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IN SILICO STUDIES: MOMENTOUS TOOL FOR DRUG DISCOVERY AND DRUG DESIGNING IN PHARMACY

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ABSTRACT

In previous years the conventional studies were followed for the drug designing and different animal models, bacterial isolates and in some extreme cases human volunteers were in practice for the declaration of pharmacological response of natural or synthesized moieties. Although these all resources are still an important part of research but the outcome of these studies can be given strength by the computer simulation, "*in silico* studies" that is the advancement of computer technology and an offshoot of computational chemistry. It predicts the interaction of drug within the body, also with pathogens and provide the action of drug at receptor site. All these facts led to estimate the level of information in pharmacy professionals and the chance of acceptance of computer softwares in pharmaceutical studies as a core. For this purpose a survey based study was conducted among the pharmacy students belonging to different private and public sector universities that helped to establish statistical idea about the decisive factors and implementation of this modern practice. One hundred students participated in this study that were asked to answer10-point questionnaire. Descriptive statistics on sample characteristics was calculated and response was summarized as percentages of Positive or Negative. Forty eight students (48%) had knowledge about *in silico* studies but only 27% of them had tried to make use of it. Majority of the students (79%) agreed about its benefits and 74% consider *in silico* studies expensive. Overall survey revealed the strong positivism for adopting this technique in Pharmacy and Pharmaceutical researches.

Key words: *In silico*, *In vivo*, *In vitro*, Computational chemistry, Pharmacy.

AIMS AND OBJECTIVES

To develop awareness among Pharmacists and Medical specialist about the use of latest advanced methods of research " *in silico*" as that it should be taken as a regular part of pharmaceutical studies.

INTRODUCTION

In silico studies includes software techniques that help to analyze and integrate biological and medical data from a variety of sources. Specifically, it characterizes the use of computational models or simulations for making predictions and eventually responsible for providing new discoveries with advances in therapeutics. The research studies about the drug can be effectively performed by applying software tools of computational chemistry. It is common in the areas of molecular pharmacology and structural biology for both natural and synthetic moieties [1]. Although the *in-silico* studies of natural products are conducted in a different way as that of synthetic compounds [2]. Most of these methods are used parallel with the *in vivo* and *in vitro* data analysis for accurate modeling and optimization of elementary pharmacological properties of molecules like absorption, distribution, metabolism, excretion and toxicity 'ADMET' [3]. The diversity of the developed mathematical and biophysical models in this field approaches the pharmacological problems distinctively, as like a pharmacophore is the 3D arrangement of molecule responsible for bioactivity. Successful applications of the use of pharmacophores in virtual screening helps to identify the hits for a variety of targets hence the pharmacophore-based approaches have considerable resourcefulness to be used with biological targets [4,5]. Target-based virtual screening methods provide a good estimate of the expected conformation, orientation and binding affinity of the molecule (docking) [6,7]. Moreover computational methods have materialized as an influential approach for the prediction of human PK. In this regard, a variety of useful *in silico* ADME models have been developed for the screening of large data [8] and different predictive models of Database for Pharmacokinetics (PK/DB) are used in research for the evaluation of ADME properties, including human oral bioavailability, plasma protein binding, human intestinal absorption, blood-brain barrier permeation and water solubility [9,10]. These successful approaches have made *in silico* a rapidly growing area globally.

METHADOLOGY

The study was presented in January 2012 till April 2012. A cross sectional survey was carried out. The population size was 100. The population was the pharmacy undergraduate students of different universities like fifty students (50%) were selected from Dow University of Health Science, twenty (20%) were from Zia-ud-Din Medical University and thirty (30%) from Karachi University. Thus these groups were found to cover both private and public sector pupils (table-1&2) and the students were asked to respond 10-point questionnaire (table-3). Descriptive statistics on sample characteristics was calculated and response was summarized as percentages of Positive or Negative in order to evaluate the execution and significance of *in silico* technique.

Criteria

1. The population consists of Pakistani students.
2. All the students were Pharm. D. undergraduate of Dow University of Health Sciences, Zia-ud-Din Medical University and of Karachi University.

Data Collection

A questionnaire consisting of ten questions about the knowledge and implementation of *in silico* (Computer simulation technique of drug designing) formerly developed and was disseminated for the purpose of estimating the response from population.

Data Analysis

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

RESULTS AND DISCUSSION:

As multidimensional research is vastly growing all over the world and it has become a need for the encroachment and novelty. Hence *in silico* study should be included in the pharmaceutical studies, for opening the access of bright prospect. The conducted survey about the awareness of *in silico* studies was reflecting satisfaction of students towards the ethical status of this technique, its merits and possible placement and replacement over other laborious tools as *in vitro* and *in vivo*. Results showed strong willingness of the majority of study population to accept it as a supportive method for research in the field of drug discovery essential for enhanced Pharmaceutical formulations (figure-1). One hundred students participated in this study. Forty eight students (48%) had knowledge about *in silico*

studies but only 27% of them had tried to make use of it. Overall 20% out of 100 participants had tried to use of *in silico* studies. Majority of the students (79%) agreed about its benefits, on the other hand 74% believed that *in silico* studies are expensive. Eighty percent of the students indicated positively for inclusion of these studies in regular course of Pharmacy. Opinion of seventy five percent population indicated that this technique should be adopted as an effective target in pharmaceutical research (figure-2).

Table: 1-Population Size

University	Number of Students
Dow University of Health Sciences	50
Karachi University	30
Zia-ud-Din University	20

Table: 2-Response of Population Towards *In Silico* Studies

Reservation	Positive Respondent	Negative Respondent
Deliberation concerning *in silico* tools (Q. Do you have any idea about *in silico* studies)	48	52

Table: 3- An Overview of Questionnaire among the Population

S. No.	Questions	Criteria of Response	Answer of Positive Respondents (%)	Answer of Negative Respondents (%)
1.	Have you ever tried to make use of *in silico* technique?	Agree	13(27.1)	7(13.5)
		Disagree	35(72.9)	45(86.5)
2.	Is it expensive?	Agree	32(66.6)	42(80.7)
		Disagree	16(33.3)	10 (19.2)
3.	Do you agree about its benefits?	Agree	48(100)	31(59.6)
		Disagree	-	21(40.4)
4	Is it helpful as a research tool?	Agree	46(95.8)	41(78.8)
		Disagree	2(4.2)	11(21.2)

5	Do you agree to get result within short interval of time comparing with *in vitro* and *in vivo* methodologies?	Agree	40(83.3)	39(75)
		Disagree	8(16.7)	13(25)
6	Do you agree that its results are more accurate than *in vitro* and *in vivo* methodologies?	Agree	31(64.6)	34(65.4)
		Disagree	17(35.4)	34(65.4)
7	*In silico* is effective to a target classification of absorption, distribution etc?	Agree	32(66.7)	43(63.5)
		Disagree	16(33.3)	43(63.5)
8	Can it be easily perform individually?	Agree	21(43.8)	26(50)
		Disagree	27(56.3)	26(50)
9	Is it true that it needs no laboratories equipments except computer	Agree	23(47.9)	25(48.1)
		Disagree	25(52.1)	27(51.1)

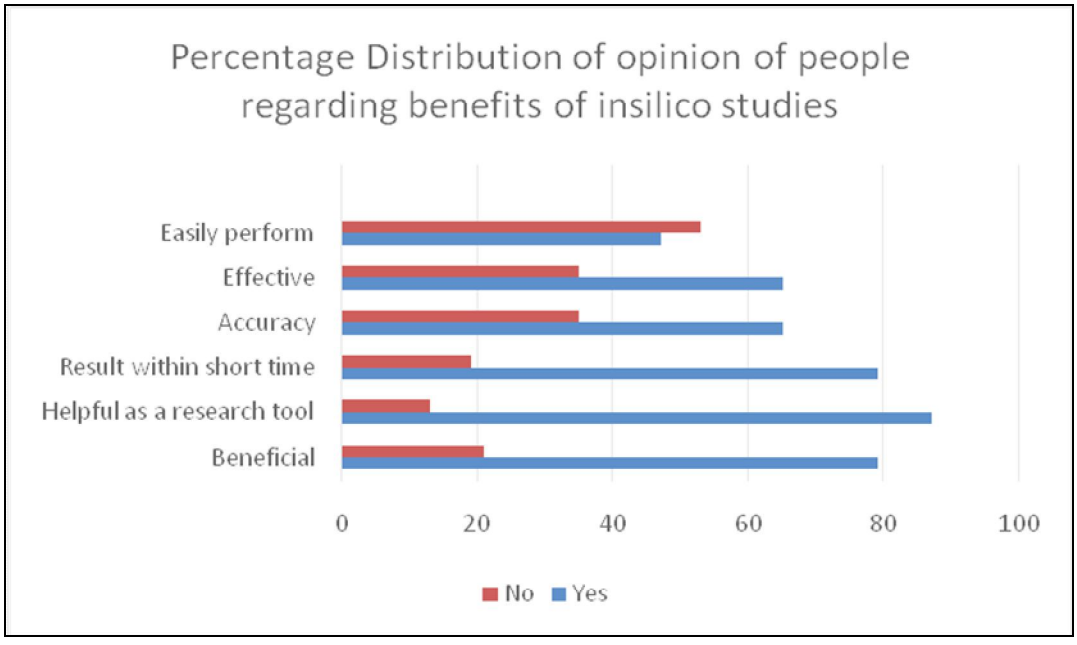

Figure -1: -Opinion of Population on the subject of *in silico* studies

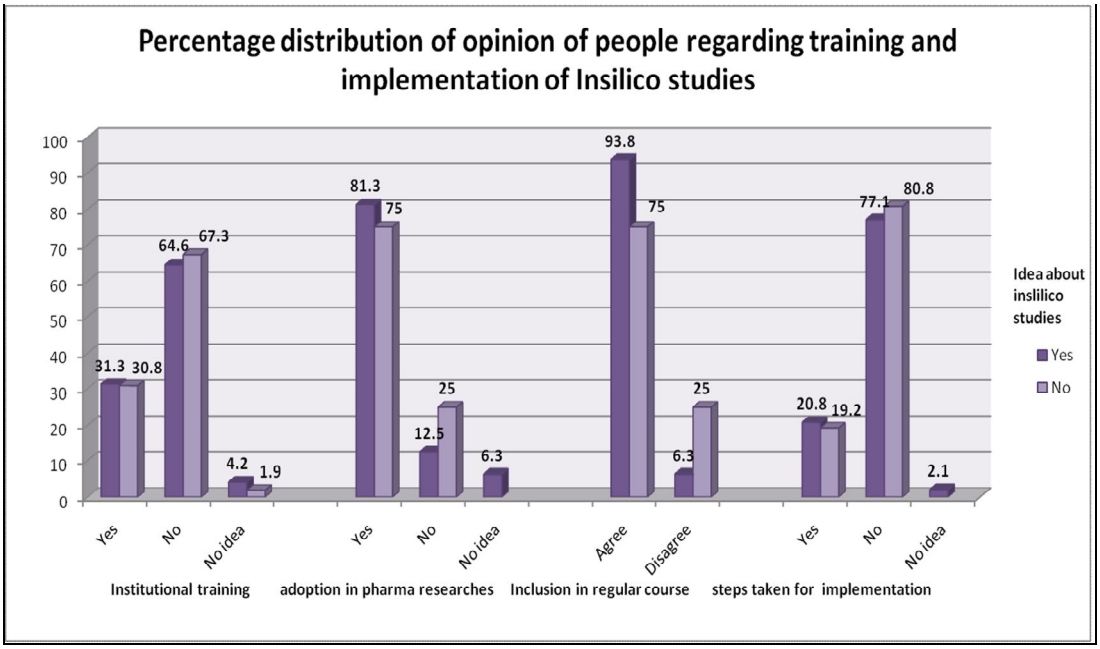

Figure -2: -Opinion of Population about the implementation of *in silico* studies

CONCLUSION

The survey results show positive response and willingness of the major population towards *in silico* studies. Hence it is concluded that these studies will be proof a milestone for drug designing and will be accepted with open hands by researchers.

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