

Test Material: Telone

MRID: 44536505

Title: Method Validation Report for GRM 94.15 - Determination of Residues of *cis*- and *trans*-3-Chloroallyl Alcohol in Water by Capillary Gas Chromatography with Mass Selective Detection

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Title: Independent Laboratory Validation of Method GRM 94.15 - Determination of Residues of *cis*- and *trans*-3-Chloroallyl Alcohol in Water by Capillary Gas Chromatography with Mass Selective Detection

EPA PC Code: 029001

OCSPP Guideline: 850.6100

For CDM Smith

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Date: 6/15/15

Analytical method for telone transformation products cis- and trans-3-chloroallyl alcohol in water

Reports: ECM: EPA MRID No.: 44536505. Duebelbeis, D.O., and A.D. Thomas. 1997. Method Validation Report for GRM 94.15 - Determination of Residues of *cis*- and *trans*-3-Chloroallyl Alcohol in Water by Capillary Gas Chromatography with Mass Selective Detection. Report prepared, sponsored, and submitted by Global Environmental Chemistry Laboratory - Indianapolis Lab, DowElanco, Indianapolis, Indiana; 44 pages. DowElanco Study ID: RES94133. Final report issued December 12, 1997.
ILV: EPA MRID No. 44536507. Duebelbeis, D.O., and B.A. Sorenson. 1997. Independent Laboratory Validation of Method GRM 94.15 - Determination of Residues of *cis*- and *trans*-3-Chloroallyl Alcohol in Water by Capillary Gas Chromatography with Mass Selective Detection. Report prepared by Global Environmental Chemistry Laboratory - Indianapolis Lab, DowElanco, Indianapolis, Indiana, and Quality Management & Analytical Services, Inc. (QMAS), Walhalla, North Dakota, sponsored and submitted by Global Environmental Chemistry Laboratory - Indianapolis Lab, DowElanco, Indianapolis, Indiana; 33 pages. QMAS Study No.: QMAS95014. DowElanco Study No.: RES95081. Final report issued January 23, 1997.

Document No.: MRIDs 44536505 & 44536507

Guideline: 850.6100

Statements: ECM: The study was conducted in compliance with USEPA Good Laboratory Practice (GLP) standards, with minor exceptions (p. 3 of MRID 44536505). Signed and dated Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-4). The certification of the authenticity of the study report is included in the Quality Assurance Statement (p. 4).
ILV: The study was conducted in compliance with USEPA GLP standards, with minor exceptions (p. 3 of MRID 44536507). Signed and dated Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-4). The certification of the authenticity of the study report is included in the Quality Assurance Statement (p. 4).

Classification: This analytical method is classified as unacceptable. The ILV was not conducted independently of the ECM originating laboratory. Though the ILV was conducted at a different laboratory, the ECM and ILV are conducted by the same study director. The experimental design of the ILV was inadequate to produce a successful validation of the ECM, with insufficient performance data at the LOQ (n = 2) and no performance data at 10x LOQ. The total number of ILV trials conducted was not reported. For both the ECM and ILV, water matrices were not characterized. The registrant failed to verify that the independent laboratory performed the ILV with a water matrix of the most difficult analytical sample condition to analyze to demonstrate how well the method performs. The ILV did not verify the LODs for the analytes.

PC Code: 029001

Reviewer:

Andrew Shelby, Physical Scientist

Signature: 

Date: May 10, 2016

For both MRIDs, page citations in this review refer to the uppermost set of page numbers located in the top right corner of each page of the MRID.

Executive Summary

DowElanco Analytical Method GRM 94.15, is designed for the quantitative determination of telone transformation products cis- and trans-3-chloroallyl alcohol (CAAL, derivatized to the respective 3-chloroallyl isobutyl carbonate) in water using GC/MS. The method is quantitative for the analytes at the stated LOQ of 0.10 ng/mL ($\mu\text{g/L}$). The LOQ is less than the lowest toxicological level of concern in water. No major modifications were made by the independent laboratory. The independent laboratory failed to validate the method for analysis of cis- and trans-3-CAAL in pond water (uncharacterized) because insufficient performance data were reported at the LOQ ($n = 2$) and no performance data were reported at 10x LOQ. The ILV did not verify the LODs for the analytes. For both the ECM and ILV, water matrices were not characterized. The registrant failed to verify that the independent laboratory performed the ILV with a water matrix of the most difficult analytical sample condition to analyze to demonstrate how well the method performs. The ILV was not conducted independently of the ECM originating laboratory, and the total number of ILV trials conducted was not reported.

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						
cis-3-CAAL ¹	44536505	44536507		Water ²	23/03/1995 ³	DowElanco	GC/MS	0.10 ng/mL ($\mu\text{g/L}$)
trans-3-CAAL								

1 CAAL = chloroallyl alcohol; transformation product of telone.

2 Uncharacterized surface (ECM validation) and pond (ILV) water matrices were used (p. 9 of MRID 44536505; p. 8 of MRID 44536507). Surface water for ECM validation obtained near Immokalee, Florida. Source location for pond water used in ILV was not reported.

3 Appendix A, p. 17 of MRID 44536505.

I. Principle of the Method

Water (40.0 mL) was fortified with cis- and trans-3-chloroallyl alcohol (CAAL) in acetone for procedural recoveries (p. 8; Appendix A, pp. 20-21, 23 of MRID 44536505). Uncharacterized surface water from a site near Immokalee, Florida, was used for the validation (p. 9). Water samples (40.0 mL) are partitioned with 15 mL of methyl-t-butyl ether (MTBE), 15 g of sodium chloride, and 10 μL of 1-propanol by shaking (reciprocating shaker, *ca.* 180 excursion/minute) for 15 minutes (1-propanol is critical to reduce evaporative losses of CAAL; Appendix A, pp. 18, 23). Phases are separated by centrifugation (1,000 rpm, 3 minutes; Appendix A, p. 24). The organic (MTBE) phase is applied, through anhydrous magnesium sulfate (*ca.* 2 g), to a silica gel SPE column preconditioned with MTBE. The sample is pulled through the column by vacuum (*ca.* 2 mL/minute), with eluate collection. The remaining aqueous phase is again partitioned with 15 mL of MTBE by shaking for 5 minutes and the resulting organic phase applied to the silica gel SPE column, with all eluates combined. The sample is combined with hexane (*ca.* 3 mL) and anhydrous sodium sulfate (*ca.* 0.1 g), then taken to near dryness using a flask equipped with a Micro Snyder

distilling column on a hot plate (Appendix A, pp. 19, 24). Residues are reconstituted with hexane (*ca.* 1 mL) and concentrated to *ca.* 0.5 mL under a gentle nitrogen stream (N-Evap, ambient temperature). Residues are reconstituted to 1.0 mL with hexane, amended with anhydrous sodium sulfate (*ca.* 0.1 g), then derivatized to the respective *cis*- and *trans*-3-chloroallyl isobutyl carbonates (CAIBC) with isobutyl chloroformate (25 μ L) in the presence of pyridine (25 μ L) at 70°C for 15 minutes (Appendix A, pp. 17, 25). Upon cooling, samples are treated with 1.0 mL of 0.1N hydrochloric acid, vortexed (5 seconds), centrifuged (2,500 rpm, 5 minutes) and the upper hexane layer taken for GC/MS analysis.

Samples are analyzed using an Hewlett-Packard 5971A Mass Selective Detector (MSD) equipped with an Hewlett-Packard 5890 (II) GC system (Appendix A, pp. 22-23 of MRID 44536505). The following GC conditions were used: J&W Scientific fused silica capillary, Durabond-17 (DB-17) liquid phase column (0.18 mm x 20 m, 0.3 μ m film thickness, injector temperature 230°C), temperature program [65°C (hold for 1 min.), 5°C/min. to 150°C (0 min. hold), 20°C/min. to 260°C (0 min. hold)]. Injection volume was 2 μ L. The following MSD conditions were used: electron impact ionization and selected ion monitoring (SIM). Analytes were identified using two ions; one for quantitation (Q) and one for confirmation (C). Ions monitored were *m/z* 136 (Q) and *m/z* 75 (C) for both *cis*- and *trans*-3-CAIBC. Identification is considered positive when the confirmation ion ratio [(peak area at *m/z* 136)/(peak area at *m/z* 75)] of the sample is \pm 20% of the average confirmation ion ratio found for the calibration standards (Appendix A, pp. 25-26). Retention times for *cis*- and *trans*-3-CAAL (as CAIBC) were 13.43-13.44 and 13.28-13.29 minutes, respectively (Appendix A, Figure 5, p. 39; Figures 7-8, pp. 41-42; Figure 10, p. 44).

ILV: Sources of the test compounds and water matrix used for the ILV were not reported (p. 8; Appendix A, pp. 29-30 of MRID 44536507). The water matrix was described as pond water, but characterization was not provided. The independent laboratory performed the extraction method as written, with the following exception: a sand bath was used for heating during the Synder column evaporation step as the evaporation flasks were not flat-bottomed (pp. 10-11; Appendix A, p. 33). In addition to minor instrument adjustments, the following GC/MSD conditions were modified: the end of the temperature program was held at 260°C for 3 minutes and ions monitored were *m/z* 136.1 (Q) and *m/z* 101.1 (C); the make/model of the MSD was not specified (Appendix A, p. 31). Confirmation ion ratios were calculated as [(peak area at *m/z* 101)/(peak area at *m/z* 136)] (Figure 3, p. 19; Figures 5-7, pp. 21-23; Figures 9-10, pp. 25-26). Retention times for *cis*- and *trans*-3-CAAL (as CAIBC) were 12.05-12.06 and 11.91-11.93 minutes, respectively (Figures 3-10, pp. 19-26).

LOQ and LOD: In the ECM and ILV, the LOQ for both *cis*- and *trans*-3-CAAL was 0.10 ng/mL (μ g/L; Appendix A, p. 17 of MRID 44536505; p. 8 of MRID 44536507). In the ECM, the LODs for *cis*- and *trans*-3-CAAL were calculated as 0.024 ng/mL and 0.023 ng/mL, respectively (p. 12; Appendix A, p. 28; Tables III-IV, pp. 33-34 of MRID 44536505). In the ILV, the LODs were not specified.

II. Recovery Findings

ECM (MRID 44536505): Mean recoveries and relative standard deviations (RSDs) were within guidelines (mean 70-120%; RSD \leq 20%) for analysis of cis- and trans-3-CAAL in Florida surface water (uncharacterized) at fortification levels of 0.10 ng/mL (μ g/L, LOQ, n = 8) and 0.52 ng/mL (5x LOQ, n = 3; Appendix A, Tables I-II, pp. 31-32 and DER Attachment 2). At fortification levels of 2.5x (0.1039-0.1043 ng/mL), 10x (1.039-1.043 ng/mL), 25x (2.598-2.608 ng/mL), and 50x (5.195-5.215 ng/mL) LOQ, only two recoveries were reported for each fortification level; therefore, meaningful statistics (mean, standard deviation, RSD) for the recovery results per analyte/fortification level/water matrix could not be generated. All individual recovery results were within 70-120%. Confirmation ion ratio results were only provided for one LOQ (0.10 ng/mL) fortified sample for both cis- and trans-3-CAAL and were \pm 3% of the average standard confirmation ratio (Appendix A, Figure 7, p. 41; Figure 10, p. 44).

ILV (MRID 44536507): Only two recoveries were reported for each fortification level; therefore, meaningful statistics (mean, standard deviation, RSD) for the recovery results per analyte/fortification level/water matrix could not be generated. Individual recovery results were within 70-120% for both cis- and trans-3-CAAL in pond water (uncharacterized) at fortification levels of 0.10 ng/mL (LOQ) and 0.50 ng/mL (5x LOQ; p. 8; Tables I-II, pp. 15-16). Performance data at 10x LOQ were not reported. Confirmation ion ratio results were only provided for one LOQ (0.10 ng/mL) and one 5x LOQ (0.50 ng/mL) fortified sample for both cis- and trans-3-CAAL and were \pm 12% of the average standard confirmation ratio (Figures 5-6, pp. 21-22; Figures 9-10, pp. 25-26). The total number of trials conducted was not reported; documented communications indicate at least two trials were performed (Appendix A, p. 33). The independent laboratory found the following Snyder column evaporation steps to be critical: flow hood drafts may cause condenser over-cooling resulting in extended evaporation time and poor analyte recoveries, and the Snyder column should be rinsed with hexane immediately after removing the flask from heat to prevent significant analyte losses (Appendix A, p. 32). Confirmation ion m/z 75 was not used because of background interference; confirmation ion m/z 101, as per the ECM (Appendix A, p. 28 of MRID 44536505), yielded an acceptable signal-to-noise ratio and was substituted.

Table 2. Initial Validation Method Recoveries for Telone Transformation Products cis- and trans-3-Chloroallyl Alcohol (CAAL) in Surface Water¹

Analyte	Fortification Level (ng/mL)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%)	Relative Standard Deviation (%)
cis-3-CAAL	0.10 (LOQ) ²	8	73-91	83	7	9
	0.2608	2	81, 86	-- ³	--	--
	0.5215	3	84-89	87	3	3
	1.043	2	79, 83	--	--	--
	2.608	2	92, 88	--	--	--
	5.215	2	75, 76	--	--	--
trans-3-CAAL	0.10 (LOQ) ⁴	8	70-93	83	7	9
	0.2598	2	82, 87	--	--	--
	0.5195	3	84-90	87	3	3
	1.039	2	82, 86	--	--	--
	2.598	2	96, 91	--	--	--
	5.195	2	80, 79	--	--	--

Data (uncorrected recovery results) were obtained from Appendix A, Tables I-II, pp. 31-32 of MRID 44536505 and DER Attachment 2 (mean, SD, RSD).

1 Uncharacterized surface water collected from a site near Immokalee, Florida (p. 9).

2 Fortification level was 0.1043 ng/mL (Appendix A, Table I, p. 31). Two fortifications made at 0.0209 ng/mL (20% of LOQ) had recoveries of 95% (0.01987 ng/mL) and 92% (0.01927 ng/mL).

3 Not applicable; meaningful statistics could not be generated because n = 2.

4 Fortification level was 0.1039 ng/mL (Appendix A, Table II, p. 32). Two fortifications made at 0.0209 ng/mL (20% of LOQ) had recoveries of 92% (0.01928 ng/mL) and 82% (0.01722 ng/mL).

Table 3. Independent Validation Method Recoveries for Telone Transformation Products cis- and trans-3-Chloroallyl Alcohol (CAAL) in Pond Water¹

Analyte	Fortification Level (ng/mL)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%)	Relative Standard Deviation (%)
cis-3-CAAL	0.10 (LOQ)	2	110, 100	-- ²	--	--
	0.50	2	104, 103	--	--	--
trans-3-CAAL	0.10 (LOQ)	2	103, 108	--	--	--
	0.50	2	88, 90	--	--	--

Data (uncorrected recovery results) were obtained from Tables I-II, pp. 15-16 of MRID 44536507.

1 Uncharacterized; source location was not reported (p. 8).

2 Not applicable; meaningful statistics could not be generated because n = 2.

III. Method Characteristics

In the ECM and ILV, the LOQ for both cis- and trans-3-CAAL was 0.10 ng/mL ($\mu\text{g/L}$; Appendix A, p. 17 of MRID 44536505; p. 8 of MRID 44536507). In the ECM, the LODs for cis- and trans-3-CAAL were calculated as 0.024 ng/mL and 0.023 ng/mL, respectively (p. 12; Appendix A, p. 28; Tables III-IV, pp. 33-34 of MRID 44536505). In the ILV, the LODs were not specified. Following the method of Keith, L.H., *et al.* (see section V. **References** below), the LOD and LOQ for determination of telone transformation products cis- and trans-3-chloroallyl alcohol in water were calculated using the standard deviation from the 0.10 ng/mL (LOQ) recovery results (Appendix A, p. 28; Tables III-IV, pp. 33-34 of MRID 44536505). The LOD was calculated as three times the standard deviation ($3s$), and the LOQ was calculated as ten times the standard deviation ($10s$) of the recovery results. Matrix blank values ($n = 7$) were 0.0000 ng/mL (Appendix A, Tables I-II, pp. 31-32). Calculated LOQ values were 0.079 ng/mL and 0.075 ng/mL for cis- and trans-CAAL, respectively.

Table 4. Method Characteristics for Telone Transformation Products cis- and trans-3-Chloroallyl Alcohol (CAAL)¹ in Surface Water

		cis-3-CAAL	trans-3-CAAL
Limit of Quantitation (LOQ)		0.10 ng/mL ($\mu\text{g/L}$)	
Limit of Detection (LOD)		0.024 ng/mL	0.023 ng/mL
Linearity (calibration curve r^2 and concentration range) ²	ECM:	Q ion: $r^2 = 0.9998$ (0.05215-10.43 ng/mL in water)	Q ion: $r^2 = 0.9998$ (0.05195-10.39 ng/mL in water)
	ILV:	Q ion: $r^2 = 0.9987$ (0.05-1.00 ng/mL)	Q ion: $r^2 = 0.9966$ (0.05-1.00 ng/mL)
Repeatable	ECM:	Yes at LOQ ($n = 8$). Fortifications at 2.5x, 5x, 10x, 25x, and 50x LOQ performed at $n = 2$ or 3.	
	ILV:	Undetermined. Fortifications at LOQ and 5x LOQ performed at $n = 2$. No performance data at 10x LOQ.	
Reproducible		Undetermined. ILV performed at $n = 2$ at LOQ and 5x LOQ.	
Specific ³	ECM:	Yes, no interferences were detected at analyte retention times (Appendix A, Figure 6, p. 40; Figure 9, p. 43). Matrix was uncharacterized Florida surface water.	
	ILV:	No interferences detected at analyte retention times for Q ion at m/z 136 and C ion at m/z 101 (Figure 4, p. 20; Figure 8, p. 24). Background interference was detected for C ion at m/z 75 (Appendix A, p. 32). Matrix was uncharacterized pond water; source location was not reported.	

Data were obtained from p. 9; Appendix A, p. 17; Tables I-IV, pp. 31-34; Figures 3-4, pp. 37-38; Figure 6, p. 40; Figure 9, p. 43 of MRID 44536505; p. 8; Tables I-II, pp. 15-16; Figures 1-2, pp. 17-18; Figure 4, p. 20; Figure 8, p. 24; Appendix A, p. 32 of MRID 44536507.

Linearity is satisfactory when $r^2 \geq 0.995$.

1 Derivatized as cis- and trans-3-chloroallyl isobutyl carbonate (CAIBC; Appendix A, p. 17 of MRID 44536505).

2 Calibration curve r^2 values determined using power regression equation (Appendix A, Figures 3-4, pp. 37-38 of MRID 44536505; Figures 1-2, pp. 17-18 of MRID 44536507).

3 For the ECM validation, confirmation ion ratio results were only provided for one LOQ (0.10 ng/mL) fortified sample for both cis- and trans-3-CAAL and were $\pm 3\%$ of the average standard confirmation ratio (Appendix A, Figure 7, p. 41; Figure 10, p. 44 of MRID 44536505). For the ILV, confirmation ion ratio results were only provided for one LOQ (0.10 ng/mL) and one 5x LOQ (0.50 ng/mL) fortified sample for both cis- and trans-3-CAAL and were $\pm 12\%$ of the average standard confirmation ratio (Figures 5-6, pp. 21-22; Figures 9-10, pp. 25-26 of MRID 44536507). A confirmatory method is typically not required where GC/MS and LC/MS methods are used as the primary method.

IV. Method Deficiencies and Reviewer's Comments

1. The ILV was not conducted independently of the ECM originating laboratory. The study director of the ECM validation, and author of the method and ECM validation study report, D.O. Duebelbeis, was also the study director of the ILV and co-author of the ILV study report (pp. 1, 3, 5; Appendix A, p. 17 of MRID 44536505; pp. 1, 3, 5 of MRID 44536507).
2. The experimental design of the ILV was inadequate to produce a successful validation of the ECM. For the ILV, only two recoveries were reported for both the LOQ and 5x LOQ fortification levels, with no performance data at 10x LOQ (Tables I-II, pp. 15-16 of MRID 44536507). 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 10x LOQ for each analyte and matrix.
3. For the ILV, the total number of trials conducted to yield acceptable recovery results was not reported; documented communications indicate at least two trials were performed (Appendix A, p. 33 of MRID 44536507).
4. For both the ECM validation and ILV, the surface (ECM) and pond (ILV) water matrices were not characterized. The registrant failed to verify that the independent laboratory performed the ILV with a water matrix of the most difficult analytical sample condition to analyze to demonstrate how well the method performs.
5. The ILV did not verify the LODs for the analytes as determined by the ECM validation.
6. For the ECM validation at fortification levels >LOQ (2.5x, 5x, 10x, 25x, and 50x LOQ), only two or three recoveries were reported for each fortification level (Appendix A, Tables I-II, pp. 31-32 of MRID 44536505).
7. For the ILV, chromatograms for reagent blank samples were not provided (Figures 4-6, pp. 20-22; Figures 8-10, pp. 24-26 of MRID 44536507). For the calibration standards, only chromatograms of 0.10 ng/mL (in water matrix, 4.0 ng/mL standard) cis- and trans-3-CAAL standards were provided (calibration standard range 0.05-1.00 ng/mL in water matrix; Figures 1-3, pp. 17-19; Figure 7, p. 23).
8. For the ECM validation, chromatograms for reagent blank and spiked samples, other than LOQ, were not provided (Appendix A, Figures 6-7, pp. 40-41; Figures 9-10, pp. 43-44 of MRID 44536505). For the calibration standards, only chromatograms of 0.10 ng/mL (in water matrix, 4.2 ng/mL standard) cis- and trans-3-CAAL standards were provided (calibration standard range 0.05-10.4 ng/mL in water matrix; Appendix A, Figures 3-5, pp. 37-39; Figure 8, p. 42).

In the ECM study report, the study authors described r^2 as both correlation coefficient and coefficient of determination (p. 11; Appendix A, p. 28; Figures 3-4, pp. 37-38). The reviewer verified that the r^2 values reported in the ECM and ILV study reports are coefficients of determination (r^2 ; DER Attachment 2).

9. The independent laboratory performed the extraction method as written, with the following exception: a sand bath was used for heating during the Snyder column evaporation step as the evaporation flasks were not flat-bottomed (pp. 9-11; Appendix A, p. 33 of MRID 44536507). In addition to minor instrument adjustments, the following GC/MSD conditions were modified: the end of the temperature program was held at 260°C for 3 minutes and ions monitored were m/z 136.1 (Q) and m/z 101.1 (C; Appendix A, p. 31). Confirmation ion ratios were calculated as [(peak area at m/z 101)/(peak area at m/z 136)] (Figure 3, p. 19; Figures 5-7, pp. 21-23; Figures 9-10, pp. 25-26). The independent laboratory found the following Snyder column evaporation steps to be critical: flow hood drafts may cause condenser over-cooling resulting in extended evaporation time and poor analyte recoveries, and the Snyder column should be rinsed with hexane immediately after removing the flask from heat to prevent significant analyte losses (Appendix A, pp. 32-33). Confirmation ion m/z 75 was not used because of background interference; confirmation ion m/z 101, as per the ECM (Appendix A, p. 28 of MRID 44536505), yielded an acceptable signal-to-noise ratio and was substituted. None of the modifications are considered substantial changes to the ECM.
10. It was reported for the ILV that a set of seven samples (one reagent blank, two matrix controls, and four fortified samples) required *ca.* 16 person hours (2 calendar days) to complete (Appendix A, p. 32 of MRID 44536507).

V. References

- Keith, L.H.; Crummett, W.B.; Deegan, J.; Libby, R.A.; Taylor, J.T.; Wentler, G., "Principles of Environmental Analysis", *Anal. Chem.*, 1983, **55**, pp. 2210-2218 (Appendix A, p. 30 of MRID 44536505).
- 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**cis- and trans-3-Chloroallyl alcohol (CAAL)**

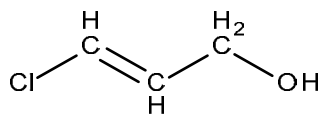
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CAS Name: 3-Chloro-2-propen-1-ol

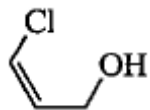
CAS Number: 29560-84-7
cis- : 4643-05-4
trans- : 4643-06-5

SMILES String: C(/C=C/Cl)O

3-CAAL



cis-3-CAAL



trans-3-CAAL

