

Use of FTIR Spectroscopy and Chemometrics with Respect to Storage Conditions of Moldavian Dragonhead Oil

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Table S1. Positions of the maxima of absorption spectra and assignment to the relevant vibrations as recorded for Moldavian dragonhead oil samples stored at 7°C (refrigerated), in an O₂ atmosphere and a clear bottle, respectively: a – immediately after pressing, b – two weeks after pressing, c – four weeks after pressing – 8 weeks after pressing.

FTIR				Type and origin of vibrations
Position of bands [cm ⁻¹]				
a	b	c	d	
3010	3010	3009	3010	$\nu(\text{=C-H}_m, \text{cis-})$
2958	2958	2956	2959	$\nu_{as}(\text{-C-H}_{vst}, \text{-CH}_a)$
2924	2926	2926	2923	and
2854	2854	2856	2856	$\nu_s(\text{-C-H}_{vst}, \text{-CH}_a)$ (aliphatic groups in triglycerides)
1743	1743	1744	1741	$\nu(\text{-C=O}_{vst})$ in esters
1706	1711	1708	1701	$\nu(\text{-C=O}_{vw})$ in acids
1653	1652	1657/1696	1650/1677	
-	-	1606	1620	
-	-	-	1556	$\nu_{vw}(\text{-C=C-}, \text{cis-})$
-	-	-	1514	
-	-	-	-	
1458	1460	1458	1457	$\delta_{vw}(\text{-C-H})$ w CH ₂ and in CH ₃ groups, deformation (scissoring)
-	-	-	-	$\nu_{vw}(\text{-C-H}, \text{cis-})$ deformation (ring)
1371	1374	1372	1369	$\nu_{w, m, vw}(\text{-C-H}, \text{-CH}_3)$ and deformation
1310	1308	1308	1311	$\delta_m(\text{-C-H}, \text{-CH}_3)$
1268	1266	1268	1270	$\nu_m(\text{-C-O})$ or $\delta_m(\text{-CH}_2-)$
1234	1238	1234	1239	$\nu_m(\text{-C-O})$ or $\delta_m(\text{-CH}_2-)$
1162	1164	1159	1164	$\nu_m(\text{-C-O})$
1100	1096	1100	1096	
-	1068	1063	1064	$\nu_{m, vw}(\text{-C-O})$
1032	1032	1032	1029	
975	974	974	972	$\delta_w(\text{-HC=CH-}, \text{trans-})$ out-of-plane deformation

ν – stretching vibrations, δ – deformation vibrations, s – symmetric, as – asymmetric, st – strong, w – weak.

Table S2. Positions of the maxima of absorption spectra and assignment to the relevant vibrations as recorded for Moldavian dragonhead oil samples stored at 7°C (refrigerated), in an argon atmosphere and a dark bottle, respectively: a – immediately after pressing, b – two weeks after pressing, c – four weeks after pressing – 8 weeks after pressing.

FTIR				Type and origin of vibrations
Position of bands [cm ⁻¹]				
a	b	c	d	
3012	3007	3008	3013	$\nu(\text{=C-H}_m, \text{cis-})$
2952	2964	2952	2959	$\nu_{as}(\text{-C-H}_{vst}, \text{-CH}_a)$
2926	2926	2926	2928	and
2853	2855	2855	2857	$\nu_s(\text{-C-H}_{vst}, \text{-CH}_a)$ (aliphatic groups in triglycerides)
1744	1744	1744	1744	$\nu(\text{-C=O}_{vst})$ in esters
1709	1723	1715	1702	$\nu(\text{-C=O}_{vw})$ in acids
1654	1654	1663	1679/1696	
-	-	1638	1618/1651	
-	-	1595	1559	$\nu_{vw}(\text{-C=C-}, \text{cis-})$
-	-	-	1537	
-	-	-	1515	
1460	1460	1460	1461	$\delta_{vw}(\text{-C-H})$ w CH ₂ and in CH ₃ groups, deformation (scissoring)
-	-	-	1434	$\nu_{vw}(\text{-C-H}, \text{cis-})$ deformation (ring)
1371	1381	1370	1370/1392	$\nu_{w, m, vw}(\text{-C-H}, \text{-CH}_3)$ and deformation
1308	1311	1305	1315	$\delta_m(\text{-C-H}, \text{-CH}_3)$
1272	1270	1270	1270	$\nu_m(\text{-C-O})$ or $\delta_m(\text{-CH}_2-)$

1239	1233	1237	1231	$\nu_m(-C-O)$ or $\delta_m(-CH_2-)$
1160	1163	1162	1165	$\nu_m(-C-O)$
1098	1095	1100	1100	
1065	-	1072	1065	$\nu_{m,vw}(-C-O)$
1029	1038	1031	1029	
967	964	969	967	$\delta_w(-HC=CH-, trans-)$ out-of-plane deformation

ν – stretching vibrations, δ – deformation vibrations, s – symmetric, as – asymmetric, st – strong, w – weak

Table S3. Positions of the maxima of absorption spectra and assignment to the relevant vibrations as recorded for Moldavian dragonhead oil samples stored at 7°C (refrigerated), in an O₂ atmosphere and a dark bottle, respectively: a – immediately after pressing, b – two weeks after pressing, c – four weeks after pressing – 8 weeks after pressing.

FTIR				Type and origin of vibrations
Position of bands [cm ⁻¹]				
a	b	c	d	
3006	3009	3012	3009	$\nu(=C-H_m, \textit{cis-})$
2957	2961	2960	2958	$\nu_{as}(-C-H_{vst}, -CH_a)$
2926	2927	2922	2927	and
2854	2853	2853	2857	$\nu_s(-C-H_{vst}, -CH_a)$ (aliphatic groups in triglycerides)
1742	1742	1744	1741	$\nu(-C=O_{vst})$ in esters
1708	1708	1708	1704	$\nu(-C=O_{vw})$ in acids
1653	1649	1659	1679	
-	1607	-	1618/1653	
-	-	1597	1556	$\nu_{vw}(-C=C-, \textit{cis-})$
-	-	-	1561	
-	-	-	1520	
1458	1457	1458	1457	$\delta_{vw}(-C-H)$ w CH ₂ and in CH ₃ groups, deformation (scissoring)
-	-	-	1435	$\nu_{vw}(-C-H, \textit{cis-})$ deformation (ring)
1374	1350/1374	1350/1375	1366	$\nu_{w, m, vw}(-C-H, -CH_3)$ and deformation
1310	1311	1313	1310	$\delta_m(-C-H, -CH_3)$
1268	1268	1268	1277	$\nu_m(-C-O)$ or $\delta_m(-CH_2-)$
1237	1237	1239	1222	$\nu_m(-C-O)$ or $\delta_m(-CH_2-)$
1163	1164	1161	1163	$\nu_m(-C-O)$
1097	1103	1097	1094	
1069	1068	1068	1068	$\nu_{m,vw}(-C-O)$
1027	1029	1029	1026	
971	967	975	973	$\delta_w(-HC=CH-, \textit{trans-})$ out-of-plane deformation

ν – stretching vibrations, δ – deformation vibrations, s – symmetric, as – asymmetric, st – strong, w – weak.