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

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Commercial citrus pectinLemonGrapefruit IntegroPectinV(OH)Polysaccharides [1,2]; water [1,2]; polyshenols [3]334732953293v (OH)Polysaccharides [1,2]; water [1,2]; polyphenols [3]292429252931v= (CH3); v wePectin backbone [1]; arabinose and galactose [1]292429252873v= (CH3); v (CH)Pectin backbone [1]; pyranose rings [1]2675(s)2671(s)vv (OH)Free carboxylic acids [1,2]2675(s)2671(s)vv (OH)Free carboxylic acids [1,2]2675(s)2671(s)vv (OH)Free carboxylic acids [1,2]2675(s)2671(s)v (CO)-atrCarboxylic acid adise, [1,2]2675(s)2671(s)v (CO)-atrCarboxylic acid adise, [1,2]2675(s)17131715v (CO)-atrMethyl esterified carboxylic groups of galacturonic acid [1,2,4,7]173717131715v. (C=O)Carboxylic acid adimers [1,2]17371674(s)vv (C=O)Methyl esterified varboxylic groups of carotenoids [1,2,4,7]1674(s)1715v. (C=O)Nonesterified hydrogenated acid: carbonyl and conjugated keto groups [1]; formyl groups of carotenoids [1]; arbinylig pos of carotenoids [3]; arboxylic acid groups with strong H bonds [10]16071631(s) δ (H-O); v (C=O)Aromatic skeleton and keto groups [3,9,13-15]160715941596v (C=C); v (C=O)Aromatic skeleton and keto groups [3,9,13-15]160715941596v (C=C);	ν̃ (cm ⁻¹)			Vibrational mode	Identification
itrus pectinIntegroPectinIntegroPectin3347vV(OH)Polysaccharides [1,2]; water [1,2]; polyphenols [3]32953293v. (OH)Polysaccharides [1,2]; water [1,2]; polyphenols [3]292429252931v. (CH); v. (CH)Pectin backbone [1]; znbinose and galactose [1]28652873v. (CH); v. (CH)Pectin backbone [1]; pyranose rings [1]2675(s)2671(s)v (OH)Free carboxylic acids [1,2] carboxylic acids [1,2]2675(s)2671(s)v (OH)Free carboxylic acids [1,2] carboxylic acid dimers [1,2] satellite17372502(s)2499(s)v (CO)O-H, carboxylic acid dimers [1,2] satellite17371715v. (C=O) carboxylic acid dimers [1,2] satelliteCarboxylic acid dimers [1,2] rec carboxylic acid groups of galacturonic acid [1,2,4-7]17131715v. (C=O) carboxylate and nonconjugated keto groups [1] formyl groups of carotenoids [3,8-9]16071674(s)v (C=O) v (C=O); v (C=O)Nonesterlifed hydrogenated acidic carboxylic acid groups [1] formyl groups of carotenoids [3,2-9] v (C=O); v (C=O)160715941596v (C=O) v (C=O)Aromatic skeleton and keto groups [3,9,13-15]160715941596v (C=O) v (C=O)Aromatic skeleton and keto groups [3,9,13-15]160715941596v (C=O) v (C=O)Aromatic skeleton and keto groups [3,9,13-15]160715941596v (C=O) v (C=O)Aromatic skeleton and keto groups [3,9,13-15]1607	Commercial	Lemon	Grapefruit		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	citrus pectin	IntegroPectin	IntegroPectin		
32953293 v (OH)Polysaccharides [1,2]; water [1,2]; polyphenols [3]292429252931 v_{sc} (CH2); v_{sm} (CH2); v (CH)Pectin backbone [1]; parabinose rings [1]2675(s)2671(s) v (OH)Free carboxylic acids [1,2] Pectin backbone [1]; pyranose rings [1]2675(s)2671(s) v (OH)Free carboxylic acids [1,2] Pectin backbone [1]; pyranose rings [1]2675(s)2671(s) v (OH)Free carboxylic acids [1,2] rec arboxylic acids [1,2]2675(s)2671(s) v (CO)-H, satelliteCarboxylic acids [1,2] rec arboxylic acids [1,2]2772502(s)2499(s) v (CO)-H, satelliteCarboxylic acid dimers [1,2] satellite173717131715 v_{s} (C=O) acid and nonconjugated keto groups of carotenoids [1,2,4-7]Methyl esterified carboxylic groups of galacturonic acid [1,2,4-7]173717131715 v_{s} (C=O) w (C=O) w (C=O)Carboxylate and nonconjugated keto groups of carotenoids [1,2,11,12], phenols and flavonoids [3,8-9]1674(s) v (C=O) w (C=O)Nonesterified carboxylic acid groups with strong H bonds [10] (1,2,4-7]16071631(s) δ (H±O); v (C=C) v_{m} (COO); v (C=C)160715121518 δ_{p} (CH0; v (C=O) Aromatic skeleton and keto groups [3,9,13-15]160715121518 δ_{p} (CH); v (C=O) Aromatic skeleton and keto groups [3,9,13-15]160715121518 δ_{p} (CH); v (C=O) Aromatic skeleton and keto groups [3,9,13-15] <tr< td=""><td>3347</td><td></td><td></td><td>ν (OH)</td><td>Polysaccharides [1,2]; water [1,2]</td></tr<>	3347			ν (OH)	Polysaccharides [1,2]; water [1,2]
2924 2925 2931 vs. (CH2); vs. (CH3) Pectin backbone [1]; arabinose (CH3); vs. (CG3); vs. (CG3); vs. (CG3); vs. (CG3); vs. (CH3); vs. (CG3); vs. (CH3);		3295	3293	ν (OH)	Polysaccharides [1,2]; water [1,2];
292429252931 v_{sc} (CH2); v_{sc} and galactose [1]Pectin backbone [1]; arabinose and galactose [1]28652873 v_{c} (CH2); v_{c} (CH)Pettin backbone [1]; pyranose rings [1]2675(s)2671(s) v_{c} (CH2); v_{c} (CH)Free carboxylic acids [1,2] ree carboxylic acids [1,2]2675(s)2671(s) v_{c} (CH2); v_{c} (CH2) (CSO)Free carboxylic acids [1,2] ree carboxylic acids [1,2]2675(s)2671(s) v_{c} (CO)Free carboxylic acids [1,2] red probability acid dimers [1,2] satellite2675(s)2671(s) v_{c} (CO)-IF, groups of galacturonic acid [1,24-7]173717131715 v_{c} (C=O) ster173717131715 v_{c} (C=O)1674(s) v_{c} (C=O) w (C=O) w (C=O)Carboxylate and nonconjugated keto groups of carotenoids [1,1,12], phenols and flavonoids [3,8-9]16071674(s) v_{c} (C=O) w (C=O)Nonesterfifed hydrogenated acidic carbonyl and conjugated keto groups [1]; formyl groups of carotenoids [8]; carboxylic acid groups of probyglacturonic acid [1,7,11,12]16071631(s) δ (H:O); v (C=O) v_{s} (COO); v (C=O)Aromatic skeleton and keto groups [3,9,13-15]160715941596 v (C=O) v_{s} (COO); v (C=O)Aromatic skeleton and keto groups [3,9,13-15]15121518 δ_{w} (CH3); δ (CH2); v (CCO) v_{s} (COO)Aromatic compounds [3,9,16-18]; ester methyl groups [3,9,15-18]; arotenoid compounds [3,9,16-18]; ester methyl groups [3,4]; ring v_{v} (CCO): δ_{w} (VCO):					polyphenols [3]
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2924	2925	2931	vas (CH2); vas	Pectin backbone [1]; arabinose
$\begin{array}{cccccccccccccccccccccccccccccccccccc$				(CH3); v (CH)	and galactose [1]
2675(s)2671(s)v (OH)Free carboxylic acids [1,2]2602(s)2499(s)v (OH)Free carboxylic acid [1,2]2502(s)2499(s)v (CO)O-H,Carboxylic acid imers [1,2]1737v (C=O)Methyl esterified carboxylic groups of galacturonic acid [1,2,4-7]17131715v (C=O)Methyl esterified carboxylic groups of carboxylate and nonconjugated keto groups [1]; formyl groups of carboxylate and nonconjugated keto groups [3,8-9]1674(s)v (C=O)_addNonesterified hydrogenated acidic carbonyl and conjugated keto groups [3]; arboxylic acid groups of carboxylate and nonconjugated keto groups [3]; pennolic acids [3-9] v (C-C); v (C=C)16071631(s) δ (H:O); v (C=C); v (C=O) vas (COO); v (C=C)Phenyl and uracyl groups [7]; v (C=C); v (C=O)160715941596v (C=O) adom and keto groups [3,9,13-15]15121518 $\delta_{\rm p}$ (CH); v (C=C)Phenyl rings [3,9,15]; carotenoid compounds [8]1459(s)		2865	2873	ν _s (CH ₃); ν (CH)	Pectin backbone [1]; pyranose rings [1]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2675(s)	2671(s)		ν (OH)	Free carboxylic acids [1,2]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			2658(s)	ν (OH)	Free carboxylic acids [1,2]
1737 v (C=O) _{estr} Methyl esterified carboxylic groups of galacturonic acid [1,2,4-7] 1713 1715 v, (C=O) Carboxylate and nonconjugated keto groups of carotenoids [1,2,11,12], phenols and flavonoids [3,8-9] 1674(s) v (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] 1607 v (C=C); v (C=C) 1607 v (C=C); v (C=C) 1594 1596 v (C=O) Aromatic skeleton and keto groups [3,9,13–15] 1578(s) v (C=C); v (C=O) Aromatic skeleton and keto groups [3,9,13–15] 1512 1518 δ_{p} (CH); v (C=C) 1512 1518 δ_{p} (CH); v (C=C) 1441 1436(s) 1438(s) δ_{s} (CH); p (CH) 1397 1399 δ_{c} (COH); COCH; Methyl groups [3,4]; ring v (COO); δ_{c} Aromatic compounds [3,9,16-18]; 1578(s) v (C=C) 1594 1439(s) 1438(s) δ_{s} (CH); p (CH) 1594 1438(s) δ_{s} (CH); p (CH) 1594 1438(s) 1438(s) δ_{s} (CH); p (CH) 1594 1438(s) 1438(s) δ_{s} (CH); p (CH) 1595 1438 (CH); p (CH) 1595 14397 1399 p (COH); COOH; methyl groups [3,9,13]; ring 1402 1397 1399 p (COH); COOH; methyl groups [3,9,13]; ring 1402 1397 1399 p (COH); p (CH) 1402 1397 1399 p (COH); p (CH) 1402 1397 1399 p (CH)		2502(s)	2499(s)	v (CO)O-H,	Carboxylic acid dimers [1,2]
$155 \qquad $	1737			$v (C=O)_{optor}$	Methyl esterified carboxylic
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1757			V (C-O)ester	groups of galacturonic acid
17131715 v_s (C=O)Carboxylate and nonconjugated keto groups of carotenoids [1,2,11,12], phenols and flavonoids [3,8-9]1674(s)v (C=O)_seldNonesterified hydrogenated acidic carbonyl and conjugated keto groups [1]; formyl groups of carotenoids [8]; carboxylic acid groups with strong H bonds [10]16071631(s) δ (H-O); v (C=C); v (C=C); v (C=C)Phenyl and uracyl groups [7]; v (C-C); v (C=C)1607 v_{ss} (COO); v (C=C)water [1]; phenolic acids [3-9] v (C=C); v (C=O)1607 v_{ss} (COO); v (C=C)Carboxylate groups of polygalacturonic acid [1,7,11,12] Aromatic skeleton and keto groups [3,9,13-15]15041596v (C=O)Aromatic skeleton and keto groups [3,9,13-15]15121518 δ_{p} (CH); v (C=O)Phenyl rings [3,9,15]; carotenoid compounds [8]1459(s) δ_{ss} (CH3); δ (CH2); v (C=C)Pectin backbone [12–16]; aromatic compounds [9,17–19])14411436(s)1438(s) δ_{ss} (CH3); ρ (CH2)Aromatic compounds [3,9,16-18]; 1* overtone; ester methyl groups in v (C-C)140213971399 δ (COO); δ_{ss} (VCO); δ_{ss} (VCO); v (COO); δ_{ss} vibration [3,9,12]; carboxylate					[1,2,4–7]
keto groups of carotenoids [1,2,11,12], phenols and flavonoids [3,8-9] 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 (H2O); v (C=C); Phenyl and uracyl groups [7]; v (C-C); v (C=C) v (C=C); v (C=C) vas (COO); v (C-C) 1594 1596 1578(s) v (C=C); v (C=O) 1578(s) v (C=C); v (C=O) 1578(s) v (C=C); v (C=O) 1578(s) v (C=C); v (C=O) 1512 1518 $\delta_{\rm p}$ (CH); v (C=C) Phenyl rings [3,9,15]; carotenoid groups [3,9,13–15] 1512 1518 $\delta_{\rm p}$ (CH); v (C=C) Phenyl rings [3,9,15]; carotenoid compounds [8] 1459(s) 1438(s) $\delta_{\rm as}$ (CH3); δ (CH2); v (C=C); v as (COO) 1441 1436(s) 1438(s) $\delta_{\rm as}$ (CH3); ρ (CH2) Pectin backbone [12–16]; v (C=C); v as (COO) aromatic compounds [3,9,16-18]; 1 st overtone; v (C=C) 20 20 20 20 20 20 20 20 20 20		1713	1715	vs (C=O)	Carboxylate and nonconjugated
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$					keto groups of carotenoids
$ \begin{array}{cccc} & & & & & & & & & & & & & & & & & $					[1,2,11,12], phenols and
$1674(s) \qquad v (C=O)_{acd} \qquad Nonesterified hydrogenatedacidic carbonyl and conjugatedketo groups [1]; formyl groups ofcarotenoids [8]; carboxylic acidgroups with strong H bonds [10]1631(s) \qquad \delta (H_2O); v (C=C); \qquad water [1]; phenolic acids [3-9]v (C-C); v (C=C) \qquad water [1]; phenolic acids [3-9]v (C-C); v (C=C) \qquad water [1]; phenolic acid [1,7,11,12]1594 1596 v (C=O) \qquad Aromatic skeleton and ketogroups [3,9,13-15]1512 1518 \delta_{p} (CH); v (C=C) Phenyl rings [3,9,15]; carotenoidcompounds [8]1459(s) \sum_{i=1}^{1512} 1518 \qquad \delta_{p} (CH); v (C=C) \qquad Phenyl rings [3,9,15]; carotenoidcompounds [8]1441 1436(s) 1438(s) \sum_{i=1}^{3} (CH_3); \delta (CH_2); \qquad Aromatic compounds [3,9,16-18];1st overtone; ester methyl groups inv (C-C) galacturonic and rhannose ringsof pectin [1,2,11,12,19]1402 1397 1399 \sum_{i=1}^{3} (COO); \delta_{ip} (VC); \delta_{ip} (VC); ioraten (3,9,12]; carboxylate$					flavonoids [3,8-9]
$ \begin{array}{cccc} \mbox{acidic carbonyl and conjugated} \\ \mbox{keto groups [1]; formyl groups of} \\ \mbox{carotenoids [8]; carboxylic acid} \\ \mbox{groups with strong H bonds [10]} \\ \mbox{istrong H bonds [10]} \\ \mbox{vice} \mb$		1674(s)		v (C=O) _{acid}	Nonesterified hydrogenated
keto groups [1]; formyl groups of carotenoids [8]; carboxylic acid groups with strong H bonds [10] 1631(s) δ (H2O); v (C=C); Phenyl and uracyl groups [7]; v (C-C); v (C=C) water [1]; phenolic acids [3–9] vss (COO'); v (C-C) Carboxylate groups of polygalacturonic acid [1,7,11,12] 1594 1596 v (C=O) Aromatic skeleton and keto groups [3,9,13–15] 1578(s) v (C=C); v (C=O) Aromatic skeleton and keto groups [3,9,13–15] 1512 1518 δ_{ip} (CH); v (C=C) Phenyl rings [3,9,15]; carotenoid compounds [8] 1459(s) $V (C=C); v_{as}$ (COO 1459(s) δ_{as} (CH3); δ (CH2); Pectin backbone [12–16]; v (C=C); v_{as} (COO aromatic compounds [9,17–19]) 1441 1436(s) 1438(s) δ_{as} (CH3); ρ (CH2) Aromatic compounds [3,9,16-18]; 1 st overtone; v (C-C) galacturonic and rhamnose rings of pectin [1,2,11,12,19] 1402 1397 1399 δ (COH)COOH; Methyl groups [3,4]; ring v, (COO); δ_{bs} vibration [3,9,121]; carboxylate					acidic carbonyl and conjugated
$ \begin{array}{ccc} \operatorname{arotenoids}[8]; \operatorname{carboxylic} \operatorname{acid} \\ \operatorname{groups} \operatorname{with} \operatorname{strong} \operatorname{H} \operatorname{bonds}[10] \\ \operatorname{product} \operatorname{product}$					keto groups [1]; formyl groups of
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$					carotenoids [8]; carboxylic acid
$1631(s) \qquad \delta (HsO); v (C=C); \qquad Phenyl and uracyl groups [7];v (C-C); v (C=C) \qquad water [1]; phenolic acids [3–9]vas (COO); v (C-C) 1594 1596 v (C=O) Aromatic skeleton and ketogroups [3,9,13–15]1578(s) v (C=C); v (C=O) Aromatic skeleton and ketogroups [3,9,13–15]1512 1518 \delta_{p} (CH); v (C=C) Phenyl rings [3,9,15]; carotenoidcompounds [8]1459(s)\delta_{as} (CH3); \delta (CH2); Pectin backbone [12–16];v (C=C); v as (COOaromatic compounds [9,17–19])1441 1436(s) 1438(s) \delta_{as} (CH3); \rho (CH2) Aromatic compounds [3,9,16-18];1st overtone; ester methyl groups inv (C-C) galacturonic and rhamnose ringsof pectin [1,2,11,12,19]1402 1397 1399 \delta (COH)COOH; Methyl groups [3,4]; ringvs (COO-); \delta_{lp} vibration [3,9,12]; carboxylate$					groups with strong H bonds [10]
1607 1607 1607 1594 1594 1596 1578(s) 1578(s) 1578(s) 1578(s) 1578(s) 1578(s) 1578(s) 1578(s) 1578(s) 1578(s) 1578(s) 1578(s) 1578(s) 1512 1518 1518 1518 1518 1518 1518 1518 1519 1518 1518 1519 1518 1518 1519 1518 1519 1518 1519 1518 1519 1518 1519 1518 1519 1518 1519 1518 1519 1518 1519 1518 1519 1518 1518 1519 1518 1519 1518 15			1631(s)	δ (H ₂ O); ν (C=C);	Phenyl and uracyl groups [7];
1607 v_{as} (COO'); v (C-C)Carboxylate groups of polygalacturonic acid [1,7,11,12] Aromatic skeleton and keto groups [3,9,13–15]15941596v (C=O)Aromatic skeleton and keto groups [3,9,13–15]1578(s)v (C=C); v (C=O)Aromatic skeleton and keto groups [3,9,13–15]15121518 δ_{ip} (CH); v (C=C)Phenyl rings [3,9,15]; carotenoid compounds [8]1459(s) δ_{as} (CH3); δ (CH2); v (C=C); vas (COO-)Pectin backbone [12–16]; v (C=C); vas (COO-)14411436(s)1438(s) δ_{as} (CH3); ρ (CH2) (C=C)Aromatic compounds [3,9,16-18]; 1st overtone; v (C-C)140213971399 δ (COH)COOH; v(SOO-); δ_{IP} Methyl groups [3,4]; ring vibration [3,9,12]; carboxylate				v (C-C); v (C=C)	water [1]; phenolic acids [3–9]
1594 1596 v (C=O) Aromatic skeleton and keto	1607			v_{as} (COO-); v (C-C)	Carboxylate groups of
15941596 v (C=O)Aromatic skeleton and keto groups [3,9,13–15]1578(s) v (C=C); v (C=O)Aromatic skeleton and keto groups [3,9,13–15]15121518 δ_{ip} (CH); v (C=C)Phenyl rings [3,9,15]; carotenoid compounds [8]1459(s) δ_{as} (CH ₃); δ (CH2); v (C=C); v_{as} (COO-)Pectin backbone [12–16]; aromatic compounds [9,17–19])14411436(s)1438(s) δ_{as} (CH ₃); ρ (CH2)Aromatic compounds [3,9,16-18]; ester methyl groups in v (C-C)140213971399 δ (COH)COOH; v_s (COO-); δ_{ip} Methyl groups [3,4]; ring vibration [3,9,12]; carboxylate		4504	4504		polygalacturonic acid [1,7,11,12]
$\begin{array}{cccc} & & & & & & & & & \\ 1578(s) & & & & & & & & \\ 1578(s) & & & & & & & & & \\ 1578(s) & & & & & & & & & \\ 1512 & & & & & & & & & \\ 1512 & & & & & & & & & \\ 1512 & & & & & & & & & \\ 1512 & & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1512 & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1459(s) & & & & & & & & \\ 1438(s) & & & & & & & & \\ 1438(s) & & & & & & & & & \\ 1438(s) & & & & & & & & & \\ 1438(s) & & & & & & & & & \\ 1438(s) & & & & & & & & & & \\ 1438(s) & & & & & & & & & & & \\ 1438(s) & & & & & & & & & & & \\ 1438(s) & & & & & & & & & & & & \\ 1438(s) & & & & & & & & & & & & \\ 1438(s) & & & & & & & & & & & & & & \\ 1438(s) & & & & & & & & & & & & & \\ 1438(s) & & & & & & & & & & & & & & & & \\ 1438(s) & & & & & & & & & & & & & & & & & & \\ 1441 & & & & & & & & & & & & & & & & & $		1594	1596	v (C=O)	Aromatic skeleton and keto
$1578(s) \qquad v (C=C); v (C=O) \qquad \text{Aromatic skeleton and keto} \\ \text{groups [3,9,13-15]} \\ 1512 \qquad 1518 \qquad \delta_{ip} (CH); v (C=C) \qquad \text{Phenyl rings [3,9,15]; carotenoid} \\ \text{compounds [8]} \\ 1459(s) \qquad \delta_{as} (CH_3); \delta (CH_2); \\ v (C=C); v_{as} (COO) \\ i \qquad \text{aromatic compounds [9,17-19]} \\) \\ 1441 \qquad 1436(s) \qquad 1438(s) \qquad \delta_{as} (CH_3); \rho (CH_2) \\ 1^{st} \text{ overtone;} \\ v (C-C) \\ \text{galacturonic and rhamnose rings} \\ of pectin [1,2,11,12,19] \\ 1402 \qquad 1397 \qquad 1399 \qquad \delta(COH)COOH; \\ v_{s} (COO); \delta_{ip} \qquad vibration [3,9,12]; carboxylate \\ \end{array}$					groups [3,9,13–15]
$1512 1518 \delta_{ip} (CH); v (C=C) Phenyl rings [3,9,15]; carotenoid compounds [8] 1459(s) \delta_{as} (CH_3); \delta (CH_2); Pectin backbone [12–16]; v (C=C); v_{as} (COO aromatic compounds [9,17–19]) 1441 1436(s) 1438(s) \delta_{as} (CH_3); \rho (CH_2) Aromatic compounds [3,9,16-18]; 1^{st} overtone; ester methyl groups in v (C-C) galacturonic and rhamnose rings of pectin [1,2,11,12,19] 1402 1397 1399 \delta(COH)COOH; Methyl groups [3,9,12]; carboxylate$			1578(s)	v (C=C); v (C=O)	Aromatic skeleton and keto
15121518 δ_{ip} (CH); v (C=C)Phenyl rings [3,9,15]; carotenoid compounds [8]1459(s) δ_{as} (CH3); δ (CH2); v (C=C); v_{as} (COO-)Pectin backbone [12–16]; aromatic compounds [9,17–19])14411436(s)1438(s) δ_{as} (CH3); ρ (CH2)Aromatic compounds [3,9,16-18]; ester methyl groups in v (C-C)140213971399 δ (COH)COOH; v_s (COO-); δ_{ip} Methyl groups [3,4]; ring vibration [3,9,12]; carboxylate		1 = 1 0	1=10		groups [3,9,13–15]
$1459(s)$ $1459(s)$ $1459(s)$ $1438(s)$ $1438(s)$ $1438(s)$ $\frac{\delta_{as}}{CH_3}; \delta (CH_2); Pectin backbone [12–16]; aromatic compounds [9,17–19]) 1441 1436(s) 1438(s) \frac{\delta_{as}}{CH_3}; \rho (CH_2) Aromatic compounds [3,9,16-18]; 1^{st} overtone; ester methyl groups in v (C-C) galacturonic and rhamnose rings of pectin [1,2,11,12,19] 1402 1397 1399 \delta(COH)COOH; Methyl groups [3,4]; ring v_s (COO^-); \delta_{lp} v ibration [3,9,12]; carboxylate$		1512	1518	δ_{ip} (CH); V (C=C)	Phenyl rings [3,9,15]; carotenoid
1439(s) ∂_{as} (CH3); δ (CH2);Fectin backbone [12–16]; aromatic compounds [9,17–19]14411436(s)1438(s) δ_{as} (CH3); ρ (CH2)Aromatic compounds [3,9,16-18]; ester methyl groups in v (C-C)140213971399 δ (COH)COOH;Methyl groups [3,4]; ring v (COC); δ_{hp}	14EO(a)			δ (CII), δ (CII),	Compounds [8]
14411436(s)1438(s) δ_{as} (CH ₃); ρ (CH ₂)Aromatic compounds [3,9,16-18]; ester methyl groups in v (C-C)140213971399 δ (COH)COOH;Methyl groups [3,4]; ring v (COC); δ_{ip}	1459(S)			O_{as} (CH3); O (CH2);	Pectin backbone [12–16];
14411436(s)1438(s) δ_{as} (CH ₃); ρ (CH ₂)Aromatic compounds [3,9,16-18]; ester methyl groups in y (C-C)140213971399 δ (COH)COOH; y _s (COO ⁻); δ_{lp} Methyl groups [3,4]; ring vibration [3,9,12]; carboxylate				$V(C=C); Vas(COO^2)$	aromatic compounds [9,17–19]
14411436(s)1436(s) ∂_{4s} (CH3); β (CH2)Aromatic compounds [3,9,16-18]; ester methyl groups in galacturonic and rhamnose rings of pectin [1,2,11,12,19]140213971399 δ (COH)COOH; v_s (COO-); δ_{ip} Wethyl groups [3,4]; ring vibration [3,9,12]; carboxylate	1 / / 1	1426(a)	1429(a)) $\delta (CH_{1}) \circ (CH_{2})$	A romatic compounds [2.0.16.19].
1st overtone;ester methyl groups in galacturonic and rhamnose rings of pectin [1,2,11,12,19]140213971399 $\delta(COH)COOH;$ Methyl groups [3,4]; ring vibration [3,9,12]; carboxylate	1441	1436(S)	1438(S)	$O_{as}(C\Pi_3); \rho(C\Pi_2)$	Aromatic compounds [3,9,16-18];
140213971399 $\delta(COH)COOH;$ Methyl groups [3,4]; ring vibration [3,9,12]; carboxylate				1^{st} overtone;	ester metnyl groups in
1402 1397 1399 δ(COH)COOH; Methyl groups [3,4]; ring v _s (COO ⁻); δ _{ip} vibration [3,9,12]; carboxylate				V (C-C)	of postin [1,2,11,12,10]
v_s (COC); δ_{ip} vibration [3,9,12]; carboxylate	1402	1307	1300	S(COH)COOH.	$\begin{array}{l} \text{Mothal groups [2,4]; ring} \\ \end{array}$
	1402	1077	1077	$v_{c}(COO) \cdot \delta_{c}$	vibration [3912], carboxylato
$(CH) \cdot \lambda_1 (CH_2)$ not in a tar groups [2, 4]				$V_{\rm s}$ (CH) $\lambda_{\rm s}$ (CH)	p_{101} p_{1
$(C11), 0s (C11s) \qquad \text{pecult ester groups } [2-4]$ $1361 \qquad 1367 \qquad 1367 \qquad \delta_s (CH_s), \delta_s (CH_s) = \text{Exter methyl groups in}$	1361	1367	1367	$\chi \subset I I$, Us $\chi \subset I I$ $\lambda_{a} (CH_{a}) \cdot \lambda_{a} (CH_{a}) \cdot$	Feter methyl groups [2-4]
$\beta_{\rm s}$ (CH2), $\delta_{\rm s}$ (CH2), δ_{\rm	1001	1007	1007	$\beta_{s}(CH_{2}), \delta_{s}(CH_{3}), \beta_{s}(CH_{3}), \delta_{s}(CH_{3})$	alacturonic and rhampose rings
μ s (CIII), σ (OII), galacturonic and Mannose Ings δ_{in} (COH), of portion [1, 2, 12, 16]: flavoroide				$\lambda_{\rm m}$ (COH).	of pectin [1 2 12 16], flavonoide
δ_{ar} (CH ₂). δ_{a} (CH ₂) [9 17_10], have notices				$\delta_{\rm op}$ (CH ₂)· $\delta_{\rm o}$ (CH ₂)	[9 17_19]

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

1ĩ (cm-1)			Vibrational mode	Identification
1228	1227	1221		Ruranoss in postic ring [2.0.20]:
1526	1327	1551	$0 (CH); V_{s} (COO);$	ryranose in pectic ring [2,9,20];
			ω (CH2);	Inetoxyphenolic substitutions
			0 ip (C-O-H)	[12]; alconol nydroxyl groups in
		1000		pyranose ring [1]
		1296	$\rho_{\rm s}$ (CH); ν (CO-O);	Aromatic ethers [9,12,17–19]
			$v_{ip}(OH)$	
1264	1261(s)		β (OH); ν (C-O-C)	Esters; hydroxyl groups of
				polysaccharides [1,3,12,16,19,20]
		1250(s)	v (C-O)	Polyols (hydroxyflavonoids) [16–
				19]
1222	1222	1225	v (C(CH ₃) ₂);	Aromatic ethers [3,8,9,17–20];
			v (CO-O);	metoxyphenolic substitutions [8];
			ν _{ip} (OH);	alcohol hydroxyl groups in
			δ _{ip} (C-O-H)	pyranose ring [1,2]
		1200(s)	v (C(CH ₃) ₂);	cyclic C-C bonds in the pectin
			v (C-C)	ring [1,2,4,5,11,12,16]; flavonoids
				[3,16–19]
		1176	ρas (CH); ν (C-O);	cyclic C-C bonds in the pectin
			ν (C-C); δ (HCC)	ring [1,2,4,5,11,12,16]; flavonoids
				[3,16-19]
1142	1142	1140	v(C-O-C); v(C-C);	Glycosidic bond in
			vas (O-C-O)	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);	Pyranose and glycoside
			v (C-O-C): v (C-C)	[1.2.15.20]: pectin ring
				[2,11,12,19]: uronic acid [3,7]
1072	1070	1067(s)	$v(C-O) \cdot o(CO)$	Pyranose and glycoside
1072	1070	1007 (8)	v (C-O-C): v (C-C)	[1 2 12 19]: arabinose and
			v (C-OH)	galactose [7]
1047	1046	1045	v (C OII)	Pyranose and glycoside
1017	1040	1045	v (C O), p (CO),	[1 2 11 12 19]: arabinose and
			v (C-OH);	galactose [7]: flavonoide
			$v (C-C): o (CH_2)$	[3 9 15 19]
1013	1010	1012	v(C-C); p(C-G)	Polysaccharides [2 3 7 20]: pactin
1015	1010	1012	v (C-C), v (C-C)	$(C_2 C_3 C_2 C_2 C_1 C_1)$ [12 10]
				(C2-C3, C2-O2, C1-O1) [12,17],
	966	970	γ (-CH) γ (CH ₂)	Polycaccharidas [1, 2, 7, 20]:
	200	570	γ (-CII), β (CII3),	arabinoso and galactoso [7]:
			V(C-C)trans,	flavonoide [2 9 15, 19]
$OE_{1}(c)$			$\delta(C-O)$, $\delta(CCH)$,	Deluce scherides in postin [1
954(5)			0 (C=0); 0 (CCH);	2 7 201, senster side [8]
014	024	010		5,7,20]; carotenoids [8]
914	924	717	μ (CII3); α -	Ester methyl groups [1,12,20];
			anomeric linkage;	glucose and fructose [1,2,12];
			$0_{\text{op}} (= CH)$ trans;	pnenyi moletles [3,9,15–18];
			p (Pn); τ (HCC)	pectin [2,6,19]; flavonoids
	000			[3,9,15–19]
	909		v (C-C); δ_{op} (CH);	Aromatic compounds [3,9,15–
			о (ССН); о (СОН)	19]; pectins [1,2,3,6,19]

ν̃ (cm⁻¹)			Vibrational mode	Identification
883	883	886	β (CH); δ (CCH); δ (COH); γ (=CH);	Methylene groups[1,12,20]; vinilydiene groups of terpenoids
			δ_{op} (C=CH ₂)	[21]
		864(s)	ρ (CH ₂); δ _{ip} (CH);	Pyranose [1,2,11,12,19]; phenols
			ρ (CH ₂); β (C-Cring)	[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
90F	005	010		compounds [3,9,15,19]
805	805	812	ρ (CH2); o_{ip} (C-H);	Pyranose [1,2,11,12,19]
780(c)	783	779(c)	$p_{op}(CH)$	Puranoso [1 2 11 12 10], six
700(5)	765	779(8)	ω (C11), p (C112), δ_{in} (C-H):	membered ring of polyphenols
			ν (COH):	[3 9 15 19]
			δ_{op} (=CH) cis	
758	761	759	δ_{op} (=CH) <i>cis</i> ; breath	Breathing ring [1,12]
743			βop CHcis; Qip CH2	
	709	712	ρ (CH2); γ (COH);	six-membered ring of
			δ _{op} (=CH);	polyphenols [3,9,15,19];
			δ_{op} (=CH)cis	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);	Glycoside linkage [1,2]; acidic
			δ _{op} (=CH);	pectins [1,2,3,6,19]
			vs (C-O-C)	
	659	660	β (C-C-O); γ (C-O)	Phenols [3,9,15,19]

 \tilde{v} (cm⁻¹) = wavenumber; v = 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-li	near least-squares fitting of the 1800-1470 cm-
region.	

Lemon IntegroPectin		Grapefruit IntegroPectin			Vibrational mode	Reference	
ν̃ (cm-1)	w	Α	ν̃ (cm-1)	W	Α		
1750	20.6	1.29	1750	21.2	1.35	v (C=O) _{ester}	[1,2,4–7]
1723	39.5	7.65	1722	40.3	8.87	Vs (C=O)carboxylate and nonconj. keto groups	[1-3,8-9,11,12]
1689	71.5	14.53	1678	58.3	8.01	v (C=O) _{acid}	[1,8,10]
			1637	23.5	2.69	δ (H ₂ O); v (C=C) _{uracyl} ; v (C-C) _{phenyl}	[1,3–9]
			1613	22.7	1.55	Vas (COO ⁻)carboxylate	[1,7,11,12]
1594	67.5	22.82	1591	55.9	17.90	u (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{v} (cm⁻¹) = wavenumber; w = width; A = integrated area.

Commercial pectin		citrus	Lemon IntegroPectin			Grapefruit IntegroPectin			Vibrational mode	Reference
vĩ (cm⁻¹)	w	Α	vĩ (cm⁻¹)	w	Α	ν̃ (cm⁻¹)	w	Α		
						1181	18.17	0.78	ρas (CH); ν (C-O); ν (C-C)pectin ring; δ(HCC)flavon	[1– 5,11,12,16 –19]
1145	30.85	4.30	1141	25.90	2.58	1139	23.81	2.68	v (C-O- C)glycosidic bond; v (C-C) pectin ring	[1,2,7,11,1 2,20]
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– 3,7,11,12,1 5,19,20]
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 (CH3)flavon.	[1–3, 7,9,11,12,1 9]
1016	34.70	14.10	1012	36.87	17.60	1015	36.18	20.90	v (C-C); v (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 <i>trans;</i> ρ (CH ₃) _{flavon.}	[1–3,7,9, 15–20]

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

 \tilde{v} (cm⁻¹) = wavenumber; w = width; A = integrated area.

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