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Notes and Comments

Chemical composition of leaf and branch extracts of the wild tomato *Solanum habrochaites* (Solanaceae)

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Secondary plant metabolites can cause repellence, food and oviposition deterrence, sterilization, metabolism blockage, and interference in the development and death of insects (Saeidi et al., 2012). The wild tomato *Solanum habrochaites* Knapp & Spooner (Solanaceae) is resistant to pests (Saeidi et al., 2012) such as *Manduca sexta* L. (Lepidoptera: Sphingidae), *Heliothis zea* Boddie (Lepidoptera: Noctuide) and *Leptinotarsa decemlineata* Say (Coleoptera: Chrysomelidae) (Williams et al., 1980), *Tuta absoluta* Meyrick (Lepidoptera: Gelechiidae) (Leite et al., 2001), *Keiferia lycopersicella* Walsingham (Lepidoptera: Gelechiidae) and *Spodoptera exigua* Hübner (Lepidoptera: Noctuidae) (Lin et al., 1987). The high density of type IV glandular trichomes (Simmons and Gurr, 2005) with synthesis, storage and secretion of secondary metabolites (Ben-Israel et al., 2009) is related to the resistance of this plant to insects.

The objective was to identify bioactive constituents of *Solanum habrochaites* extracts, a wild tomato species resistant to pests and with potential, for the development of formulations that can be used in pest management.

The research was carried out at the chemistry department of the "Universidade Federal de Viçosa (UFV)" and at the "Instituto de Biotecnologia Aplicada à Agropecuária (BIOAGRO/UFV)" in Viçosa, Minas Gerais State, Brazil.

Leaves and branches of *S. habrochaites* were collected in an area of the UFV, dried in a ventilated oven at 40 °C, cold macerated and extracted with 98% ethanol (3 L) for seven days. This procedure was carried out in triplicate and the ethanolic extracts were combined, dried with anhydrous sodium sulfate (Na_2SO_4) and the solvent removed in a rotary evaporator, obtaining 58.936 grams of crude extract of *S. habrochaites*.

Extractions and chromatographic procedures were performed with previously distilled analytical grade solvents. Vacuum and open column chromatographic separations were performed with silica gel 60 (70-230 or 230-400 mesh) as the stationary stage. Analytical thin layer chromatography was performed using 0.25 mm thick silica gel 60GF254 plates under ultraviolet light (254 and 366 nm) followed by immersion in an acidic vanillin solution. Gas chromatography, coupled with mass spectrometry, was performed in a Shimadzu chromatograph, model CG-EM QP 5000A, equipped with a Supelco DB-5 capillary column (30m x 0.25mm x 0.25µm), under the operating conditions of: method by electron impact (70 eV); scan mode, m/z 30.00 to 700.00; carrier gas flow (He) 1.6 mL min-1; split ratio 1:2, temperature programming from T1= 40 ºC for 2 min., gradient from 20 ºC min-1 to T2= 300 ºC; injector and detector temperatures of 290ºC. The chemical constituents of the leaf and branch extracts of *S. habrochaites* were identified by comparing their mass spectra with data from the equipment library and their calculated retention index with values from literature. Only compounds with mass spectra at least with 90% similarity with data from the equipment library were considered identified.

The tridecan-2-one, besides the 6,10,14-trimethylpentadecan-2-one, pentadecane-2-one and 9,12,15-octadecatrienal (Figure 1) are among the 14 molecules identified in the dichloromethane extract of *S. habrochaites* with higher insecticidal potential. Methylketones (6,10,14-trimethylpentadecan-2-one, pentadecan-2-one and tridecan-2-one), long chain fatty acid esters (ethyl docosanoate, ethyl hexadecanoate and ethyl octadecanoate), one long chain aldehyde (9,12,15-octadecatrienal), one long chain fatty acid (hexadecanoic acid), one straight-chain alkane (heptacosane) and a series of long chain hydrocarbons (docosane, octacosane, pentacosane, squalene, and tricosane) were identified in the leaf and branch extracts of *S. habrochaites*. Hexadecanoic acid, hexadecyl acetate, docosane, tetracosane, pentacosane, and octacosane were, respectively, the main constituents of the essential

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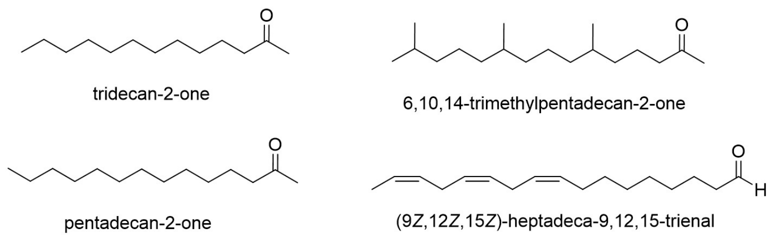

Figure 1. Structural formula of methylketones and aldehyde potentially involved in the insecticidal activity of ethanolic extract from *Solanum habrochaites* collected in Viçosa, Minas Gerais State, Brazil.

oil of leaves, flowers and fruits of *Moringa oleifera* Lam. (Brassicales: Moringaceae) (Chuang et al., 2007). The identification of the 6,10,14-trimethylpentadecan-2-one, the long-chain aldehyde 9,12,15-octadecatrienal, methyl ketones, pentadecan-2-one, tridecan-2-one, in addition to low polarity aldehydes, esters of long-chain fatty acids and hydrocarbons in the dichloromethane extract of *S. habrochaites* leaves and branches is similar to that reported in those of *Couroupita guianensis* Aubl. (Lecythidaceae) with insecticidal potential (Baskar et al., 2015). The tridecan-2-one induces the enzymatic activity of the cytochrome P450 in the midgut of insects and thus with insecticide potential. The identification of these molecules in the leaf and branch extracts of *S. habrochaites* confirms the variability of chemical compounds in plants (Figueiredo et al., 2008). Tridecan-2-one in *S. habrochaites* is among the major methylketones of essential oils from plants, such as for *Cladanthus mixtus* L. (Elouaddari et al., 2013). Heptacosane, octacosane, pentacosane, squalene, and tricosane have been reported in seed oil of *Aerva javanica* Burm. f. (Caryophyllales: Amaranthaceae).

Fourteen molecules were identified in the dichloromethane extract of *S. habrochaites*, most with insecticidal potential, mainly the tridecan-2-one, besides the 6,10,14-trimethylpentadecan-2-one, pentadecane-2-one and 9,12,15-octadecatrienal.

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