

# A Study on the Teaching of Drug Design Course in Pharmacy - Taking Chifeng University as an Example

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**Abstract:** The course of drug design is a new interdisciplinary subject developed from multiple disciplines, with the research methods of innovative new drugs as the main content. It covers a wide range of knowledge points. Taking teaching this course to the Pharmaceutical students in Chifeng University as an example, this paper makes a preliminary exploration from many aspects such as clarifying the teaching objectives, Selection of the teaching contents, having a good first class, diversified teaching design models, diversified assessment methods, making full use of network resources and moral education throughout the whole process, aiming to provide reference for the training of innovative Drug Development staff in the future.

**Keywords:** drug design course, teaching objectives, teaching design, assessment methods, moral education

## 1. Introduction

Drug design<sup>[1]</sup> is a new interdisciplinary discipline with innovative new drug research methods as the main content, which is developed from Medicine, Mathematics, Physics, Organic Chemistry, Biochemistry, Molecular Biology, Cell Biology, Pharmacology, Pharmacokinetics, Informatics, Computer science and other disciplines.

Drug design is an important compulsory course for pharmacy majors. At present, the Pharmaceutical students in Chifeng University are using the third edition of the textbook of drug design compiled by Fang Hao and published by the People's Medical Publishing House. This textbook takes Chemical Biology as the main line, drug discovery as the goal, combines the traditional theories and methods of drug design with modern frontier science and technology, and contains case studies or drug research and development examples. This textbook covers many knowledge points of drug design, such as life science basis of drug design, drug design based on cell signal transduction pathway, drug design based on bioactive peptide, drug design based on enzymatic principle, drug design based on nucleic acid principle, drug design based on metabolic principle, drug design based on molecular hybrid principle, drug design based on combinatorial chemistry technology, drug design based on chemical genomics, drug design based on target structure, drug design based on ligand structure, drug- likeness and their applications in drug design.

Due to the wide range of knowledge points covered by drug design, it will be difficult for Pharmaceutical students to learn. Therefore, teachers' education and teaching methods are particularly important. This article takes the pharmacy major of Chifeng University as an example to explore the teaching of drug design.

## 2. A Study on the teaching of Drug Design Course

### 2.1. Clarify teaching objectives

In the teaching process, it is particularly important to clarify the teaching objectives<sup>[2]</sup>. In terms of knowledge objectives, students should understand the development direction of drug design and the procedures of new drug research and development, be familiar with the discovery approaches of new drugs or lead compounds, and master the theory, methods and technologies of drug design and discovery by studying this course. In terms of ideological goals, students should have a firm and correct political direction, develop morally, intellectually, physically and aesthetically in an all-round way, and be able to

constantly improve their sense of national defense, national security, patriotism and collectivism. In terms of ability objectives, we should cultivate students' innovative thinking and independence, enable students to have life-long learning awareness and independent learning ability, provide the ability basis for becoming staffs in new drug research and development in the future to meet the need of new drug research and development in China .

## ***2.2. Selection of teaching content***

The total period of Drug Design Course for Pharmaceutical students in Chifeng University is 32. Due to the limited class hours and many chapters, the teaching content should be appropriately selected. According to the teaching objectives of the course, some representative chapters are selected for key teaching during the teaching process. During the teaching process, the basic concepts, basic principles, basic methods and specific examples of drug design will be introduced. In the course of teaching, we will not only introduce the traditional methods to discover new drugs, but also introduce the latest design methods in combination with current research methods.

### ***2.2.1. Life science basis of drug design***

Introduce the biological targets of drug action, including the definition, classification and quantity of biological targets, the structure and function of biological macromolecules. Introduce the interaction between drugs and biological macromolecule targets, including the chemical nature, adaptation relationship and basic theory of interaction. Introduce the transmembrane transport of biomembrane and drugs, including the basic structure and function of biomembrane, transport mechanism and regulation, and molecular pharmacology affecting membrane transport.

### ***2.2.2. Drug design based on cell signal transduction pathway***

Introduce cell signal transduction, including the material basis of signal and signal transduction, chemical signal molecules, cell signal receiving system, the third messenger, drug intervention on signal transduction system. Introduce relevant cases of drug design based on regulating the second messenger, including drug design for regulating cAMP and cGMP signal pathways, drug design for regulating calcium, drug design for regulating kinase system. Introduce the related cases of drug design based on the regulation of the third messenger, such as the drug design of vitamin D receptor ligands.

### ***2.2.3. Drug design based on bioactive peptides***

Introduce the structure and function of peptide compounds, including the structural characteristics of peptide compounds, some important endogenous bioactive peptides in the body. Introduce the design principles and methods of peptide likeness compounds, including the design of configuration limiting amino acids, the modification of peptide chain skeleton, dipeptide segment analogues, the restriction of overall molecular conformation, the molecular simulation of peptide secondary structure, etc. Introduce the cases of peptide likeness compounds in drug design, such as the design process of  $\beta$ -secretase inhibitors.

### ***2.2.4. Drug design based on enzymatic principle***

Introduce the basic knowledge of enzymatic reaction, including the theory of enzymatic reaction, the activation and inhibition of enzymes. Introduce the design principle of enzyme inhibitors, including the development and classification of enzyme inhibitors, the rational design of enzyme inhibitors. Introduce the relevant cases of enzyme inhibitors, including the design of HIV reverse transcriptase inhibitors and tyrosine kinase inhibitors.

### ***2.2.5. Drug design based on nucleic acid principle***

Introduce the biosynthesis of nucleic acid, the design examples of metabolic antagonistic anti-tumor and antiviral drugs, the design of nucleoside antiviral drugs, and the design of antisense nucleic acid and siRNA drugs.

### ***2.2.6. Drug design based on metabolic principle***

Introduce the relationship between drug metabolism and new drug design, including the discovery of lead compounds and how to optimize lead compounds. Introduce the basic principle of prodrug design, including the basic concept of prodrug, the purpose and method of prodrug design, the application of prodrug design principle and biological precursor drugs. Introduce the basic concept of soft drugs, the design principle and specific application of soft drugs, the design and application of active target prodrug and passive target prodrug, etc.

### 2.2.7. Drug design based on molecular hybrid principle

Introduce the principle of molecular hybrid principle and twin drug, including the concept of molecular hybrid principle, the classification of twin drug, the specific application of twin drug principle, the overview of multi target drugs, including multi target drugs, design strategies, and the specific application of multi target drugs in various diseases (Tumor, Alzheimer's disease, Schizophrenia, Diabetes, Hypertension, AIDS).

### 2.2.8. Drug design based on combinatorial chemistry technology

Introduce the basic principles of combinatorial chemistry, including the basic concepts and principles of combinatorial chemistry, introduces the construction of combinatorial chemistry library, including the design, construction method, synthesis technology, etc. Introduce high throughput screening technology, including the composition of high throughput screening technology, computer virtual screening and the basic process of high throughput screening for drug discovery.

### 2.3. Have a good first lesson

In the teaching process of the first class, namely introduction, in addition to introducing the basic situation, development process and domestic and foreign curriculum of drug design, it is also necessary to introduce the current situation of new drug research and development, the prospects, opportunities and significance of new drug development to students, so that students can fully realize that the rational design of drug molecules is one of the important ways of new drug discovery. In the first class, we played the case videos related to drug design such as the past life and present life of paclitaxel to the society. In this process, students realized that learning drug design could provide a theoretical basis for rational drug design in the future, which greatly improved students' interest and enthusiasm in learning.

### 2.4. Diversified teaching design mode

The traditional knowledge based whole process teaching mode and the characteristics of this course's complex knowledge points will lead to students' low enthusiasm for learning this course. In order to improve students' autonomy in learning, we should actively develop a variety of teaching modes. For example, in the multimedia assisted teaching process, brainstorming cases<sup>[3]</sup>, flipped classroom and other methods are integrated to enrich the teaching mode and enhance the teaching effect.

Taking the study of the chapter of drug design based on combinatorial chemistry technology as an example, The teaching process and time allocation are shown in Table 1. The first is the student group presentation, the group presentation is a must for each class, and the presentation requirements are arranged in advance on the learning pass, mainly to show cases related to drug design. Before each presentation, the leader of the presentation group is required to upload the presentation content to the learning pass, and other group students will score on the learning pass, the Scoring criteria for group presentation is shown in Table 2. After the presentation, brief discussion and summary will be conducted.

Table 1: The teaching plan of drug design based on combinatorial chemistry technology

Teaching process	Time allocation(min)
Group presentation	20min
Review the content of the last lesson and give feedback on the assignment	10min
Introduce the teaching objectives of this chapter	5min
Introduce the content of this chapter	40min
Randomly select students to make a brief summary of the content of this course	10min
Teacher's summary and supplement	5min

Table 2: The Scoring criteria for group presentation

Scoring criteria	Proportion	Excellent	Good	Pass	Fail	score
On site explanation	40%	Rigorous logic, strong persuasion, natural expression, gesture and speech are integrated, and the connection is natural. Speak clearly and fluently, and dress generously, naturally and appropriately.	The logic is more rigorous, the expression is basically natural, the gesture and speech are integrated, and the connection is basically natural. Mandarin is fluent, and clothes are generous, natural and decent.	There is a certain degree of logic, the expression is not very natural, the gesture and speech can still cooperate, and the connection is interrupted. The pronunciation of some characters in Mandarin is not accurate, and the clothes are ordinary.	Poor logic, nervous expression, nonstandard pronunciation of Putonghua, frequent interruption of explanations, and unnatural attitude.	
Display Content	40%	All the references displayed are related to the theme of the disease, with prominent emphasis and appropriate details	Most of the references displayed are related to the theme of the disease, with more emphasis and appropriate details	Some of the references displayed are related to the theme of the disease, with less emphasis and less detail	Most of the references presented has nothing to do with the subject of the disease, and the emphasis is not prominent and the details are not appropriate	
Display form	20%	The typesetting is beautiful, the theme is prominent, the color scheme, animation design, switching effects, hyperlinks and action buttons are properly used.	The typesetting basically meets the requirements, with certain themes, color schemes, animation design, switching effects, hyperlinks and action buttons.	The typesetting basically meets the requirements, with a certain theme, color scheme, animation design, switching effects, hyperlinks and action buttons.	The typesetting does not meet the requirements, there is no theme, and the slide production is monotonous.	

Then review the content of the last lesson and give feedback on the assignment.

Then introduce the teaching objectives of this chapter: master the concept and basic principles of combinatorial chemistry, the basic process and link of drug design based on combinatorial chemistry technology, the concept and system composition of high-throughput screening; Be familiar with the construction methods and technologies of the combinatorial library, the advantages and disadvantages of different methods, the identification methods of possible active compounds in the combinatorial library, and the detection technologies in the high-throughput screening system; Understand the design of combinatorial library, dynamic combinatorial chemistry, and the development of combinatorial chemistry.

The content of this chapter was introduced from the screening case of the antimalarial drug target Plasmapin II inhibitor and the key knowledge points were taught: during the explanation, the students were shown the Nobel Prize winning video of Tu Youyou, a famous Chinese pharmacist, and introduced the discovery and development process of artemisinin and its derivative dihydroartemisinin. At the same time, the class was just in time for the International Anti Malaria Day, so that the students could

understand that the older generation of pharmacists were serious in their work and research, Practice the spirit of perseverance in scientific research, and encourage students to inherit the fine tradition and patriotism of hard study, hard work, innovation and patriotic dedication. In the process of teaching knowledge points, questions and answers, discussion and other methods are used to enrich the teaching mode and enhance the teaching effect.

After class summary, randomly select students to make a brief summary of the content of this course, and then teachers will supplement it. On the one hand, it can test students' mastery of knowledge, on the other hand, it can also exercise students' ability to summarize language expression.

### **2.5. Diversified assessment methods**

The training objective of the pharmacy major of Chifeng University is to cultivate applied, compound and innovative pharmaceutical professionals. The traditional assessment method is generally composed of usual performance and final exam scores. The usual performance are composed of attendance and classroom performance. The proportion of usual performance is 20%, and the final exam scores account for 80%. As a result, students will suddenly study in the final exam. They do not really master knowledge and use knowledge to solve problems in the later stage, and the training effect is relatively poor. Based on these problems, we adopt the method of process assessment in the teaching process to assess the teaching effect in various forms. The proportion of assessment methods is shown in Table 3, in the new assessment method, the usual performance account for 20%, the periodical achievement tests account for 20%, the group presentations account for 20%, the individual assignments account for 10%, and the final tests account for 30%. The usual performance consists of attendance and class performance, which includes the number of times students participate in class discussions, and the accuracy of answering questions. Periodical achievement tests regularly check the students' mastery of knowledge so that teachers can adjust the teaching progress according to the students' mastery of knowledge. On the one hand, group presentation can enhance students' ability to review and summarize literature cases, on the other hand, it can exercise students' strong sense and ability of teamwork, share information with other members, coordinate and cooperate enhance students' ability to correctly handle personal and team relationships. On the one hand, individual homework tests students' mastery of knowledge points, on the other hand, it is also to enhance students' ability to think independently. Diversified assessment methods can achieve a comprehensive evaluation of students' learning effects.

*Table 3: The proportion of assessment methods*

Assessment method	The proportion (%)
Usual performance	20%
Periodical achievement tests	20%
Group presentations	20%
Individual assignments	10%
Final exam	30%

### **2.6. Make full use of network resources**

This course adopts online and offline hybrid teaching in the teaching process, and network resources play an important role in the course teaching process. As an indispensable tool in mixed teaching, Chaoxing Xuexi Tong plays an important role in the teaching process. At present, Chaoxing Xuexi Tong has all the functions such as regular attendance, roll call in class, preemptive answering, online homework (you can establish an assignment library), online examination (you can randomly select test questions when you establish an examination paper library, publish the exam and choose the items out of order when you publish the exam). In addition, Chaoxing Xuexi Tong can be used as a repository to store the learning materials uploaded by teachers (teaching plans, syllabus, electronic textbooks, chapter courseware, chapter case videos) and analyze the students' learning of these materials. There are also some online resources available on the Chaoxing Xuexi Tong, which make the boring classroom lively and interesting in various forms. For example, the homework presented by the group is uploaded to the Chaoxing Xuexi Tong for scoring, and the Chaoxing Xuexi Tong will automatically summarize according to the scoring situation and scoring proportion. Each group of students can see the scoring situation of each group and the final equal score, which increases students' interest and enthusiasm in learning.

### **2.7. Moral education runs through the whole curriculum**

It can constantly improve the concept of national defense, national security awareness, patriotism and collectivism. Moral education is essential for each course, but the moral education of natural science should not be copied mechanically, and should be implemented in invisible moral education, which can achieve the infiltration of moistening things silently. For example, when the students watched the Nobel Prize winning video of Tu Youyou, a famous Chinese pharmacologist, and introduced the discovery and development of artemisinin and its derivative dihydroartemisinin, they did not need too much words to understand that the older generation of pharmacists were serious in their work and research, practiced the spirit of persevering scientific research, and the fine tradition of innovation, patriotic dedication and patriotism, Moral education naturally permeates into the curriculum.

### **3. Conclusions**

Reforms are the driving force behind development. Education must also be constantly improved. Only in this way can we meet today's society's needs for the cultivation of innovative talents.

Drug design plays a very important role in the cultivation of innovative talents in pharmacy. This paper makes a preliminary exploration from the following aspects: clear teaching objectives, good first class, diversified teaching design models, diversified assessment methods, making full use of network resources and moral education throughout the whole process, etc., aiming to provide reference for the training of innovative Drug Development staff in the future.

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