

1. Spectroscopic devices. Distortion of spectroscopic measurements. Aparatic function. Means for elimination of data distrotron	1		2					3	2	
2. Spectral data processing software packages. Device manufacturers' software packages: OPUS, Omnic, etc. and peculiarities of working with them. Universal data processing packages: Origin, Matlab.	1		4					5	4	
3. Data formats. Problems of spectral data storage. File formats and incompatibilities. ASCII data format. Universal spectral data format JCAMP-DX, its structure and data compression capabilities.	1							1	2	
4. One-dimensional Fourier transform. Spectrum recording and analysis using Fourier transform. Pros and cons. Fourier Transform spectrometer "hardware function". Apodization functions and their purpose. Phase correction. Use of Fourier transform for filtering spectral noises and interference signals.	2		6					9	20	
5. Two-dimensional Fourier transform. Optical representation of two-dimensional Fourier Transform. Usage of Fourier transform for analysis and modification of images.	2		4					6	16	
6. Principles of statistical data analysis. Supervised and unsupervised statistical methods	1								4	
7. Principle Component Analysis (PCA). Mathematical foundations of PCA. Illustration of the PCA method for a small number of variables. Application of PCA to the analysis of complex spectral data.	2		4					6	10	
8. Cluster analysis. Principles of data clustering. Methods of dividing data into clusters: hierarchical, central, etc. Strictly and loosely defined clusters. Application of clusters for data analysis, examples from the analysis of spectra of biological-medical samples.	2		4					6	12	
9. Regression analysis. Partial least squares regression	1		4					6	11	
10. Two-dimensional correlation spectral analysis. The idea and principles of 2D spectral analysis. Application of 2D analysis to identify spectral changes.	2		4					6	11	
11. Imaging of spectral data. Spectral maps 4D data arrays. Principles of tomography.	1									
Total	16		32					48	92	

Assessment strategy	Weight %	Deadline	Assessment criteria
Seminar reports	50	study semester	During the seminar, the results of independently performed tasks are presented. Report is assessed according to the tasks performed: quality and accuracy of the information provided (5 points), presentation style and presentation (2 points), answers to additional questions (3 points). A 10-point system is used.
Examination	50	exam session	5 theoretical and practical tasks. Each correctly answered question is evaluated with 2 points, incorrectly with 0 points. A final 10-point system is used.

Author	Publishing year	Title	Issue of a periodical or volume of a publication; pages	Publishing house or internet site
Required reading				
V. Šablinskas, J. Čeponkus.	2014	Modernioji molekulių virpesinė spektrometrija		https://www.ff.vu.lt/external/ff/files/institutai/ChFI/Students/Modernioji_molekulių_virpesinė_spektrometrija.pdf
V. Balevičius.	2008	Skaitmeninė Optika		Vilnius, BMK
D. Navakauskas	2008	Skaitmeninis signalų apdorojimas taikant MATLAB		Vilnius, Technika
Recommended reading				