Supplementary information for

A New Water-Soluble Bactericidal Agent for the Treatment of Infections Caused by Gram-Positive and Gram-Negative Bacterial Strains

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Table S1. ATR-FTIR absorption bands of grapefruit and lemon pectin and their attribution (observed maxima).

$\tilde{\nu}$ (cm^{-1})			Vibrational mode	Identification
Commercial citrus pectin	**Lemon IntegroPectin**	**Grapefruit IntegroPectin**		
3347			ν (OH)	Polysaccharides [1,2]; water [1,2]
	3295	3293	ν (OH)	Polysaccharides [1,2]; water [1,2]; polyphenols [3]
2924	2925	2931	ν_{as} (CH_2); ν_{as} (CH_3); ν (CH)	Pectin backbone [1]; arabinose and galactose [1]
	2865	2873	ν_s (CH_3); ν (CH)	Pectin backbone [1]; pyranose rings [1]
2675(s)	2671(s)		ν (OH)	Free carboxylic acids [1,2]
		2658(s)	ν (OH)	Free carboxylic acids [1,2]
	2502(s)	2499(s)	ν (CO)O-H, satellite	Carboxylic acid dimers [1,2]
1737			ν (C=O)$_{ester}$	Methyl esterified carboxylic groups of galacturonic acid [1,2,4–7]
	1713	1715	ν_s (C=O)	Carboxylate and nonconjugated keto groups of carotenoids [1,2,11,12], phenols and flavonoids [3,8-9]
	1674(s)		ν (C=O)$_{acid}$	Nonesterified hydrogenated acidic carbonyl and conjugated keto groups [1]; formyl groups of carotenoids [8]; carboxylic acid groups with strong H bonds [10]
		1631(s)	δ (H_2O); ν (C=C); ν (C-C); ν (C=C)	Phenyl and uracyl groups [7]; water [1]; phenolic acids [3–9]
1607			ν_{as} (COO^-); ν (C-C)	Carboxylate groups of polygalacturonic acid [1,7,11,12]
	1594	1596	ν (C=O)	Aromatic skeleton and keto groups [3,9,13–15]
		1578(s)	ν (C=C); ν (C=O)	Aromatic skeleton and keto groups [3,9,13–15]
	1512	1518	δ_{ip} (CH); ν (C=C)	Phenyl rings [3,9,15]; carotenoid compounds [8]
1459(s)			δ_{as} (CH_3); δ (CH2); ν (C=C); ν_{as} (COO^-)	Pectin backbone [12–16]; aromatic compounds [9,17–19]
1441	1436(s)	1438(s)	δ_{as} (CH_3); ρ (CH_2) 1st overtone; ν (C-C)	Aromatic compounds [3,9,16-18]; ester methyl groups in galacturonic and rhamnose rings of pectin [1,2,11,12,19]
1402	1397	1399	δ(COH)COOH; ν_s (COO^-); δ_{ip} (CH); δ_s (CH_3)	Methyl groups [3,4]; ring vibration [3,9,12]; carboxylate pectin ester groups [2–4]
1361	1367	1367	δ_s (CH_2); δ_s (CH_3); β_s (CH_3); δ (OH); δ_{ip} (COH); δ_{op} (CH_3); δ_s (CH_3)	Ester methyl groups in galacturonic and rhamnose rings of pectin [1,2,12,16]; flavonoids [9,17–19]

$\tilde{\nu}$ (cm^{-1})			Vibrational mode	Identification
1328	1327	1331	δ (CH); ν_s (COO^-); ω (CH_2); δ_{ip} (C-O-H)	Pyranose in pectic ring [2,9,20]; metoxyphenolic substitutions [12]; alcohol hydroxyl groups in pyranose ring [1]
		1296	ρ_s (CH); ν (CO-O); ν_{ip} (OH)	Aromatic ethers [9,12,17–19]
1264	1261(s)		β (OH); ν (C-O-C)	Esters; hydroxyl groups of polysaccharides [1,3,12,16,19,20]
		1250(s)	ν (C-O)	Polyols (hydroxyflavonoids) [16–19]
1222	1222	1225	ν ($C(CH_3)_2$); ν (CO-O); ν_{ip} (OH); δ_{ip} (C-O-H)	Aromatic ethers [3,8,9,17–20]; metoxyphenolic substitutions [8]; alcohol hydroxyl groups in pyranose ring [1,2]
		1200(s)	ν ($C(CH_3)_2$); ν (C-C)	cyclic C-C bonds in the pectin ring [1,2,4,5,11,12,16]; flavonoids [3,16–19]
		1176	ρ_{as} (CH); ν (C-O); ν (C-C); δ (HCC)	cyclic C-C bonds in the pectin ring [1,2,4,5,11,12,16]; flavonoids [3,16-19]
1142	1142	1140	ν (C-O-C); ν (C-C); ν_{as} (O-C-O)	Glycosidic bond in polysaccharide ring [1,2,11,12,20]; cyclic C-C bonds in the pectin ring [7,12]
1094	1096	1096	ν (C-O); ν (C-OH); ν (C-O-C); ν (C-C)	Pyranose and glycoside [1,2,15,20]; pectin ring [2,11,12,19]; uronic acid [3,7]
1072	1070	1067(s)	ν (C-O); ϱ (CO); ν (C-O-C); ν (C-C) ν (C-OH)	Pyranose and glycoside [1,2,12,19]; arabinose and galactose [7]
1047	1046	1045	ν (C-O); ρ (CO); ν (C-O-C); ν (C-OH); ν (C-C); ρ (CH_3)	Pyranose and glycoside [1,2,11,12,19]; arabinose and galactose [7]; flavonoids [3,9,15,19]
1013	1010	1012	ν (C-C); ν (C-O)	Polysaccharides [2,3,7,20]; pectin (C2-C3, C2-O2, C1-O1) [12,19]; uronic acid [7]
	966	970	γ (=CH); ρ (CH_3); ν(C=C)*trans*;	Polysaccharides [1-3,7,20]; arabinose and galactose [7]; flavonoids [3,9,15–19]
954(s)			δ (C=O); δ (CCH); δ (COH)	Polysaccharides in pectin [1–3,7,20]; carotenoids [8]
914	924	919	ρ (CH_3); α-anomeric linkage; δ_{op} (=CH)*trans*; β (Ph); τ (HCC)	Ester methyl groups [1,12,20]; glucose and fructose [1,2,12]; phenyl moieties [3,9,15–18]; pectin [2,6,19]; flavonoids [3,9,15–19]
	909		ν (C-C); δ_{op} (CH); δ (CCH); δ (COH)	Aromatic compounds [3,9,15–19]; pectins [1,2,3,6,19]

$\tilde{\nu}$ (cm^{-1})			Vibrational mode	Identification
883	883	886	β (CH); δ (CCH); δ (COH); γ (=CH); δ_{op} (C=CH_2)	Methylene groups[1,12,20]; vinilydiene groups of terpenoids [21]
		864(s)	ρ (CH_2); δ_{ip} (CH); ρ (CH_2); β (C-C_{ring})	Pyranose [1,2,11,12,19]; phenols [3,9,15–19]
845			ρ (CH_2)	Pectin
829	832	831	γ (OH); δ_{op} (CH)	Six-membered ring of polyphenols [3,9,15,19]; α-glycosidic linkages [7]; phenolic compounds [3,9,15,19]
805	805	812	ρ (CH_2); δ_{ip} (C-H); β_{op} (CH)	Pyranose [1,2,11,12,19]
780(s)	783	779(s)	ω (CH); ρ (CH_2); δ_{ip} (C-H); γ (COH); δ_{op} (=CH) *cis*	Pyranose [1,2,11,12,19]; six-membered ring of polyphenols [3,9,15,19]
758	761	759	δ_{op} (=CH)$_{cis}$; breath β_{op} CH_{cis}; ϱ_{ip} CH_2	Breathing ring [1,12]
743				
	709	712	ρ (CH_2); γ (COH); δ_{op} (=CH); δ_{op} (=CH)cis	six-membered ring of polyphenols [3,9,15,19]; vibrations of pyranoid ring [1,2,11,12,19]
		703	δ_{op} (=CH)	Pectin [1,2,3,6,19]
	684	686(s)	ω (C=O); δ_{op} (=CH); ν_s (C-O-C)	Glycoside linkage [1,2]; acidic pectins [1,2,3,6,19]
	659	660	β (C-C-O); γ (C-O)	Phenols [3,9,15,19]

$\tilde{\nu}$ (cm^{-1}) = wavenumber; ν = stretching, δ = bending/scissoring, ϱ = rocking, β = deformation modes, ω = wagging, breath = breathing, γ = out of plane ring vibrations, τ = twisting; as and s = asymmetric and symmetric; ip and op = in plane and out of plane, respectively.

Table S2. Results of the spectral deconvolution by non-linear least-squares fitting of the 1800-1470 cm^{-1} region.

Lemon IntegroPectin			Grapefruit IntegroPectin			Vibrational mode	Reference
$\tilde{\nu}$ (cm^{-1})	w	A	$\tilde{\nu}$ (cm^{-1})	w	A		
1750	20.6	1.29	1750	21.2	1.35	ν (C=O)$_{ester}$	[1,2,4–7]
1723	39.5	7.65	1722	40.3	8.87	ν_s (C=O)$_{carboxylate\ and\ nonconj.\ keto\ groups}$	[1–3,8–9,11,12]
1689	71.5	14.53	1678	58.3	8.01	ν (C=O)$_{acid}$	[1,8,10]
			1637	23.5	2.69	δ (H_2O); ν (C=C)$_{uracyl}$; ν (C-C)$_{phenyl}$	[1,3–9]
			1613	22.7	1.55	ν_{as} (COO^-)$_{carboxylate}$	[1,7,11,12]
1594	67.5	22.82	1591	55.9	17.90	ν (C=O)$_{aromatic\ skeleton\ and\ keto\ groups}$	[3,9,13–15]
1511	19.5	0.666	1516	15.7	0.77	δ_{ip} (CH); ν (C=C)	[3,8,9,15]

$\tilde{\nu}$ (cm^{-1}) = wavenumber; w = width; A = integrated area.

Table S3. Results of the spectral deconvolution by non-linear least-squares fitting of the 1200-950 cm^{-1} region.

Commercial pectin			citrus Lemon IntegroPectin			Grapefruit IntegroPectin			Vibrational mode	Reference
$\tilde{\nu}$ (cm^{-1})	w	A	$\tilde{\nu}$ (cm^{-1})	w	A	$\tilde{\nu}$ (cm^{-1})	w	A		
						1181	18.17	0.78	ρ_{as} (CH); ν (C-O); ν $(C\text{-}C)_{pectin\ ring}$; $\delta(HCC)_{flavon.}$	[1–5,11,12,16–19]
1145	30.85	4.30	1141	25.90	2.58	1139	23.81	2.68	ν $(C\text{-}O\text{-}C)_{glycosidic\ bond}$; ν (C-C) pectin ring	[1,2,7,11,12,20]
1097	30.75	8.75	1099	27.32	8.22	1098	30.93	9.46	ν (C-O); ν(C-O-C); ν (C-OH); ν (C-C)	[1–3,7,11,12,15,19,20]
1069	20.00	4.90	1070	21.30	6.42	1067	26.12	9.64	ν (C-O); ρ (CO); ν (C-O-C); ν (C-OH); ν (C-C)	[1,2,7,12,19];
1049	17.11	3.20	1047	18.47	5.20	1045	20.37	6.53	ν (C-O); ρ (CO); ν (C-O-C); ν (C-OH); ν (C-C); ρ $(CH_3)_{flavon.}$	[1–3,7,9,11,12,19]
1016	34.70	14.10	1012	36.87	17.60	1015	36.18	20.90	ν (C-C); ν (C-O)	[2,3,7,12,19,20]
966	45.52	8.50	967	28.70	5.30	970	34.61	8.92	γ (=CH); C=C *trans*; ρ $(CH_3)_{flavon.}$	[1–3,7,9,15–20]

$\tilde{\nu}$ (cm^{-1}) = wavenumber; w = width; A = integrated area.

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