently introduced course "Computer Aided Drug Design" effectively exposes students to the realm of drug design, specifically focusing on computational tools. The course will remain available to third-year undergraduate students as an elective. Additionally, the effective use of PBL in this course argues for the inclusion of more PBL-based courses in the biotechnology curriculum and encourages the use of more active teaching methods in biotechnology education.

V. CONCLUSION

One of the unique and key courses in Biotechnology under pharmaceutical specialization is computer-aided drug design, which aims to teach students the fundamental theories, concepts, and computational abilities used in the pharmaceutical industry. The use of PBL mode in the computer-aided drug design course process makes difficult subjects simple to comprehend and makes it easy to apply foundational knowledge to real-world situations. Additionally, positive teaching outcomes are observed, and students' desire for independent learning is stimulated. PBL method teaching change in CADD course is an ongoing process. The objectives of the PBL style teaching reform in the CADD course will only be met with constant improvement in teaching practices.

ACKNOWLEDGMENT

I acknowledge the Department of Biotechnology and School of Bio, Chemical and Processing Engineering, Kalasalingam Academy of Research and Education, Krishnankoil in providing constant support and motivation.

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