Short Communication

N'-Isopropylornnicotine in Burley Tobacco (*Nicotiana tabacum*)Masashi MIYANO, Hajime MATSUSHITA,
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More than twenty pyridine alkaloids have been identified in tobacco leaves. Some of them having both pyridine and pyrrolidine rings in their molecules may be considered as the derivatives of nornicotine (3-(2'-pyrrolidyl)pyridine). In spite of a number of *N'*-acyl and *N'*-carboalkoxy derivatives of nornicotine having been reported,^{1,2)} no *N'*-alkyl derivatives other than nicotine have been isolated as the tobacco alkaloids. During our studies on basic compounds of air-cured tobacco, a new minor alkaloid was found in one of the fractions reported in a previous paper³⁾ and identified as one of *N'*-alkylornnicotine, *N'*-isopropylornnicotine (**I**).

The basic fraction of aged burley tobacco was fractionated on an alumina column.³⁾ The ether/methanol (95: 5) eluate was subjected to GC-MS analysis using a glass capillary column. This procedure revealed that an unidentified compound was eluted from the capillary column between nicotine and nornicotine. The mass spectrometric data of this compound were as follows (relative intensities in parentheses); *m/e*: 190 (9), 176 (14), 175 (100), 161 (7), 147 (8), 132 (46), 130 (47), 117 (33), 112 (33), 105 (18), 92 (25), 78 (14), 70 (61), 65 (22), 56 (22), 51 (19), 43 (38), 41 (46).

The fragment peaks at *m/e* 78 and 51 in the mass spectrum of the compound suggested the compound has a pyridine ring and this suggestion was supported with the intense ion peak at *m/e* 112 (*M*-78) that was supposed to be due to the loss of the pyridine ring from

the molecule.⁴⁾ The major peak at *m/e* 70 suggested the compound has a pyrrolidine ring.⁴⁾ The fragment ion peak at *m/e* 147 together with the data mentioned above supported the fact that the compound has a nornicotine moiety in its structure. The fragment ion peaks at *m/e* 175 (*M*-15), 161 (*M*-29) and 147 (*M*-43) suggested the presence of a *C*₃-alkyl group attached to the nornicotine moiety, and from the most abundant peak at *m/e* 175, an isopropyl was assumed for the group. The abundant peaks at *m/e* 132, 130 and 117 are characteristic for *N'*-alkylornnicotine other than nicotine.⁵⁾ Therefore, *N'*-isopropylornnicotine (**I**) was presumed for the compound.

The above structure assignment was confirmed by comparing the mass spectrum and the retention time in gas chromatography of the compound with those of *N'*-isopropylornnicotine prepared by the reaction of nornicotine with isopropyl bromide. The nornicotine used was isolated from tobacco leaves. Gas chromatography was carried out with a Hitachi Model 063 gas chromatograph equipped with a flame ionization detector and with a glass capillary column (10% PEG-20 M, 0.25 mm×30 m). GC-MS was carried out with a NEVA Model TE-600 equipment using the same column.

Recently, many minor tobacco alkaloids have been found by many workers^{1~3)} utilizing newly-developed analytical equipments. These new alkaloids, including *N'*-formylanabasine and *N'*-formylanatabine³⁾ as well as nornicotine derivatives, are characterized by the substitution on the nitrogen of the ring other than pyridine.¹⁾ *N'*-Isopropylornnicotine is another *N'*-substituted compound. Hitherto, many *N'*-methyl substituted pyridine alkaloids such as nicotine, *N'*-methylanabasine and *N'*-methylanatabine have been reported,¹⁾ but no

other *N'*-alkylated alkaloids have been identified in tobacco leaves. This is the first case that a *N'*-alkyl pyridine alkaloid except for *N'*-methyl derivatives was identified in tobacco leaves.

REFERENCES

- 1) I. Schmeltz and D. Hoffmann, *Chem. Rev.*, **77**, 295 (1977).
 - 2) H. Matsushita, Y. Tsujino, D. Yoshida, A. Saito, T. Kisaki, K. Kato and M. Noguchi, *Agric. Biol. Chem.*, **43**, 193 (1979).
 - 3) M. Miyano, H. Matsushita, N. Yasumatsu and K. Nishida, *Agric. Biol. Chem.*, **43**, 1607 (1979).
 - 4) D. F. Glenn and W. B. Edwards III, *J. Org. Chem.*, **43**, 2860 (1978).
 - 5) Our preliminary work on some *N'*-alkyl derivatives prepared.
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