Eco-Friendly Extraction of Pectin and Essential Oils from Orange and Lemon Peels

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Supplementary Electronic Information

Table S1. Assignments of the DRIFT spectra (observed maxima) of pectin samples extracted via two processes (P1 and P2) from fresh peels (F) and waste residues (W) of lemon (L) and orange (O)

Wavenumber / cm^{-1}						**Assignment**
FL-P1	**FL-P2**	**WL-P1**	**FO-P1**	**FO-P2**	**WO-P2**	
~3500$_{sh}$		~3500$_{sh}$				νO-H
3344$_{VS,br}$	3270$_{m,br}$	3290$_{VS,br}$	3302$_{m,br}$	3325$_{m,br}$	3314$_{S,br}$	νO-H
2932$_{VS}$	2932$_{m}$	2938$_{VS}$	2931$_{w}$	2933$_{w}$	2932$_{w}$	$\nu CH+\nu_{as}CH_3+\nu_{as}CH_2$
2893$_{VS}$	2891$_{m,sh}$	2904$_{VS}$	2894$_{w}$	2894$_{w,sh}$	2891$_{w,sh}$	$\nu CH+\nu_{s}CH_3$
~2700$_{sh}$	~2700$_{sh}$	~2700$_{sh}$	~2700$_{sh}$	~2700$_{sh}$		ν(CO)O-H, satellite
~2500$_{sh}$	~2500$_{sh}$	~2500$_{sh}$	~2500$_{sh}$	~2500$_{sh}$		ν(CO)O-H, satellite
1740$_{S}$	1745$_{w}$	1727$_{S}$	1742$_{w}$	1745$_{w}$	1742$_{vw}$	$\nu(C{=}O)_{ester}$
1670$_{S}$	1670$_{w}$					$\nu(C{=}O)_{acid}$
1606$_{S}$	1606$_{m}$	1605$_{S}$	1606$_{m}$	1605$_{w}$	1604$_{w}$	$\nu_{as}COO^{-}$
1506$_{m}$	1512$_{vw,sh}$	1515$_{w}$	1516$_{vw}$	1515$_{vw}$	1514$_{vw}$	δCH_2
1436$_{VS,sh}$	1437$_{m,sh}$	1457$_{m}$				$\delta_{as}CH_3$
1419$_{VS}$	1414$_{m}$	1413$_{S}$	1412$_{m}$	1413$_{w}$	1413$_{m}$	$\nu_{s}COO^{-}$
1362$_{VS}$	1363$_{m}$	1356$_{S}$	1373$_{m}$	1367$_{w}$	1366$_{m}$	$\delta_{s}CH_3$
1264$_{S}$	1260$_{m}$	1258$_{m,sh}$	1258$_{w}$	1257$_{w}$	1257$_{m}$	$\nu(C\text{-}O\text{-}C)_{ester}$
1230$_{S,sh}$	1238$_{m}$	1235$_{m}$	1235$_{w,sh}$	1240$_{w}$	1238$_{w}$	$\delta(C\text{-}O\text{-}H)_{ip,pyranose}$
1140$_{VS}$	1138$_{S}$	1138$_{S,sh}$	1141$_{S,sh}$	1141$_{m,sh}$	1139$_{m,sh}$	$\nu(C\text{-}O\text{-}C)_{pyranose} + \nu(C\text{-}O\text{-}C)_{glycoside} + \nu(C\text{-}OH)_{pyranose} + \nu(C\text{-}C)_{pyranose}$
1098$_{VS}$	1099$_{VS}$	1099$_{S}$	1099$_{VS}$	1099$_{VS}$	1100$_{VS}$	
	1071$_{VS}$		1070$_{VS}$	1074$_{VS}$		
1049$_{VS}$	1048$_{VS}$	1052$_{VS}$	1053$_{VS}$	1054$_{VS}$	1052$_{VS}$	
1031$_{VS}$	1031$_{VS}$	1033$_{VS,sh}$	1037$_{VS}$	1033$_{VS}$	1032$_{VS}$	
920$_{w}$	918$_{w}$	919$_{vw}$	918$_{w}$	919$_{vw}$	920$_{w}$	$\rho(CH_3)_{ester}$
		895$_{vw}$	899$_{vw}$	901$_{vw,sh}$		$\rho CH_2 + \delta_{ip}(C\text{-}H)_{pyranose} + \rho CH_2$
868$_{vw}$	868$_{vw}$	868$_{vw}$	867$_{w}$	867$_{w}$	867$_{w}$	
818$_{w}$	818$_{w}$	817$_{m}$	818$_{m}$	818$_{w}$	818$_{w}$	
776$_{w}$	776$_{m}$	777$_{m}$	777$_{m}$	777$_{m}$	777$_{w}$	

Table S2. Results of the spectral deconvolution by non-linear least squares fitting of the 1900-950 cm^{-1} region: $\tilde{\nu}$ - wavenumber (cm^{-1}); FWHM - full width at half maximum; A - integrated area.

FL-P1			FL-P2			WL-P1			FO-P1			FO-P2			WO-P2			Assignment
$\tilde{\nu}$	FWHM	A	$\tilde{\nu}$	FWHM	A	$\tilde{\nu}$	FWHM	A	$\tilde{\nu}$	FWHM	A	$\tilde{\nu}$	FWHM	A	$\tilde{\nu}$	FWHM	A	
1753	25	6.97	1752	27	4.58	1750	22	1.48	1750	32	5.39	1749	24	3.91	1749	29	2.48	$\nu(C=O)_{ester}$
1731	52	30.49	1727	47	13.71	1726	71	58.95	1721	67	16.71	1725	59	11.76	1722	57	5.46	
1676	31.2	10.2	1676	29.7	6.0	1666	52.2	12.0	1668	30.0	2.2	1667	25.5	1.6	1667	30.0	1.1	$\nu(C=O)_{acid}$
1610	116	116.07	1610	94	52.54	1606	81	59.16	1607	82	37.70	1608	65	27.40	1605	69	18.71	$\nu_{as}COO^-$
1512	33	7	1510	34	5	1516	23	5	1515	21	2	1515	16	1	1515	16	1	
1461	66	42	1460	54	18	1456	52	19	1451	66	22	1449	54	17	1459	33	2	$\delta_{as}(CH_3)$
1415	48	12.4	1418	48	10.5	1414	41	8.8	1408	41	5.5	1408	35	5.3	1417	96	31.6	ν_sCOO^-
-	-	-	-	-	-	1357	171	113	1370	19	0	1371	20	1	1367	25	1	$\delta_s(CH_3)$
1359	137	118	1355	147	81	-	-	-	1351	133	56	1348	107	45	1333	69	16	$\delta(C\text{-}O\text{-}H)_{ip,pyranose}$
1266	15	0.3	1266	16	0.3	1268	24	0.9	1269	25	0.9	1268	20	0.7	1256	75	20.4	$\nu(C\text{-}O\text{-}C)_{ester}$
1235	105	64.3	1234	87	33.6	1229	76	31.4	1235	84	28.4	1236	70	25.9	1224	28	2.0	$\delta(C\text{-}O\text{-}H)_{ip,pyranose}$
1190	20	2	1189	21	2	1184	34	9	1187	25	2	1187	21	2	1192	33	4	$\nu(C\text{-}C)_{pyranose}$
1147	44	28.6	1145	43	25.1	1149	39	16.5	1142	49	29.5	1142	42	28.0	1141	50	21.6	$\nu(C\text{-}O\text{-}C)_{pyranose}$
1101	51	46.4	1100	46	39.7	1106	62	46.2	1102	37	24.6	1101	30	25.1	1103	32	14.5	
1075	25	6.1	1077	20	4.1	-	-	-	1078	19	3.5	1078	17	5.6	1078	19	3.3	
1050	42	38.1	1059	35	25.4	1059	58	41.5	1056	52	52.6	1053	42	52.4	1053	61	53.4	$\nu(C\text{-}O\text{-}C)_{glycoside}$
1028	27	7.8	1037	35	15.1	-	-	-	1030	14	0.8	1030	14	2.3	1029	15	1.4	$\nu(C\text{-}OH)_{pyranose} + \nu(C\text{-}C)_{pyranose}$
1006	38	31.9	1013	46	38.1	1012	65	51.6	1012	43	30.1	1013	26	18.8	1014	26	9.2	
980	26	13	979	33	14	978	21	5	980	27	10	983	25	13	987	33	12	$\delta(C\text{-}O\text{-}H)_{op,pyranose}$
963	13	2	1752	27	4.58	962	15	3	962	12	2	962	10	1	963	11	1	$\delta(C\text{-}O\text{-}H)_{op,pyranose}$

Table S3. Assignments of the DRIFT spectra (observed maxima) of essential oils (EO) extracted from fresh peels (F) and waste residues (W) of lemon (L) and orange (O)

Wavenumber / cm^{-1}				Assignment
FL-EO	**WL-EO**	**FO-EO**	**WO-EO**	
~3400				νO-H
3082_{vw}	3084_{vw}	3084_{vw}	3083_{vw}	$\nu_{as}=CH_2$
3072_{vw}	3073_{vw}	3072_{vw}	3073_{vw}	$\nu_{s}=CH_2$
	3047_{vw}	3046_{vw}	3046_{vw}	ν=CH
$3007_{vw,sh}$	3010_{vw}	3010_{w}	3010_{w}	ν=CH
2963_{S}	2965_{S}	2966_{S}	2965_{S}	$\nu_{as}CH_3$
2924_{VS}	2922_{VS}	2921_{VS}	2919_{VS}	$\nu_{as}CH_2$
2874_{m}	$2875_{S,sh}$	$2875_{S,sh}$	$2875_{S,sh}$	$\nu_{s}CH_3$
2855_{m}	2856_{m}	2856_{S}	2856_{S}	$\nu_{s}CH_2$
	2835_{m}	2835_{m}	2835_{m}	
1740_{w}				νC=O
1717_{w}				
1679_{m}				
1645_{w}	1645_{w}	1644_{w}	1644_{w}	νC=C
$1447_{m,sh}$	1452_{w}	1452_{m}	1452_{m}	δCH
1437_{m}	1437_{m}	1437_{m}	1437_{m}	$\delta_{as}CH_3$
1377_{m}	1376_{w}	1375_{w}	1376_{w}	$\delta_{s}CH_3$
1232_{w}				ν_{as}C-O-C
1196_{vw}				ν_{s}C-O-C
1155_{vw}	1155_{vw}	1155_{vw}	1155_{vw}	νC-C
1148_{vw}	1147_{vw}	1147_{vw}	1147_{vw}	
914_{w}	914_{w}	914_{w}	914_{w}	ρCH_3
887_{m}	887_{m}	887_{S}	887_{S}	$\delta_{op}=CH_2$
798_{vw}	797_{w}	797_{w}	797_{w}	δ_{op}=CH