

**MINISTRY OF HEALTH OF UKRAINE**  
**BOGOMOLETS NATIONAL MEDICAL UNIVERSITY**

**GUIDELINES**  
**to lectures**

Academic discipline	Fundamentals of chemical metrology
Branch of knowledge	22 “Health care”
Specialty	226 “Pharmacy, industrial pharmacy”
Specialization	226.01 “Pharmacy”
Department	Analytical, physical and colloid chemistry

**Approved** at the meeting of Analytical, Physical and Colloid Chemistry Department  
Proceedings N 1 dated 29 August 2024

**Considered and approved by** cyclical methodological commission of specialty 226  
“Pharmacy, industrial pharmacy”  
Proceedings N 1 dated 30 August 2024

**Author: Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and  
Colloid Chemistry Department, PhD in Chemistry, Associate Professor

## CONTENTS

Lecture N 1 “Metrology as a science of measurement” .....	3
Lecture N 2 “Role of chemical metrology in pharmacy and medicine” .....	6
Lecture N 3 “Errors of measurement: general concepts and classification” .....	9
Lecture N 4 “Errors in chemical analysis” .....	12
Lecture 5 “Metrological characteristics of pharmaceutical analysis” .....	15
Lecture N 6 “Validation of analytical procedures and tests” .....	18
Lecture N 7 “Main ideas of correlation and regression analyses” .....	21
Lecture N 8 “Basic concepts of probability theory. Probability distributions for discrete and continuous random variables” .....	24
Lecture N 9 “Chemometrics as an interdisciplinary scientific discipline. Review of main chemometric methods” .....	27
Lecture N 10 “Application of chemometric methods in pharmacy and medicine” .....	30

## Lecture N 1 “Metrology as a science of measurement”

**Type of lecture:** traditional (informational).

### **Competencies:**

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).

2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### **Purposes:**

1) didactic purpose – to form systematized knowledge about the main stages of metrology development; to reveal the concepts of “physical quantity” and “measurement”;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### **Tasks of the lecture:**

1) to know the subject, object and tasks of metrology;

2) to be able to classify quantities and measurements.

### **Lecture plan:**

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	Present information on the need for a targeted policy aimed at the effective functioning of metrology systems, standardization and certification.	Reveal the relevance of the topic of the lecture; familiarize students with the lecture plan.	5 minutes
Main part	1. The main stages of the development of metrology:	Acquire knowledge about the development	30 minutes

	<p>reveal the content of the six stages of the development of metrology.</p> <p>2. Measurement and physical quantity: definition of concepts; classification of measurements; measurement in chemical analysis; classification of quantities.</p>	<p>of metrology as a science of measurement.</p> <p>Acquire knowledge about the concepts of “measurement” and “physical quantity”; to realize the importance of measurement in the field of chemistry and pharmacy.</p>	
Results	Highlight the importance of measurement in the field of chemistry and pharmacy.	Summarize the presented material; emphasize the definition, role and main purpose of metrology.	5 minutes
Answers to questions	Active dialogue / discussion.	Explain the most difficult and unclear points of the lecture.	5 minutes

### Recommended literature:

#### *Basic*

1. Introduction to Statistics in Metrology / S. Crowder et al. Cham : Springer International Publishing, 2020, P. 1-34. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

2. Taylor, J. K., Cihon, C. Statistical techniques for data analysis (second edition). Chapman and Hall/CRC, 2004, P. 1-7. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Additional*

1. Barwick V. J., Prichard E. (eds.). Eurachem Guide: Terminology in Analytical Measurement – Introduction to VIM 3 (2011). P. 1-6. URL: [https://www.eurachem.org/images/stories/Guides/pdf/TAM\\_2023\\_EN.pdf](https://www.eurachem.org/images/stories/Guides/pdf/TAM_2023_EN.pdf) (date of access: 25.07.2024).

#### *Information resources*

- <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/department-medical-general-chemistry/>
- <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

### Questions for student self-preparation for the lecture:

- Concepts of “metrology”, “measurement” and “physical quantity”.
- Object, subject and tasks of metrology.

**The methodical instruction is developed by Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor

## Lecture N 2 “Role of chemical metrology in pharmacy and medicine”

**Type of lecture:** traditional (informational).

### **Competencies:**

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).

2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### **Purposes:**

1) didactic purpose – to reveal the meaning of chemical metrology in accordance with the needs and interests of the health care industry; to form systematized knowledge about the key aspects of the role of chemical metrology in pharmacy and medicine;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### **Tasks of the lecture:**

1) to know the areas of application of chemical metrology in pharmacy and medicine;

2) to be able to identify the tasks and significance of metrology in the relevant fields of pharmacy and medicine.

### **Lecture plan:**

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	Present current data on the role of chemical metrology in the pharmaceutical industry.	Reveal the relevance of the topic of the lecture; familiarize students with the lecture plan.	5 minutes
Main part	1. Fields of application of chemical metrology in	Reveal the meaning and main tasks of the	30 minutes

	<p>pharmacy:</p> <p>1) statistical processing of analysis results;</p> <p>2) metrological substantiation of pharmaceutical analysis methods;</p> <p>3) obtaining validation characteristics of pharmaceutical analysis methods.</p> <p>2. Metrology in medicine. Emphasize the need to ensure the unity of measurements in medical practice.</p>	<p>metrology of pharmaceutical analysis:</p> <p>Reveal the importance of metrology in the field of medicine.</p>	
Results	To single out the importance of chemical metrology for pharmacy (medicine).	Summarize the presented material; emphasize the need knowledge and understanding of the basics of chemical metrology for the professional training of future masters of pharmacy.	5 minutes
Answers to questions	Active dialogue / discussion.	Explain the most difficult and unclear points of the lecture.	5 minutes

### Recommended literature:

#### *Basic*

1. Riffenburg R. H., Gillen D. L. Statistical in Medicine (fourth edition). Academic press, 2020, P. 1-28. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Additional*

1. Statistics and Chemometrics for Analytical Chemistry (seventh edition) / J. N. Miller, J.C. Miller and R. D. Miller : Pearson, 2018, P. 75-99. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Information resources*

- <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/department-medical-general-chemistry/>
- <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

**Questions for student self-preparation for the lecture:**

1. The main tasks of metrology of pharmaceutical analysis.
2. Analyze the list of categories of legally regulated measuring equipment subject to periodic verification, and to single out measuring equipment related to pharmacy / medicine.

**The methodical instruction is developed by Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor



## Lecture N 3 “Errors of measurement: general concepts and classification”

**Type of lecture:** traditional (informational).

### Competencies:

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).

2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### Purposes:

1) didactic purpose – to reveal the essence and meaning of the measurement error; analyze the classification of errors; demonstrate and analyze the algorithms for checking the homogeneity of the sample using the Q-test and Grubb’s test;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### Tasks of the lecture:

1) to know the classification of errors;

2) to be able to identify the type of error;

3) to know the peculiarities of applying the Q-test, Grubb’s test and rule of the huge error;

4) to be able to identify outliers.

### Lecture plan:

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	Present information on the need to study the obtained experimental data in order to assess errors and make appropriate corrections to	Reveal the relevance of the topic of the lecture; familiarize students with the lecture plan.	5 minutes

	the final result.		
Main part	<p>1. Classification of errors: according to the method of expression; depending on the value of the measured quantity; according to the nature of behavior over time and according to the mode of measurements.</p> <p>2. Checking the homogeneity of the sample: algorithms for checking the homogeneity of the sample using the Q-test, Grubb's test and rule of the huge error.</p>	<p>Acquire knowledge about the classification of measurement errors and the ability to identify the type of error.</p> <p>Master the skills to determine the presence / absence of mistakes (gross errors) in the results of chemical analysis.</p>	30 minutes
Results	To single out the fact that the homogeneity of the sample is a necessary condition for ensuring the reliability of statistical processing of the results of quantitative analysis.	Summarize the presented material; emphasize the practical value of knowledge about the classification of errors and the ability to exclude gross errors from a sample of experimental results.	5 minutes
Answers to questions	Active dialogue / discussion.	Explain the most difficult and unclear points of the lecture.	5 minutes

### Recommended literature:

#### *Basic*

1. Statistics and Chemometrics for Analytical Chemistry (seventh edition) / J. N. Miller, J.C. Miller and R. D. Miller : Pearson, 2018, P. 1-14, 49-52. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

2. Taylor, J. K., Cihon, C. Statistical techniques for data analysis (second edition). Chapman and Hall/CRC, 2004, P. 100-107. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Additional*

1. Barwick V. J., Prichard E. (eds.). Eurachem Guide: Terminology in Analytical Measurement – Introduction to VIM 3 (2011). P. 6-16. URL: [https://www.eurachem.org/images/stories/Guides/pdf/TAM\\_2023\\_EN.pdf](https://www.eurachem.org/images/stories/Guides/pdf/TAM_2023_EN.pdf) (date of access: 25.07.2024).

2. Ellison S. L. R., Williams A. Eurachem/Citac Guide: Quantifying Uncertainty in Analytical Measurements (third ed, 2012). URL:

[https://www.eurachem.org/images/stories/Guides/pdf/QUAM2012\\_P1.pdf](https://www.eurachem.org/images/stories/Guides/pdf/QUAM2012_P1.pdf) (date of access: 25.07.2024).

3. Pereira P. Eurachem/CITAC Guide “Assessment of Performance and Uncertainty in Qualitative Chemical Analysis” – A Medical Laboratory Perspective. *Standards*. 2022. Vol. 2, no. 2. P. 194–201. URL: <https://doi.org/10.3390/standards2020014> (date of access: 25.07.2024).

*Information resources*

1. <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/department-medical-general-chemistry/>

2. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

**Questions for student self-preparation for the lecture:**

1. Classification of errors.
2. The concept of “error” and “outlier”.
3. Algorithms for Q-test, Grubb’s test and rule of the huge error.

**The methodical instruction is developed by Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor

## Lecture N 4 “Errors in chemical analysis”

**Type of lecture:** traditional (informational).

### **Competencies:**

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).

2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### **Purposes:**

1) didactic purpose – to analyze the specifics of chemical analysis as a metrological discipline; reveal the causes and sources of errors in chemical analysis;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### **Tasks of the lecture:**

1) to know the specifics of chemical analysis as a metrological discipline;

2) to know the causes and sources of errors in chemical analysis;

3) to be able to determine and predict possible causes and sources of errors when performing experimental research.

### **Lecture plan:**

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	Present information that chemical analysis studies methods and means of measuring the chemical properties of substances and the composition of samples.	Reveal the relevance of the topic of the lecture; familiarize students with the lecture plan.	5 minutes
Main part	1. Specificity of chemical	Form an understanding	30

	<p>analysis as a metrological discipline: measurement of various parameters; application of various measurement methods; use of standard samples of substances; non-linear dependencies; processing of complex multidimensional data.</p> <p>2. Causes of errors in chemical analysis: systematic and random errors; instrumental errors; methodical errors; computational errors; personal errors.</p>	<p>of the specifics of chemical analysis as a metrological discipline.</p> <p>Acquire knowledge about the main causes and sources of errors in chemical analysis; to form the ability to determine and predict possible causes and sources of errors when performing experimental research.</p>	minutes
Results	To single out the opinion that in chemical analysis, it is important to take into account the errors that may occur at various stages of the analysis.	Summarize the presented material; emphasize the importance of the ability to identify and predict possible causes and sources of errors when performing experimental research.	5 minutes
Answers to questions	Active dialogue / discussion.	Explain the most difficult and unclear points of the lecture.	5 minutes

### Recommended literature:

#### *Basic*

1. Statistics and Chemometrics for Analytical Chemistry (seventh edition) / J. N. Miller, J.C. Miller and R. D. Miller : Pearson, 2018, P. 1-14. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

2. Introduction to Statistics in Metrology / S. Crowder et al. Cham : Springer International Publishing, 2020, P. 23-33. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Additional*

1. Bettencourt da Silva R., Ellison S. L. R. (eds.). Eurachem/CITAC Guide: Assessment of performance and uncertainty in qualitative chemical analysis. First

Edition. Eurachem, 2021. 48 p. URL: [https://www.eurachem.org/images/stories/Guides/pdf/AQA\\_2021\\_EN\\_v01a.pdf](https://www.eurachem.org/images/stories/Guides/pdf/AQA_2021_EN_v01a.pdf) (date of access: 25.07.2024).

2. Ellison S. L. R., Williams A. Eurachem/Citac Guide: Quantifying Uncertainty in Analytical Measurements (third ed, 2012). URL: [https://www.eurachem.org/images/stories/Guides/pdf/QUAM2012\\_P1.pdf](https://www.eurachem.org/images/stories/Guides/pdf/QUAM2012_P1.pdf) (date of access: 25.07.2024).

3. Pereira P. Eurachem/CITAC Guide “Assessment of Performance and Uncertainty in Qualitative Chemical Analysis” – A Medical Laboratory Perspective. *Standards*. 2022. Vol. 2, no. 2. P. 194–201. URL: <https://doi.org/10.3390/standards2020014> (date of access: 25.07.2024).

#### *Information resources*

1. <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/department-medical-general-chemistry/>
2. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

#### **Questions for student self-preparation for the lecture:**

1. Characteristics of chemical analysis as a metrological discipline.
2. Concepts of “systematic error”, “random error”, “instrumental error”, “methodical error”, “personal error”, “computational error”.

**The methodical instruction is developed by Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor

## Lecture 5 “Metrological characteristics of pharmaceutical analysis”

**Type of lecture:** traditional (informational).

### **Competencies:**

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).

2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### **Purposes:**

1) didactic purpose – to analyze the formulas for calculating the main metrological characteristics of the analysis method; to form systematized knowledge regarding their practical significance; to develop the ability to interpret the results of calculations;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### **Tasks of the lecture:**

1) to know the formulas for calculating the main metrological characteristics of the analysis method;

2) to be able to calculate the main metrological characteristics of the analysis method;

3) to be able to present the results of quantitative analysis using statistical processing;

4) to be able to interpret the results of calculations.

### **Lecture plan:**

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	Present information that metrological characteristics of the	Reveal the relevance of the topic of the lecture; familiarize students	5 minutes

	analysis method are established by statistical processing of the obtained experimental sample.	with the lecture plan.	
Main part	Demonstrate formulas for calculating the main metrological characteristics of the analysis method and analyze them using specific examples, namely: sample mean, standard deviation, variance, standard deviation of the mean value, relative variance, relative standard deviation, relative standard deviation of the mean result, confidence interval.	Acquire knowledge and skills regarding the calculation of the main metrological characteristics of the analysis method and presenting the results of quantitative analysis.	30 minutes
Results	Highlight significance statistical processing of quantitative chemical analysis results.	Summarize the presented material; to emphasize the importance and relevance of the acquired knowledge for the work of research and / or innovative nature of future masters of pharmacy.	5 minutes
Answers to questions	Active dialogue / discussion.	Explain the most difficult and unclear points of the lecture.	5 minutes

### Recommended literature:

#### *Basic*

1. European Pharmacopoeia / European Directorate for the Quality of Medicines & HealthCare of the Council of Europe. – tenth edition, volume 1. Strasbourg : Council of Europe, 2019. Section 5.3. Statistical analysis of results of biological assays and tests. P. 683-713. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

2. Taylor, J. K., Cihon, C. Statistical techniques for data analysis (second edition). Chapman and Hall/CRC, 2004, P. 47-52. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Additional*

1. Statistics and Chemometrics for Analytical Chemistry (seventh edition) / J. N. Miller, J.C. Miller and R. D. Miller : Pearson, 2018, P. 16-34. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).



*Information resources*

1. <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/department-medical-general-chemistry/>
2. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

**Questions for student self-preparation for the lecture:**

1. Formulas for calculating the main metrological characteristics of the analysis method.
2. Presentation of the results of quantitative analysis.

**The methodical instruction is developed by Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor

## Lecture N 6 “Validation of analytical procedures and tests”

**Type of lecture:** traditional (informational).

### **Competencies:**

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).

2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### **Purposes:**

1) didactic purpose – to form systematized knowledge regarding the validation of analytical methods and tests; analyze analytical tests and methods that are subject to validation; explain validation characteristics and requirements; to be aware of the importance of validation of analytical methods and tests for pharmacy and medicine;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### **Tasks of the lecture:**

1) to know analytical tests and methods that are subject to validation;

2) to know validation characteristics and requirements;

3) to be able to determine the list of necessary validation characteristics for various tests and methods.

### **Lecture plan:**

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	To present information that method validation is an extremely important process in scientific research, pharmacy and medicine.	Reveal the relevance of the topic of the lecture; familiarize students with the lecture plan.	5 minutes

	Validation is the procedure of checking the accuracy, reliability and suitability of a technique or instrument used to measure, evaluate or control data.		
Main part	<p>1. Analytical tests and methods subject to validation: identification tests; quantitative tests to determine impurities; limit test for impurity control.</p> <p>2. Validation characteristics and requirements: correctness, precision; specificity; detection limit; limit of quantification; linearity; range of application.</p>	<p>Acquire knowledge regarding the appointment and practical application of analytical methods and tests subject to validation.</p> <p>Acquire knowledge about the practical significance of validation characteristics and requirements, as well as the ability to determine the list of necessary validation characteristics for various tests and methods.</p>	30 minutes
Results	Highlight the importance of validation of analytical methods and tests in pharmacy and medicine, which consists in ensuring scientific validity, accuracy and confidence in measurements and results.	Summarize the presented material; to emphasize the importance and relevance of the acquired knowledge for the work of research and / or innovative nature of future masters of pharmacy.	5 minutes
Answers to questions	Active dialogue / discussion.	Explain the most difficult and unclear points of the lecture.	5 minutes

### Recommended literature:

#### *Basic*

1. B. Magnusson and U. Örnemark (eds.). Eurachem Guide: The Fitness for Purpose of Analytical Methods – A Laboratory Guide to Method Validation and Related Topics, (2nd ed. 2014). URL:

[www.eurachem.org/images/stories/Guides/pdf/MV\\_guide\\_2nd\\_ed\\_EN.pdf](http://www.eurachem.org/images/stories/Guides/pdf/MV_guide_2nd_ed_EN.pdf) (date of access: 25.07.2024).

*Additional*

1. Barwick V. J. and Prichard E. (eds.). Eurachem Guide: Terminology in Analytical Measurement – Introduction to VIM 3 (2011). P. 18-22. URL: [https://www.eurachem.org/images/stories/Guides/pdf/TAM\\_2023\\_EN.pdf](https://www.eurachem.org/images/stories/Guides/pdf/TAM_2023_EN.pdf) (date of access: 25.07.2024).

*Information resources*

1. <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/departament-medical-general-chemistry/>
2. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

**Questions for student self-preparation for the lecture:**

1. Analytical tests and methods subject to validation.
2. Validation characteristics and requirements.

**The methodical instruction is developed by Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor

## Lecture N 7 “Main ideas of correlation and regression analyses”

**Type of lecture:** traditional (informational).

### Competencies:

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).  
2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### Purposes:

1) didactic purpose – to form systematized knowledge about the basics of regression and correlation analysis; analyze the linear regression equation and calculate its parameters; analyze types of non-linear regression; analyze the correlation coefficient calculation; analyze the detection limit calculation; to realize the practical significance of the considered methods;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### Tasks of the lecture:

- 1) to know the basics of regression analysis;
- 2) to be able to calculate parameters of linear regression;
- 3) to know the types of non-linear regression;
- 3) to know the basics of correlation analysis;
- 4) to be able to calculate the correlation coefficient;
- 5) to be able to calculate the limit of detection.

### Lecture plan:

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	Present information that when using many chemical and physico-	Reveal the relevance of the topic of the lecture; familiarize students	5 minutes

	chemical methods of quantitative analysis, a certain value can be directly measured $in$ , which is a linear function of the desired concentration (quantity) $h$ substance or element to be determined.	with the lecture plan.	
Main part	<p>1. Linear and non-linear regressions: demonstrate appropriate graphical dependencies and mathematical equations; calculation of linear regression parameters and correlation coefficient.</p> <p>2. Statistical assessment of the detection limit: concept and meaning of this validation characteristic; calculation of the detection limit.</p>	<p>Master the knowledge of the basics of regression and correlation analysis and the skills to perform the necessary calculations.</p> <p>Acquire knowledge about the practical significance of knowledge of the basics of regression analysis and the ability to calculate the limit of detection.</p>	30 minutes
Results	Highlight the significance of linear dependence for many chemical and physicochemical methods of quantitative analysis and the practical value of the detection limit as a validation characteristic.	Summarize the presented material; to emphasize the importance and relevance of the acquired knowledge for the work of research and / or innovative nature of future masters of pharmacy.	5 minutes
Answers to questions	Active dialogue / discussion.	Explain the most difficult and unclear points of the lecture.	5 minutes

### Recommended literature:

#### *Basic*

1. Statistics and Chemometrics for Analytical Chemistry (seventh edition) / J. N. Miller, J.C. Miller and R. D. Miller : Pearson, 2018, P. 120-150. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Additional*

1. Introduction to Statistics in Metrology / S. Crowder et al. Cham : Springer International Publishing, 2020, P. 63-68. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

2. Taylor, J. K., Cihon, C. Statistical techniques for data analysis (second edition). Chapman and Hall/CRC, 2004, P. 126-133. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

*Information resources*

1. <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/department-medical-general-chemistry/>

2. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

**Questions for student self-preparation for the lecture:**

1. Linear and non-linear regressions.

2. Detection limit: definition, practical significance, calculation.

**The methodical instruction is developed by Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor

## Lecture N 8 “Basic concepts of probability theory. Probability distributions for discrete and continuous random variables”

**Type of lecture:** traditional (informational).

### **Competencies:**

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).

2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### **Purposes:**

1) didactic purpose – to form systematized knowledge about the basics of probability theory; analyze the distribution laws of discrete random variables; analyze the distribution laws of continuous random variables;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### **Tasks of the lecture:**

1) to know the main theorems of probability theory;

2) to be able to perform calculations according to Bernoulli's formula;

3) to know the main characteristics of the binomial distribution and the Poisson distribution;

4) to know the main characteristics of the exponential distribution and the normal distribution law.

### **Lecture plan:**

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	Present information that the theory of probabilities is the basis for the justification of	Reveal the relevance of the topic of the lecture; familiarize students with	5 minutes



	mathematical and applied statistics. Give examples of the use of discrete statistical distributions in pharmaceutical analysis.	the lecture plan.	
Main part	<p>1. Basic concepts of the theory of probabilities: probabilities of events; basic theorems of probability theory (addition theorem for incompatible events, addition theorem for compatible events, theorems of multiplication of probabilities); consecutive independent trials, Bernoulli's formula.</p> <p>2. Laws of distribution of discrete random variables: binomial distribution and Poisson distribution.</p> <p>3. Distribution laws of continuous random variables: exponential (exponential) distribution, normal distribution law.</p>	<p>Acquire knowledge about the basics of the theory of probabilities; master the skills to correctly apply the basic theorems of probability theory and perform calculations according to the Bernoulli formula.</p> <p>Master the knowledge of the main characteristics of the binomial distribution and the Poisson distribution, as well as analyze their application in pharmaceutical analysis.</p> <p>Acquire knowledge about the main characteristicsexponential distribution and normal distribution law, as well as analyze their significance and practical value.</p>	30 minutes
Results	Highlight the importance and relevance of the considered issues in modern conditions, when in the foreground the creation of new medicines is preceded by a computer one modeling of their structure and prediction of properties.	Summarize the presented material; emphasize the need knowledge and understanding of the basics of mathematical statistics for the professional training of future masters of pharmacy.	5 minutes
Answers to	Active dialogue / discussion.	Explain the most difficult	5

questions		and unclear points of the lecture.	minutes
-----------	--	------------------------------------	---------

### **Recommended literature:**

#### *Basic*

1. Riffenburg R. H., Gillen D. L. Statistical in Medicine (fourth edition). Academic press, 2020, P. 51-88. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

2. Introduction to Statistics in Metrology / S. Crowder et al. Cham : Springer International Publishing, 2020, P. 59-77. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Additional*

1. Taylor, J. K., Cihon, C. Statistical techniques for data analysis (second edition). Chapman and Hall/CRC, 2004, P. 185-188. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Information resources*

1. <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/department-medical-general-chemistry/>

2. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

### **Questions for student self-preparation for the lecture:**

1. Random events and probabilities of events.
2. Functions of random variables.

**The methodical instruction is developed by Yaroslava Pushkarova – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor**

## Lecture N 9 “Chemometrics as an interdisciplinary scientific discipline. Review of main chemometric methods”

**Type of lecture:** traditional (informational).

### **Competencies:**

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).

2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### **Purposes:**

1) didactic purpose – to form systematized knowledge about the main tasks of chemometrics and the main chemometric methods; analyze the principles of basic chemometric methods;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### **Tasks of the lecture:**

1) to know aspects of implementation of basic chemometric methods;

2) to know the practical application of basic chemometric methods;

3) to be able to propose the necessary chemometric method for solving the relevant problems of quantitative analysis.

### **Lecture plan:**

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	Present the information that chemometrics is science at the junction of applied mathematics and chemistry and is currently a modern and effective means of solving a	Reveal the relevance of the topic of the lecture; familiarize students with the lecture plan.	5 minutes

	wide range of problems.		
Main part	<p>1. The main areas of application of chemometrics: creation and management of chemistry databases; prediction of properties of chemical compounds and materials; pharmacophores and pharmacophore search; molecular similarity and search by molecular similarity; virtual screening, computer synthesis, visualization and research of chemical space, molecular design of chemical compounds with given properties.</p> <p>2. Overview of the main chemometric methods: principal component analysis; principal component regression; classification and regression trees; formal independent modeling of class analogies; method of support vectors; partial least-squares regression; artificial neural networks; cluster analysis; discriminant analysis.</p>	<p>Acquire knowledge about the main fields of application of chemometrics as an interdisciplinary science; to realize the significance of chemometrics for pharmaceutical analysis.</p> <p>Acquire knowledge about the principles of application and algorithms of operation of the main chemometric methods.</p>	30 minutes
Results	Highlight the significance of chemometrics in the creation of new medicinal products, in the investigation of the authenticity of medicinal products, in solving the problems of identification and classification.	Summarize the presented material; to emphasize the importance and relevance of the acquired knowledge for the work of research and / or innovative nature of future masters of pharmacy.	5 minutes
Answers to questions	Active dialogue / discussion.	Explain the most difficult and unclear points of the lecture.	5 minutes

### **Recommended literature:**

#### *Basic*

1. Statistics and Chemometrics for Analytical Chemistry (seventh edition) / J. N. Miller, J.C. Miller and R. D. Miller : Pearson, 2018, P. 235-261. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Additional*

1. European Pharmacopoeia / European Directorate for the Quality of Medicines & HealthCare of the Council of Europe. – tenth edition, volume 1. Strasbourg : Council of Europe, 2019. – Section 5.21. Chemometric methods applied to analytical data. P. 817-836. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

2. Gummadi S., Chandaka P. K. Chemometrics Approach to Drug Analysis – An Overview. *American Journal of PharmTech Research*. 2019. Vol. 9, no. 1. P. 1–13. URL: <https://doi.org/10.46624/ajptr.2019.v9.i1.001> (date of access: 25.07.2024).

#### *Information resources*

1. <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/department-medical-general-chemistry/>

2. <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

### **Questions for student self-preparation for the lecture:**

1. Tasks of chemometry and its practical application.
2. Basic chemometric methods.

**The methodical instruction is developed by Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor

## Lecture N 10 “Application of chemometric methods in pharmacy and medicine”

**Type of lecture:** traditional (informational).

### **Competencies:**

– **integral competence:** ability to solve tasks of research and/or innovative nature in the field of pharmacy;

– **general competencies (GC):**

1. Ability for abstract thinking, analysis and synthesis (GC 01).

2. Knowledge and understanding of the subject area; understanding of professional activity (GC 02).

3. Ability to work in a team (GC 06).

– **professional competences of the specialty (PC):**

1. Ability to integrate knowledge and solve complex problems of pharmacy / industrial pharmacy in broad or multidisciplinary contexts (PC 01).

2. The ability to collect, interpret and apply data necessary for professional activity, carrying out research and implementation of innovative projects in the field of pharmacy (PC 02).

### **Purposes:**

1) didactic purpose – to analyze the tasks and problems of pharmaceutical analysis that can be solved or optimized with the help of chemometric methods;

2) educational purpose – to contribute to the formation of a scientific outlook;

3) developmental purpose – to develop intellectual abilities, thinking, independence.

**Lecture equipment:** multimedia system, appropriate software.

### **Tasks of the lecture:**

1) to know the practical application of basic chemometric methods in the field of pharmacy and medicine;

3) to be able to propose the necessary chemometric method for solving the relevant problems of pharmaceutical analysis.

### **Lecture plan:**

Stage of the lecture	Content of stages	Educational purpose of the stage	Time
Introduction	Present information that chemometric methods are successfully and effectively used in the pharmaceutical industry from establishing quality control specifications for	Reveal the relevance of the topic of the lecture; familiarize students with the lecture plan.	5 minutes

	raw materials, powders and dosage forms to controlling various processes and stages of production.		
Main part	Application of chemometric methods in pharmacy: prediction of various types of activity of chemical compounds; prediction of toxicity; control of the pharmaceutical production process; identification and classification.	Acquire knowledge about the practical application of basic chemometric methods in the field of pharmacy and medicine.	30 minutes
Results	Highlight the importance of chemometric methods in modern conditions of powerful development of instrumental methods of analysis, the need to process multidimensional experimental data arrays and practical requests for mass analysis of samples of complex composition in new subject areas.	Summarize the presented material; to emphasize the importance and relevance of the acquired knowledge for the work of research and / or innovative nature of future masters of pharmacy.	5 minutes
Answers to questions	Active dialogue / discussion.	Explain the most difficult and unclear points of the lecture.	5 minutes

### Recommended literature:

#### *Basic*

1. European Pharmacopoeia / European Directorate for the Quality of Medicines & HealthCare of the Council of Europe. – tenth edition, volume 1. Strasbourg : Council of Europe, 2019. – Section 5.21. Chemometric methods applied to analytical data. P. 817-836. URL: <https://likar.nmu.kiev.ua/md/course/view.php?id=7412> (date of access: 25.07.2024).

#### *Additional*

1. Gummadi S., Chandaka P. K. Chemometrics Approach to Drug Analysis – An Overview. *American Journal of PharmTech Research*. 2019. Vol. 9, no. 1. P. 1–13. URL: <https://doi.org/10.46624/ajptr.2019.v9.i1.001> (date of access: 25.07.2024).

#### *Information resources*

- <https://nmuofficial.com/en/zagalni-vidomosti/kafedri/department-medical-general-chemistry/>
- <https://likar.nmu.kiev.ua/md/course/view.php?id=7412>

**Questions for student self-preparation for the lecture:**

1. What modern conditions contribute to the development of chemometric methods?
2. Application of chemometric methods in pharmaceutical analysis.

**The methodical instruction is developed by Yaroslava Pushkarova** – Associate Professor of Analytical, Physical and Colloid Chemistry Department, PhD in Chemistry, Associate Professor