

Development of essential oil diffusion matrices using non-ionic surfactants-supported NADES and hydrophobic NADES

Samir Scandar^{1,2}, Natali Rianika Mustafa², Claudia Zadra¹, Maria Carla Marcotullio^{1,*} and Young Hae Choi^{2,*}

¹ Department of Pharmaceutical Sciences, Via del Giochetto, Ed. B, University of Perugia, 06122 Perugia, Italy

² Natural Products Laboratory, Institute of Biology Leiden, Leiden University, 2333 BE Leiden, The Netherlands

* Corresponding Authors: mariacarla.marcotullio@unipg.it, y.choi@chem.leidenuniv.nl,

Table S1. Screening test conducted to identify the optimal HLB ratio for hydrophilic NADES formulations, N3 based on various Tween20:Span 80 HLB values.

Tween 20	Tween 80	Triton X 100	PEG 400	PEG 200	Span 80	Span 20	Span 65	
16.7	15	13.4	9.7	8	4.3	8.6	2.1	

NADES 3 – N3											
	Range	% Span 80	% Tween 20	T0	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7
1	4.3	3000	0								
2	5	2831	169								
3	6	2589	411								
4	7	2347	653								
5	8	2105	895								
6	9	1863	1137								
7	10	1621	1379								
8	11	1379	1621								
9	12	1137	1863								
10	13	895	2105								
11	14	653	2347								
12	15	411	2589								
13	16	169	2831								
14	16.7	0	3000								

Colors of the cells indicate the % of phase separation:

0% separation	30% separation	60% separation	90% separation	100% separation	Heat: MW irradiation 600W; *Clear: see Figure S2
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Table S2. Screening test conducted to identify the optimal HLB ratio for hydrophilic NADES formulations, N5 based on various Tween20:Span 80 HLB values.

Tween 20	Tween 80	Triton X 100	PEG 400	PEG 200	Span 80	Span 20	Span 65	
16.7	15	13.4	9.7	8	4.3	8.6	2.1	

NADES 5 – N5											
	Range	% Span 80	% Tween 20	T0	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7
1	4.3	3000	0	+ heat							
2	5	2831	169	+ heat	Clear						
3	6	2589	411	+ heat	Clear						
4	7	2347	653	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
5	8	2105	895	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
6	9	1863	1137	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
7	10	1621	1379	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
8	11	1379	1621	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
9	12	1137	1863	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
10	13	895	2105	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
11	14	653	2347	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
12	15	411	2589	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
13	16	169	2831	+ heat							
14	16.7	0	3000	+ heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear

Colors of the cells indicate the % of phase separation:



	0% separation		30% separation		60% separation		90% separation		100% separation	Heat: MW irradiation 600W; *Clear: see Figure S2
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Table S3. Screening test conducted to identify the optimal HLB ratio for hydrophilic NADES formulations, N1 based on various Tween20:Span 80 HLB values.

Tween 20	Tween 80	Triton X 100	PEG 400	PEG 200	Span 80	Span 20	Span 65
16.7	15	13.4	9.7	8	4.3	8.6	2.1

NADES 1 – N1											
	Range	% Span 80	% Tween 20	T0	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7
1	4.3	3000	0	+heat							
2	5	2831	169	+heat							
3	6	2589	411	+heat							
4	7	2347	653	+heat							
5	8	2105	895	+heat							
6	9	1863	1137	+heat							
7	10	1621	1379	+heat							
8	11	1379	1621	+heat							
9	12	1137	1863	+heat							
10	13	895	2105	+heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
11	14	653	2347	+heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
12	15	411	2589	+heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
13	16	169	2831	+heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear
14	16.7	0	3000	+heat	Clear	Clear	Clear	Clear	Clear	Clear	Clear

Colors of the cells indicate the % of phase separation:

	0% separation		30% separation		60% separation		90% separation		100% separation	Heat: MW irradiation 600W; *Clear: see Figure S2
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Table S4. 21 Volatile headspace compounds (mean peak area \pm SD) of *Lavandula angustifolia* extracted by headspace and analyzed by GCMS at various incubation times of 0.0, 0.5, 1.0, 4.0, 24.0, 48.0, 72.0, and 96.0 hours for control (C) samples.

Compounds	T 0.0 mean	\pm SD	T 0.5 mean	\pm SD	T 1.0 mean	\pm SD	T 4.0 mean	\pm SD	T 24.0 mean	\pm SD	T 48.0 mean	\pm SD	T 72.0 mean	\pm SD	T 96.0 mean	\pm SD
α -thujene	1729.33	25.42	3607.00	102.09	3318.33	60.50	3607.67	46.70	2065.33	706.09	2864.25	208.60	2912.75	44.67	3361.75	44.67
α -phellandrene	16767.33	8785.43	25878.67	3715.53	22946.00	4623.80	22177.67	42.03	15834.67	6241.22	15030.00	6509.84	16969.50	1463.03	25016.25	1463.03
α -pinene	29654.67	12522.75	42489.33	363.36	41608.67	2099.84	44469.00	271.18	34082.33	7187.53	22457.00	17204.77	36270.75	2783.36	40039.00	2783.36
camphene	13893.00	3433.38	16977.33	2299.86	18195.00	901.63	19014.33	406.04	15057.00	2808.65	14512.75	5177.32	16292.75	1618.32	18257.75	1618.32
β -thujene	3093.67	1026.95	3824.67	85.78	3982.00	166.96	3717.67	118.80	2976.00	414.35	2951.25	833.84	3312.25	242.47	3445.50	242.47
β -pinene	12290.67	1030.05	23212.00	1574.22	23918.00	998.98	25822.67	916.64	21860.00	3759.27	20448.00	4754.66	20821.50	1873.83	4533.00	1873.83
3-octanone	11378.00	4856.68	17669.67	1280.17	17654.33	1034.84	20026.33	377.50	14728.67	3422.70	14733.50	2722.03	15066.00	862.42	15842.50	862.42
β -myrcene	15576.00	6631.79	23212.00	1574.22	23822.00	960.93	25754.00	1088.81	21652.00	3577.86	20447.25	4754.96	20505.25	1687.05	19722.25	1687.05
3-carene	8930.00	3612.29	13411.33	370.17	13752.33	1090.96	14583.67	530.41	9777.00	7538.98	14733.50	2722.03	9930.00	446.76	9321.50	446.76
β -cymene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3713.50	112.98
o-cymene	3683.33	1417.83	5677.33	513.75	5370.67	316.11	5807.00	289.68	3965.00	524.13	4166.75	940.46	5462.25	915.21	7220.75	915.21
d-limonene	4412.00	543.04	8663.00	229.42	8693.33	348.01	9358.00	99.51	7772.33	1013.55	7541.25	1117.65	7716.00	861.50	8169.25	861.50
eucalyptol	6727.67	136.39	10065.67	1229.74	13088.33	404.54	13458.33	115.85	9355.33	1182.79	8897.00	1206.71	9746.75	1339.72	10833.50	1339.72
trans- β -ocimene	83890.00	37919.77	123822.00	128.18	131514.67	1444.57	141542.00	1953.95	113718.33	163.93	97403.00	183.28	92818.50	342.27	42411.00	342.27
β -ocimene	27671.33	11012.60	41246.67	1984.84	42678.00	1453.04	44974.67	1163.36	45535.67	7011.76	29918.25	18630.05	29669.25	4842.03	5831.25	4842.03
Linalool	27711.67	14283.06	42462.33	437.26	48937.67	2013.17	51444.33	4970.95	46277.00	3331.40	46522.00	3821.80	43212.50	4146.12	43135.75	4146.12
trans-2-pinanol	0.00	0.00	2241.67	62.55	2472.67	102.51	2672.33	151.85	2184.33	311.37	2327.25	498.95	2048.00	271.89	2375.75	271.89
(+)-camphor	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	845.50	22.72	886.25	118.98	1095.50	118.98
(-)-4-terpineol	3538.33	2658.12	6335.67	628.45	7366.33	1182.48	6753.00	1165.03	6711.67	913.30	7569.75	740.79	6160.75	1429.16	5106.75	1429.16
linalyl acetate	11085.00	578.09	30464.33	2048.70	33356.33	1640.60	35130.00	4868.80	32609.33	2951.13	32613.75	1039.43	29184.75	4535.55	13035.00	4535.55
(Z,Z)- α -farnesene	0.00	0.00	0.00	0.00	730.33	40.43	353.33	22.59	953.00	192.32	969.75	211.32	608.00	232.26	769.00	232.26

Table S5. 22 Volatile headspace compounds (mean peak area \pm SD) of *Lavandula angustifolia* extracted by headspace and analyzed by GCMS at various incubation times of 0.0, 0.5, 1.0, 4.0, 24.0, 48.0, 72.0, and 96.0 hours for N1 samples

Compounds	T 0.0 mean	\pm SD	T 0.5 mean	\pm SD	T 1.0 mean	\pm SD	T 4.0 mean	\pm SD	T 24.0 mean	\pm SD	T 48.0 mean	\pm SD	T 72.0 mean	\pm SD	T 96.0 mean	\pm SD
α -thujene	0.0	0.0	0.0	0.0	0.0	0.0	487.2	67.3	1440.3	155.9	1698.0	114.3	1769.0	175.6	2321.5	234.8
α -phellandrene	164.4	19.7	160.8	37.7	476.0	69.8	4187.2	78.7	9912.3	166.2	11207.0	431.3	12642.7	125.9	11606.0	378.3
α -pinene	441.6	43.1	677.6	69.5	1428.8	18.6	9502.2	475.9	18757.7	1067.7	20935.3	1156.9	22813.0	362.7	23546.0	111.0
camphene	413.4	24.3	535.8	36.7	1635.0	35.8	7396.0	380.4	6861.3	527.4	7339.8	388.2	7442.7	239.0	7479.5	194.5
β -phellandrene	0.0	0.0	0.0	0.0	0.0	0.0	1832.8	205.4	2246.8	45.9	2594.0	93.4	2183.7	198.3	1772.8	32.3
β -pinene	0.0	0.0	0.0	0.0	0.0	0.0	3068.0	43.3	4313.8	210.1	3972.3	122.2	3814.3	382.0	3742.0	60.1
3-octanone	0.0	0.0	0.0	0.0	9489.2	56.2	13773.6	220.1	15740.8	488.9	16883.5	272.9	14454.0	368.9	11564.0	111.7
β -myrcene	0.0	0.0	0.0	0.0	0.0	0.0	11040.4	260.1	12588.9	123.1	14583.5	237.6	13340.5	227.0	12401.0	146.7
3-carene	499.2	62.2	808.0	94.1	2267.2	27.5	6893.0	395.5	8158.0	214.7	8769.0	187.7	8115.0	35.4	7341.0	26.4
hexylacetate	0.0	0.0	0.0	0.0	1651.0	51.5	6624.4	62.6	5838.8	727.9	6231.8	482.1	4714.0	635.6	4377.0	412.0
o-cymene	0.0	0.0	0.0	0.0	7759.6	14.4	16542.6	102.6	17203.8	1849.7	18614.0	562.1	18103.0	1400.0	18967.3	698.6
d-limonene	0.0	0.0	0.0	0.0	0.0	0.0	5440.4	227.0	6017.3	505.7	6732.3	103.9	5832.7	5.7	5536.0	96.2
eucalyptol	2245.0	35.2	4229.0	21.2	8513.4	21.4	11614.2	571.1	13679.8	664.6	15455.3	847.4	13342.0	1868.5	11709.5	4.9
trans- β -ocimene	9360.8	284.4	10442.8	384.0	25665.2	0.0	85786.0	1033.8	97151.5	3087.2	90941.0	3360.2	69638.0	608.1	56644.5	281.3
β -ocimene	6048.2	54.2	8953.4	14.1	9221.6	65.2	16113.4	1265.1	37426.5	519.6	38413.0	522.1	28894.0	2256.6	19718.8	272.2
γ -terpinene	0.0	0.0	0.0	0.0	2136.4	524.0	4522.0	1010.5	4026.5	236.0	3917.5	416.5	2559.3	218.5	1805.0	11.3
linalool	24447.0	165.7	27491.6	1858.4	40364.4	1434.9	41608.4	135.8	46421.8	1934.9	48336.0	410.0	37998.3	691.1	28883.5	74.2
(+)-camphor	712.8	111.5	1366.0	196.4	1336.4	177.7	1445.2	213.9	1727.6	418.0	3869.8	2624.0	3446.3	3526.5	2945.2	270.3
(-)-4-terpineol	3847.8	35.9	4676.6	153.5	5521.6	222.6	8055.4	570.8	5497.8	310.6	3067.8	36.2	2653.0	14.4	1930.3	4.2
linalyl acetate	23300.2	506.9	25989.2	817.9	37098.4	549.7	43265.0	963.9	40494.8	346.2	37454.3	132.2	28445.3	287.0	27575.5	135.1
trifluoroacetyl-lavandulol	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2666.5	199.7	3533.3	729.4	2580.0	98.0	3114.8	389.6
(Z,Z)- α -farnesene	478.4	86.8	472.8	60.0	373.0	93.4	659.2	337.1	602.3	183.0	566.5	50.4	497.0	39.9	457.0	180.8

Table S7. 18 Volatile headspace compounds (mean peak area \pm SD) of *Lavandula angustifolia* extracted by headspace and analyzed by GCMS at various incubation times of 0.0, 0.5, 1.0, 4.0, 24.0, 48.0, 72.0, and 96.0 hours for N5 samples.

Compounds	T 0.0 mean	\pm SD	T 0.5 mean	\pm SD	T 1.0 mean	\pm SD	T 4.0 mean	\pm SD	T 24.0 mean	\pm SD	T 48.0 mean	\pm SD	T 72.0 mean	\pm SD	T 96.0 mean	\pm SD
α -thujene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	674.60	39.26	741.60	114.77	1960.00	374.90	1524.25	28.34
α -phellandrene	0.00	0.00	0.00	0.00	0.00	0.00	1042.60	42.31	3046.60	1250.47	4465.00	267.55	8541.50	141.53	7699.75	245.10
α -pinene	0.00	0.00	0.00	0.00	758.20	250.08	4205.40	1741.42	13731.00	681.45	19008.80	932.41	24645.25	272.48	23613.25	315.81
camphene	0.00	0.00	0.00	0.00	467.20	413.05	2531.60	341.35	8129.60	634.65	10884.60	1872.30	12760.50	868.97	11618.75	329.13
β -phellandrene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1253.00	182.82	1636.60	310.19	1777.75	351.32	1397.75	57.41
β -pinene	0.00	0.00	0.00	0.00	0.00	0.00	695.80	99.25	1647.60	341.77	2340.80	262.71	2852.50	157.47	2267.00	163.58
β -myrcene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	12784.72	1887.73	14664.69	424.21	13423.85	319.58	12401.00	374.98
3-carene	0.00	0.00	0.00	0.00	0.00	0.00	1733.60	130.99	5116.60	630.51	6950.60	345.62	6909.00	34.42	4888.50	583.89
o-cymene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	240.00	103.85	420.40	102.78	15245.25	657.87	11521.75	378.94
d-limonene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	280.80	84.36	1195.60	144.72	3871.25	559.45	1439.25	86.90
eucalyptol	544.00	756.18	2253.40	685.27	5643.60	427.10	4761.40	133.63	10550.40	422.52	11671.80	223.26	7302.25	306.85	5888.50	46.34
trans- β -ocimene	0.00	0.00	0.00	0.00	0.00	0.00	1527.80	326.38	5231.60	327.56	5245.40	670.09	6435.25	47.38	227.50	43.93
β -ocimene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	450.40	109.98	681.60	279.46	402.75	17.00	403.00	57.58
linalool	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6095.50	77.98	4111.00	94.87
(+)-camphor	0.00	0.00	0.00	0.00	875.00	244.66	956.80	433.49	3137.99	259.93	6296.34	517.68	6072.60	420.12	4832.05	431.97
(-)-4-terpineol	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2648.00	15.45	1930.25	12.89
linalyl acetate	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5127.50	27.77	6217.50	47.05
(z,z)- α -farnesene	0.00	0.00	775.00	448.72	776.60	301.44	390.00	67.99	323.40	54.67	168.80	40.71	0.00	0.00	0.00	0.00

Table S8. 4 Volatile headspace compounds (mean peak area \pm SD) of *Lavandula angustifolia* extracted by headspace and analyzed by GCMS at various incubation times of 0.0, 0.5, 1.0, 4.0, 24.0, 48.0, 72.0, and 96.0 hours for N9 samples.

Compounds	T 0.0 mean	\pm SD	T 0.5 mean	\pm SD	T 1.0 mean	\pm SD	T 4.0 mean	\pm SD	T 24.0 mean	\pm SD	T 48.0 mean	\pm SD	T 72.0 mean	\pm SD	T 96.0 mean	\pm SD
α -phellandrene	401.60	82.40	512.00	92.04	529.40	65.11	686.00	180.20	710.8	75.69	711.80	116.40	750.20	92.49	796.60	68.04
α -pinene	1682.40	125.80	2310.40	152.73	2397.40	225.08	2606.20	141.56	2833	402.40	2990.20	320.94	3702.40	297.34	3606.80	357.39
camphene	569.00	134.86	663.60	117.62	880.20	232.12	1101.00	90.17	1092.2	84.86	1200.20	177.67	1388.80	65.03	1521.40	96.73
eucalyptol	229.40	49.60	298.40	116.98	643.40	188.31	691.40	159.03	698.4	107.40	766.00	100.57	812.60	126.19	775.20	193.98

Table S9. Emulsifier families, types, chemical names, and hydrophilic-lipophilic balance (HLB) value

	Emulsifier family	Type	Chemical name	HLB
(A)	Span	80	Sorbitan monooleate	4.3
(B)	Tween	20	Polyoxyethylene (20) sorbitan monolaurate	16.7
(C)	Span	20	Sorbitan monolaurate	8.6
(D)	PEG-200	N/A	Polyethylene glycol 200	8.2
(E)	Triton X 100	N/A	Polyethylene Glycol-p-isooctylphenyl Ether	13.5

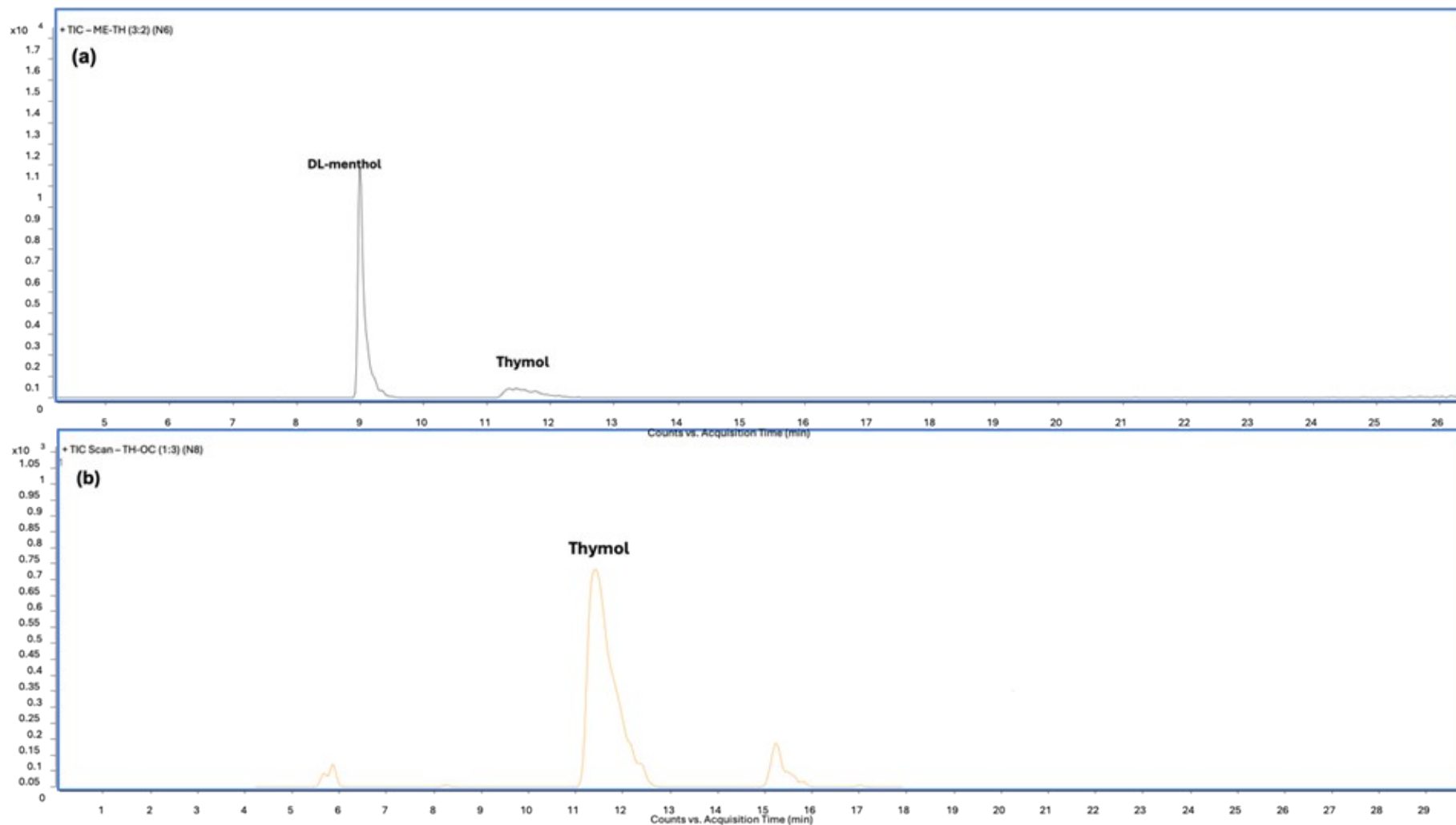
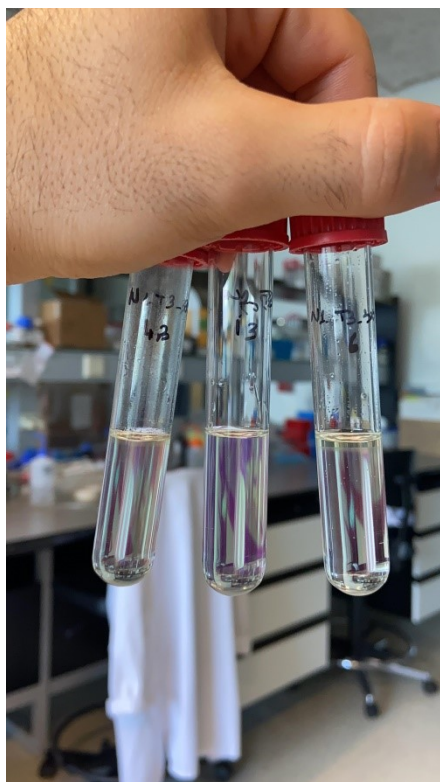
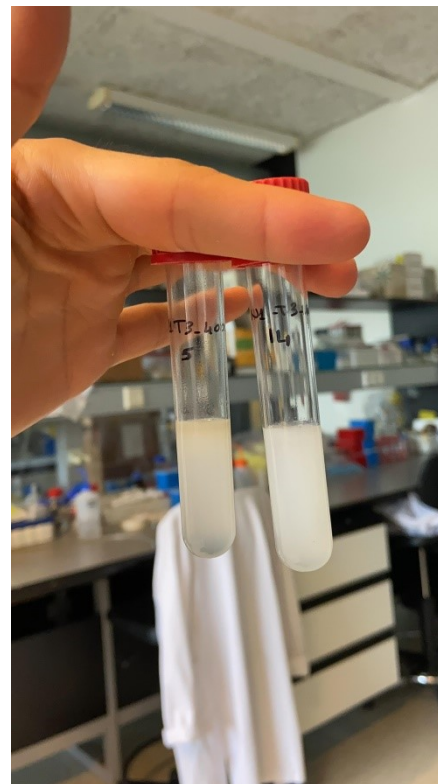


Figure S1. Total ion chromatograms for the volatile compounds of the two hydrophobic NADES: (a) Menthol-Thymol (3:2) (N6), (b) Thymol-Octanoic Acid (1:3) (N8)



a



b

Figure S2. Example of N1 phase separation; **a)** Clear formulation with different phase separations (60, 30, 90%, from left to right); **b)** Example of not clear formulation with phase separation.

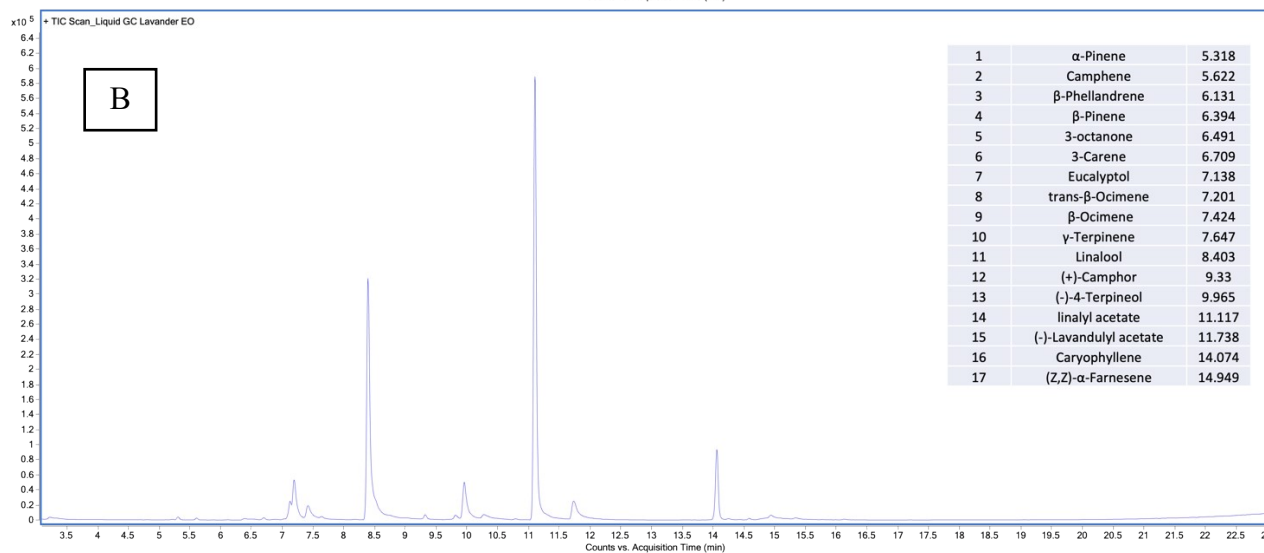
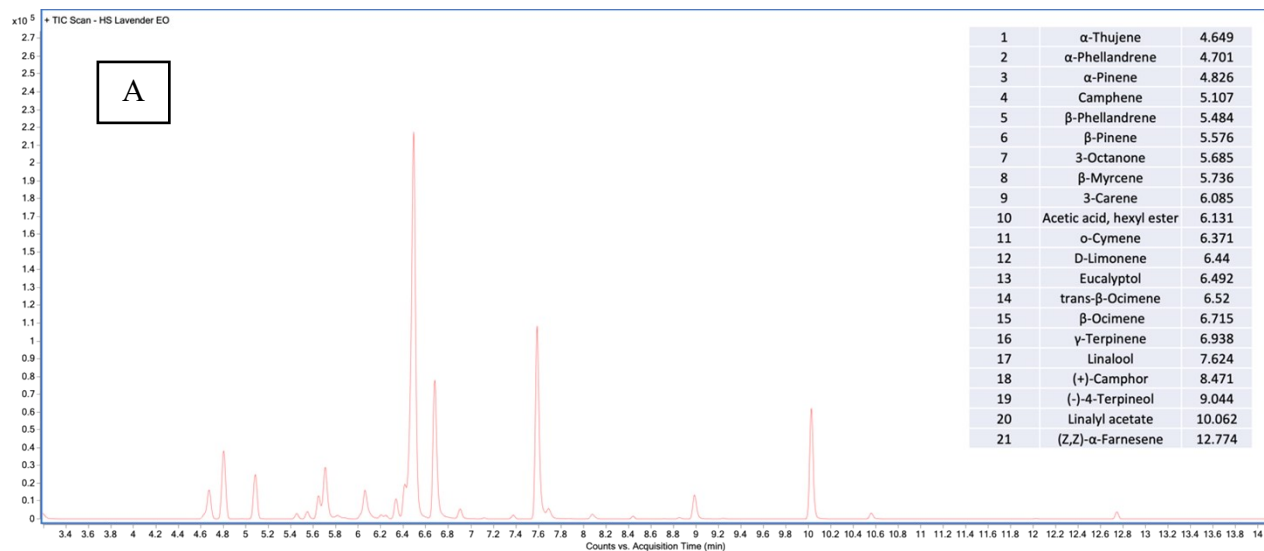


Figure S3. *Lavandula angustifolia* essential oil (LEO) Total Ion Chromatograms (TIC) profile showing: (A) Headspace GC/MS injection with a total of 21 identified peaks (used as control (C) in this study), and (B) Liquid GC/MS injection with a total of 17 identified compounds