

Nanoemulsions and solid microparticles containing pentyl cinnamate to control *Aedes aegypti*

Supplementary material

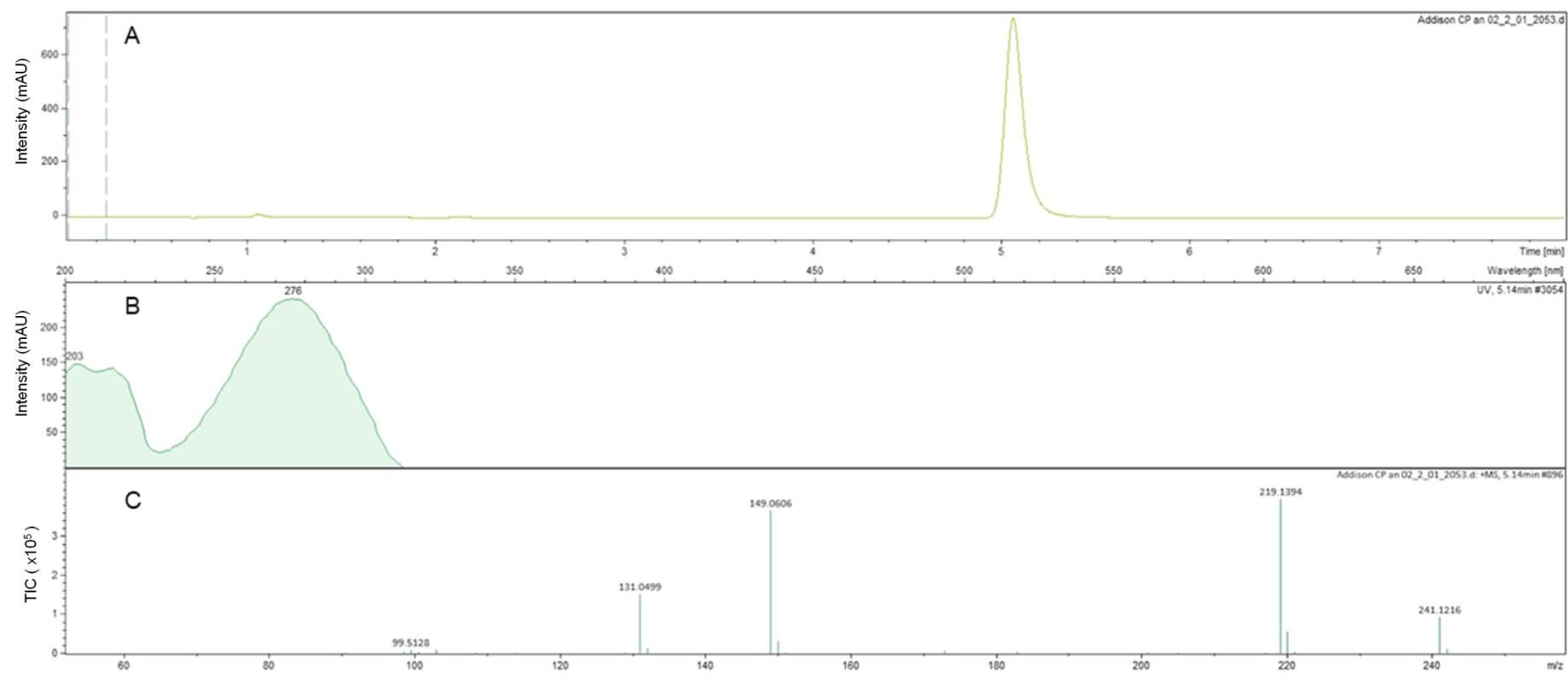


Figure S1. LC-MS/MS spectrum of pentyl cinnamate. In A: Total ion chromatogram obtained by the isocratic method in LC-MS/MS (ESI-QTOF), B and C: UV and mass spectrum spectrum for peak at 5.1 min, respectively. $[M+H]^+$ m/z 219.1394 (calcd. for $[C_{14}H_{19}O_2]^+$ m/z 219.1385, error 4.1 ppm).

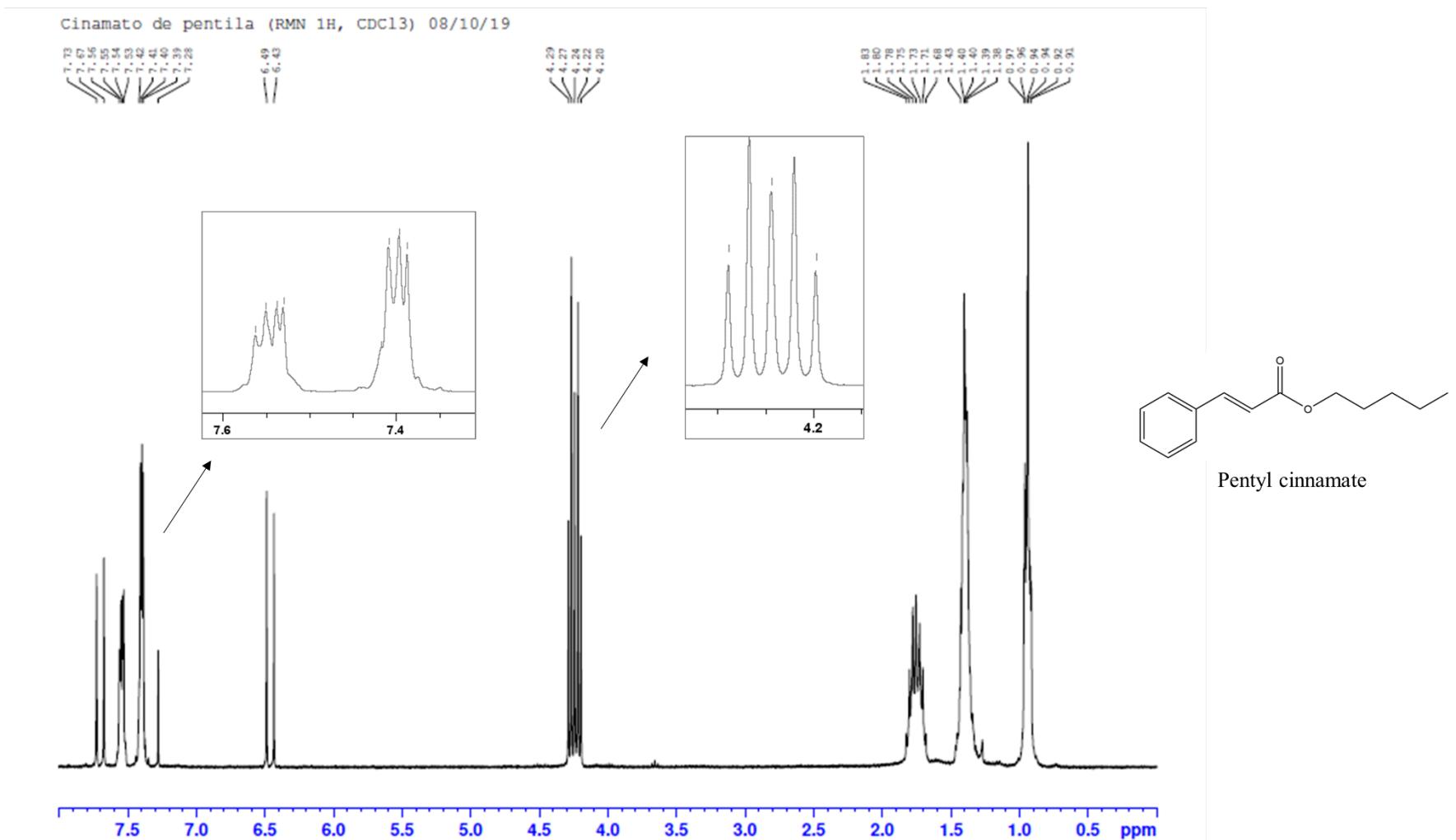


Figure S2. ¹H NMR (300 MHz) spectrum of pentyl cinnamate (PC) in CDCl₃.

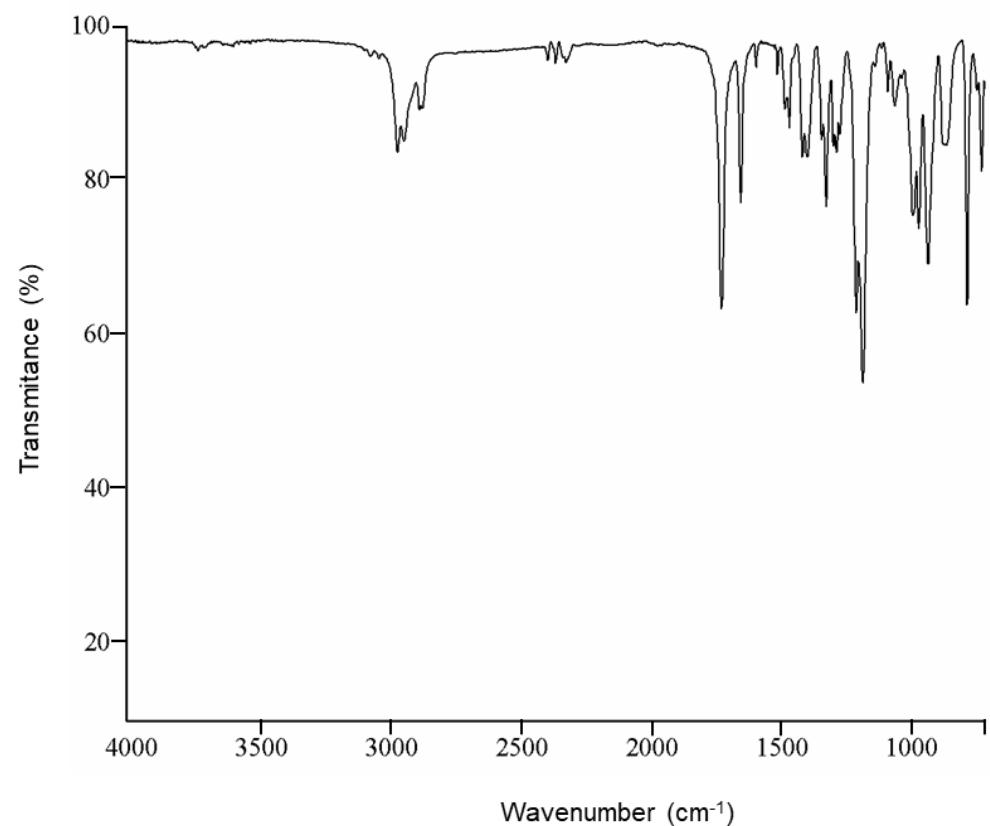


Figure S3. FTIR-ATR spectrum of pentyl cinnamate (PC) obtained in the range of 700-4000 cm^{-1} .

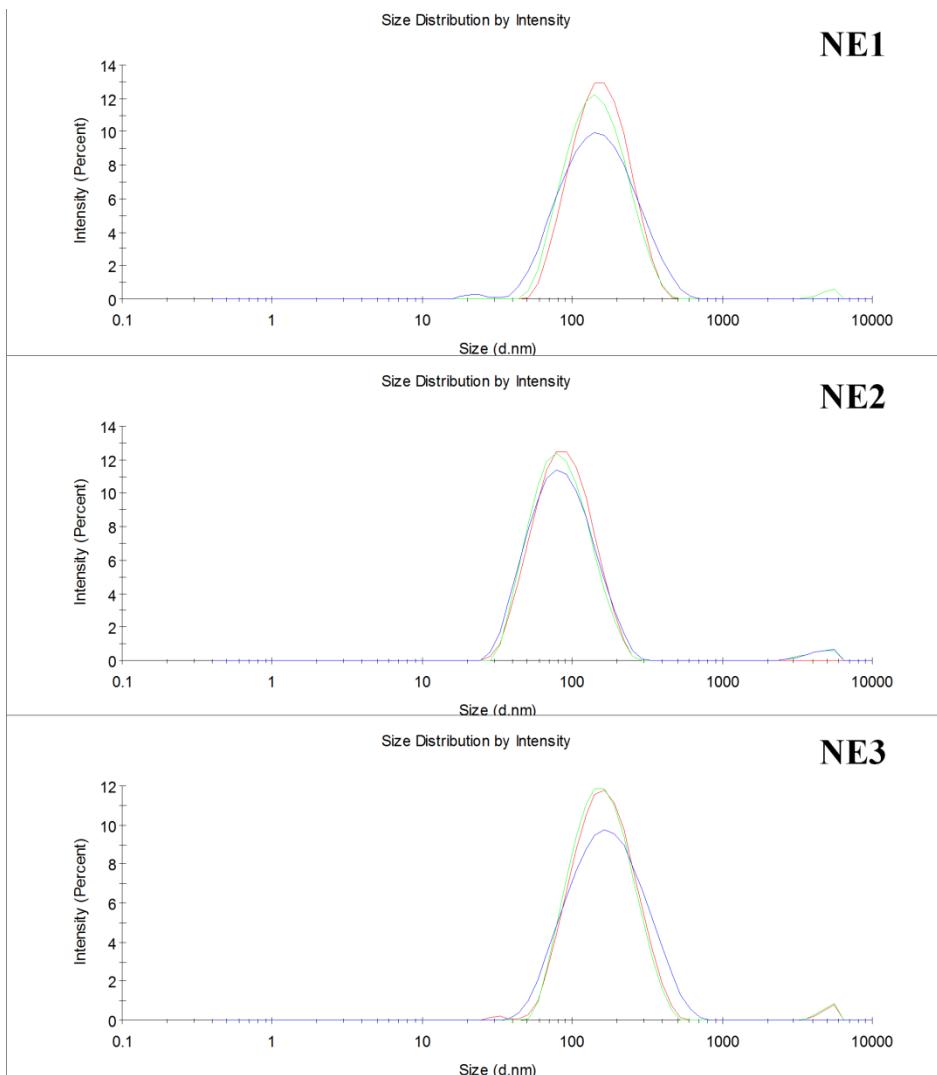


Figure S4. Size distribution of nanoemulsions NE1, NE2 and NE3 obtained by Dynamic light scattering (DLS).

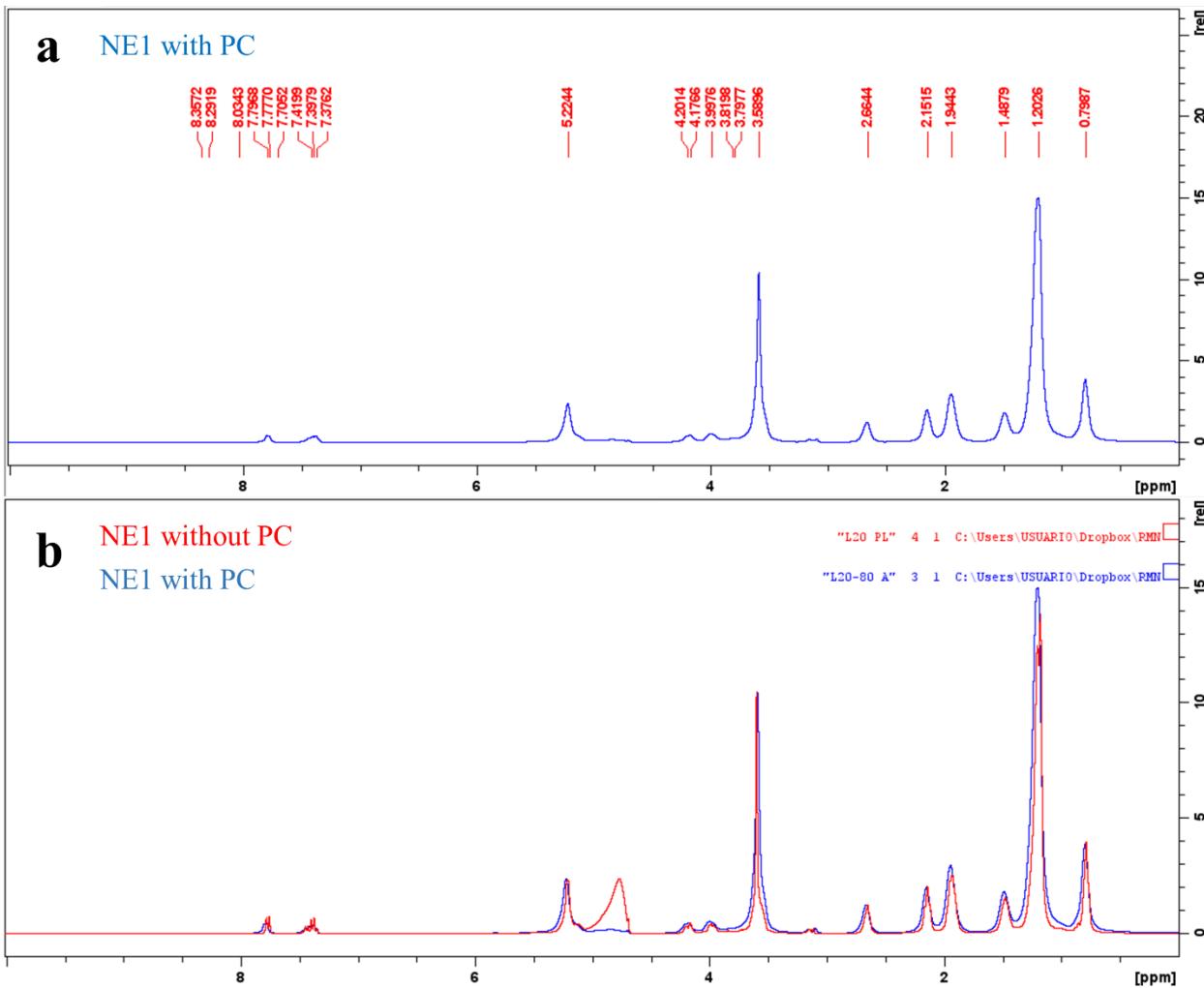


Figure S5. (a) ^1H NMR (300 MHz) spectra of NE1 with PC in D_2O and (b) superposition of ^1H NMR (300 MHz) spectra of NE1 with PC (blue) and without PC (red) in D_2O

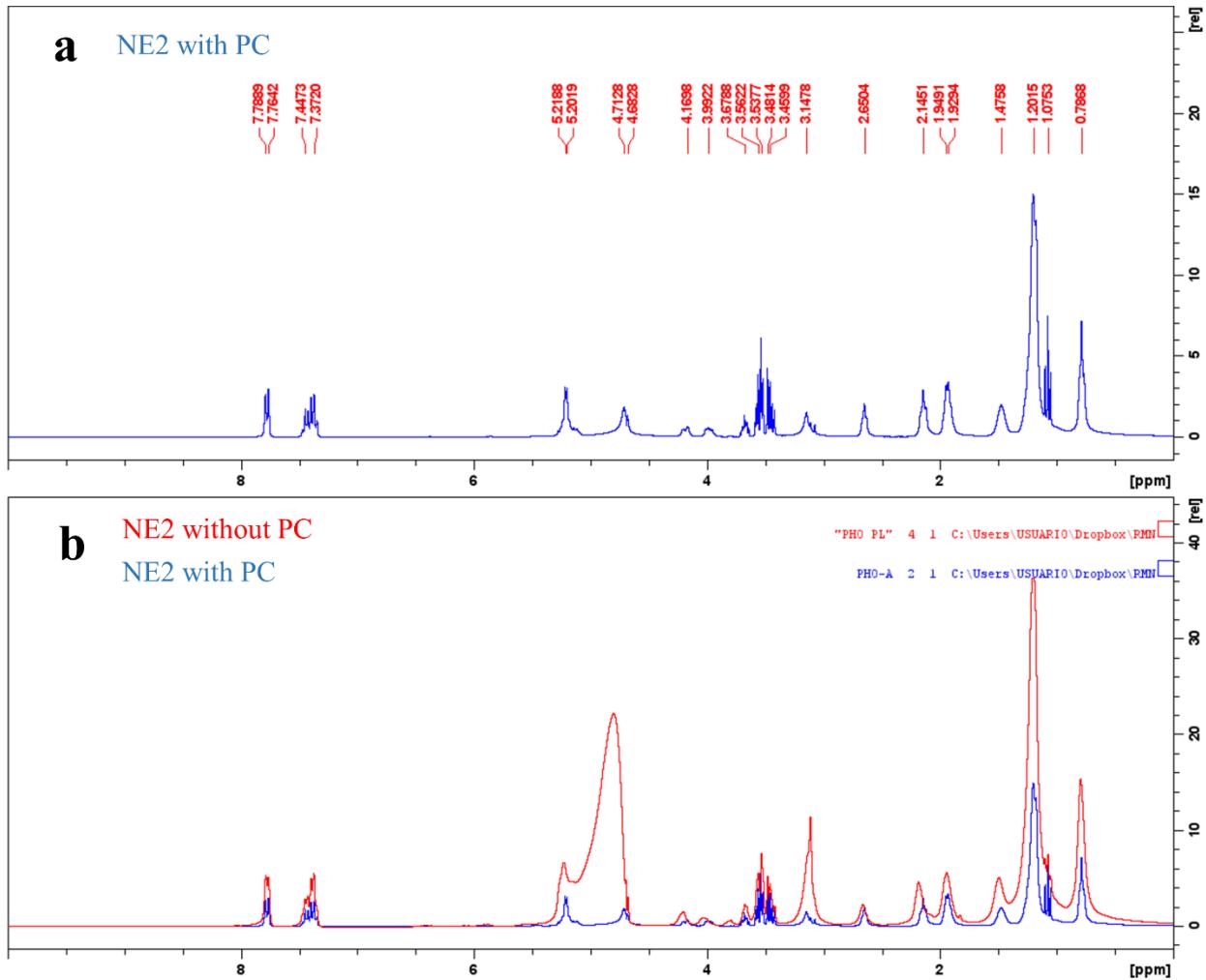


Figure S6. (a) ^1H NMR (300 MHz) spectra of NE2 with PC in D_2O and (b) superposition of ^1H NMR (300 MHz) spectra of NE2 with PC (blue) and without PC (red) in D_2O

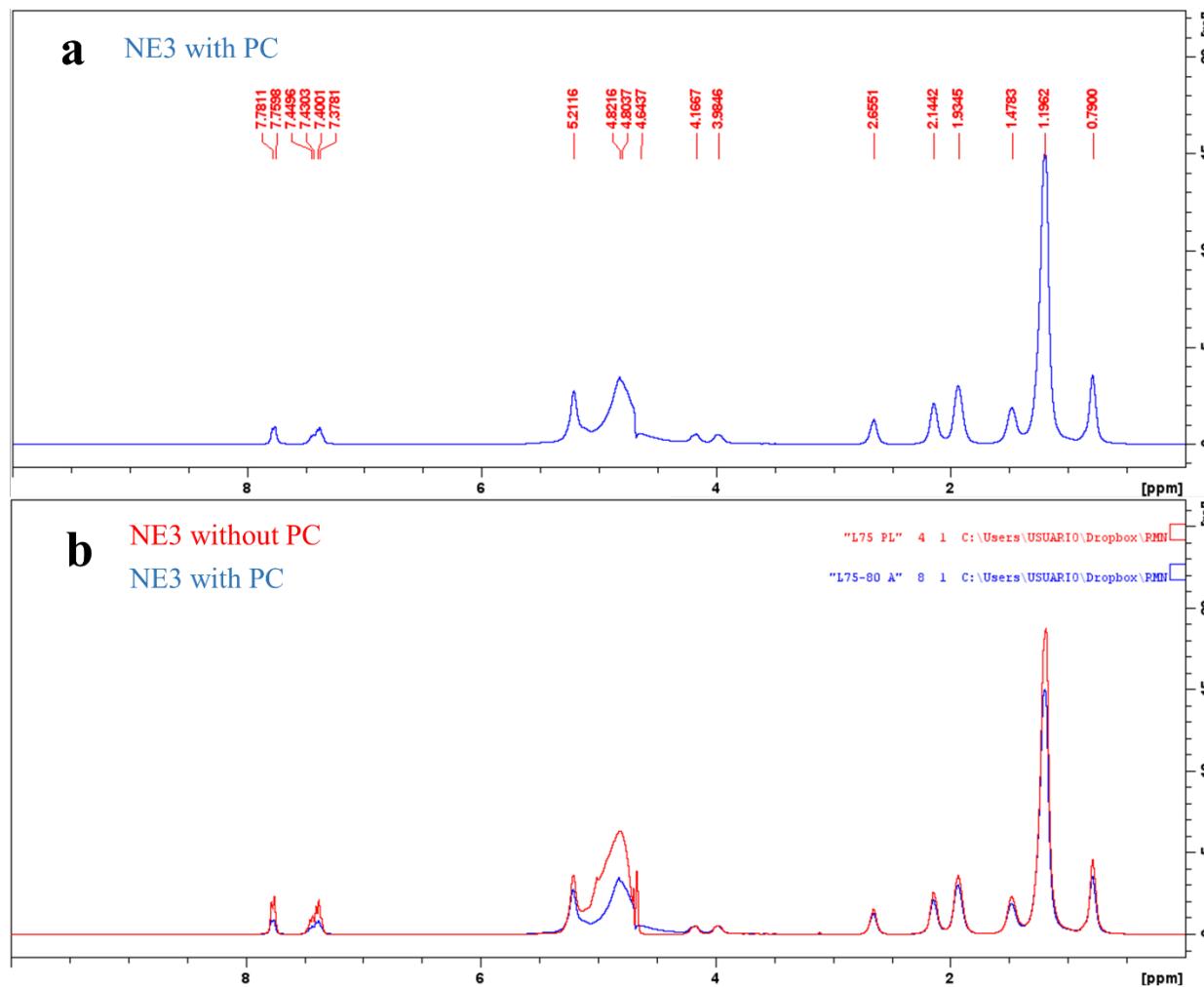


Figure S7. (a) ^1H NMR (300 MHz) spectra of NE3 with PC in D_2O and (b) superposition of ^1H NMR (300 MHz) spectra of NE3 with PC (blue) and without PC (red) in D_2O

Table S1 Composition of the nanoemulsions with the best results of particle size and PDI.

Sample	Sunflower oil (%)	Lecithin (%)	Tween 80 (%)	Water (%)	T. (°C)
NE1 A	5.0	1.5	1.5	91.5	60.0
NE1 B	5.0	1.75	1.25	91.5	25.0
NE2 A	0.0	5.0	0.0	94.5	25.0
NE2 B	0.0	5.0	0.5	94.0	50.0
NE3 A	5.0	1.5	0.0	93.0	25.0
NE3 B	5.0	1.5	0.5	92.5	60.0

Table S2 NMR data assignments for PC (CDCl_3 300/75 MHz)

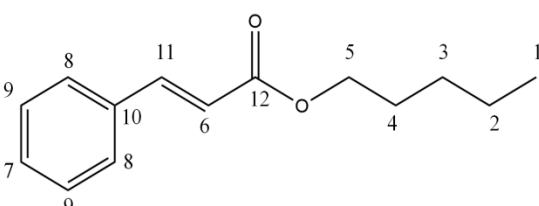
Pentil cinnamate		
Carbon signal	δ ^1H	δ ^{13}C
1	0.93 (3H, t, $J=7.2$ Hz)	14.1
2	1.38 - 1.43 (4H, m)	22.4
3		28.2
4	1.68 - 1.83 (2H, q, $J=6.8$ Hz)	28.5
5	4.20 - 4.29 (2H, m, $J= 6.8$ Hz)	64.8
6	6.46 (1H, d, $J=16$ Hz)	118.4
7	7.39 - 7.42 (3H, m)	128.1
8		129.0
9	7.53 - 7.55 (2H, dd)	130.3
10	-	134.5
11	7.70 (1H,d , $J=16$ Hz)	144.6
12	-	167.2

Table S3 Chemical shift (ppm) obtained by ^1H NMR (300 MHz) spectra of nanoemulsions NE1, NE2 and NE3 with PC and without PC.

Peak	NE1	NE1 with PC	NE2	NE2 with PC	NE3	NE3 with PC
1	7.781	7.787	7.786	7.788	7.779	7.781
2	7.755	7.762	7.763	7.764	7.756	7.759
3	7.473	-	7.449	7.447	7.450	7.449
4	7.449	7.449	7.428	-	7.428	7.430
5	7.426	7.427	7.397	-	7.399	7.400
6	7.398	7.397	7.374	7.372	7.376	7.378
7	7.373	7.374	5.227	5.218	5.207	5.211
8	7.350	7.349	-	5.201	5.010	-
9	5.216	5.213	4.800	-	4.816	4.821
10	5.206	-	-	4.712	4.806	4.803
11	4.771	4.766	-	4.682	4.697	-
12	-	4.695	4.203	-	4.667	4.643
13	4.196	4.196	-	4.169	4.194	-
14	4.165	4.163	4.026	3.992	4.165	4.166
15	4.004	4.001	3.674	3.678	3.986	3.984
16	3.987	3.984	3.661	-	2.653	2.655
17	3.968	3.965	3.560	3.562	2.142	2.144
18	3.951	-	3.533	3.537	1.931	1.934
19	3.598	3.599	3.478	3.481	1.476	1.478
20	-	3.149	3.457	3.459	1.184	-
21	-	3.112	-	3.147	-	1.196
22	2.651	2.649	3.112	-	0.788	0.790
23	2.142	2.139	2.664	2.650		
24	2.120	-	2.185	-		
25	1.948	1.928	-	2.145		

26	1.930	-	1.942	1.949		
27	1.478	1.474	-	1.929		
28	1.203	1.200	1.497	-		
29	1.177	1.175	-	1.475		
30	0.787	0.785	1.203	1.201		
31			1.073	1.075		
32			0.794	-		
33			-	0.786		

Table S4 Larvicidal activity of PC and nanoemulsions on larvae of *Aedes aegypti* after 24, 48 and 72 h.

Sample	Mortality (%)			Larvicidal Assay (LC ₅₀ µg/mL)		
	24 h	48 h	72 h	24 h	48 h	(CI)
PC	100	-	-	22.0 (20.0 to 24.0)	20.2 (17.9 to 22.5)	19.9 (16.4 to 22.9)
NE1	37.3	74.7	88.0	> 50.0	24.7 (19.3 to 32.7)	19.4 (19.1 to 19.9)
NE2	54.7	74.7	89.3	> 50.0	<6.25	<6.25
NE3	72.0	96.0	98.6	33.8 (30.7 to 37.2)	16.3 (13.5 to 19.9)	11.9 (9.8 to 15.3)
DMSO	0	0	0	nd	nd	nd

nd – not determined; LC - Lethal concentration; CI - Confidence interval.

Table S5 Tonset of decomposition of PC and solid microparticles.

Sample	Tonset (°C)
PC	97.0
MP1 PL	167.0
MP1 AT	181.0
MP2 PL	181.0
MP2 AT	180.0
MP3 PL	192.0
MP3 AT	177.0

* PL: solid microparticles without PC; AT: solid microparticles with PC.

Table S6 DSC data of PC and solid microparticles MP1, MP2 and MP3.

Sample	Peak (°C)	Heat (J/g)	Peak (°C)	Heat (J/g)	Peak (°C)	Heat (J/g)
PC	254.70	-	-	-	-	-
MP1 PL	83.48	143.70	231.36	3.10	233.45	3.31
MP1 AT	70.19	181.77	214.57	0.81	216.12	2.63
MP2 PL	67.89	198.66	230.19	5.49	233.44	0.58
MP2 AT	69.00	156.13	215.17	14.92	-	-
MP3 PL	84.14	176.89	230.42	1.17	236.83	13.36
MP3 AT	83.09	-	214.12	-	-	-

* PL: solid microparticles without PC; AT: solid microparticles with PC.