RAMAN SPECTROSCOPY FOR CHARACTERIZATION OF PLANT BIOACTIVE COMPONENTS USED AS NUTRACEUTICALS

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Background: Infrared (IR) and Raman spectroscopy are complementary vibrational spectroscopy techniques, which may provide important composition-related informations of complex plant/food samples. Generally, vibrational measurements can be performed directly on plant tissues or on samples isolated from the plant material by distillation or extraction. Evaluation of biological tissues without extraction, which can lead to degradation of the bioactive components (ex., antioxidants), short time of analysis, a high degree of precision, use in order to perform fast quality checks of raw materials or continuous controlling of the production, are advances of application of Raman spectroscopy to analysis of nutraceutical compounds.

Materials and methods:

This technique allow to obtain spectra (Raman fingerprints) which present characteristic key Raman bands of individual bioactive components (Table 1,2 and 3). These bands provide information about the chemical composition of the investigated samples as primary (proteins and amino acids, lipids and fatty acids, carbohydrates) and secondary metabolites (flavonoids, polyphenols and other phenolic substances, terpenoids (mono-, sesqu-, and tetraterpenes), alkaloids, nitrile compounds, iridoids) present.

Table 1: Selected Characteristic Raman Vibrational Modes Resulting From Plant Lipids and Carbohydrates*

Analyte	Wave Number (cm^{-1})	Vibrational Mode
Lipids/Fatty acids	3008	=C-H
	2970	$-CH_3$
	2940	$=CH_2$
	1670	C=C trans
	1660	C=C cis
Carbohydrates		
α-Glucose	847	(C–O–C) skeletal mode
β-Glucose	898	(C–O–C) skeletal mode
β-Fructose	868	(C–O–C) skeletal mode
Sucrose	1462	$d(CH_2)$
Maltose	847	(C–O–C) skeletal mode

CONCLUSION

The ability for rapid monitoring of various plant bioactive components makes Raman spectroscopy one of techniques with future more wide application in the nutraceutical field. As the existed demand to solve complex issues of nutraceuticals is increased recently, investigation of the changes in the functionality of these specific substances with the addition or loss of nutraceutical compounds (both in foods and in model Systems) by using multidisciplinary approach, Raman spectroscopy can play important role in it.

Table 2: Selected Characteristic Raman Vibrational Modes Resulting From Plant Proteins*

Analyte	Wave Number (cm^{-1})	Vibrational Mode
Cystine	510	S-S stretch
Cystine	525	S-S stretch
Methionine	630–670 700–745 2550–2580	C-S stretch C-S stretch S-H stretch
Tyrosine	850/830	Resonance between ring fundamental and overtone
Tryptophan	760, 880, 1360	Indol ring
Phenylalanine	1006	Ring breathe
Histidine	1409	N-Deuteroimidazole
Aspartic acid	1400–1430	C=O stretch of carboxyl group
Glutamic acid	1700–1750	C=O stretch of carboxyl or ester group
Amide I	1655–1685	Amide C=O stretch, N-H wagging
Amide III	1235–1280	N-H in-plane bend, C-N stretch

Table 3: Selected Characteristic Raman Vibrational Modes Resulting From Some Plant Terpene Compounds*

Analyte	Wave Number (cm^{-1})	Vibrational Mode
Citronellol	1674; 1382	C=C; $-CH_3$
Geranyl acetate	1679	C=C
Limonene	1678 1645	(cyclohexane C=C) (ethylene C=C)
α-Pinene	1659 666	C=C δ(ring)
α-Bisabolol	1677 1436	C=C $\delta(CH_2)$
β-Caryophyllene	1671; 1632	C=C
β-Carotene	1524; 1157	C=C; C-C
Lutein	1527; 1157	C=C; C-C
Lycopene	1510; 1156	C=C; C-C

*Critical Reviews in Food Science and Nutrition, 52:853–875 (2012); Vibrational Spectroscopy, 43: 13-25 (2007); Food Chemistry, 338:128115 (2021)