

Characterization of essential oils extracted from different aromatic plants by FTIR spectroscopy

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ABSTRACT

Four essential oils isolated from dried leaves of parsley, lovage, basil and thyme were investigated by FTIR spectroscopy. The analysis of recorded spectra revealed that the main compounds of tested essential oils dominate their vibrational spectra.

Keywords: FTIR analysis, essential oils, aromatic plants, dried leaves

Introduction. Essential oils components are mono- and sesquiterpenes including carbohydrates, phenols, alcohols, ethers, aldehydes, and ketones that are responsible for the biological activity of aromatic plants as well as for their fragrance (Soković *et al.*, 2010).

Aim. This study aimed to analyze the FTIR spectra of four essential oils extracted from dried leaves of aromatic plants.

Materials and methods. For the experiment, dried leaves of parsley, lovage, basil, and thyme were purchased from a Romanian Company. Essential oils were extracted by hydrodistillation (50 g of dried leaves with 750 mL distilled water) using a Clevenger-type apparatus (for 3 hours). The extracts were dried over anhydrous sodium sulphate and stored at 4°C until analysis (Semeniuc *et al.*, 2017). A Shimadzu Fourier Transform Infrared Spectrophotometer (IRPrestige-21) equipped with a Horizontal Attenuated Total Reflectance (HATR) accessories was used to collect FTIR spectra. Essential oils (1000 µL/sample) were deposited on HATR plates with ZnSe and the FTIR spectra were recorded in the range

of 4000-650 cm⁻¹ by accumulating 64 scans per spectrum with a resolution of 4 cm⁻¹. Data were then processed using the IR Solution software (Shimadzu) and Origin 7SR1 software (OriginLab Corporation).

Results and Discussion. Figure 1 shows the overlap diagram of acquired FTIR spectra.

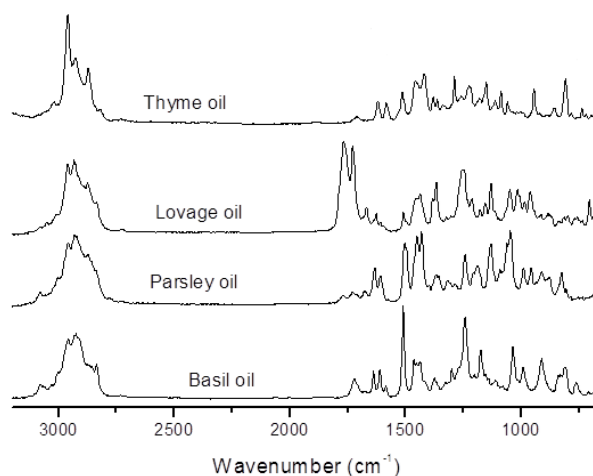


Fig. 1. Overlay of the FTIR spectra of parsley EO, lovage EO, basil EO, and thyme EO

Tab. 1. Wavenumbers of measured peaks for parsley, lovage, basil, and thyme essential oils

Stretching frequency (cm ⁻¹)*	Parsley EO	Lovage EO	Basil EO	Thyme EO	β -phellandrene	estragole	<i>o</i> -cymene
Zone 1 3700-3200 cm ⁻¹	-	-	-	-	-	-	-
Zone 2 3200-2700 cm ⁻¹	2835, 2924, 2966, 3001, 3030, 3064, 3078	2835, 2873, 2931, 2960	2757, 2872, 2931, 2956, 3003, 3078, 3122	2821, 2872, 2924, 2958, 3018	2879, 2919, 2992, 3063, 3108	2850, 2915, 2942, 3006, 3034, 3086	2818, 2880, 2940, 2967, 3031, 3057, 3065, 3074, 3112, 3160
Zone 3 2300-2000 cm ⁻¹	-	-	-	-	-	-	-
Zone 4 1850-1650 cm ⁻¹	1676, 1730, 1770	1668, 1730, 1768	1674, 1720	1710, 1888	1651, 1770	-	1700, 1724, 1800, 1838
Zone 5 1680-1450 cm ⁻¹	1450, 1504, 1575, 1608, 1633	1510, 1608	1452, 1463, 1510, 1585, 1610, 1639	1458, 1515, 1583, 1618	1457, 1475, 1608	1470, 1510, 1610, 1638	1461, 1495, 1583, 1611
Fingerprint region below 1450 cm ⁻¹	671, 686, 736, 754, 786, 806, 825, 877, 912, 956, 991, 1047, 1061, 1091, 1132, 1192, 1282, 1367, 1398, 1431	690, 705, 736, 758, 799, 815, 839, 895, 916, 960, 995, 1016, 1049, 1114, 1132, 1157, 1178, 1211, 1247, 1259, 1305, 1325, 1366, 1382, 1436	686, 707, 763, 806, 831, 912, 993, 1035, 1080, 1111, 1176, 1203, 1244, 1300, 1375, 1438	696, 721, 738, 783, 808, 858, 885, 945, 1004, 1020, 1037, 1060, 1112, 1153, 1180, 1226, 1259, 1288, 1340, 1381, 1419	679, 702, 763, 775, 796, 819, 828, 880, 924, 942, 971, 989, 1020, 1045, 1076, 1097, 1120, 1156, 1172, 1201, 1210, 1230, 1249, 1250, 1285, 1294, 1324, 1375, 1391, 1424, 1445	760, 822, 914, 994, 1042, 1102, 1174, 1246, 1290, 1442	758, 788, 860, 892, 939, 990, 1035, 1085, 1110, 1154, 1180, 1225, 1280, 1302, 1342, 1360, 1377, 1423

*Source: http://web.chem.ucla.edu/~harding/ec_tutorials/tutorial46.pdf; [http://webbook.nist.gov/cgi/cbook.cgi?ID=C555102&Mask=80](http://webbook.nist.gov/cgi/cbook.cgi?ID=C555102&Mask=80;); <http://webbook.nist.gov/cgi/cbook.cgi?ID=C140670&Units=SI&Mask=384>; <http://webbook.nist.gov/cgi/cbook.cgi?ID=C527844&Type=IR-SPEC&Index=1>

The spectrum itself is divided into 5 zones and an area known as the fingerprint region (see Table 1). FTIR spectra of parsley, lovage, basil and thyme essential oils exhibit absorptions in 3 zones and the fingerprint region. Based on ITEX/GC-MS data, the main components of these essential oils are listed in Table 1.

A comparison of spectral features between tested essential oils and standard substances from literature clearly shows that their main compounds dominate the vibrational spectra. The four spectra show very similar profiles since their key bands, listed in Table 1, are characteristic of essential oils. The compounds found in essential oils at low concentrations have not significantly influenced their FTIR spectra. The spectral regions, with useful molecular structural information, were identified in the 640-1840 and 2770-3070 cm⁻¹ ranges. The IR bands are dominated by a very intense C=O stretching vibration at 1744 cm⁻¹. The C-H bending vibrations are present in the FTIR

spectra at 1466 cm⁻¹, whereas the C-C and C-O stretching vibrations are shown at 1097 and 1161 cm⁻¹, respectively. In the high wavenumber range, the -CH₂ stretching vibrations are shown by the peaks at 2853 and 2923 cm⁻¹, whereas the band at 3008 cm⁻¹ is assigned to the =C-H stretching vibration.

Conclusion. The current study shows that the spectra of tested essential oils present very similar profiles and the main constituents found in essential oils by ITEX/GC-MS analysis dominate the resulting vibrational spectra.

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