

Supplementary Information

Insecticidal and Acaricidal Activity of Essential Oils Rich in (*E*)-Nerolidol from *Melaleuca leucadendra* Occurring in the State of Pernambuco (Brazil) and Effects on Two Important Agricultural Pests

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Isolation of (*E*)-nerolidol ((*E*)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol)

Essential oil (300 mg) of *M. leucadendra* was subjected to column chromatography with silica gel column (70-230 mesh). Gradient elution was applied using hexane and ethyl acetate mixtures in various ratios (100:0, 75:25, 65:35, 50:50 and 0:100) with increasing polarities, as the mobile phase. In total, eighteen fractions (10 mL each) were collected, of which 6 to 10 corresponded to (*E*)-nerolidol. These fractions were combined and the solvent was removed under reduced pressure using a rotator evaporator to produce pure (*E*)-nerolidol.

(*E*)-Nerolidol data

Pale yellow oil; $[\alpha]_D^{25} +13.3$ (*c* 1, CH₂Cl₂); IR (KBr) ν_{max} / cm⁻¹ 3389, 3085, 2968, 2924, 2855, 1670, 1641, 1450, 1411, 1375, 1108, 994, 919, 837, 689; EI/MS, *m/z* (rel. int) [M]⁺: 69 (100), 41 (86), 93 (69), 107 (31), 55 (35), 81 (29), 136 (17), 161 (17), 121 (18), 148 (7), 179 (5), 189 (4), 204 (1); ¹H NMR (300 MHz, CDCl₃) δ 5.92 (dd, 1H, *J* 17.4, 10.8, CH), 5.20 (dd, 1H, *J* 17.3, 1.2, CH₂), 4.99 (dd, 1H, *J* 10.8, 1.2, CH₂), 5.18-5.03 (m, overlapping with, 1H, CH), 5.03-5.13 (m, overlapping with, 1H, CH), 2.20-2.01 (m, 2H, CH₂), 1.96-1.58 (m, 2H, CH₂), 1.94-1.58 (m, 2H, CH₂), 1.67 (s, 3H, CH₃), 1.59 (s, 3H), 1.58 (s, 3H, CH₃), 1.55 (m, 2H, CH₃), 1.27 (s, 3H, CH₃); ¹³C NMR (75 MHz, CDCl₃) δ 144.98 (C-2), 135.54 (C-7), 131.41 (C-11), 124.17 (C-6) 124.17 (C-10), 111.64 (C-1), 73.48 (C-3), 41.97 (C-4), 39.65 (C-8), 27.84 (C-13), 26.58 (C-9), 25.67 (C-12), 22.67 (C-5), 17.65 (C-15), 15.97 (C-14).

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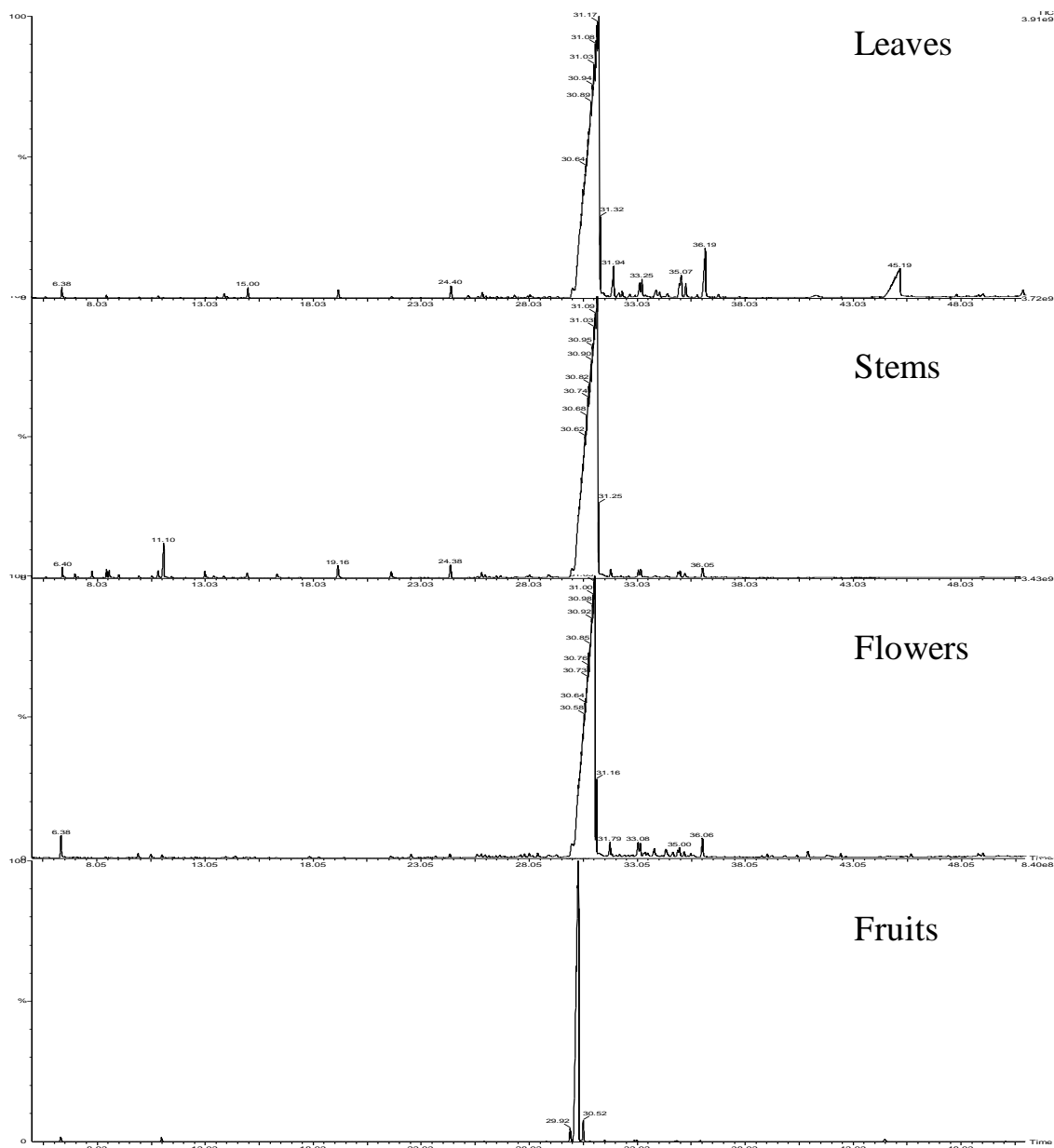


Figure S1. GC-MS chromatogram of volatile oil from leaves, stems, flowers and fruits of *M. leucadendra* obtained using DB-5 column.

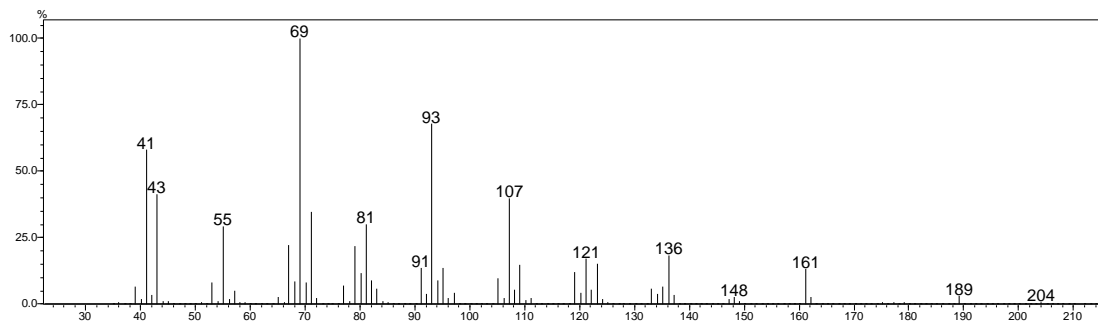


Figure S2. EIMS spectrum of (*E*)-nerolidol.

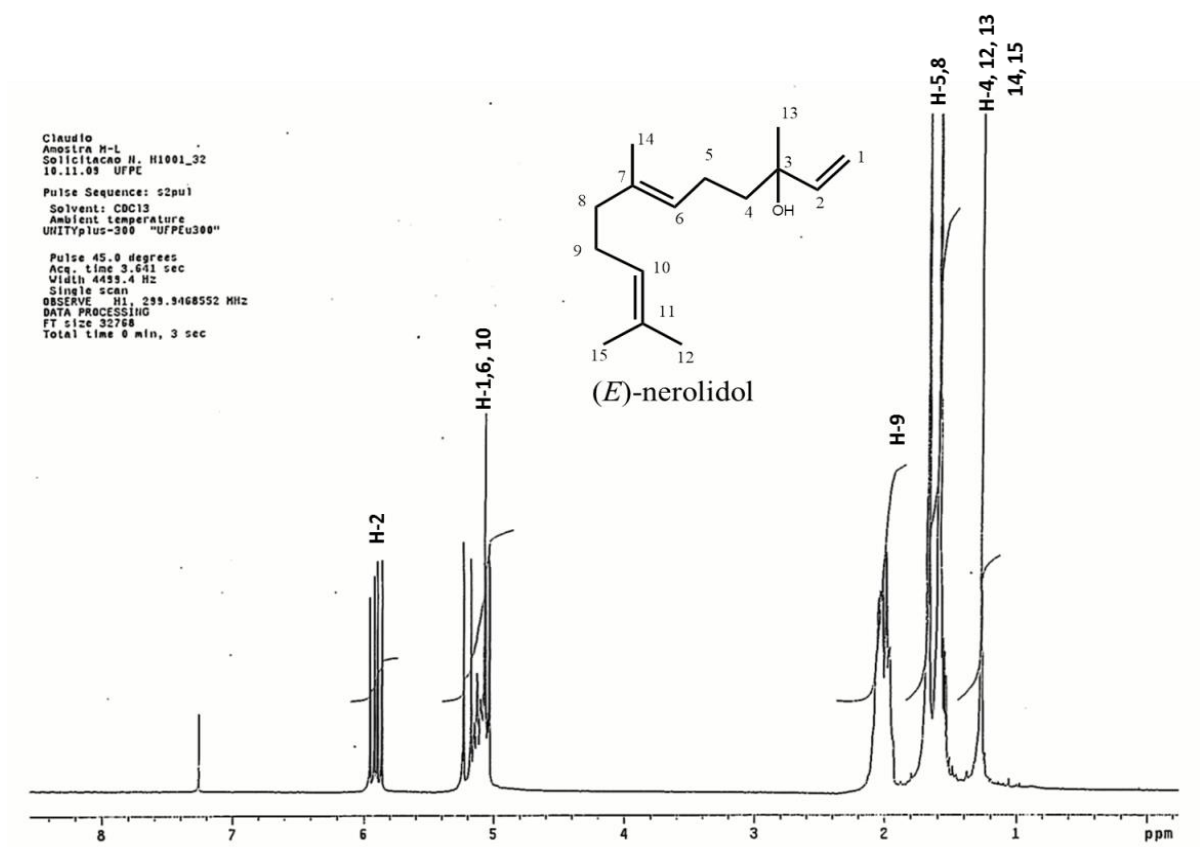


Figure S3. ^1H NMR (300 MHz, CDCl_3) spectrum of (*E*)-nerolidol.

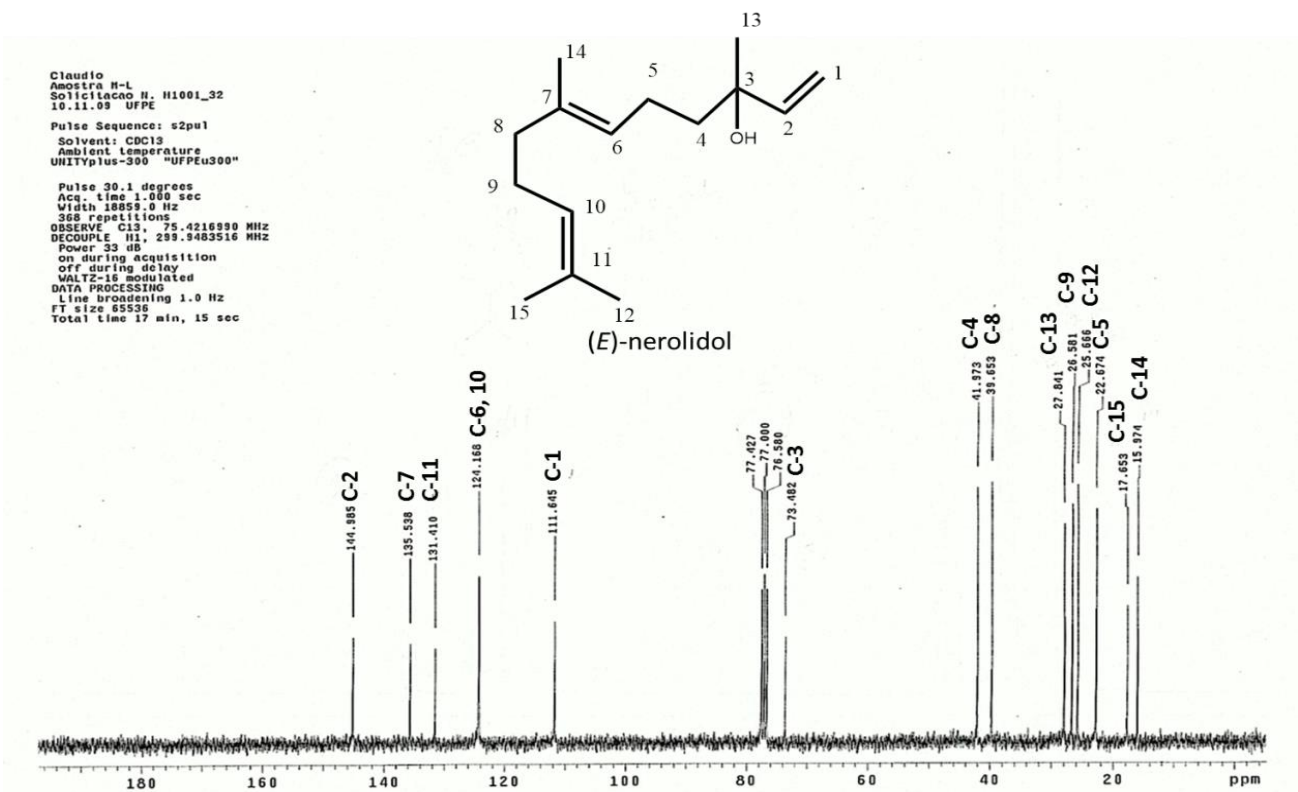


Figure S4. ^{13}C NMR (75 MHz, CDCl_3) spectrum of (*E*)-nerolidol.

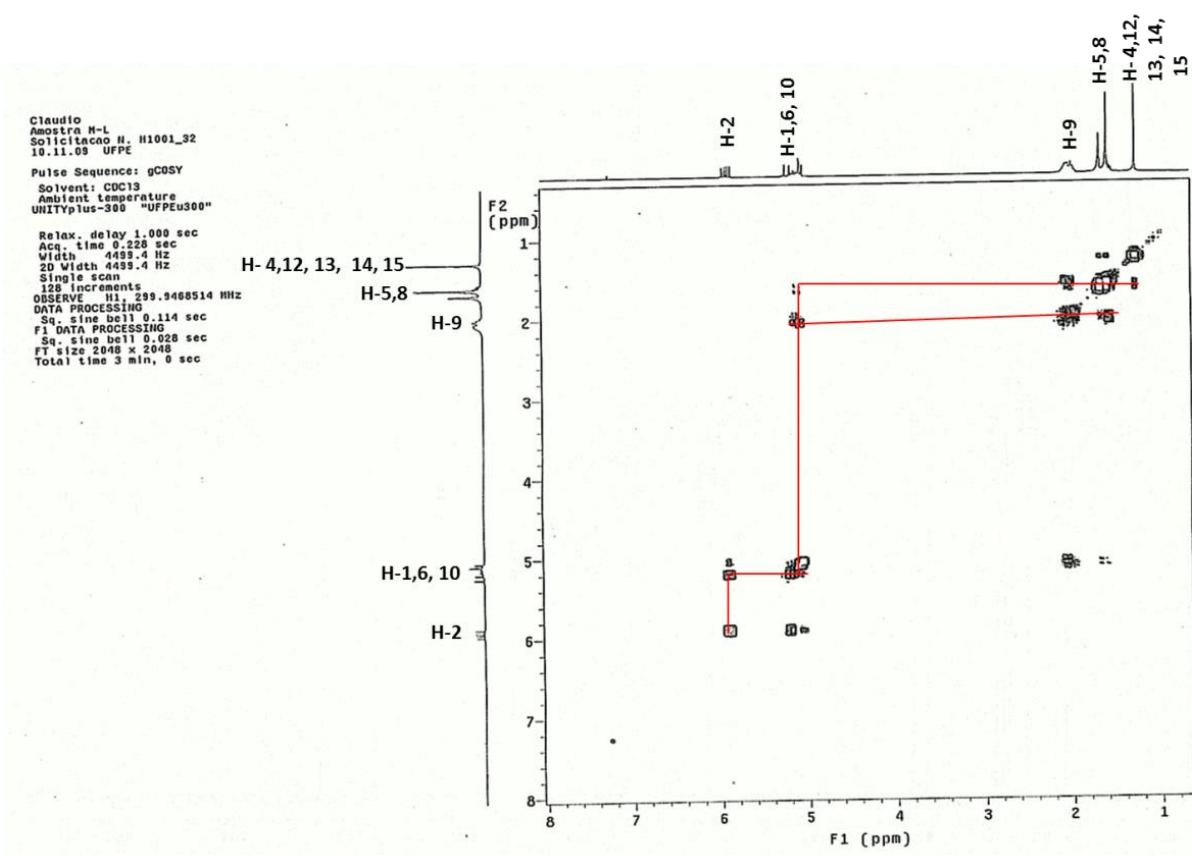


Figure S5. COSY spectrum of (*E*)-nerolidol.

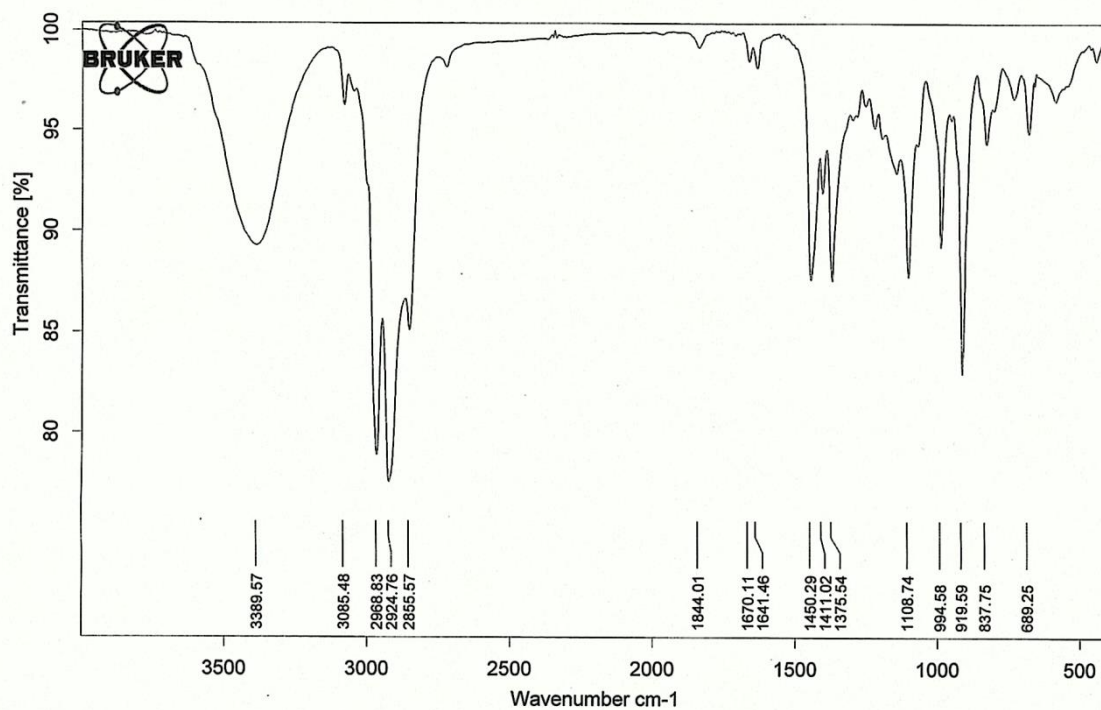


Figure S6. Infrared spectrum (KBr) of (*E*)-nerolidol.