

Spectroscopic techniques for the identification and quantitation of organic compounds in the agrifood field

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4 CFU	Activities	Lectures	20 hours
		Laboratory	4 hours
		Seminars	4 hours

Objectives

The course will provide basic theoretical and practical information on the main spectroscopic techniques used for detection and quantitation of organic compounds with agricultural and food interest. Laboratory activities will include practical sessions on interpretation of spectroscopic data.

Learning outcome

The student will gain a basic knowledge of the most common spectroscopic techniques, will be able to choose the most appropriate technique for a particular problem, and will be able to solve simple analytical problems in the agrifood field using spectroscopic techniques.

Topics (with the indication of the n of hours/topic)

Infrared (IR) spectroscopy. Basic theory. Vibrational frequencies of main functional groups. Applications of IR spectroscopy in the agrifood field. (2 h)

Ultraviolet (UV) spectroscopy: Basic theory. Main chromophoric groups in organic compounds. (2 h)

Circular dichroism (CD) for the analysis of chiral compounds. (2 h)

Mass spectrometry (MS). Basic theory. Ion Sources. Analyzers. High-resolution mass spectrometry. (4 h)

Tandem mass spectrometry (MS2). Instrumentation. Mechanisms of fragmentations and their structural meaning. (2 h)

Hyphenated techniques: Gas chromatography coupled to mass spectrometry (CG-MS). Liquid chromatography coupled to mass spectrometry (LC-MS). Liquid chromatography coupled to ultraviolet spectroscopy (HPLC-UV). Some applications in the agrifood field. (4 h)

Nuclear magnetic resonance (NMR) spectroscopy. Basic theory. Nuclear Overhauser Effect (NOE). One- and two-dimensional NMR spectra. Application of 1D- and 2D-NMR in the agrifood field. (4 h)

Evaluation

The final exam will involve structural determination of a small organic molecule from its spectroscopic data.

Recommended readings

Silverstein, Webster, Kiemle. Spectrometric Identification of Organic Compounds. Casa Editrice Ambrosiana.

Randazzo. Guida Pratica alla Interpretazione di Spettri NMR. Loghia.

