

Chitosan/Polyvinyl alcohol/ Tea Tree Essential Oil composite films for Biomedical Applications

Jorge Iván Castro ¹, Carlos Humberto Valencia-Llano ², Mayra Eliana Valencia Zapata ³, Yilmar Joan Restrepo ³, José Herminul Mina Hernandez ³, Diana Paola Navia-Porras ⁴, Yamid Valencia ⁵, Cesar Valencia ⁵ and Carlos David Grande-Tovar ^{6,*}

¹ Grupo de Investigación SIMERQO, Departamento de Química, Universidad del Valle, Calle 13 No. 100-00, 76001 Cali, Colombia; jorge.castro@correounivalle.edu.co (J.I.C.);

² Grupo Biomateriales Dentales, Escuela de Odontología, Universidad del Valle, Calle 4B No. 36-00, 76001 Cali, Colombia; carlos.humberto.valencia@correounivalle.edu.co

³ Grupo de Materiales Compuestos, Escuela de Ingeniería de Materiales, Facultad de Ingeniería, Universidad del Valle, Calle 13 No. 100-00, 760032 Santiago de Cali, Colombia; valencia.mayra@correounivalle.edu.co (M.E.V.Z.); yilmar.restrepo@correounivalle.edu.co; jose.mina@correounivalle.edu.co (J.H.M.H.).

⁴ Grupo de Investigación Biotecnología, Facultad de Ingeniería, Universidad de San Buenaventura Cali, Carrera 122 # 6-65, Cali 76001, Colombia

⁵ Área de Investigación, Desarrollo e Innovación, Disproquin S.A.S., Calle 93 Número 7u-2a, Vía Cali-Juanchito 760021, Colombia

⁶ Grupo de Investigación de Fotoquímica y Fotobiología, Facultad de Ciencias, Universidad del Atlántico, Carrera 30 Número 8-49, 081008 Puerto Colombia, Colombia

* Correspondence: carlosgrande@mail.uniatlantico.edu.co; Tel.: +57-53-599-484

Supplementary Materials

Table S1. Volatile compounds expressed as area percentage identified in the *Melaleuca alternifolia* essential oil

	Compound	RT	Relative amount (%)
Monoterpenes hydrocarbons	α -Thujene	15.96	1.1
	α -Pinene	16.35	2.7
	Sabinene	18.06	0.1
	β -Pinene	18.33	0.8
	β -Myrcene	18.72	0.8
	α -Phellandrene	19.54	0.5
	α -Terpinene	20.08	9.4
	<i>p</i> -Cymene	20.39	4.7
	Limonene	20.57	1.0
	1,8-cineole	20.75	3.9
	γ -Terpinene	21.91	18.4
Monoterpenes oxygenated	Terpinolene	22.93	3.7
	<i>p</i> -Cymenene	23.09	0.1
	Linalool	23.37	0.1
	<i>cis-p</i> -Ment-2-en-1-ol	24.50	0.2

	<i>trans-p</i> -Ment-2-en-1-ol	25.34	0.1
	Terpinene-4-ol	27.09	35.5
	α -Terpineol	27.41	3.5
	<i>Trans</i> -piperitol	27.80	0.1
Sesquiterpenes oxygenated	A mixture of compounds	29.53	0.1
	C ₁₀ H ₁₆ O+C ₁₀ H ₁₈ O+N.I.		
	A mixture of compounds <i>trans</i> -ascaridol	30.19	0.1
	glicol+C ₁₀ H ₁₄ O		
	N.I.	30.80	0.1
Sesquiterpenes no oxygenated	C ₁₀ H ₁₈ O ₂	31.83	0.1
	α -cubebene	32.81	0.1
	Isodene	33.82	0.1
	α -copaene	34.02	0.2
	α -gurjunene	35.26	0.6
	<i>trans</i> - β -Caryophellene	35.75	0.6
	C ₁₅ H ₂₄	36.00	0.1
	α -Maaliene	36.29	0.1
	Aromadendrene	36.44	1.8
	Seline-5,11-diene	36.65	0.2
	<i>Trans</i> -muurola-3,5-diene	36.74	0.2
	α -humulene	37.01	0.2
	Aloaramadendrene	37.18	0.7
	<i>Trans</i> -cadine-1(6),4-diene	37.47	0.4
	γ -muurolene	37.54	0.1
	δ -selinene	37.98	0.3
	Viridiflorene	38.17	1.5
	Bicyclgermacrene	38.32	0.7
	δ -cadidine	38.95	1.6
	Mixture of compounds: <i>cis</i> -calamenene+zonarene	39.13	0.7
	<i>Trans</i> -cadine-1,4-diene	39.42	0.3
	<i>epi</i> -globulol	40.42	0.1
	A mixture of compounds: Maaliol-Palustrol	40.68	0.1
	Espatulenol	40.84	0.2
	Globulol	41.14	0.5
	Mixture of compounds:	41.41	0.4

Viridiflorol+cubeban- 11-ol		
Rosifoliol	41.70	0.2
C ₁₅ H ₂₄ O	42.18	0.2
1- <i>epi</i> -cubenol	42.25	0.3
Cis-cadin-4-en-7-ol	42.66	0.7

Table S2. Physical-chemical analysis of the emulsions before and after adding PVA

Sample	Solids (%) *	pH*	Apparent viscosity (cP) (1/100) *	Density (g/mL)	Particle Size*		observation
					D ₅₀ (μm)	D ₉₈ (μm)	
CS	1.65 ^b ± 0.018	2.76 ^a ± 0.004	35 ^a	1.00	N/A	N/A	
CS/TTEO 0.5%	2.45 ^a ± 0.018	2.82 ^a ± 0.013	35 ^{ab} ± 0.023	1.00	0.78 ^a ± 0.004	1.56 ^a ± 0.004	
CS/TTEO 1.0%	2.10 ^a ± 0.060	2.81 ^a ± 0.004	35 ^{ab} ± 0.045	1.00	1.04 ^a ± 0.004	1.98 ^a ± 0.004	
CS/TTEO 1.5%	2.08 ^a ± 0.022	2.81 ^a ± 0.011	35 ^b ± 0.021	1.00	1.01 ^a ± 0.007	1.99 ^a ± 0.004	
CS	1.65 ^b ± 0.040	2.75 ^a ± 0.004	35 ^a ± 0.0032	1.00	N/A	N/A	Measurement was
CS/TTEO 0.5%	2.43 ^a ± 0.022	2.81 ^a ± 0.007	35 ^{ab} ± 0.002	1.00	0.50 ^a ± 0.007	0.98 ^a ± 0.000	performed after
CS/TTEO 1.0%	2.07 ^a ± 0.020	2.83 ^a ± 0.016	35 ^{ab} ± 0.005	1.00	0.69 ^a ± 0.007	1.22 ^a ± 0.011	homogenization at 3000 psi
CS/TTEO 1.5%	2.09 ^a ± 0.064	2.81 ^a ± 0.009	35 ^b ± 0.021	1.00	0.89 ^a ± 0.011	1.62 ^a ± 0.018	for 10 minutes.
CS	1.66 ^b ± 0.03	7.43 ^a ± 0.009	106 ^a ± 0.0012	1.00	N/A	N/A	Measurement performed
CS/TTEO 0.5%	2.46 ^a ± 0.04	7.44 ^a ± 0.007	74 ^{ab} ± 0.444	1.00	1.29 ^a ± 0.140	3.16 ^a ± 0.160	after PVA addition to the
CS/TTEO 1.0%	2.05 ^a ± 0.01	7.44 ^a ± 0.009	66 ^{ab} ± 0.002	1.00	1.43 ^a ± 0.031	3.44 ^a ± 0.069	CS/TTEO emulsion was
CS/TTEO 1.5%	2.10 ^a ± 0.06	4.55 ^a ± 0.013	28 ^b ± 0.444	1.00	1.60 ^a ± 0.024	3.38 ^a ± 0.049	added and homogenized
							again at 3000 psi for 10
							minutes.
CS	2.74 ^b ± 0.056	2.92 ^a ± 0.011	42 ^a ± 0.003	1.00	N/A	N/A	Measurement performed two
CS/TTEO 0.5%	4.00 ^a ± 0.064	2.95 ^a ± 0.004	43 ^{ab} ± 0.009	1.00	0.45 ^a ± 0.024	2.37 ^a ± 0.020	years later without
CS/TTEO 1.0%	3.95 ^a ± 0.040	3.01 ^a ± 0.004	40 ^{ab} ± 0.012	1.00	0.32 ^a ± 0.018	0.82 ^a ± 0.018	homogenization
CS/TTEO 1.5%	3.90 ^a ± 0.013	3.15 ^a ± 0.011	42 ^b ± 0.003	1.00	0.52 ^a ± 0.004	1.42 ^a ± 0.018	

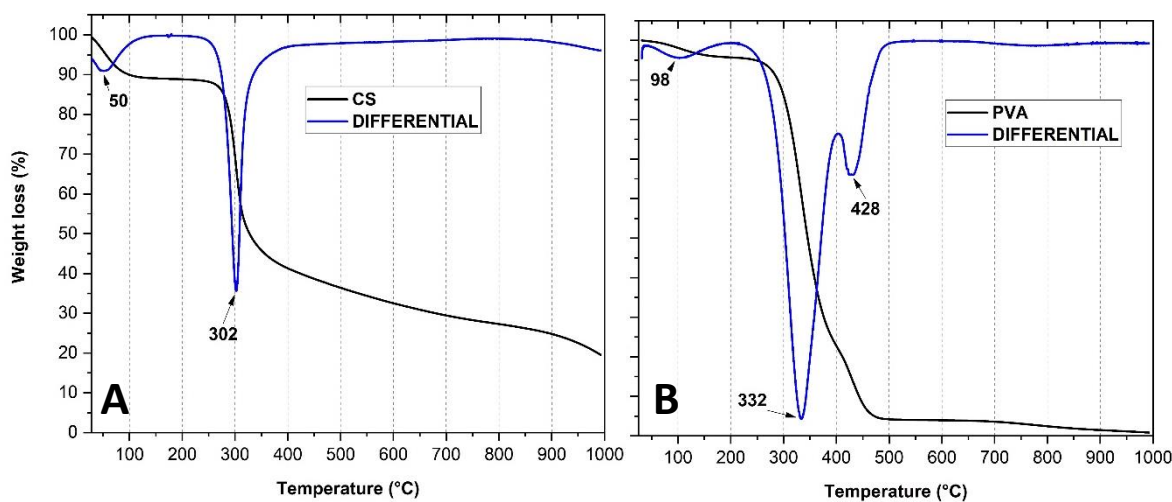


Figure S1. TGA and differential curves for CS and PVA