oxygenase Systems and in Mammals. *J. Agric. Food Chem.* **1977**, *25*, 1–9.
Langseth, W. Determination of Diphenyltin and Dialkyltin Homologues by HPLC with Morin in the Eluent. *Talanta* **1984**, *31*, 975–978.
Maguire, R. J.; Tkacz, R. J. Degradation of the Tri-*n*-butyltin species in Water and Sediment from Toronto Harbor. *J. Agric. Food Chem.* **1985**, *33*, 947–953.
Mazaev, V. T.; Korolev, A. A. Experimental Basis for the Maximum Permissible Concentration of Dichlorodibutyltin in Reservoir Waters. *Prom. Zagryaz. Vodoemov* **1969**, *9*, 15–37.
Mueller, M. D. Tributyltin Detection at Trace Levels in Water and Sediments Using GC with Flame-Photometric Detection and GC–MS. *Fresenius' Z. Anal. Chem.* **1984**, *317*, 32–36.
Sasaki, K.; Ishizaka, T.; Suzuki, T.; Saito, Y. Determination of Tri-*n*-Butyltin and Di-*n*-Butyltin Compounds in Fish by Gas Chromatography with Flame Photometric Detection. *J. Assoc. Off. Anal. Chem.* **1988a**, *71*, 360–363.
Sasaki, K.; Suzuki, T.; Saito, Y. Determination of Tri-*n*-butyltin and Di-*n*-butyltin Compounds in Yellowtails. *Bull. Environ. Contam. Toxicol.* **1988b**, *41*, 888–893.
Takami, K.; Yamamoto, H.; Okumura, T.; Sugimae, A.; Nakamoto, M. Application of "Clean-up" Cartridge for Gas Chromatographic Determination of Di- and Tri-*n*-butyltin in Fish. *Anal. Sci.* **1987**, *3*, 63–67.
Wada, O.; Manabe, S.; Iwai, H.; Arakawa, Y. Recent Progress in the Study of Analytical Methods, Toxicity, Metabolism and Health Effects of Organotin Compounds. *Jpn. J. Ind. Health* **1982**, *24*, 24–54.
WHO. *Environmental Health Criteria 15: Tin and organotin compounds*; World Health Organization: Geneva, 1980.
Yu, T.; Arakawa, Y. High-Performance Liquid Chromatographic Determination of Dialkyltin Homologues Using Fluorescence Detection. *J. Chromatogr.* **1983**, *258*, 189–197.

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Insect Juvenile Hormone Mimics: Synthesis of Some 5-Oxa-3,8,12-trimethyltridecenoates

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Syntheses of some 5-oxahomofarnesanes have been described and shown to be active at micrograms/nymph against *Dysdercus koenigii*, and the activity is comparable with that of methoprene (Altozar IGR; ZR 515). Stress was also laid on the separation of *Z* and *E* isomers, thereby confirming their structural integrity.

Insect growth regulators (IGRs) are potent growth regulators (Williams, 1956) of certain essential processes in the life cycle of insects. Many insects are remarkably sensitive to the external application of suitable IGRs at critical stages in their life cycle. Though the question of structure–activity relationship in the area of juvenile hormone (JH) mimics is very complex because of a large number of variables (Slama et al., 1974), the compounds with optimum activity are as a rule based on the farnesane skeleton. Oxafarnesanes and oxahomofarnesanes have been reported as juvenoids. However, the methods of synthesis are either patented or low yielding. The detailed JH activity studies of 4-oxafarnesanes along with their synthesis have been reported in the literature (Patwardhan et al., 1976). Jarolim and Sorm (1974) have reported the synthesis of oxahomofarnesanes and have mentioned the separation of *Z* and *E* isomers on a silica gel column, but no further evidence has been attributed to confirm their structural identity. We report herein a novel approach to the synthesis of these oxahomofarnesanes (Scheme I) starting with the easily accessible citronellol (1) and their separation. However, the method of separation of *E* and *Z* isomers as reported by the authors failed in our hands. Hence, the separation was carried out on a silica gel column impregnated with silver nitrate (10–15%) to afford the pure *E* and *Z* isomers. The salient features of our approach are (i) preparation of propargyl ether, (ii) catalytic hydration of terminal acetylene to the desired methyl ketone, and (iii) separation of *E* and *Z* isomers on a silica gel column impregnated with silver nitrate.

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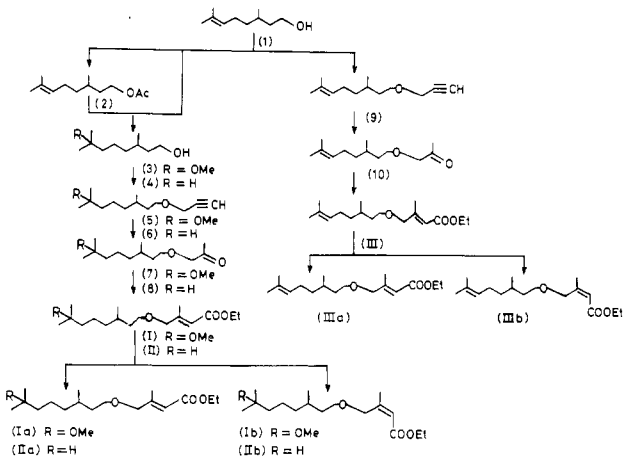
Scheme I



EXPERIMENTAL SECTION

IR spectra were recorded on a Perkin-Elmer Infracord spectrophotometer (Model 783). ^1H NMR spectra were obtained in $CDCl_3$ with tetramethylsilane as the internal reference in a Varian A-60A spectrometer. GLC was carried out on a Schimadzu GC-7A chromatograph fitted with hydrogen flame detector and glass columns. HPLC analyses were performed on a Water Associates instrument (Model ALC/GPC 244) equipped with a solvent delivery system (Model 6000 A) and U6K injector and detector (Model 440).

7-Methoxycitronellol (3). To a stirred suspension of mercuric acetate (16.0 g, 0.05 mol) was added citronellyl acetate (**2**; 9.8 g, 0.05 mol) in dry methanol (130 mL). The reaction mixture was stirred for 0.5 h at ambient temperature to complete the meth-

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oxymercuration stage. A solution of sodium hydroxide (6.0 g) in water (50 mL) was added followed by the addition of sodium borohydride (0.950 g) in portions. Reduction of the carbon–mercury bond was almost instantaneous. In order to facilitate the hydrolysis of the acetate group, the mixture was stirred overnight at ambient temperature. Mercury was removed by filtering the mixture through a short pad of Celite. The filtrate was concentrated; ether and brine were added to the residue. Usual workup followed by distillation of the residue afforded 8.5 g (90%) of **3**: bp 88–90 °C (0.2 mm); IR (film) 3380, 2940, 1460, 1380, 1365, 1070 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.9 (d, 3, J = 7 Hz, $-CH_3$), 1.13 (s, 6, 2 CH_3), 2.86 (s, 1, D_2O exchangeable, $-CH_2OH$), 3.16 (s, 3, $-OCH_3$), 3.63 (t, 2, J = 6 Hz, $-CH_2OH$). Anal. Calcd for $C_{11}H_{24}O_2$: C, 70.21; H, 12.76. Found C, 70.40; H, 12.50.

7,11-Dimethyl-11-methoxy-4-oxadodec-1-yne (5). To a stirred suspension of sodium hydride (50% dispersion in oil; 0.96 g, 0.04 mol) in tetrahydrofuran (10 mL) was added a solution of methoxycitronellol (**3**; 3.76 g, 0.02 mol) in tetrahydrofuran (20 mL) over a period of 30 min. The reaction mixture was cooled to 0 °C, and a solution of propargyl bromide (2.6 g, 0.022 mol) in tetrahydrofuran (20 mL) was added dropwise over a period of 20 min. It was stirred at 0 °C for 30 min and the temperature raised to 50 °C. Stirring was continued for further 1 h. The progress of the reaction was monitored by IR (disappearance of the 3380-cm^{-1} band (OH) and appearance of the 2100-cm^{-1} band (C≡CH) indicated the formation of alkyne). This was then diluted with water (100 mL), acidified (2 N HCl, pH neutral), and extracted with ether (3 × 50 mL). The ether extract was washed with water and brine and dried (Na_2SO_4). Removal of solvent followed by distillation of the residue gave 3.9 g (85%) of **5**: bp 85–6 °C (0.5 mm); GLC, 3% OV-17, 150 °C, 40 mL/min N_2, R_t = 5.5 min; IR (film) 3300, 2960, 2930, 2860, 2100, 1460, 1380, 1100 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.89 (d, 3, J = 8 Hz, $-CH_3$), 1.13 (s, 6, 2 CH_3), 2.4 (m, 1, $-OCH_2C{\equiv}CH$), 3.15 (s, 3, $-OCH_3$), 3.53 (t, 2, J = 6 Hz, $-CH_2OCH_2C{\equiv}CH$), 4.1 (dist s, 2, $-OCH_2C{\equiv}CH$).

7,11-Dimethyl-4-oxadodec-1-yne (6): bp 78–80 °C (1.5 mm); GLC, 3% OV-17, 150 °C, 40 mL/min N_2, R_t = 2.55 min; IR (film) 3300, 2950, 2920, 2860, 2110, 1460, 1100 cm^{-1}: ^1H NMR ($CDCl_3$) δ 0.88 (dd, 9, J = 7 Hz, 3 CH_3), 2.42 (t, 1, J = 2 Hz, $-CH_2C{\equiv}CH$), 3.56 (t, 2, J = 6 Hz, $-CH_2OCH_2C{\equiv}CH$), 4.15 (d, 2, J = 2 Hz, $-OCH_2C{\equiv}CH$).

7,11-Dimethyl-4-oxadodec-10-en-1-yne (9): bp 72–4 °C (0.6 mm); GLC, 3% OV-17, 150 °C, 40 mL/min N_2, R_t = 3.28 min; IR (film) 3300, 2960, 2920, 2860, 2110, 1455, 1375, 1100 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.88 (d, 3, J = 7 Hz, $-CH_3$), 1.62, 1.7 (2 s, 6, 2 CH_3), 2.42 (d, 1, J = 2 Hz, $-CH_2C{\equiv}CH$), 3.49 (t, 2, J = 6 Hz, $-CH_2OCH_2C{\equiv}CH$), 4.15 (d, 2, J = 2 Hz, $-OCH_2C{\equiv}CH$), 5.1 (br, 1, $-C{=}CH$).

7,11-Dimethyl-11-methoxy-4-oxadodecan-2-one (7). To a stirred solution of aqueous methanol (70%, 12 mL), mercuric sulfate (20 mg), and concentrated sulfuric acid (24 μL), was added a solution of alkenyl ether **5** (1.94 g, 0.01 mol). The bath temperature was slowly raised to 70 °C, and stirring was continued for further 5 h. The reaction mixture was cooled, diluted with water (50 mL), and extracted with ether (3 × 50 mL). The ether extract was washed with water and brine and dried (Na_2SO_4). Removal of solvent followed by distillation of the residue gave 1.7 g (80%) of **7**: bp 130–2 °C (8 mm) [lit. bp 145–50 °C (12 mm) (Jarolim and Sorm, 1974)]; GLC, 3% OV-17, 150 °C, 40 mL/min N_2, R_t = 6.72 min; IR (film) 2960, 2920, 2860, 1720, 1460, 1355, 1130 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.88 (d, 3, J = 7 Hz, $-CH_3$), 1.15 (s, 6, 2 CH_3), 2.18 (s, 3, $-COCH_3$), 3.17 (s, 3, $-OCH_3$), 3.53 (t, 2, J = 7 Hz, $-CH_2OCH_2COCH_3$), 4.02 (s, 2, $-OCH_2COCH_3$).

7,11-Dimethyl-4-oxadodecan-2-one (8): bp 125–7 °C (5 mm) [lit. bp 140–45 °C (10 mm) (Jarolim and Sorm, (1974)]; GLC, 3% OV-17, 150 °C, 40 mL/min N_2, R_t = 5.16 min; IR (film) 2960, 2920, 2870, 1720, 1460, 1355, 1125 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.88 (dd, 9, J = 7 Hz, 3 CH_3), 2.18 (s, 3, $-COCH_3$), 3.53 (t, 2, J = 7 Hz, $-CH_2O$), 4.02 (s, 2, $-OCH_2$).

7,11-Dimethyl-4-oxadodec-10-en-2-one (10): bp 130–2 °C (8 mm) [lit. bp 145–50 °C (12 mm) (Jarolim and Sorm, 1974)]; GLC, 3% OV-17, 150 °C, 40 mL/min N_2, R_t = 6.72 min; IR (film) 2960, 2920, 2860, 1720, 1460, 1355, 1130 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.88 (d, 3, J = 7 Hz, $-CH_3$), 1.61, 1.68 (2 s, 6, 2 CH_3), 2.18 (s, 3, $-COCH_3$), 3.53 (t, 2, J = 7 Hz, $-CH_2OCH_2COCH_3$), 4.02 (s, 2, $-OCH_2COCH_3$), 5.11 (br, 1, $-C{=}CH$).

Table I. Spectral Characteristics of 3,8,12-Trimethyltridecenoates

compd	C-2 H	C-3 Me	C-4 H
Ia *E*	5.77	1.97 (s)	4.58 (d, J = 6 Hz)
Ib *Z*	5.96	2.1 (s)	3.84 (d, J = 6 Hz)
IIa *E*	5.77	1.98 (s)	4.58 (d, J = 6 Hz)
IIb *Z*	5.95	2.1 (s)	3.96 (d, J = 6 Hz)
IIIa E	5.76	1.96 (s)	4.58 (d, J = 6 Hz)
IIIb *Z*	5.97	2.1 (s)	3.96 (d, J = 6 Hz)

Table II. Retention Time for Oxahomofarnesanes Using MeOH–H_2O (4:1 v/v) as Eluant (Flow Rate 1.8 mL/min)

oxahomofarnesane	ret time, min
I (mixture of *E* and *Z*)	27.78, 31.88 (70:30)
Ia *E*	27.78
Ib *Z*	31.88
II (mixture of *E* and *Z*)	11.4, 12.81 (62:38)
IIa *E*	11.4
IIb *Z*	12.81
III (mixture of *E* and *Z*)	19.78, 22.66 (60:40)
IIIa *E*	19.78
IIIb *Z*	22.66

General Procedure for the Preparation of 5-Oxa-2-tridecenoate. To a stirred suspension of sodium hydride (50% dispersion in oil; 0.24 g, 0.01 mol) in tetrahydrofuran (5 mL) at 0 °C was added a solution of triethyl phosphonoacetate (1.12 g, 0.005 mol) in tetrahydrofuran (10 mL). The reaction mixture was stirred at 0 °C for 0.5 h when a clear solution resulted (also indicated by the ceasing of hydrogen evolution); thereafter, a solution of the alkoxy ketone (0.005 mol) in tetrahydrofuran (10 mL) was added dropwise over a period of 0.5 h and the temperature maintained at 0 °C for further 2 h. Usual workup afforded a residue consisting of *Z* and *E* isomers in the ratio of 40:60 in 80% yield.

Ethyl 3,8,12-trimethyl-12-methoxy-5-oxa-2-tridecenoate (I): IR (film) 2960, 2930, 2860, 1715, 1660, 1460, 1380, 1360, 1315, 1220, 1150, 1110, 1040, 860 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.88 (d, 3, J = 7 Hz, $-CH_3$), 1.13 (dd, 6, J = 6 Hz, 2 CH_3), 2.07, 1.92 [2 s (due to *Z* and *E*), 3, $-CH_3$], 3.15 (s, 3, $-OCH_3$), 3.44 (t, 2, J = 7 Hz, $-CH_2O$), 3.9, 4.5 [2 s (due to *Z* and *E*), 2, $-OCH_2$], 4.15 (q, 2, J = 6 Hz, $-COOCH_2CH_3$), 5.85, 5.65 [2 br s (due to *Z* and *E*), 1, $-C{=}CHCOOCH_2CH_3$]; UV (MeOH) λ_{max} 212.1 nm; mass spectrum, m/e 314 (M^+).

Ethyl 3,8,12-trimethyl-5-oxa-2-tridecenoate (II): IR (film) 2950, 2860, 1710, 1660, 1440, 1375, 1315, 1220, 1150, 1110, 1040, 860 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.88 (dd, 9, J = 6 Hz, 3 CH_3), 1.3 (t, 3, J = 7 Hz, $-COOCH_2CH_3$), 2.1, 1.96 [2 s (due to *Z* and *E*), 3, $-CH_3$], 3.48 (t, 2, J = 6 Hz, $-CH_2O$), 3.94, 4.57 [2 s, (due to *Z* and *E*), 2, $-OCH_2$], 4.19 (q, 2, J = 7 Hz, $-COOCH_2CH_3$), 5.95, 5.75 [2 br s (due to *Z* and *E*), 1, $-CH$]; UV (MeOH) λ_{max} 215.5 nm; mass spectrum, m/e 284 (M^+).

Ethyl 3,8,12-trimethyl-5-oxa-2,11-tridecadienoate (III): IR (film) 2950, 2920, 2860, 1710, 1660, 1440, 1375, 1315, 1220, 1150, 1110, 1040, 860 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.89 (d, 3, J = 7 Hz, $-CH_3$), 1.29 (t, 3, J = 7 Hz, $-COOCH_2CH_3$), 1.61, 1.69 (2 s, 6, 2 CH_3), 2.1, 1.96 [2 s (due to *Z* and *E*), 3, $-CH_3$], 3.47 (t, 2, J = 6 Hz, $-CH_2O$), 3.96, 4.58 [2 s (due to *Z* and *E*), 2, $-OCH_2$], 4.19 (q, 2, J = 6 Hz, $-COOCH_2CH_3$), 5.11 (br, 1, $-C{=}CH$), 5.97, 5.76 [2 br s (due to *Z* and *E*), 1, $-CH$]; UV (MeOH) λ_{max} 213.1 nm; mass spectrum, m/e 282 (M^+).

The *E* and *Z* isomers of oxahomofarnesanes I–III were separated on a silica gel column impregnated with silver nitrate (10–15%) (eluant PE–EtOAc (5–10%)) to furnish the pure *E* and *Z* isomers. The characteristic NMR signals and HPLC retention times have been indicated in Tables I and II.

Bioassay Procedure. Compounds I–III were tested for JH activity with freshly molted last instar nymphs of red cotton bug, *Dysdercus koenigii*, as test insects. Test compounds I–III were dissolved in acetone, and 1 μL of the acetone solution was topically applied on the dorsal side of each nymph. Acetone solvent treated insects served as controls. Treated nymphs were allowed to feed on cotton seeds and water. The insects that successfully molted were classified, and percent JH activity was assessed. Methoprene, a known JH analogue, was used as a standard compound for

Table III. Juvenile Hormone Activity of Oxahomofarnesanes

compd	dose, μg/nymph	% JH act.
I	1.0	68
II	1.0	65
III	1.0	65
methoprene	0.2	75

comparison. Ten insects were used for each concentration, and it was repeated three times. From the experimental data (Table III) it is evident that synthetic oxahomofarnesanes I–III had activity comparable to that of methoprene.

HPLC Separation. Oxahomofarnesanes I–III have been separated by high-performance liquid chromatography using a μ-Bondapak C_{18} column (stainless steel, 300 mm × 3.9 mm (i.d.)) with particle size 10 μm under varying conditions of eluant concentration (methanol–water). Adequate resolution of the above mixtures was observed with methanol–water (4:1), and the retention times have been shown in Table II.

RESULTS AND DISCUSSION

Acetylation of citronellol (1) with acetic anhydride in pyridine at room temperature gave citronellyl acetate (2). This was subjected to oxymercuration–demercuration reaction (Brown and Rei, 1969) to afford 7-methoxycitronellol (3). This on subjection to a O-alkylation reaction with propargyl bromide provided alkynyl ether **5** in more than 80% yield. The next step involved conversion of the terminal acetylene to the corresponding methyl ketone **7**. This was brought about by a mercuric sulfate catalyzed reaction (Thomas et al., 1938) in 80% yield.

Following a similar sequence of reactions, citronellol (1) and dihydrocitronellol (4) were converted to their corresponding oxa ketones **6** and **10**, respectively. Compounds I–III were prepared in a 60:40 *E*:*Z* ratio over 80% yield by a Wittig–Horner reaction between respective methyl ketones and triethyl phosphonoacetate. The isomers were exclusively separated on a silica gel column impregnated with silver nitrate to afford the corresponding *E* and *Z* isomers, which were designated with suffixes a and b, respectively. These were in more than 98% purity as confirmed by its GLC analysis. The structures of the *Z* and *E* isomers of I–III were fully characterized on the basis of their NMR spectra, and the characteristic ^1H NMR signals are shown in Table I. It is evident from the table that the chemical shift values of proton signals at C-2 and C-3 methyls of *Z* isomers fall downfield whereas C-4 fall upfield compared to that of *E* isomers.

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Registry No. (±)-1, 26489-01-0; (±)-2, 67650-82-2; (±)-3, 120444-95-3; (±)-4, 59204-02-3; (±)-5, 120411-85-0; (±)-6, 120411-86-1; (±)-7, 120411-87-2; (±)-8, 120411-88-3; (±)-9, 120411-89-4; (±)-10, 120444-96-4; (±)-Ia, 120411-90-7; (±)-Ib, 120411-93-0; (±)-IIa, 120411-91-8; (±)-IIb, 120411-94-1; (±)-IIIa, 120411-92-9; (±)-IIIb, 120411-95-2.

LITERATURE CITED

Brown, H. C.; Rei, M. H. The solvomercuration–demercuration of representative olefins in the presence of alcohols. Convenient procedures for the synthesis of ethers. *J. Am. Chem. Soc.* **1969**, *91*, 5646.

Jarolim, V.; Sorm, F. Synthesis of some 5-oxa analogs of acyclic juvenoids. *Collect. Czech. Chem. Commun.* **1974**, *39*, 587–595.

Patwardhan, S. A.; Gupta, A. S.; Sukh Dev. Some 4-oxafarnesane insect juvenile hormone mimics. *Agric. Biol. Chem.* **1976**, *40*(4), 697.

Slama, K.; Romanuk, M.; Sorm, F. *Insect Hormones and Bioanalogues*; Springer-Verlag: New York, 1974; p 194.

Thomas, R. J.; Campbell, K. N.; Hennion, G. F. Catalytic hydration of alkylacetylenes. *J. Am. Chem. Soc.* **1938**, *60*, 718.

Williams, C. M. The Juvenile Hormone of Insects. *Nature* **1956**, *178*, 212.

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Identification of Hydrolysis Products of the Fungicide Vinclozolin by Spectroscopic and X-ray Crystallographic Methods

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The hydrolysis of vinclozolin [3-(3,5-dichlorophenyl)-5-methyl-5-vinyloxazolidine-2,4-dione], a dicarboximide fungicide, at 20 °C in 0.1 M phosphate buffers of pH 5.0, 7.0, and 9.0 gives three products, identified as 2-[[(3,5-dichlorophenyl)carbamoyl]oxy]-2-methyl-3-butenoic acid (M1), 3′,5′-dichloro-2-hydroxy-2-methylbut-3-enanilide (M2), and 3,5-dichloroaniline (M3). The identity of M3 was confirmed by gas chromatography–mass spectrometry. M1 and M2 were isolated from a 0.1 M phosphate buffer of pH 7.0 after incubation at 35 °C for 7 days. After purification, their identities were confirmed by solid-probe mass spectrometry and proton and ^{13}C NMR spectrometry. Furthermore, the identity of M1 was confirmed by unambiguous evidence from X-ray crystallography of its ethyl ester.

Vinclozolin [3-(3,5-dichlorophenyl)-5-methyl-5-vinyloxazolidine-2,4-dione] (Figure 1a) was introduced by BASF AG of Germany in 1975 under the code number BAS 35204F. Its fungicidal properties against *Botritis cinerea* were first reported by Pommer and Mangold (1975) and by Hess and Locher (1975). Subsequent research showed that vinclozolin is effective in the control of diseases in grapes, fruits, vegetables, ornamentals, hops, rapeseed, and turfgrass caused by *Botritis spp.*, *Sclerotinia spp.*, and *Monilinia spp.* (Spencer, 1982). Since its introduction vinclozolin has been widely used in Europe for the control of fungal diseases. This fungicide is currently registered in the United States, but not in Canada.

Little was known about the degradation of vinclozolin in the environment. Clark (1983) reported that the oxazolidine ring of vinclozolin was opened in ethanolic and

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