

Figure S6. ^1H NMR (500 MHz, CDCl_3) spectrum of the crude essential oil from specimen RN-3 (chemotype: limonene).

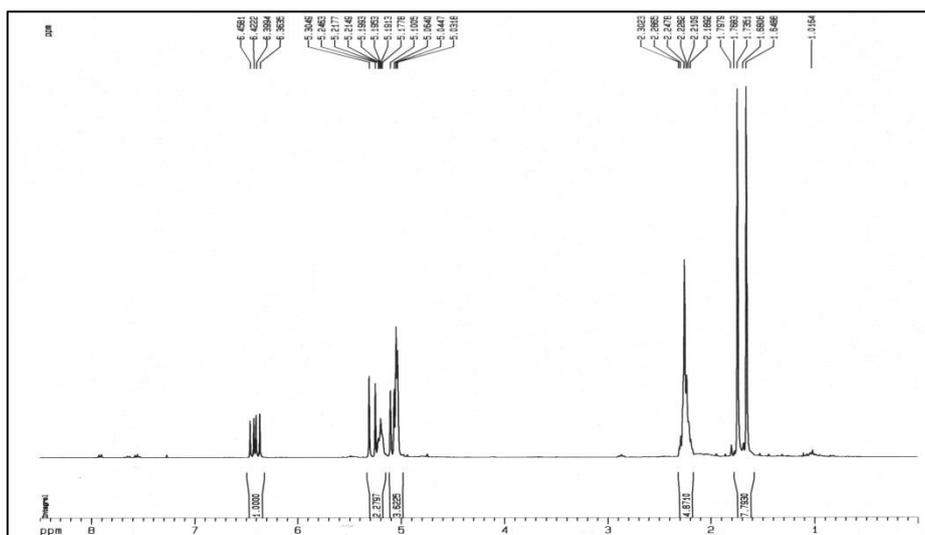


Figure S7. ^1H NMR (300 MHz, CDCl_3) spectrum of the crude essential oil from specimen BA-4 (chemotype: myrcene).

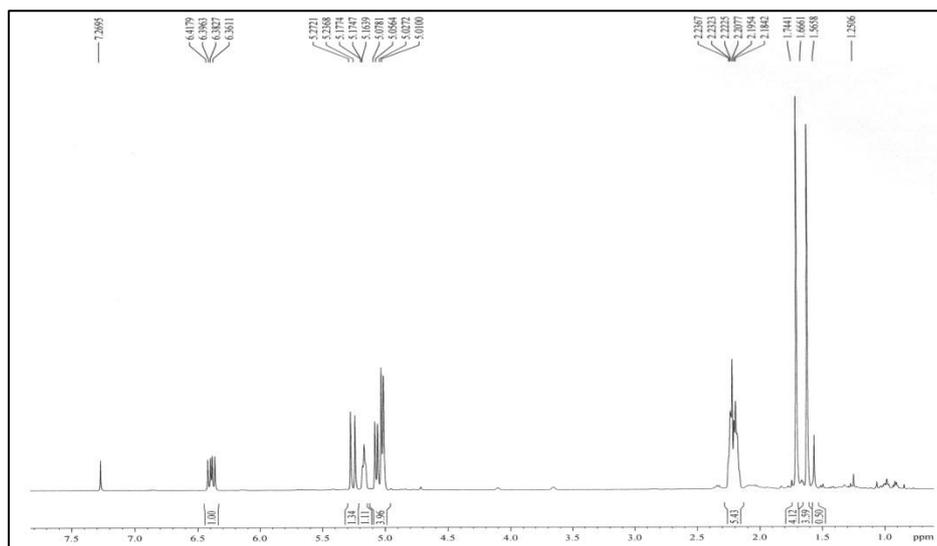


Figure S8. ^1H NMR (500 MHz, CDCl_3) spectrum of the crude essential oil from specimen RN-2 (chemotype: myrcene).

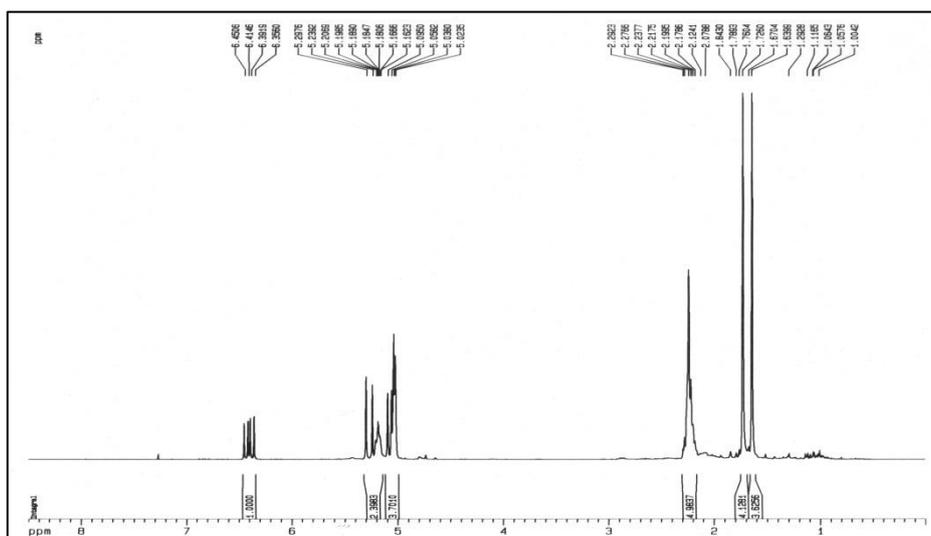


Figure S9. ^1H NMR (500 MHz, CDCl_3) spectrum of the crude essential oil from specimen PE-1 (chemotype: myrcene).

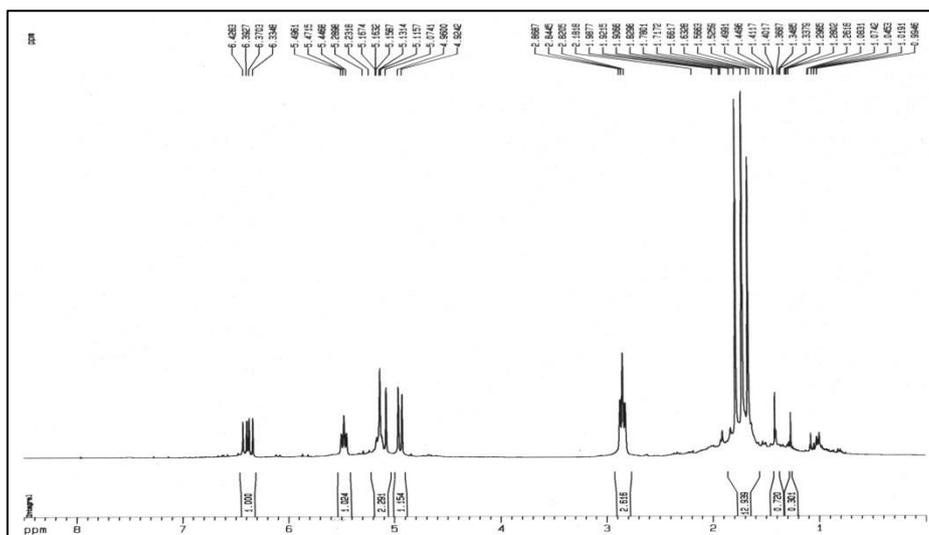


Figure S14. ^1H NMR (300 MHz, CDCl_3) spectrum of the crude essential oil from specimen CE-6 (chemotype: (*E*)- β -ocimene).

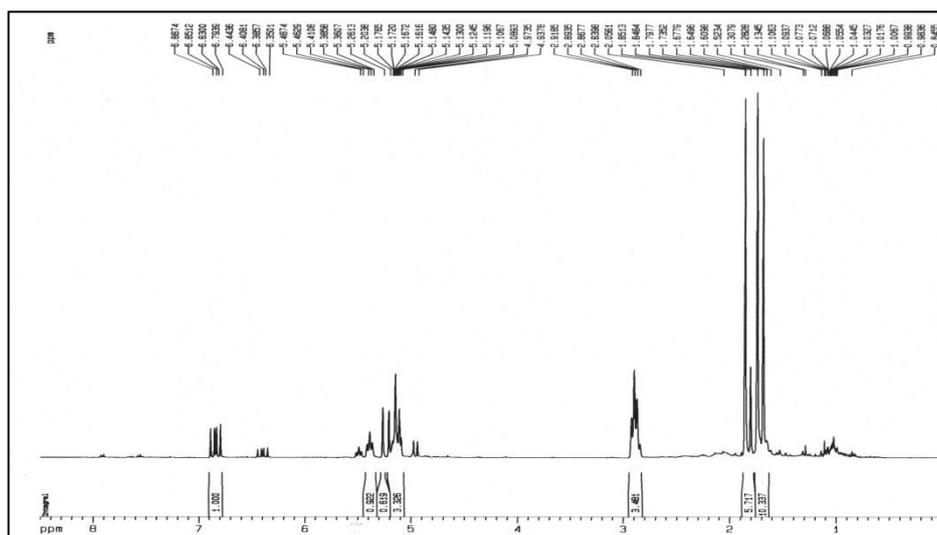


Figure S15. ^1H NMR (300 MHz, CDCl_3) spectrum of the crude essential oil from specimen BA-2 (chemotype: (*Z*)- β -ocimene).

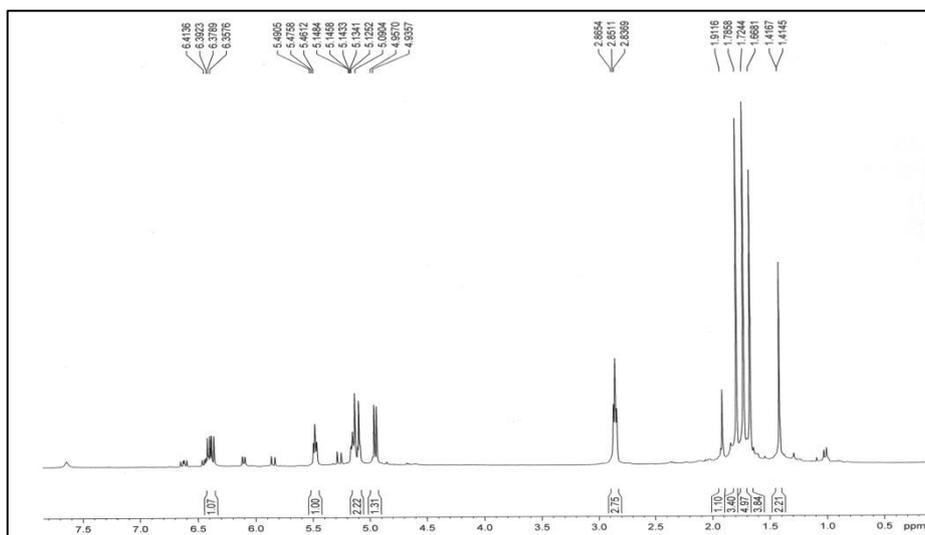


Figure S18. ¹H NMR (500 MHz, CDCl₃) spectrum of the crude essential oil from specimen CE-32 (chemotype: (*E*)-β-ocimene).

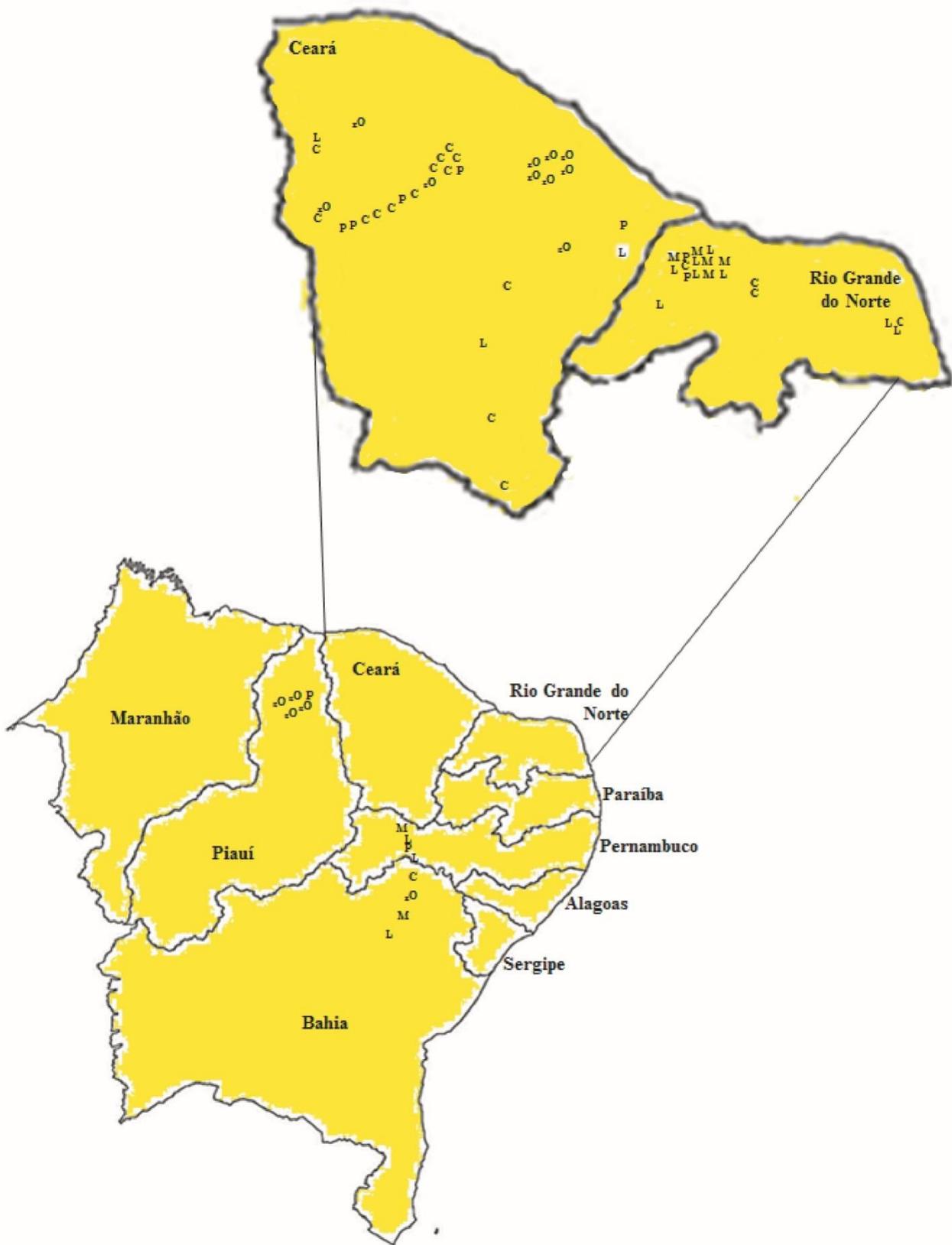


Figure S19. Map of the Northeast of Brazil (highlighting Ceará and Rio Grande do Norte States) detailing the collection points of leaves from wild specimens of “aroeiras-do-sertão” (chemotypes: myrcene (M), α -pinene (P), limonene (L), Δ^3 -carene (C), (Z)- β -ocimene (zO) and (E)- β -ocimene (E)).

Table S1. Experimental data of essential oils from leaves of 62 wild specimens of “aroeira-do-sertão” from locations at different states of Northeastern Brazil

Sample	Locality	Geographical coordinates		Date of collection	Weight (leaves) / g	Oil volume / mL	Yield / (% m/v)	Major constituent
		S	W					
Ceará State								
CE-1	Acarape	04°14.014'	38°37.656'	04/02/2010	410	0.8	0.19	(Z)- β -ocimene
				04/12/2010	455	0.5	0.12	(Z)- β -ocimene
CE-2	Acarape	04°14.001'	38°37.614'	04/02/2010	630	1.4	0.22	(Z)- β -ocimene
CE-3	Acarape	04°13.830'	38°37.655'	04/02/2012	530	0.9	0.16	Δ^3 -carene
				04/12/2010	390	0.3	0.07	Δ^3 -carene
CE-4	Russas	05°00.928'	37°47.817'	01/26/2010	1065	3.2	0.30	α -pinene
				01/29/2011	385	1.2	0.31	α -pinene
				02/10/2012	3000	9.3	0.31	α -pinene
CE-5	Acarape	04°13.897'	38°37.637'	02/04/2010	430	0.8	0.18	(Z)- β -ocimene
CE-6	Acarape	04°13.897'	38°37.637'	02/04/2010	465	0.8	0.17	(Z)- β -ocimene
CE-7	Tabuleiro do Norte	05°15.887'	38°03.746'	05/04/2010	635	1.4	0.22	limonene
CE-8	Crateús	05°12.315'	40°36.914'	05/11/2010	530	0.5	0.09	Δ^3 -carene
				05/21/2010	645	0.5	0.07	Δ^3 -carene
CE-9	Crateús	05°12.315'	40°36.914'	05/11/2010	580	0.5	0.08	(Z)- β -ocimene
				05/21/2010	1005	0.3	0.03	(Z)- β -ocimene
CE-10	highway BR-020	04°01.874'	38°59.483'	05/25/2010	575	0.8	0.13	α -pinene
CE-11	highway BR-020	04°09.157'	39°07.619'	05/25/2010	650	0.7	0.10	(E)- β -ocimene
CE-12	highway BR-020	04°25.743'	39°19.940'	05/25/2010	930	0.5	0.05	Δ^3 -carene
CE-13	highway BR-020	04°44.471'	39°28.181'	05/26/2010	690	1.4	0.20	α -pinene
CE-14	highway BR-020	04°55.910'	39°37.665'	05/26/2010	560	0.7	0.12	Δ^3 -carene
CE-15	highway BR-020	05°12.659'	39°47.765'	05/22/2010	575	0.5	0.08	Δ^3 -carene
CE-16	highway BR-020	05°12.659'	39°47.765'	05/22/2010	775	0.7	0.09	Δ^3 -carene
CE-17	highway BR-020	05°12.659'	39°47.765'	05/22/2010	610	0.9	0.14	α -pinene
CE-18	highway BR-116	05°25.617'	40°12.200'	05/26/2010	560	0.8	0.14	(E)- β -ocimene
CE-19	highway BR-116	05°15.646'	40°31.047'	05/26/2010	550	0.7	0.12	Δ^3 -carene
CE-20	highway BR-116	07°50.219'	39°05.221'	06/26/2010	430	0.6	0.13	limonene
CE-21	highway BR-116	05°17.113'	38°10.659'	06/26/2010	535	1.2	0.22	Δ^3 -carene
CE-22	highway BR-116	04°43.370'	38°05.182'	06/26/2010	505	0.6	0.12	Δ^3 -carene
CE-23	Cajueiro Jaburuna	03°53.408'	40°57.913'	08/28/2010	535	0.3	0.06	Δ^3 -carene
CE-24	Cajueiro Jaburuna	03°53.408'	40°57.913'	08/28/2010	565	0.3	0.06	limonene
CE-25	Paramoti	04°09.151'	39°07.196'	03/19/2011	775	1.5	0.19	Δ^3 -carene
CE-26	Paramoti	04°09.151'	39°07.196'	03/19/2011	780	1.6	0.20	Δ^3 -carene
CE-27	Paramoti	04°09.151'	39°07.196'	03/19/2011	740	1.5	0.20	Δ^3 -carene
CE-28	Paramoti	04°09.151'	39°07.196'	03/19/2011	530	0.7	0.14	α -pinene
CE-29	Paramoti	04°09.143'	39°06.954'	03/19/2011	905	1.3	0.14	Δ^3 -carene
CE-30	Paramoti	04°09.016'	39°06.553'	03/19/2011	1005	1.5	0.14	Δ^3 -carene
CE-31	Sobral	03°44.430'	40°29.665'	03/26/2011	665	0.7	0.10	(Z)- β -ocimene
CE-32	Acarape	05°02.992'	37°44.688'	01/19/2013	240	0.6	0.25	(E)- β -ocimene

Table S2. Experimental data of essential oils from leaves of 62 wild specimens of “aroeira-do-sertão” from locations at different states of Northeastern Brazil (cont.)

Sample	Locality	Geographical coordinates		Date of collection	Weight (leaves) / g	Oil volume / mL	Yield / (% m/v)	Major constituent
		S	W					
Rio Grande do Norte State								
RN-1	Baraúna	05°09.498'	37°26.055'	01/29/2010	380	0.8	0.21	limonene
RN-2	Baraúna	05°01.356'	37°43.371'	01/29/2010	725	2.0	0.27	myrcene
				05/04/2010	535	0.4	0.07	myrcene
				01/26/2011	1150	3.1	0.27	myrcene
				02/10/2012	3000	3.7	0.12	myrcene
RN-3	São José de Mipibu	06°08.785'	35°13.681'	01/29/2010	350	0.5	0.14	limonene
RN-4	São José de Mipibu	06°08.785'	35°13.681'	01/29/2010	595	1.1	0.18	Δ^3 -carene
RN-5	São José de Mipibu	06°08.785'	35°13.681'	01/29/2010	735	0.6	0.08	Δ^3 -carene
RN-6	Apodi	05°13.371'	37°49.310'	04/05/2010	545	0.9	0.16	limonene
RN-7	Baraúna	05°01.628'	37°42.397'	04/05/2010	595	1.1	0.18	Δ^3 -carene
				01/27/2011	1015	3.4	0.33	Δ^3 -carene
RN-8	Baraúna	05°02.938'	37°44.721'	05/04/2010	710	1.0	0.14	limonene
				01/27/2011	990	3.6	0.36	limonene
RN-9	Baraúna	05°02.989'	37°44.708'	09/22/2010	220	0.3	0.15	myrcene
RN-10	Baraúna	05°02.259'	37°41.768'	01/21/2011	720	1.0	0.13	limonene
RN-11	Mossoró	05°09.136'	37°26.048'	08/08/2013	780	1.9	0.24	Δ^3 -carene
RN-12	Mossoró	05°06.497'	37°26.591'	08/08/2013	940	2.1	0.22	Δ^3 -carene
RN-13	Baraúna	05°02.969'	37°44.835'	08/08/2013	875	1.2	0.13	limonene
RN-14	Baraúna	05°05.686'	37°35.260'	01/30/2014	1020	3.1	0.30	α -pinene
RN-15	Baraúna	05°05.668'	37°35.436'	01/30/2014	1020	2.8	0.30	α -pinene
RN-16	Baraúna	05°02.462'	37°41.491'	01/30/2014	1010	3.4	0.33	limonene
RN-17	Baraúna	05°02.260'	37°41.767'	01/30/2014	785	1.7	0.21	α -pinene
Bahia State								
BA-1	highway BR-116	11°12.046'	40°02.402'	06/25/2010	685	1.4	0.20	Δ^3 -carene
BA-2	highway BR-116	10°51.381'	40°06.722'	06/25/2010	615	1.0	0.16	(Z)- β -ocimene
BA-3	highway BR-116	09°42.874'	40°10.229'	06/25/2010	585	1.5	0.25	myrcene
BA-4	highway BR-116	09°41.892'	40°22.228'	06/25/2010	475	0.6	0.12	limonene
Pernambuco State								
PE-1	highway BR-116	09°09.728'	40°21.940'	06/25/2010	395	0.6	0.15	myrcene
PE-2	highway BR-116	08°53.853'	40°02.685'	06/26/2010	400	0.4	0.10	limonene
PE-3	highway BR-116	08°36.790'	39°40.126'	06/26/2010	280	0.5	0.17	α -pinene
PE-4	highway BR-116	08°32.387'	08°14.593'	06/26/2010	495	0.4	0.08	limonene
Piauí State								
PI-1	highway BR-222	03°58.651'	41°20.707'	03/26/2011	745	0.6	0.08	(E)- β -ocimene
PI-2	highway BR-222	03°57.449'	41°17.137'	03/26/2011	840	0.7	0.08	α -pinene
PI-3	Piripiri	70°58.220'	59°24.197'	01/23/2014	645	1.7	0.26	(E)- β -ocimene
PI-4	Piracuruca	03°43.498'	41°40.883'	01/23/2014	845	2.0	0.23	(E)- β -ocimene
PI-5	Piracuruca	03°43.498'	41°40.883'	01/23/2014	666	0.7	0.10	(E)- β -ocimene

Table S2. ^{13}C NMR data (ppm, 125 MHz, CDCl_3) representative of the major constituents of the essential oils from the whole fresh leaves of *M. urundeuva*, and comparison with literature data^{1,2}

C	OEFA CE-3	Δ^3 -Carene	OEFA RN-8	Limonene	OEFA RN-2	Myrcene	OEFA CE-4	α -Pinene	OEFA CE-2	(Z)- β - Ocimene	OEFA CE- 32 ^a
C-1	131.4	131.3	150.3	150.2	146.3	146.1	144.7	144.4	133.8	133.8	141.7
C-2	119.7	119.4	133.8	133.7	139.2	139.0	116.2	116.0	132.1	132.1	133.7
C-3	28.5	28.3	120.8	120.6	131.9	131.7	47.2	47.1	132.1	131.8	132.4
C-4	25.0	24.3	108.5	108.4	124.3	124.1	40.9	40.8	129.8	129.9	126.4
C-5	23.8	23.7	41.1	41.1	115.8	115.6	38.1	38.0	122.7	122.8	122.4
C-6	21.0	20.8	31.0	30.9	113.2	113.0	31.6	31.5	113.6	113.4	110.6
C-7	18.8	18.5	30.8	30.6	31.6	31.5	31.4	31.3	26.6	26.6	27.5
C-8	16.9	16.7	28.1	28.0	26.9	26.8	26.5	26.4	25.8	25.7	25.8
C-9	16.9	16.6	23.6	23.5	25.8	25.7	23.1	23.0	19.9	19.8	24.5
C-10	13.3	13.2	20.9	20.9	17.8	17.7	21.0	20.8	17.8	17.7	11.9

^a ^{13}C NMR data for (*E*)- β -ocimene has not been reported previously.

References

1. Chang, C. W. J.; Flament, I.; Matson, J. A.; Nishida, T.; Ohloff, G.; Wehrli, F. W.; Weinheimer, A. J.; *Progress in the Chemistry of Organic Natural Products*, vol. 36; Herz, W.; Grisebach, H.; Kirby, G. W., eds.; Springer-Verlag: New York, USA, 1979.
2. Pouchert, C. J.; Behnke, J.; *The Aldrich Library of ^{13}C and ^1H FT-NMR Spectra*, vol. 1, 1st ed.; Aldrich Chemical Co.: Milwaukee, 1983.