

Hecker) and Mrs. Jost and Dr. Kramer (Pharm. Chem. Institut, Universität Heidelberg, Prof. Neidlein) for running the ms and <sup>1</sup>H-nmr spectra, respectively.

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Received 10 June 1985

## ESSENTIAL OILS FROM BRAZILIAN COMPOSITAE

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Chemical and pharmacological screening of odoriferous and medicinal plants of the northeastern region of Brazil has been underway in our laboratories since 1975. In previous papers, we have reported the chemical composition of oils of regional species belonging to the Rutaceae, Verbenaceae, and Euphorbiaceae families (1-3).

In this paper, we describe the chemical composition of the essential oils from four species of the Asteraceae family (Compositae) (Table 1). Among the species studied, only *Bidens bipinnata* L. and *Pectis apodocephala* Baker have popular uses, the former being used as a diuretic and the latter as a sedative (4). In addition, *B. bipinnata* is used in the People's Republic of China against rheumatism, weakness, and furunculosis, showing also anticancer and anti-inflammatory activities (5).

TABLE 1. Essential Oils from Compositae Species from Northeastern Brazil, General Data

File <sup>a</sup>	Species	Voucher <sup>b</sup>	Common name	Part studied	Yield (%)
403	<i>Bidens bipinnata</i> L.	5843	Carrapicho de cavalo	Aerial	0.15
421	<i>Pectis apodocephala</i> Baker	5045	Cha de moca	Leaves	0.07
272	<i>Verbesina diversifolia</i> D.C.	8673	Camara branco	Leaves	0.10
220	<i>Wedelia scaberrima</i> Benth	7168	Camara de flexa	Leaves	0.10

<sup>a</sup>Library file number for the Chemical Analysis in Departamento de Química Orgânica e Inorgânica, Universidade Federal do Ceará, Brazil.

<sup>b</sup>Herbarium "Prisco Bezerra." Departamento de Biologia, Universidade Federal do Ceará, Brazil.

Results obtained by *gc/ms* coupled to computer library search programs of the species studied are presented in Table 2. It can be seen that: (a) the major constituents of the oil of *B. bipinnata* are thymol,  $\beta$ -caryophyllene,  $\gamma$ -cadinene,  $\gamma$ -elemene, and  $\alpha$ -humulene; polyacetylenes found in essential oils of other *Bidens* species (6,7) were not detected in the present study of *B. bipinnata*. (b) The chief constituents of the oil of *P. apodocephala*, are neral and geranial (citral);  $\beta$ -pinene, carvone, and cineol were found to be the major monoterpenes in the essential oils of other plants of the genus *Pectis* in former studies (11-14). (c) The major terpenes in the essential oil of *Verbesina diversifolia* D.C. are  $\gamma$ -muurolene and  $\gamma$ -elemene. Previous reports of studies of the essential oils from the *Verbesina* genus were not found; however, the presence of bornyl ferulate and coumarate, epicampherol, and rupesterol as its cinnamate has been reported in *Verbesina rupestris* (15-16). (d)  $\alpha$ -Pinene is the chief compound present in the essential oil of *Wedelia scaberrima* Benth. Two biologically active kaurenic diterpenes isolated from extracts of this species were reported in a recent work, but no references to volatile compounds were made (17).

TABLE 2. Chemical Composition of Essential Oils of Compositae Species from Northeastern Brazil

No. Compound	Kovat Index	<i>Bidens bipinnata</i>	<i>Pectis apodocephala</i>	<i>Verbesina diversifolia</i>	<i>Wedelia scaberrima</i>
1 $\alpha$ -Pinene . . . . .	927	4.07	4.44	7.86	36.66
2 Camphene . . . . .	937	—	—	4.63	—
3 $\beta$ -Pinene . . . . .	967	0.80	—	5.27	20.00
4 Myrcene . . . . .	981	—	—	1.38	1.64
5 1.8-Cineole . . . . .	1016	—	—	2.02	—
6 Limonene . . . . .	1020	—	5.78	—	1.06
7 Methylthymol . . . . .	1211	5.09	—	—	—
8 Neral . . . . .	1222	—	28.07	—	—
9 Geranial . . . . .	1258	—	25.05	—	—
10 Thymol . . . . .	1288	17.68	—	—	—
11 $\Delta$ -Elemene . . . . .	1328	4.26	1.25	—	—
12 $\alpha$ -Cubebene . . . . .	1335	1.44	—	1.79	4.26
13 $\alpha$ -Copaene . . . . .	1359	—	5.64	—	—
14 $\beta$ -Elemene . . . . .	1376	—	9.90	5.75	1.74
15 $\beta$ -Caryophyllene . . . . .	1414	16.80	—	—	—
16 $\alpha$ -Bergamotene . . . . .	1424	—	2.52	—	—
17 $\alpha$ -Humulene . . . . .	1443	10.50	—	—	1.07
18 $\gamma$ -Cadinene . . . . .	1450	13.95	—	—	—
19 $\gamma$ -Muurolene . . . . .	1459	—	1.14	30.47	11.80
20 $\alpha$ -Muurolene . . . . .	1461	—	1.79	—	—
21 $\gamma$ -Elemene . . . . .	1480	11.94	1.08	24.63	12.13
22 Calamenene . . . . .	1502	—	2.63	—	—
23 $\Delta$ -Cadinene . . . . .	1504	5.81	—	2.36	—
24 Guayol <sup>a</sup> . . . . .	1638	—	—	—	1.38
Total <sup>b</sup> . . . . .	—	92.34	89.29	86.16	91.74

<sup>a</sup>Tentative identification.

<sup>b</sup>Yield % of compounds identified related to 100% as full identification.

## EXPERIMENTAL

**PLANT COLLECTION.**—The plant materials were collected in Fortaleza and Ubajara, Ceara, Brazil. Botanical identifications of the species studied were made in the Herbarium of the Universidade Federal do Ceara, Brazil, where a voucher of each species is deposited under the number specified in Table 1.

**EXTRACTION.**—Ground fresh plant materials (1 kg) were extracted by steam distillation until about 2 liters of co-distillate  $H_2O$  were obtained. The separated essential oils were dried over anhydrous  $Na_2SO_4$ , filtered and kept in sealed vials for further analysis.

**ANALYSIS.**—The essential oils were analyzed on a 5995A HP GC/MS using SP 2100 (methyl-silicone) open tubular column (30m  $\times$  0.5mm i.d.), temperature programmed (50-250°, 4°/min) and helium 1 ml/min as carrier gas. All data were processed on 9825 HP microprocessor and kept on flexible diskettes for further utilization. Ms fragmentations were carried out 70 eV under electron impact.

Kovat's indices were calculated after co-injection of the essential oils with standard hydrocarbons (3).

COMPOUND IDENTIFICATION.—Compound identifications were achieved by computer library search programs (3) and confirmed by visual comparison of the full ms with published standards (18, 19).

#### ACKNOWLEDGMENTS

The authors gratefully acknowledge Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Financiadora de Estudos e Projetos (FINEP), for financial support and A. G. Fernandes e P. Bezerra (Departamento de Biologia da Universidade Federal do Ceará) for botanical identifications of the species and other helpful information and Prof. James McChesney (Fullbright, Fellow, Mississippi University) for revising the English.

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Received 12 June 1985

#### A GUAIANOLIDE FROM *CHROMOLAENA GLABERRIMA*

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In the course of our work on terpenoids in the family Compositae, we have investigated *Chromolaena glaberrima* (D.C.) King & H. Rob. (tribe Eupatorieae). In addition to two heliangolides reported previously (1), we isolated the guaianolide 8 $\beta$ -(4'-hydroxytigloyl)-oxypreupatundin. After completion of the work described here, this was reported as a new compound from *Elephantopus carolinianus* Willd. (tribe Vernonieae). The <sup>13</sup>C nmr is here reported for the first time.

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