

FTIR SPECTRAL DATA IN CORRELATION WITH MAIN ORGANOLEPTIC AND BIOCHEMICAL FEATURES OF JONATHAN POSTHARVEST APPLES

DATE PRIVIND SPECTRELE FT-IR ÎN CORELAȚIE CU PRINCIPALELE CARACTERISTICI ORGANOLEPTICE ȘI BIOCHIMICE ALE MERELOR JONATHAN DUPĂ RECOLTARE

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Abstract. Apple fruit quality is a multi-component concept, defined by organoleptic, biochemical and physiological attributes such as firmness, skin and flesh color, sugars, organic acids, pigments, phenolic compounds and volatiles, ethylene production, respiration rate. Most instrumental techniques currently required for measuring these parameters are long, expensive and involve a considerable amount of manual work. Therefore, there is a demand for new and rapid analytical methods for assessing quality attributes. Recently, Fourier transform mid-infrared (FT-IR) spectroscopy has become a well-accepted method for the determination of food constituents since it achieves high analysis speed and requires little or no sample preparation. In our study Jonathan apples were evaluated by FT-IR spectral data in order to establish main characteristics / modification after postharvest and to correlate it with apple fruit quality main parameters.

Key words: FT-IR spectral data, biochemical features, Jonathan apples.

Rezumat. Caracteristicile organoleptice, biochimice și fiziologice ale merelor (fermitatea, culoarea, conținutul de glucide, acizi organici, substanțe solubile, producția de etilenă, rata respirației) pot fi monitorizate în prezent prin tehnici instrumentale clasice dificile, costisitoare și greoaie astfel încât s-a impus necesitatea unor metode analitice rapide și precise. Astfel, spectroscopia în infraroșu cu transformată Fourier (FT-IR) este o metodă recent adoptată pentru analiza substraturilor alimentare datorită rapidității și mai ales datorită faptului că implică o minimă pregătire a probelor. Lucrarea prezintă caracteristicile spectrelor FT-IR pentru merele Jonathan după recoltare în corelație cu principalele modificări ale parametrilor organoleptici și biochimici.

Cuvinte cheie: spectre FT-IR, parametri biochimici, mere Jonathan.

INTRODUCTION

Apple fruit quality is a multi-component concept, defined by organoleptic, biochemical and physiological attributes such as firmness, skin

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and flesh color, sugars, organic acids, pigments, phenolic compounds and volatiles, ethylene production, respiration rate (Beceanu, 2010).

Most instrumental techniques currently required for measuring these parameters are expensive and involve a considerable amount of manual work. Therefore, there is a demand for new and rapid analytical methods for assessing quality attributes.

Recently, Fourier transform mid-infrared (FT-IR) spectroscopy has become a well-accepted method for the determination of food constituents since it achieves high analysis speed and requires little or no sample preparation (Trincă et al., 2012, 2013).

In our study Jonathan apples were evaluated by FT-IR spectral data in order to establish main characteristics / modification after postharvest and to correlate it with apple fruit quality main parameters.

MATERIAL AND METHOD

Jonathan apples were purchased from the city market with weight ranging between 81-103 g and normal, healthy appearance. Periodic measurements for various types of biochemical features were carried out for 60 apples (by considering the lot of ten apples stored under the same conditions of temperature and humidity).

Drying of the samples was performed by oven drying (Trincă et al., 2012). For oven drying. 5 g sample of Jonathan apple (chunks or grinded) have been subjected to drying at 90⁰ C temperature until constant mass ($\Delta < 10^{-2}$ g).

Water content was determined according to eq.(1):

$$\text{H}_2\text{O} \% = \frac{m - m_1}{m_2} \times 100 \quad (1)$$

Spectral analysis by FTIR spectroscopy highlights functional changes of the structure sample substrate in relation to the standard.

FTIR spectra were recorded in KBr pill using DIGILAB-EXCALIBUR SDS 2000 spectrometer fitted with a heating device.

Working parameters were: spectral range between 4000-400 cm⁻¹, resolution 4 cm⁻¹ and the number of scans 24.

RESULTS AND DISCUSSION

In figures 1- 4 are presented FTIR spectra for apples (chunks and grinded) in day five and day twenty.

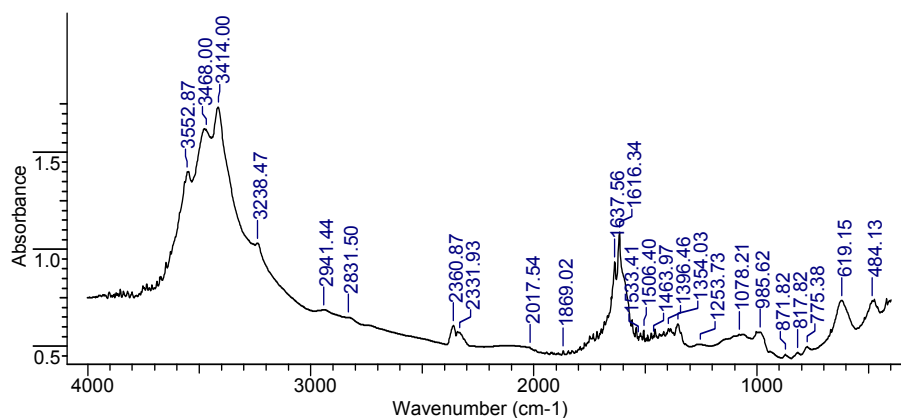


Fig. 1 - FT-IR spectral data for chunks apple day 0

The vibrational spectrum of a molecule is considered to be a unique physical property, characteristic of the molecule. As such, the infrared spectrum can be used as a fingerprint for identification by the comparison of the spectrum from an “unknown” with previously recorded reference spectra. This is the basis of computer-based spectral searching. In the absence of a suitable reference database it is possible to do a basic interpretation from first principle leading to characterization and possibly even identification of an unknown sample (Coates, 2000).

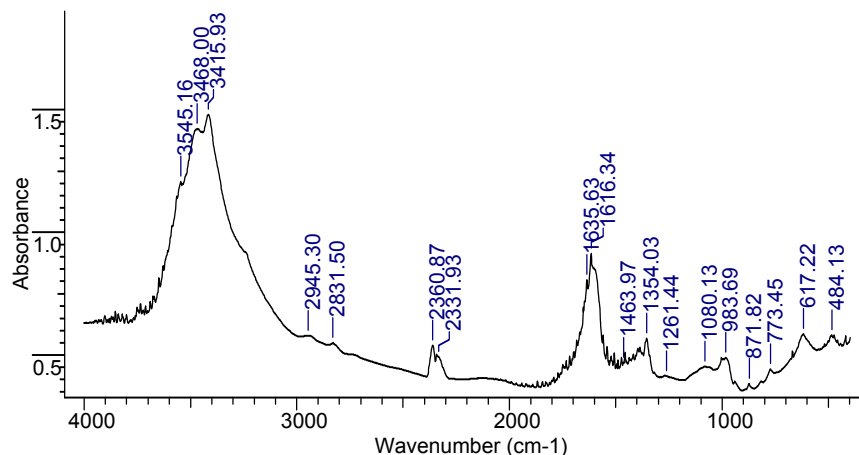


Fig. 2 - FT-IR spectral data for chunks apple day 20

This first principles approach consider that structural features of a molecule- whether they are the backbone of the molecule or the functional groups attached to the molecule- produce characteristic and reproducible signals in spectrum. First step monitoring if whether the backbone consists of linear / branched chains or unsaturation and aromatic rings in the structure. Finally, it is possible to deduce whether specific functional groups are present.

Absorptions in the region 3560–3420 cm⁻¹

The corresponding signals of water in the food substrate are given by symmetric and asymmetric bands of excitation of phenolic groups -OH present in the area 3552-3540 cm⁻¹. These signals are specific to chemical bound water from the substrate structure.

Thus, from these registered spectra can be notice that intense signals appears in the area just in the case of the samples analysed in day five. Spectra recorded for samples of day twenty day presented low intensity signals in this area maybe because of the existence of a smaller percentage of chemical bound water in raw samples. In this case the signals appear only in the aria of 3480-3420 cm⁻¹ both for apple pieces and minced samples (Chiş et al., 2010, Esbensen et. al., 2002).

Absorptions in the region 3200–2700 cm⁻¹

Well-defined and characteristic absorptions in this region are normally characteristic of carbon- and hydrogen containing species, and are assigned to various forms of C-H stretching.

Ther are there slightly signals of absorptions above 3000 cm⁻¹, which correspond to unsaturated (contains C=C) or aromatic compounds.

The signals presented in the 2935-2860 cm⁻¹ and 1470- 720 cm⁻¹ absorption area , correspond to long linear aliphatic chain compounds.

Absorption in the region 1850–1620 cm⁻¹

A major band in this region usually indicates the presence of a C=O group (carbonyl compound). The signals at the high end of the range, e.g. 1775 cm⁻¹ or above, correspond to a simple carbonyl compound, such as a ketone, an aldehyde, an ester, or a carboxylic acid.

The conjugation with another carbonyl group, or a double bond or aromatic ring, will lower the carbonyl absorption by 30–50 cm⁻¹. Therefore, conjugated aldehydes, ketones, esters, and carboxylic acids may fall into this lower end category. If conjugation with a double bond is present, then a second strong absorption should be observed nearby, between 1650 and 1600 cm⁻¹. In the case of the involvement of an aromatic ring, it is important to look for evidence of the characteristic aromatic absorptions (Max et al, 2007, Rudnitskaya et. al., 2006).

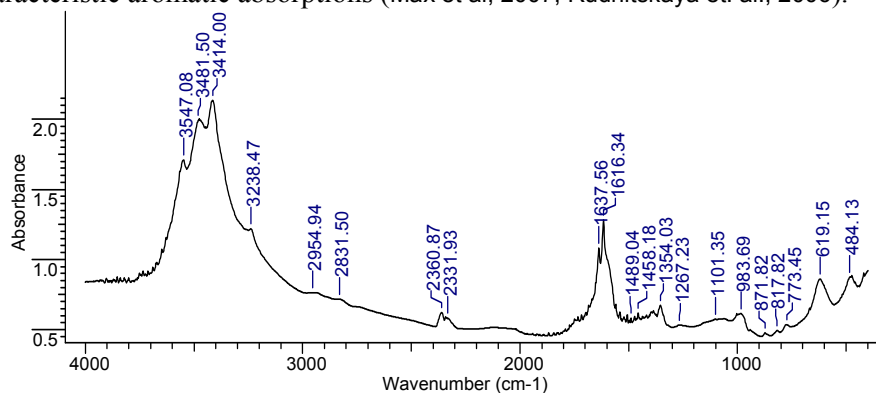


Fig. 3 - FT-IR spectral data for grinded apples, day 0

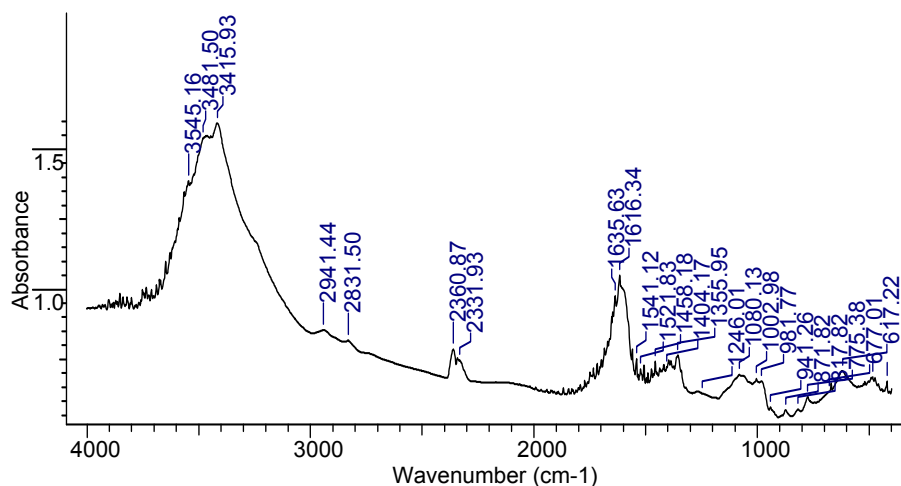


Fig. 4 - FT-IR spectral data for grinded apples, day 20

Absorption in the region 1640–480 cm⁻¹

FTIR spectra present a strong bandwidth due to water absorption bandwidth, centered around 1637 cm⁻¹.

The bands of the 885-1500 cm⁻¹ are assigned to the stretching vibration of the C - O and C - C, while the bands from 1474-cm⁻¹ are due to vibrations of groups O = C - H and C - O - H of carbohydrate components.

Characteristic bands of glucose were identified (specific maximum at 983, 1062, 1283, 1261, 1366, 1386, 1458, 1367 și 1460 cm⁻¹), fructose (specific maximum at 966, 1063, 1155, 1254, 1346, 1416 și 1456 cm⁻¹) and sucrose (specific maximum at 995, 1055, 1113, 1138, 1338 și 1464 cm⁻¹).

CONCLUSIONS

1. In our study Jonathan apples were evaluated by FT-IR spectral data in order to establish main characteristics / modification after postharvest and to correlate it with apple fruit quality main parameters.

2. FTIR analysis confirmed the presence of bound water in apple samples (bound water specific signals were more intense in day 0 while in day 20 can be noticed their absence in certain areas of absorption).

3. The results highlight the potential of FTIR spectroscopy to realise quick and efficient analyses for routine monitoring of carbohydrates in apples, as indicators of quality and authenticity

REFERENCES

1. Beceanu D., 2010 - *Tehnologia produselor horticole*, Partea I, Ed. Pim.
2. Chiș A, Fetea F., Abdelmoumen T, Socaciu C., 2010 - *Application Of FTIR Spectroscopy For A Rapid Determination Of Some Hydrolytic Enzymes Activity On*

Sea Buckthorn Substrate, Romanian Biotechnological Letters, Vol. 15, No. 6, p. 5738-5744

3. **Coates J., 2000** - Interpretation of Infrared Spectra, A Practical Approach in *Encyclopedia of Analytical Chemistry*, R.A. Meyers (Ed.), John Wiley & Sons Ltd, Chichester, p. 10815–10837,
4. **Esbensen K. H., Guyot D., Westad F., Houmøller L. P., 2002** - *Multivariate Data Analysis - in practice*, Camo Process AS.
5. **Max J.J., Chapados C., 2007** - *Glucose and fructose hydrates in aqueous solution by IR spectroscopy*, J. Phys. Chem. A, 111(14), p. 2679-2689.
6. **Rudnitskaya A, Kirsanov D, Legin A, Beullens K, Lammertyn J, Nicolai BM, Irudayaraj J., 2006** - *Analysis of apples varieties – comparison of electronic tongue with different analytical techniques*. Sensor Actuat B – Chem 28, p. 23-286.
7. **Trincă L.C., Căpraru A.M, 2013** - *Biochimia Alimentelor, Manual de lucrări practice*, Ed. Pim.
8. **Trincă L.C., Căpraru A.M., Arotăriței D., Volf I., 2012** - *Cercetări privind determinarea conținutului de apă pentru merele din soiul Jonathan prin metode clasice și inovative*, Lucrări Științifice USAMV Iași, vol.1 (55), Seria Horticultură, p. 111-116.