Phytochemistry, Vol. 20, No. 11, pp. 2587–2588, 1981.
Printed in Great Britain.

0031-9422/81/112587-02 $02.00/0
Pergamon Press Ltd.

ESSENTIAL OIL AND TERPENOIDS OF *MIKANIA MICRANTHA**

GILLES NICOLLIER and A. C. THOMPSON†

Department of Biochemistry, Mississippi State University, MS 39762; †Boll Weevil Research Laboratory, Agricultural Research, Science and Education Administration, USDA, MS 39762, U.S.A.

(*Received* 7 *March* 1981)

Key Word Index—*Mikania micrantha*; Compositae; essential oil; (−)-kauren-16-β-ol; (−)-kaur-15-en-19-oic acid; taraxasterol.

Abstract—Twenty-seven mainly terpenoid constituents were identified in the essential oil of *Mikania micrantha* whole plant. Higher terpenoids present in the same plant included two kaurene derivatives and taraxasterol.

Mikania micrantha is distributed in Loreto, Maynas, 20 km from Indiana, along a band of the Amazon river in Peru, and belongs to the genus *Mikania* of the tribe Eupatorieae. The plant was identified at the Botanical Institute of Mississippi State University. Sesquiterpenoid lactones [1–5], flavonoids [6], kaurenoid diterpenes [5,7] and triterpenoids [8,9] have been reported for several species within this genus [10–13]. No work has been done on the analysis of the essential oil or terpenoids of the species *micrantha* which has allelopathic activity in our bioassay (unpublished data).

The compounds of the essential oil of *M. micrantha* that were identified in this work are given in Table 1. The volatile monoterpenes represent 10.8 %, the oxygenated monoterpenoids 43 %, and linalol 15.1 % of the oil. Also, sesquiterpenes were present among them cadinene (7 %), and several sesquiterpenoids (21.6 %), the latter of which are responsible for the odor of the oil. The major difference between *M. micrantha* and other previously investigated species of the genus is the absence therein of aromatic terpenes or coumarin derivatives. The diterpenoids and triterpenoids constitute 18.2 % of the oil extracted from the plant.

EXPERIMENTAL

Steam distillation from an all-glass system on 1 kg of dried whole plant material for 10 hr yielded 8 g (0.8 %) of essential oil.

Table 1. Constituents of the essential oil of *Mikania micrantha*

Peak No.	Compound	Total Oil (%)	Peak No	Compound	Total Oil (%)
1.	2-Thujene	0.76	20.	Terpinene-4-ol	6.31
2.	β-Terpinene	4.11	21.	Myrthenal	0.56
3.	2-Pinene	0.23	22.	Verbenone	3.77
4.	β-Myrcene	0.27	23.	Geraniol	2.69
5.	β-Pinene	1.61	24.	Geranial	0.73
6'	*t*-Butylbenzene	0.59	25.	Thymol	0.13
7.	α-Terpinene	2.06	26.	Oxygenated terpenoid	0.22
8.	Monoterpene	0.92	27.	Oxygenated terpenoid	0.23
9.	β-Ocimeme	0.56	28.	Eugenol	0.48
10.	Linalol oxide	0.38	29.	Geranyl acetate	0.20
11.	Linalol	15.86	30.	2-Cubebene	3.91
12.	Oxygenated terpene	0.20	31.	γ-Elemene	0.37
13.	Oxygenated terpene	0.46	32.	2-Copaene	2.75
14.	Oxygenated terpene	0.32	33.	Sesquiterpene	1.22
15.	Oxygenated terpene	0.39	34.	β-Caryophylene	2.49
16.	Carveol	3.30	35.	Sesquiterpene	0.81
17.	Menthol	1.66	36.	D-Germacrene	1.82
18.	*p*-Cymeme-2-ol	2.46	37.	δ-Cadinene	7.48
19.	Oxygenated terpene	3.20	38–48.	Sesquiterpenoids	21.64

---

*Paper No. 4710 Mississippi Agricultural and Forestry Experiment Station.

The oil was sepd by chromatography on Al_2O_3 (Woelm, activity = 1, $l = 30$ cm, $\phi = 2$ cm) with hexane, hexane–C_6H_6 (1:1), C_6H_6, and C_6H_6—EtOAc (1:1). Quantitation of the components in each fraction was made on a FIGLC, equipped with a 50 m × 0.3 mm SS capillary column coated with OV-101 and programmed from 90 to 250° at 4°/min. Soxhlet extraction of dried finely powdered *M. micrantha* (400 g) for 10 hr with hexane yielded 5 g (1.3%) non-volatile multiterpenoids. Part of this residue (2 g) was placed on an Al_2O_3 column (Woelm, activity = 1, l = 30 cm, $\phi = 2$ cm) and eluted with hexane, and hexane–C_6H_6 (1:1) to give stigmasterol (100 mg, 5%) [16, 17] and (−)-kauren-16-β-ol (30 mg, 1.5%) [16, 18]. The remainder (3 g) of oil was chromatographed on Si gel column (Merck 7734, 1–40 cm, $\phi = 2.5$ cm) and the components eluted with hexane, hexane–C_6H_6 (1:1), and C_6H_6–EtOAc (1:1). The elution order was: taraxasterol acetate (200 mg, 6.7%, mp 250°, $[\alpha]_D^{25} = +100°$, MS $m/z = 468$ M^+) [16, 19]; (−)-kaur-16-en-19-oic acid (150 mg, 5%) [7, 16], and stigmasterol (200 mg, 6.7%, mp 155°, $[\alpha]_D^{25} = -47$, $m/z = 412$ M^+).

(−)-Kaur-16-en-19-oic acid was identified by MS, IR and ^{13}C NMR spectra using the ^{13}C assignments for ent-3-β-acetoxykaur-16-en-19-oic acid [14] and grandifloric acid [15] to locate all the carbon shifts. ^1H and ^{13}C NMR were made on a Varian FT-80 and Bruker 200 MHz spectrometers operating in the FT mode. ^{13}C chemical shifts were made from off-resonance and noise-decoupled ^{13}C NMR spectra.

(−)-Kaur-16-en-19-oic acid: mp 175°; $[\alpha]_D^{25} = -44°$. IR ν_{max}^{KBr} cm^{-1}: 3060, 3000–2800, 2930, 2850, 1690, 1655, 1470, 1460, 1440, 1360, 1260, 1170, 870. ^1H NMR: 0.95 (3 H, *s*, Me-20), 1.23 (3 H, *s*, Me-18), 2.05 (2 H, *m*, CH_2 – 15), 4.77 (2 H, *m*, $=CH_2-17$, $J = 2$ Hz), 11.46 (1 H, *s*, COOH – 19). ^{13}C NMR: (50.29 MHz): δ 15.72 (Me – 20), 18.55 (CH_2 – 11), 19.28 (CH_2 – 2), 22.08 (CH_2 – 6), 29.04 (Me – 18), 33.25 (CH_2 – 12), 38.08 (CH_2 – 14), 29.91 (CH_2 – 1), 39.95 (C – 10), 40.96 (CH_2 – 3), 41.50 (CH_2 – 7), 43.96 (C – 4), 44.09 (CH – 13), 44.46 (C – 8), 49.24 (CH_2 – 15), 55.50 (CH_2 – 5), 57.39 (CH – 9), 103.13 (CH_2 – 17), 155.94 (C – 16), 183.91 (COOH – 19). MS 70 eV, direct inlet m/z (rel. int.): 302 M^+ (4.4), 287 (3), 259 (6), 243 (4.4) 241 (5), 213 (5), 131 (28), 105 (29), 93 (30), 91 (63), 81 (28), 79 (47), 77, (35), 67 (32), 55 (41), 53 (26), 43 (40), 41 (100).

Acknowledgements—We thank Dr. R. Tabacchi, Institute of Chemie, Neuchatel, Switzerland for making some of the NMR spectra and Dr. S. McDaniel of the Botany Department of Mississippi State University for supplying the plant material.

REFERENCES

1. Herz, W., Subramaniam, P. S., Santhanam, K. A. and Hall, A. L. (1970) *J. Org. Chem.* **35**, 1453.
2. Herz, W., Poplawski, J. and Sharma, R. P. (1975) *J. Org. Chem.* **40**, 199.
3. Herz, W., Poplawski, J. and Sharma, R. P. (1975) *J. Org. Chem.* **44**, 199.
4. Herz, W., Srinivasan, A. and Kalyanaraman, S. P. (1975) *Phytochemistry* **14**, 233.
5. Bohlmann, F., Natu Arvid, A. and Mahanta Pradipk (1978) *Phytochemistry* **17**, 483.
6. Herz, W. and Santhanam, P. S. (1969) *Tetrahedron Letters* **39**, 3419.
7. Mathur, S. B. and Fermin Cenis, M. (1973) *Phytochemistry* **12**, 226.
8. Herz, W., Santhanam, P. S., Subramanian, P. and Schmid, J. J. (1967) *Tetrahedron Letters* 3111.
9. Kiang, A. K. (1965) *J. Chem. Soc.* 6371.
10. Dominguez, X. A., Gomez, M. E., Gomez, P. A., Villarreal, A. N. and Rombold, C. (1970) *Planta Med.* **19**, 52.
11. Alertsen, A. R. (1955) *Acta Chem. Scand.* **9**, 1975.
12. Karlsson, K., Wahlberg, I. and Enzell, C. R. (1972) *Acta Chem. Scand.* **26**, 3839.
13. Karlsson, K., Wahlberg, I. and Enzell, C. R. (1972) *Acta Chem. Scand.* **26**, 2837.
14. Piozzi, F., Savona, G. and Hanson, J. R. (1980) *Phytochemistry* **19**, 1237.
15. Ohno, N. and Mabry, T. J. (1980) *Phytochemistry* **19**, 611.
16. Stenhagen, E., Abrahamsson, S. and McLafferty, F. W. (1974) *Registry of Mass Spectral Data.* John Wiley, New York.
17. (1963) *Sadtler NMR and IR Standard Spectra*, Sadtler Research Laboratories, Philadelphia, PA.
18. Hugel, G., Lods, L., Mellor, J. M., Theobald, D. W. and Ourisson, G. (1965) *Bull. Soc. Chim. Fr.* 2882.
19. Yamagushi, K. (1970) *Spectral Data of Natural Products.* Elsevier, Amsterdam.