

Analytical method for imazalil and its metabolite T000824 (R014821; imazalil alcohol) in soil

Reports: ECM: EPA MRID No.: 49611108. Schernikau, N. 2008. Validation of an analytical method for the determination of Imazalil and T000824 (metabolite R014821) in soil. Specht Study No.: CET-0802V. Specht File Reference: G08-0015. Report prepared by Eurofins Analytik GmbH, Dr. Specht Laboratorien, Hamburg, Germany, and sponsored by Certis Europe Brussels, Brussels, Belgium, and submitted by Certis USA LLC, Columbia, Maryland; 39 pages. Final report issued March 6, 2008.

ILV: EPA MRID No. 49767603. Witte, A. 2015. INDEPENDENT LABORATORY VALIDATION (ILV) OF AN ANALYTICAL METHOD FOR DETERMINATION OF RESIDUES OF IMAZALIL AND ITS METABOLITE R014821 IN SOIL. CIP Study Code: 15A06123-01-VMS. ADAMA Reference No.: R-35756. Janssen Study No.: AGR 5375. Report prepared by CIP Chemisches Institut Pforzheim GmbH, Pforzheim, Germany, sponsored by ADAMA Makhteshim Ltd., Airport City, Israel, Certis Europe BV, Maarsse, The Netherlands, and Janssen PMP, Beerse, Belgium, and submitted by Makhteshim-Agan of North America, Inc. (d/b/a ADAMA), Raleigh, North Carolina, Certis USA LLC, Columbia, Maryland, and Janssen PMP, a division of Janssen Pharmaceutical Companies of Johnson & Johnson, Raritan, New Jersey; 38 pages. Final report issued November 5, 2015.

Document No.: MRIDs 49611108 & 49767603


Guideline: 850.6100

Statements: ECM: The study was conducted in accordance with German and OECD Good Laboratory Practice (GLP) standards (pp. 3-4 of MRID 49611108). Signed and dated No Data Confidentiality, GLP and Quality Assurance statements were provided (pp. 2-5). A statement of the authenticity of the study report was included with the GLP statement (p. 3).

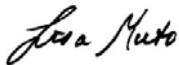
ILV: The study was conducted in accordance with German and OECD GLP standards, which are accepted by Regulatory Authorities throughout the European Community, the United States of America and Japan (pp. 3, 5 of MRID 49767603). Signed and dated No Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-3, 5, 7). A statement of the authenticity of the study report was included with the GLP statement (p. 3).

Classification: This analytical method is classified as acceptable for ECM and unacceptable for ILV. Performance data at 10×LOQ was not reported to validate the method in the ILV. ILV performance data for imazalil in sandy loam soil did not meet OCSPP guidelines requirements for repeatability at the LOQ with RSDs were 32% (Q) and 31% (C). Communication between the ILV testing facility and the method developer was not discussed in the ILV.

PC Code: 111902

Final EPA**Reviewer:**James Lin
Environmental EngineerSignature: 

Date: 8/28/17

**CDM/CSS-
Dynamac JV****Reviewers:**Lisa Muto,
Environmental ScientistSignature: 

Date: 6/14/17

Kathleen Ferguson, Ph.D.,
Environmental ScientistSignature: 

Date: 6/14/17

This Data Evaluation Record may have been altered by the Environmental Fate and Effects Division subsequent to signing by CDM/CSS-Dynamac JV personnel.

Executive Summary

This analytical method, Specht Study No. CET-0802V, is designed for the quantitative determination of imazalil and its metabolite R014821 (T000824) in soil at the LOQ of 0.001 mg/kg using LC/MS/MS. The ECM used characterized sandy loam matrices; the ILV used a different characterized sandy loam soil matrix. The specific sources of the ECM and ILV soils were not reported. Although the specific number of trials was not reported, the reviewer assumed that the method was validated after one trial with insignificant modifications to the analytical method. Performance data at 10×LOQ was not reported to validate the method in the ILV. ILV performance data for imazalil in sandy loam soil did not meet OCSPP guidelines requirements for accuracy at the LOQ [RSDs were 32% (Q) and 31% (C)]. Communication between the ILV testing facility and the method developer was not discussed in the ILV. All submitted ILV data pertaining to linearity was acceptable. All submitted ECM data pertaining to linearity, repeatability and reproducibility was acceptable. Significant baseline noise was observed in the ECM and ILV representative chromatograms; in the ILV, the baseline noise interfered with analyte peak integration.

Table 1. Analytical Method Summary

Analyte(s) by Pesticide	MRID		EPA Review	Matrix	Method Date (dd/mm/yyyy)	Registrant	Analysis	Limit of Quantitation (LOQ)
	Environmental Chemistry Method	Independent Laboratory Validation						
Imazalil	49611108 ¹	49767603 ²		Soil	06/03/2008	Certis USA LLC ³	LC/MS/MS	0.001 mg/kg
R014821 (Imazalil alcohol; T000824)								

¹ In the ECM, sandy loam soil matrix [Lufa Speyer soil type 2.3; 58.2 ± 0.8% sand 32.3 ± 1.3% silt 9.6 ± 0.8% clay; pH 6.3 ± 0.2 (0.1M CaCl₂), 1.2 ± 0.2% organic carbon] was used (USDA soil texture classification; p. 8; Appendix 4, p. 39 of MRID 49611108). The specific soil source was not reported. The soil characterization was performed by LUFA Speyer.

- 2 In the ILV, sandy loam soil matrix [Lufa Speyer soil type 2.3; 65.8% sand 24.0% silt 10.2% clay; pH 6.96 (0.1M CaCl₂), 0.87% organic carbon] was used (USDA soil texture classification; p. 14 of MRID 49767603). The specific soil source was not reported. The soil characterization was performed by LUFA Speyer.
- 3 The ILV was submitted by Makhteshim-Agan of North America, Inc. (d/b/a ADAMA), Certis USA LLC, and Janssen PMP, a division of Janssen Pharmaceutical Companies of Johnson & Johnson.

I. Principle of the Method

Soil samples (5 g) were fortified in a 50-mL Sarstedt centrifuge tube (pp. 12-14 of MRID 49611108). Water and acetonitrile (10 mL each) were added to the sequentially to the tube with shaking. For extraction, the tube was shaken vigorously by hand for 1 minute. Magnesium sulfate (4 g), sodium chloride (1.0 g), trisodium citrate dihydrate (1.0 g) and disodium hydrogen citrate (0.5 g) were added, and the sample was immediately shaken vigorously by hand for *ca.* 1 minute. After centrifugation (2 minutes at 4000 rpm), 1.7 mL of the upper acetonitrile phase was transferred to a 2 mL Eppendorf tube containing 160 mg of PSA (primary secondary amine) and 225 mg of magnesium sulfate. The sample was intensively shaken vigorously by hand for 1 minute then centrifuged (2 minutes at 6000 rpm). After 1.0 mL of the upper acetonitrile phase was transferred to another Eppendorf tube, the extract was evaporated to dryness using a gentle stream of nitrogen. The residue was reconstituted with 1.0 mL of acetonitrile:0.05% acetic acid (1:3, v:v), transferred to an autosampler vial and analyzed by HPLC/MS/MS. The method noted that the sample processing was the QuEChERS method.

Samples were analyzed for imazalil and T000824 using an Agilent Series 1200 HPLC coupled to a PE-Sciex API 4000 tandem MS equipped with an Supelco Ascentis Express C18 column (2.1 mm x 50 mm, 2.7 μ m; column temperature 30°C) using a gradient mobile phase of (A) methanol + 0.05% acetic acid and (B) water + 0.05% acetic acid [percent A:B at -1.4 to 0.0 min. 5:95, 1.0 to 3.5 min. 95:5] with MS/MS-ESI (electrospray ionization) detection in positive ion mode and multiple reaction monitoring (MRM; pp. 14-15 of MRID 49611108). Injection volume was 8 μ L. Analytes were identified using two ion transitions (quantitation and confirmation, respectively): *m/z* 297 \rightarrow 159 and *m/z* 297 \rightarrow 201 for imazalil and *m/z* 257 \rightarrow 69 and *m/z* 257 \rightarrow 125 for T000824. Expected retention times were *ca.* 1.8 minutes for imazalil and *ca.* 1.6 minutes for T000824.

In the ILV, the ECM was performed as written with insignificant modifications to the analytical instrumentation (pp. 15, 17-19, 22 of MRID 49767603). A Dionex Ultimate 3000 HPLC coupled to an AB Sciex API 5500 QTRAP MS was used for analyte identification. All other analytical parameters were the same as the ECM. Imazalil and T000824 were identified using the same two ion transitions; expected retention times were *ca.* 4.0 minutes for imazalil and *ca.* 3.6 minutes for T000824. No other modifications of the ECM were reported.

The Limit of Quantification (LOQ) for soil was 0.001 mg/kg for both analytes in the ECM and ILV (pp. 9-10, 17; Appendix 2, Tables 1-4, pp. 28-31 of MRID 49611108; pp. 10, 24 of MRID 49767603). The Limit of Detection (LOD) was reported as 0.0003 mg/kg (30% of the LOQ) in the ILV and ECM.

II. Recovery Findings

ECM (MRID 49611108): Mean recoveries and relative standard deviations (RSDs) were within guideline requirements (mean 70-120%; RSD \leq 20%) for analysis of imazalil and its metabolite T000824 (R014821; imazalil alcohol) at fortification levels of 0.001 mg/kg (LOQ), 0.01 mg/kg (10 \times LOQ) and 0.05 mg/kg (50 \times LOQ) in one soil matrix (p. 19; Appendix 2, Tables 1-4, pp. 28-31). Analytes were identified using two ion transitions; performance data (recovery results) from quantitation and confirmation analyses were comparable. Sandy loam soil matrix [Lufa Speyer soil type 2.3; 58.2 \pm 0.8% sand 32.3 \pm 1.3% silt 9.6 \pm 0.8% clay; pH 6.3 \pm 0.2 (0.1M CaCl₂), 1.2 \pm 0.2% organic carbon] was used (USDA soil texture classification; p. 8; Appendix 4, p. 39). The specific soil source was not reported. The soil characterization was performed by LUFA Speyer.

ILV (MRID 49767603): Mean recoveries and RSDs were within guideline requirements for analysis of imazalil and its metabolite T000824 (R014821; imazalil alcohol) at fortification levels of 0.001 mg/kg (LOQ) and 0.05 mg/kg (50 \times LOQ) in one soil matrix, except for imazalil RSDs at the LOQ [32% (Q) and 31% (C); Table 4, p. 23 of MRID 49767603; DER Attachment 2]. No samples were prepared at 10 \times LOQ. Analytes were identified using two ion transitions; performance data (recovery results) from quantitation and confirmation analyses were comparable. Imazalil means and RSDs at the LOQ were reviewer-calculated based on n = 5. The study author calculated statistics for n = 4 since one value was deemed to be an outlier according to Grubbs and F-test. The results calculated in the study report were 93% mean and 6.5% RSD for the quantitation ion transition and 96% mean and 5.0% RSD for the confirmation ion transition. Sandy loam soil matrix [Lufa Speyer soil type 2.3; 65.8% sand 24.0% silt 10.2% clay; pH 6.96 (0.1M CaCl₂), 0.87% organic carbon] was used (USDA soil texture classification; p. 14). The specific soil source was not reported. The soil characterization was performed by LUFA Speyer. Although the specific number of trials was not reported, the reviewer assumed that the method was validated after one trial with insignificant modifications to the analytical instrumentation (pp. 10, 17-19, 22, 23-25).

Table 2. Initial Validation Method Recoveries for Imazalil and Its Metabolite T000824 (R014821; Imazalil Alcohol) in Soil^{1,2}

Analyte	Fortification Level (mg/kg)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%)	Relative Standard Deviation (%)
Sandy Loam Soil						
Quantitation Ion Transition						
Imazalil	0.001	5	78-87	83	3.4	4.1
	0.01	5	83-86	85	1.3	1.5
	0.05	5	88-90	89	0.8	0.9
T000824 (R014821; Imazalil Alcohol)	0.001	5	81-84	83	1.2	1.4
	0.01	5	81-84	83	1.3	1.6
	0.05	5	76-82	80	2.3	2.9
Confirmation Ion Transition						
Imazalil	0.001	5	78-94	87	6.7	7.7
	0.01	5	82-87	85	2.0	2.4
	0.05	5	86-88	87	0.8	0.9
T000824 (R014821; Imazalil Alcohol)	0.001	5	79-98	87	7.7	8.9
	0.01	5	80-83	82	1.1	1.3
	0.05	5	78-84	80	2.2	2.8

Data (uncorrected recovery results, pp. 15-16) were obtained from p. 19; Appendix 2, Tables 1-4, pp. 28-31 of MRID 49611108.

1 Sandy loam soil matrix [Lufa Speyer soil type 2.3; $58.2 \pm 0.8\%$ sand $32.3 \pm 1.3\%$ silt $9.6 \pm 0.8\%$ clay; pH 6.3 ± 0.2 (0.1M CaCl₂), $1.2 \pm 0.2\%$ organic carbon] was used (USDA soil texture classification; p. 8; Appendix 4, p. 39). The specific soil source was not reported. The soil characterization was performed by LUFA Speyer.

2 Analytes were identified using two ion transitions (quantitation and confirmation, respectively): m/z 297→159 and m/z 297→201 for imazalil and m/z 257→69 and m/z 257→125 for T000824.

Table 3. Independent Validation Method Recoveries for Imazalil and Its Metabolite T000824 (R014821; Imazalil Alcohol) in Soil^{1,2}

Analyte	Fortification Level (mg/kg)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%) ³	Relative Standard Deviation (%)
Sandy Loam Soil						
Quantitation Ion Transition						
Imazalil	0.001	5 ⁴	84-168	108	34	32
	0.05	5	78-81	80	1	1.5
T000824 (R014821; Imazalil Alcohol)	0.001	5	73-79	77	3	3.7
	0.05	5	72-74	74	1	1.2
Confirmation Ion Transition						
Imazalil	0.001	5 ⁴	90-171	111	34	31
	0.05	5	78-82	80	2	2.0
T000824 (R014821; Imazalil Alcohol)	0.001	5	79-82	81	1	1.4
	0.05	5	72-74	73	1	1.1

Data (uncorrected recovery results, pp. 19-20) were obtained from Table 4, p. 23 of MRID 49767603 and DER Attachment 2.

- 1 Sandy loam soil matrix [Lufa Speyer soil type 2.3; 65.8% sand 24.0% silt 10.2% clay; pH 6.96 (0.1M CaCl₂), 0.87% organic carbon] was used (USDA soil texture classification; p. 14). The specific soil source was not reported. The soil characterization was performed by LUF A Speyer.
- 2 Analytes were identified using two ion transitions (quantitation and confirmation, respectively): m/z 297→159 and m/z 297→201 for imazalil and m/z 257→69 and m/z 257→125 for T000824.
- 3 Standard deviations were reviewer-calculated since these values were not calculated in the study report (see DER Attachment 2). Rules of significant figures was followed when reporting results.
- 4 The results reported above were reviewer-calculated based on $n = 5$ (see DER Attachment 2). The study author calculated statistics for $n = 4$ since one value was deemed to be an outlier according to Grubbs and F-test (Table 4, p. 23). The results calculated in the study report were 93% mean and 6.5% RSD for the quantitation ion transition and 96% mean and 5.0% RSD for the confirmation ion transition.

III. Method Characteristics

The LOQ for soil was 0.001 mg/kg for both analytes in the ECM and ILV (pp. 9-10, 17; Appendix 2, Tables 1-4, pp. 28-31 of MRID 49611108; pp. 10, 24 of MRID 49767603). In the ECM, the LOQ was justified by the fact that the chromatographic peaks at 0.001 mg/kg were greater than the signal equivalent to three times the background noise. In the ILV, the LOQ was defined as the lowest fortification level at which mean recoveries ranging 70% to 120% at a RSD of $\leq 20\%$ and blanks not exceeding 30% of the LOQ were achieved. The LOD was reported as 0.0003 mg/kg (30% of the LOQ) in the ILV and ECM without justification. No calculations were provided for the LOQ or LOD in the ECM or ILV.

Table 4. Method Characteristics

Analyte		Imazalil	T000824 (R014821; Imazalil Alcohol)
Limit of Quantitation (LOQ)		0.001 mg/kg	
Limit of Detection (LOD)		0.0003 mg/kg (30% of the LOQ)	
Linearity (calibration curve r^2 and concentration range) ¹	ECM	$r^2 = 1.0000$ (Q) $r^2 = 0.9998$ (C)	$r^2 = 0.9998$ (Q) $r^2 = 1.0000$ (C)
	ILV	$r^2 = 0.9995$ (Q) $r^2 = 0.9996$ (C)	$r^2 = 0.9999$ (Q) $r^2 = 0.9999$ (C)
	Concentration range	0.1-50 $\mu\text{g/L}$	
Repeatable	ECM ²	Yes at LOQ, 10 \times LOQ and 50 \times LOQ.	
	ILV ^{3,4}	No at LOQ [RSD 32% (Q) and 31% (C)] ⁵ . Yes at 50 \times LOQ.	Yes at LOQ and 50 \times LOQ.
Reproducible		No at LOQ.	Yes at LOQ.
		Could not be determined at 10 \times LOQ since no samples were prepared.	
Specific	ECM	Only control and LOQ chromatograms were presented. Analyte peaks were distinguishable, but surrounded by significant background noise at the LOQ.	
	ILV	Matrix interferences were <10% (based on peak area). Significant background noise interfered with peak integration at the LOQ.	Matrix interferences were <i>ca.</i> $\leq 3\%$ (based on peak area). Significant background noise interfered with peak integration at the LOQ for the confirmation ion.

Data were obtained from pp. 9-10, 17; p. 19; Appendix 2, Tables 1-4, pp. 28-31 (recovery data); Appendix 1, Figures A-D, pp. 21-24 (calibration curve); Appendix 3, Figures 3-4, pp. 35-36 (chromatograms) of MRID 49611108; pp. 10, 24; Table 4, p. 23 (recovery data); Appendix 2, Figures 1-4, pp. 27-30 (calibration curve); Appendix 4, Figures 9-16, pp. 33-36 (chromatograms) of MRID 49767603; DER Attachment 2. Q = Quantitation ion transition; C = Confirmatory ion transition.

- 1 Reported correlation coefficients were reviewer-calculated from r values reported in the study report (Appendix 1, Figures A-D, pp. 21-24 of MRID 49611108; DER Attachment 2). Solvent-based calibration standards were used.
- 2 In the ECM, sandy loam soil matrix [Lufa Speyer soil type 2.3; 58.2 \pm 0.8% sand 32.3 \pm 1.3% silt 9.6 \pm 0.8% clay; pH 6.3 \pm 0.2 (0.1M CaCl₂), 1.2 \pm 0.2% organic carbon] was used (USDA soil texture classification; p. 8; Appendix 4, p. 39 of MRID 49611108). The specific soil source was not reported. The soil characterization was performed by LUFA Speyer.
- 3 In the ILV, sandy loam soil matrix [Lufa Speyer soil type 2.3; 65.8% sand 24.0% silt 10.2% clay; pH 6.96 (0.1M CaCl₂), 0.87% organic carbon] was used (USDA soil texture classification; p. 14 of MRID 49767603). The specific soil source was not reported. The soil characterization was performed by LUFA Speyer.
- 4 Although the specific number of trials was not reported, the reviewer assumed that the method was validated after one trial with insignificant modifications to the analytical instrumentation (pp. 10, 17-19, 22, 23-25 of MRID 49767603).
- 5 Reported results were reviewer-calculated based on $n = 5$ (see DER Attachment 2). The study author calculated statistics for $n = 4$ since one value was deemed to be an outlier according to Grubbs and F-test (Table 4, p. 23). The results calculated in the study report were 93% mean and 6.5% RSD for the quantitation ion transition and 96% mean and 5.0% RSD for the confirmation ion transition.

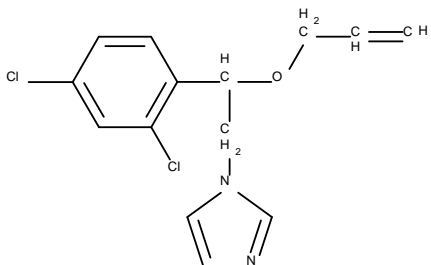
IV. Method Deficiencies and Reviewer's Comments

1. For the ILV, performance data at 10×LOQ was not reported to validate the method. A validation sample set should consist of, at a minimum, a reagent blank, two unspiked matrix control samples, five matrix control samples spike at the LOQ, and five matrix control samples spiked at 10×LOQ for each analyte and matrix. The reproducibility of the method at 10×LOQ could not be determined.
2. The ILV performance data for imazalil in sandy loam soil did not meet OCSPP guidelines requirements for repeatability at the LOQ [RSDs were 32% (Q) and 31% (C); Table 4, p. 23 of MRID 49767603; DER Attachment 2]. OCSPP Guideline 850.6100 criteria for precision states that RSDs for replicates at each spiking level are $\leq 20\%$. Imazalil means and RSDs at the LOQ were reviewer-calculated based on $n = 5$. The study author calculated statistics for $n = 4$ since one value was deemed to be an outlier according to Grubbs and F-test. The results calculated in the study report were 93% mean and 6.5% RSD for the quantitation ion transition and 96% mean and 5.0% RSD for the confirmation ion transition.
3. The communication between the ILV testing facility and the method developer was not discussed in the ILV.
4. Significant baseline noise was observed in the ECM and ILV representative chromatograms (Appendix 3, Figures 3-4, pp. 35-36 of MRID 49611108; Appendix 4, Figures 9-16, pp. 33-36 of MRID 49767603). In the ECM, the background noise created an elevated baseline with some small peaks in the area of the retention time of the analytes. At the LOQ, the analyte peaks were distinguishable from the background noise, but the base of the analyte peak was elevated from the normal baseline of the chromatogram. In the ILV, significant background noise interfered with peak integration at the LOQ for the quantitation and confirmation ions of imazalil and for the confirmation ion of T000824 (R014821; Imazalil Alcohol).
5. In the ECM, representative chromatograms were not provided for two of the three fortification levels, 10×LOQ and 50×LOQ (Appendix 3, Figures 3-4, pp. 35-36 of MRID 49611108). Representative chromatograms for the controls and each fortification level should be provided for all matrices tested so that the specificity of the method can be fully evaluated.
6. The estimation of LOQ and LOD in ECM and ILV was not based on scientifically acceptable procedures as defined in 40 CFR Part 136 ILV (pp. 9-10, 17; Appendix 2, Tables 1-4, pp. 28-31 of MRID 49611108; pp. 10, 24 of MRID 49767603). In the ECM, the LOQ was justified by the fact that the chromatographic peaks at 0.001 mg/kg were greater than the signal equivalent to three times the background noise. In the ILV, the LOQ was defined as the lowest fortification level at which mean recoveries ranging 70% to 120% at a RSD of $\leq 20\%$ and blanks not exceeding 30% of the LOQ were achieved. The LOD was reported in the ILV and ECM without justification. No calculations were provided for the LOQ or LOD in the ECM or ILV.

7. The ECM matrix and ILV matrix were both sandy loam soil matrix (Lufa Speyer soil type 2.3), but the soils were not the exact same since batch numbers and soil characterizations were different (p. 8; Appendix 4, p. 39 of MRID 49611108; p. 14 of MRID 49767603).
8. The reviewer noted the following typographical error in the ECM: the recovery of the third T000824 sample was reported as “891%” instead of “81%” (pp. 10, 19; Appendix 2, Tables 1-4, pp. 28-31 of MRID 49611108).
9. In the ILV, the study author noted that, since no matrix effects were found, solvent-based standards were used (p. 24 of MRID 49767603).
10. The extracts were found to be stable 24 hours after extraction in the ILV (pp. 11, 24-25 of MRID 49767603). Storage details were not reported.
11. The timeframe required to complete the method validation for one set was reported in the ILV as 3 hours (10 recoveries and 2 blank/control samples), without time to analyse the LC/MS/MS results (p. 17 of MRID 49767603).

V. References

- U.S. Environmental Protection Agency. 2012. Ecological Effects Test Guidelines, OCSPP 850.6100, Environmental Chemistry Methods and Associated Independent Laboratory Validation. Office of Chemical Safety and Pollution Prevention, Washington, DC. EPA 712-C-001.
- 40 CFR Part 136. Appendix B. Definition and Procedure for the Determination of the Method Detection Limit-Revision 1.11, pp. 317-319.

Attachment 1: Chemical Names and Structures**Imazalil****IUPAC Name:** (RS)-1-(β -allyloxy-2,4-dichlorophenethyl)imidazole**CAS Name:** 1-[2-(2,4-Dichlorophenyl)-2-(2-propen-1-yloxy)ethyl]-1H-imidazole**CAS Number:** 35554-44-0**SMILES String:** c1cc(Cl)cc(Cl)c1C(OCC=C)Cn2cnc2**R014821 (T000824; Imazalil alcohol)****IUPAC Name:** Alpha-(2,4-dichloro-phenyl)-1 H-imidazole-1-ethanol**CAS Name:** Not reported**CAS Number:** 24155-42-8**SMILES String:** c1cc(c(cc1Cl)Cl)C(Cn2ccnc2)O