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Phototoxic compounds in 3 *Dyssodia* species (*Asteraceae*)

(with 1 figure)

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Abstract. From the root of *Dyssodia tagetoides* T. & G. two phototoxic compounds were isolated, a polyacetylene ester and a thiophene ester, which were used as markers of the genus.

On the other hand, an intraspecific and interspecific comparison of the chromatografic profiles of *D. porophylla* (Cav.) Cav. and *D. papposa* (Vent.) Hitche stems and roots was made. The profiles showed great similarity as well as the spots corresponding to the markers thus establishing a relationship between the 3 species.

Resumen. De la raíz de *Dyssodia tagetoides* T. & G. se aislaron dos compuestos fototóxicos, un éster poliacetilénico y uno tiofénico, que se emplearon como marcadores del género.

Por otra parte, se realizó una comparación intra e interespecífica de los perfiles cromatográficos de raíz y tallos de *D. porophylla* (Cav.) Cav. y *D. papposa* (Vent.) Hitche. Los perfiles mostraron gran similitud y también las manchas correspondientes a los marcadores, estableciéndose así una relación entre las 3 especies estudiadas.

Dyssodia, a genus that belongs to the family *Asteraceae* is found mainly in the dry region of the tropics and subtropics of North and Central America. It comprises 32 species and 12 varieties (2).

In continuation of our search for phototoxic compounds in *Asteraceae*, we report here the isolation of a polyacetylene ester and a thiophene ester from the root of *Dyssodia tagetoides*. These compounds were used as markers for the chromatographic profiles of stems and roots of *D. papposa* and *D. porophylla*. Also the phototoxic activity of the hexane extracts of the three species was evaluated against *Bacillus subtilis*.

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MATERIAL & METHODS

Dyssodia tagetoides T. & G. was collected in Matehuala, San Luis Potosí; *D. porophylla* (Cav.) Cav. and *D. papposa* (Vent.) Hitche were collected in Santo Domingo Huehuetlán, Puebla Mexico. Voucher specimens were deposited at the Herbarium of Facultad de Ciencias, UNAM (FCME) (*D. tagetoides*) and at the Herbarium of the Benemérita Universidad Autónoma de Puebla (HUAP) (*D. porophylla* and *D. papposa*).

Extraction. The dry and ground stems and roots of the plants were extracted with hexane at room temperature (24 h, 3x) and the solvent was eliminated at reduced pressure.

Compound isolation. The fluorescent fractions of the root extract of *D. tagetoides* were separated on a silica gel column and chromatographed by HPLC in a Varian 85000 apparatus with a Si-10, 50 cm. X 8 mm. column. The spectroscopic analysis of the resulting compounds was carried out for structure determination.

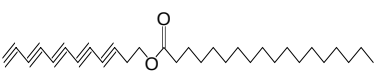
Chromatographic profiles. The profiles of *D. papposa* and *D. porophylla* stems and roots were determined on silica gel plates using as a mobile phase hexane - AcOEt 85:15; the thiophene and polyacetylene esters, isolated from *D. tagetoides* were used as markers.

Phototoxic activity. The bioassay was carried out with *Bacillus subtilis* ATCC-6051 in the usual manner (1), at a bacterial concentration of 10^7 UFC and with 0.1, 0.25 and 0.5 mg/ml of the extracts.

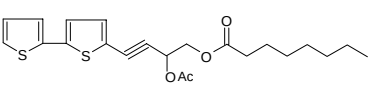
RESULTS & DISCUSSION

Two phototoxic compounds were isolated, a polyacetylene (Fig. 1a) and a thiophene (Fig. 1b) derivatives. Their structures were determined by UV, IR, PMR and MS spectroscopy; 1a could be considered the precursor of 1b.

Polyacetylene ester. UV: 220, 245, 252, 348 nm; IR: 3004 (H-C≡C), 2150, 2234 (-C≡C-), 1708 (carbonyl) cm^{-1}; PMR: 0.88 (CH_3-), 1.89 (-CH_2-),



a) Polyacetylene ester



b) Tiophene ester

Fig. 1.– Compounds isolated from *Dyssodia tagetoides*

2.48 (H-C≡C-) ppm; MS: M^+ 432, m/z 165 (polyacetylene moiety, m/z 267 (C_{18} fatty acid moiety).

Thiophene ester. UV: 196, 198, 200, 235, 335 nm; IR: 3038,3006 (aromatic), 2470 (-C≡C-), 1736, 1705 (carbonyl) cm^{-1}; PMR: 2.1 (CH_3-, acetate), 2.8 (H-C≡C-), 4.25 (H, base of the acetate), 6.8-7.2 (5 H, thiophenic) ppm; MS: M^+ 418, m/z 291 (bithienyl moiety), m/z 127 (C_8 fatty acid moiety).

Chromatographic profiles. Compounds 1**a** and 1**b** were used as chemical markers in the profiles of *D. papposa* and *D. porophylla* stems and roots. Both markers were found in the two species.

In the intraspecific comparison, root and stem profiles of the two species were identical (same number of spots and their R_f); in *D. papposa* the spots had the same concetration in both parts of the plant, *in D. porophylla* they were slightly more concentrated in roots.

The interspecific comparison showed a small difference. *Dyssodia papposa* has an intense spot at R_f 0.61 which is not present in the profile of *D. porophylla*.

This chromatografic analysis suggests that there is a close chemical resemblance between the 2 species studied, and the presence of the markers indicate also a relationship *with D. tagetoides*.

Phototoxic activity. All extracts showed bioactivity against *Bacillus subtilis* after irradiation with UV light; the stems were more active than the roots. In *D. porophylla* there was a bacterial growth inhibition of 88 and 60% respectively; *D. Papposa* had an 80 and 40% and *D. tagetoides*, 72 and 64%, with respect to the ampiciline control (0.05 mg) and at an extract concentration of 0.5 mg/ml.

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