**Research Article**

# COMPUTER-AIDED DRUG DESIGNING LEADING PHARMACY PROFESSION AND PHARMACIST TOWARDS INNOVATION

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(Received: 11 November 2012; Accepted: 22 November, 2012; Published: 29 December, 2012)
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**Abstract**: CADD , C*omputer Aided DRUG Designing* has made great advances and significant contributions to the discovery and optimization of many clinically used medicines. Previously only traditional experimentation (in-vivo and in-vitro ) was done for therapeutic purpose , for this animal and human models were used and also other laboratory tests were performed for assurance of desired pharmacological response . It was all very costly and timing consuming and many years were needed for the approval of a single drug. Now in the advanced era of computer technology, by using the CADD software time and expenses can be saved. Through computational chemistry one can discover, enhance, study and relate the biologically active molecules. In the light of these facts the present survey based study was conducted to look into the matter of awareness of CADD among Pharmacy students and also its worth in contrast with other experimental techniques that is; in vivo and in vitro , hence to observe the possibilities of its implementation in Pakistan. The study was presented in January 2012 till April 2012, the students were asked to answer13 –item questionnaire. Descriptive statistics on sample characteristics was calculated and response was summarized as percentages of YES or NO. The results indicates the source of awareness 42% and 24% as through the questionnaire surveyed and from college lectures respectively. The sources like teachers and internet stood on 3rd and 4th position respectively than we had another sources like research journals, books etc. The survey is reflecting satisfaction of students towards the ethical status of CADD, its merits and possible placement and replacement over other laborious techniques as in vitro and in vivo. Results showed strong willingness of the majority of study population to adopt CADD as a helpful and fruitful method of research in the field of drug discovery that will give a new life to Pharmacy profession.

**Key words:** CADD, C*omputer Aided DRUG Designing, In-vivo, In-vitro.*

## INTRODUCTION

The researcher and drug developers are in a new era for adopting all the computer techniques to discover, design and optimize pharmacologically active compounds. As safety, efficacy and economy are the most considered criteria during the drug discovery and remain along all the time in the journey of drug from the laboratory bench to the pharmacy shelf and at last in the hand of consumer or patient[1].The method of drug discovery which has been adopted based on the idea of screening of synthetic and natural moiety having excellent pharmaceutical agent in past and then enhancing the activity and minimizing as much as possible the side effects previously[2]. All these efforts had two major targets that are lead molecule development and lead molecule optimization. Today a variety of computational chemistry and molecular modeling are now routinely and successfully applied for drug designing [3,4]. In this regard attempts are need to made for the implementation of latest computational based techniques as like modeling, docking, binding site prediction, quantitative structure activity relationship and molecular dynamics simulation [5, 6].

The continuous advancement in molecular biology and information technology is helping for the development of a rich molecular simulation and can be applied in system biology, proteomics, molecular biology and bioinformatics. We are intended to introduce the latest developments in drug design based on computational techniques, including protein structure modeling, docking, binding site prediction, quantitative structure–activity relationship (QSAR), and molecular dynamics simulation [7-12]. There are very large number of known compounds and new ones discovered each year indicating the need for an electronic information processing for storing of

chemical information in databases and obtaining a better overview of known chemistry. The effect of a drug in the human body is a consequence of the molecular recognition between a ligand (the drug) and a macromolecule (the target). Computational chemistry can characterize the dynamics and structure of such interactions [13,14], docking, structural interaction, virtual screening, and statistical learning methods have been used to identify new inhibitors using large commercially available databases and highly selective and efficient programs[15] The technological progress of CADD brought a paradigm change to both Pharmas and research institutions: it is now possible to obtain appropriate hits within several weeks because of the contribution of CADD, the computational technologies .

The addition of computer-aided drug design (CADD) technologies to the research and drug discovery approaches could lead to a reduction of up to 50% in the cost of drug design. Designing a drug is the process of finding or creating a molecule which has a specific activity on a biological organism. Development and drug discovery is a time-consuming, expensive, and interdisciplinary process whereas scientific advancements during the past two decades have altered the way of pharmaceutical research [16].

Computer Aided Drug Design is becoming an Emerging Tool for Research and Drug Development and in the era of research and development of novel and lead compound CADD has made its place strongly and playing supportive role for the discovery of potent compounds. It has stepped inn and now it is on the high way of great success in the field of drug development [17]. The goal of the present study was to portray and to speculate the susciptabillityof coputer aided drug designing and computer simulation for the development of pharmacy profession.

**METHOD:**

For the above mentioned purpose, a survey based method was adopted through which views and knowledge of Future Pharmacist about CADD were considered. Purposely the Pharmacy students from Dow University were assessed through a 13 item questionnaire and the importance and implementation of CADD was evaluated hence to observe its worth in contrast with other experimental techniques that is in vivo and in vitro.

**Criteria:**
1. The population consists of Pakistani students.
2. All the students were from the Pharm. D. undergraduate (Dow University of Health Sciences).

**Data Collection:**

A questionnaire consisting of ten questions about the awareness of CADD (Computer Aided Drug Designing) previously developed and was distributed among one hundred students and they were asked to give response by using a two point scale that is Yes or No (Positive or Negative). In the rest of two questions one had ten options and one was open ended question.

**Data Analysis:**

The retrieved questioners were analysed by the Statistical software SPSS-17. Through which frequency, %age and cumulative %age was calculated.

**RESULT AND DISCUSSION:**

The most important implementation of this technique is to find out whether a given molecule will bind to the target and how strongly. By using molecular dynamics information of both molecule and target site conformational changes can be predicted that could help to optimize the parameters for good pharmacological response of the drug. This analytical tool helps to provide low cost resources, time, safety, and can be fruitful for improving the efficiency of products and for the discovery of new moieties

The present study was aimed towards Pharmacy undergraduate students . For this purpose opinions of under graduate professionals of Pharm. D., Dow college of Pharmacy, Dow University of Health Sciences ( n=100) were obtained through questionnaire . The students were from first till final year, like that the different brain levels were covered for approaches . In the group 20.6% were male and 79.4% were female. According to the educational year, $1^{st}$ year-11.5%, $2^{nd}$ year-17.8%, $3^{rd}$ year-27.1%, $4^{th}$ year-19.6% and $5^{th}$ year 24.3% respectively. Characteristics of sample population were summarized in table -1.

As far as the awareness is concerned 63% had a know how about that but 44% had entirely not. The source of awareness is 42% and 24% through this questionnaire and from college lectures respectively .The sources like teachers and internet stood on $3^{rd}$ and $4^{th}$ position respectively than other sources like research journals, books etc. Number and % of response was also mentioned age ( Table-2, Graph-1). The survey showed the comparatively strong attitude of students towards

the CADD, its merits and possible placement and replacement over other laborious techniques as in vitro and in vivo. Depending on these facts and values it was observed that Pharmacy graduates are in deep interest for the matter of acceptance and implementation in Pakistan.

**Table-1: Characteristics of study population (n =100)**

| Characteristic | | N (%) |
|---|---|---|
| Gender | Male | 22 (20.6) |
| | Female | 85 (79.4) |
| Educational Year | First year | 12 (11.2) |
| | Second year | 19(17.8) |
| | Third year | 29 (27.1) |
| | Fourth year | 21 (19.6) |
| | Fifth year | 26 (24.3) |

**Table- 2: Respondent's opinion about CADD**

| S. No | Questions | Positive Response | Negative Response |
|---|---|---|---|
| 1 | Before reading this were you aware of CADD (computer –aided drug design or computer –assisted drug design)? | 63 (58.9) | 44 (41.1) |
| 2 | Where did you first time get information on CADD (computer –aided drug design or computer –assisted drug design)? | 77 (72) | 30 (28) |
| 3 | Do you approve animal / human experimentation ( in vivo and in vitro ) done on ethical basis which also include volunteer approval and consent if human subject ? | 95 (88.8) | 12 (11.2) |
| 4 | Do you approve animal / human experimentation ( in vivo and in vitro) done on unethical basis which also include volunteer approval and consent if human subject , unethical cloning, unethical genetic variation, torture? | 49(45.8) | 58(54.2) |
| 5 | Do you think that CADD must completely or partially replace animal / human experimentation ( in vivo and in vitro )? | 56 (52.3) | 51 (47.7) |
| 6 | CADD is used by world's major companies, especially in the developed countries,, Did you know this before? | 102 (95.3) | 5(4.7) |
| 7 | Computer technology is leading man to a much ease and better life than in past as it justify use of cheap resources, time, safety and improve efficiency of products and / or discover new product .Do you agree? | 99 (92.5) | 8 (7.5) |
| **8** | Do you think that CADD would be helpful to mankind**?** | 83(77.6) | 24 (22.4) |

**CONCLUSION:**

Results of the present effort showed strong willingness of the majority of population to adopt CADD as a helpful and fruitful method of research in the field of drug discovery that will give a new life to Pharmacy profession.

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