Test Materials: Prometryn, Atrazine, Simazine, and Propazine

MRID: 49537101

Atrazine - Analytical Method (GRM071.01A) for the Determination of Title:

Atrazine, Simazine, Propazine, and Prometryn in Soil by LC-MS/MS

MRID: 49537102

Independent Laboratory Validation of Residue Method (GRM071.01A)

for the Determination of Atrazine, Simazine, Propazine, and Prometryn

in Soil by LC-MS/MS

080805 (prometryn)

080803 (atrazine) **EPA PC Codes:** 

080807 (simazine)

080808 (propazine)

OCSPP Guideline: 850.6100

**For CDM Smith** 

Title:

Zymme Dinai **Signature:** Primary Reviewer: Lynne Binari

**Date:** 7/28/15

**Signature:** Secondary Reviewer: Lisa Muto

**Date:** 7/28/15

**QC/QA Manager:** Joan Gaidos Signature:

**Date:** 7/28/15

## Analytical method for prometryn, atrazine, simazine, and propazine in soil

**Reports:** ECM: EPA MRID No.: 49537101. Mayer, L.C. 2014. Atrazine - Analytical

Method (GRM071.01A) for the Determination of Atrazine, Simazine, Propazine, and Prometryn in Soil by LC-MS/MS. Report prepared, sponsored, and submitted by Syngenta Crop Protection, LLC, Greensboro, North Carolina; 48 pages. Report No.: GRM071.01A. PASC Study No.: 141-1030. Task No.: TK0225755. Final

report issued December 17, 2014.

ILV: EPA MRID No. 49537102. Yang, A. (J.). 2014. Independent Laboratory Validation of Residue Method (GRM071.01A) for the Determination of Atrazine, Simazine, Propazine, and Prometryn in Soil by LC-MS/MS. Report prepared by Primera Analytical Solutions Corp., Princeton, New Jersey, sponsored and submitted by Syngenta Crop Protection, LLC, Greensboro, North Carolina; 152 pages. Report No.: PASC-REP-0505. PASC Study No.: 141-1030. Task No.:

TK0182056. Final report issued October 31, 2014.

**Document No.:** MRIDs 49537101 & 49537102

**Guideline:** 850.6100

**Statements:** ECM: No claim of compliance with USEPA Good Laboratory Practice (GLP)

standards (40 CFR Part 160) was made for this study (p. 3 of MRID 49537101). Signed and dated Data Confidentiality and GLP statements were provided (pp. 2-

3). Quality Assurance and Authenticity Certification statements were not

provided.

ILV: The study was conducted in compliance with USEPA GLP standards (p. 3 of MRID 49537102). Signed and dated Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-4). An Authenticity Certification

statement was not provided.

**Classification:** This analytical method is classified as supplemental. Two sets of performance

data were not submitted; ECM validation data were not reported. The

determinations of the LOQ and LOD were not based on scientifically acceptable procedures. Linearity of the prometryn quantitation ion analysis calibration curves was not satisfactory. Reagent blank and 10x LOQ chromatograms were not provided. The registrant did not verify that the ILV was conducted with a soil of

Signature: **4** 

the most difficult analytical sample condition. The method did not include the degradates of prometryn. The registrant is requested to submit a state-of-art

method that includes prometryn degradates.

**PC Codes:** 080805 (prometryn)

080803 (atrazine) 080807 (simazine) 080808 (propazine)

**Reviewer:** Mohammed A. Ruhman,

Senior Scientist, EFED, EPA Date: 03/20/2017

## **Executive Summary**

The analytical method, Syngenta Analytical Method GRM071.01A, is designed for the quantitative determination of prometryn, atrazine, simazine, and propazine in soil using LC/MS/MS. The method is quantitative for the analytes at the stated LOQ of 0.01 mg/kg (ppm). The LOQ is less than the current lowest toxicological level of concern in soil. The independent laboratory validated the method for analysis of prometryn, atrazine, simazine, and propazine at the LOQ and 10x LOQ in a sandy loam soil matrix after one trial. No major modifications were made by the independent laboratory. For both the ECM study report and ILV, linearity of the prometryn quantitation ion analysis calibration curves were not satisfactory, and reagent blank and 10x LOQ chromatograms were not provided. The registrant did not verify that the ILV was conducted with a soil of the most difficult analytical sample condition.

**Table 1. Analytical Method Summary** 

	MRID							Limit of
Analyte(s) by Pesticide	Environmental Chemistry Method	Independent Laboratory Validation	EPA Review	Matrix	Method Date (dd/mm/yyyy)	Registrant	Analysis	Quantitation (LOQ)
Prometryn								
Atrazine	49537101 <sup>1</sup>	49537102		Soil <sup>2</sup>	17/12/2014	Syngenta Crop	I C/MC/MC	0.01 mg/kg
Simazine	4933/101	4933/102		3011-	1//12/2014	Protection	LC/MS/MS	(ppm)
Propazine								

<sup>1</sup> No quantitative method recovery data were reported. All of the recovery results presented in the tables of the ECM study report (Tables 2-3, pp. 24-25 of MRID 49537101) are data generated by Primera Analytical Solutions Corp. for the ILV (pp. 19-22; Tables 1-8, pp. 26-33 of MRID 49537102).

## I. Principle of the Method

Soil (10 g) was fortified with a mixed standard solution of prometryn, atrazine, simazine, and propazine in acetonitrile for procedural recoveries (pp. 11, 13 of MRID 49537101). The soil used during the ECM development/validation was not characterized (Figures 9-10, p. 33; Figures 15-16, p. 36; Figures 21-22, p. 39; Figures 27-28, p. 42). The soil characterization presented in Table 1 (p. 24) of the ECM study report is for the soil matrix used in the ILV (p. 13 of MRID 49537102). Soil samples (10 g) are reflux extracted with 60 mL of acetonitrile:water (90:10, v:v) for 1 hour (p. 13; Appendix 4, p. 48). Soil and extract are separated by centrifugation (3,500 rpm, 5 minutes). Filter a 1-mL aliquot of the extract through 50 mg CEC18 sorbent (UTC, United Chemical Technologies) using either a 1-mL tube or 96-well plate format. Collect 0.6 mL of the filtrate in a LC vial or deep well titer plate. Add 0.4 mL of 0.1% aqueous acetic acid (final volume 1.0 mL). Final solvent concentration should be equivalent to acetonitrile:water + 0.1% acetic acid (40:60, v:v), or if volume is less or more than 0.5 mL add an equal volume of 0.1% aqueous acetic acid.

Samples are analyzed using a Waters Acquity UPLC system (I-Class) and an Applied Biosystems Sciex 5500 QTRAP triple quadrupole MS with TurboIonSpray interface (pp. 14-17 of MRID 49537101). The following LC conditions were used: ACE 5 C18 column (3.0 mm x 50 mm, 5.0  $\mu$ m, column temperature 30°C), mobile phase of (A) 0.1% acetic acid in ultra-pure water and (B) 0.1% acetic acid in acetonitrile [percent A:B (v:v) at 0.0 min. 95:5, 1.5-2.2 min. 5:95, 2.5-3.5 min. 95:5], and injection volume of 10  $\mu$ L. The following MS/MS conditions were used: positive ion

<sup>2</sup> Characterized sandy loam (17% clay, 4.4% organic carbon) soil was used for the ILV (p. 13 of MRID 49537102; Table 1, p. 24 of MRID 49537101).

mode, ionization temperature 500°C, and multiple reaction monitoring (MRM). Analytes are identified using two ion pair transitions; one for quantitation (Q, "primary") and one for confirmation (C). Ion transitions monitored are as follows: m/z 242.2 $\rightarrow$ 158.1 (Q) and m/z 242.2 $\rightarrow$ 200.1 (C) for prometryn, m/z 216.1 $\rightarrow$ 174.2 (Q) and m/z 216.1 $\rightarrow$ 132.0 (C) for atrazine, m/z 202.1 $\rightarrow$ 132.0 (Q) and m/z 202.1 $\rightarrow$ 103.7 (C) for simazine, and m/z 230.1 $\rightarrow$ 146.0 (Q) and m/z 230.1 $\rightarrow$ 188.0 (C) for propazine. Expected retention times are ca. 1.16, 1.23, 1.10, and 1.35 minutes for prometryn, atrazine, simazine, and propazine, respectively (Figures 5-7, pp. 31-32; Figures 10-13, pp. 33-35; Figures 16-19, pp. 36-39; Figures 22-25, pp. 39-41; Figures 28-29, pp. 42-43).

<u>ILV</u>: Test compounds and sandy loam soil were supplied by Syngenta (pp. 11-13 of MRID 49537102; Table 1, p. 24 of MRID 49537101). The soil matrix was characterized, but the source location was not reported. The independent laboratory performed the method as written with the following modifications: following reflux, a 10-mL aliquot of the extract was centrifuged in a glass tube instead centrifuging the entire soil/extract sample in a 125-mL Nalgene bottle; a Waters Sep-Pak C18 40-mg 96-well plate was used for filtration instead of the 50-mg CEC18 sorbent (UCT); samples were analyzed using a Waters Acquity UPLC System with an Applied Biosystems Sciex 4000 QTRAP triple quadrupole MS; and injection volume was increased to 20 μL (pp. 15-17; Figure 1, pp. 35-39; Figure 2, pp. 41-45; Figure 3, pp. 47-51; Figure 4, pp. 53-57; Figure 5, pp. 59-63; Figure 6, pp. 65-69; Figure 7, pp. 71-75; Figure 8, pp. 77-81; Appendix 1, Appendix A, pp. 95-145 of MRID 49537102). Expected retention times were *ca.* 1.47, 1.33-1.34, 1.20, and 1.47 minutes for prometryn, atrazine, simazine, and propazine, respectively.

<u>LOQ and LOD</u>: In the ECM and ILV, the LOQ was 0.01 mg/kg (ppm, 10 ppb) for prometryn, atrazine, simazine, and propazine (pp. 10, 20 of MRID 49537101; pp. 8, 10, 23 of MRID 49537102). For all four analytes, the ECM determined a LOD of 1.0 pg injected on the column, equivalent to 0.10 pg/ $\mu$ L (ng/mL) for a 10- $\mu$ L injection volume (p. 20 of MRID 49537101). Instrument detection limits were evaluated as part of the ILV, but were not reported (p. 17; Tables 1-8, pp. 26-33 of MRID 49537102).

### **II. Recovery Findings**

ECM (MRID 49537101): Recovery results presented in Tables 2-3 (pp. 24-25) of the study report are data generated by Primera Analytical Solutions Corp. for the ILV (Tables 1-8, pp. 26-33 of MRID 49537102) and are discussed in the following paragraph. The soil characterization presented in Table 1 (p. 24) of the study report is the soil used in the ILV (p. 13 of MRID 49537102). ECM validation method recovery data were not reported.

ILV (MRID 49537102): Mean recoveries and relative standard deviations (RSDs) were within guidelines (mean 70-120%; RSD ≤20%) for analysis of prometryn, atrazine, simazine, and propazine in sandy loam soil at fortification levels of 0.01 mg/kg (LOQ) and 0.10 mg/kg (10x LOQ; pp. 19-22; Tables 1-8, pp. 26-33). Analytes were identified and quantified using two ion transitions; quantitation and confirmation recovery results were comparable. The method was validated for all four analytes at both fortification levels in the soil matrix after one trial, with minor method modifications and equivalent instrument substitutions (pp. 15, 17-18). The sandy loam soil (17% clay, 4.4% organic carbon) matrix was supplied by Syngenta and characterized by Agvise Laboratories, Northwood, North Dakota (p. 13 of MRID 49537102; Table 1, p. 24 of MRID 49537101).

Table 2. Initial Validation Method Recoveries for Prometryn, Atrazine, Simazine, and

**Propazine in Soil** 

Analyte	Fortification	Number	Recovery	Mean	Standard	Relative Standard		
	Level (mg/kg)	of Tests	Range (%)	Recovery (%)	<b>Deviation (%)</b>	Deviation (%)		
	Quantitation Ion							
Prometryn	0.01 (LOQ)	5						
Frometryn	0.10	5						
Atrazine	0.01 (LOQ)	5						
Atrazine	0.10	5						
C:i	0.01 (LOQ)	5	No performance data were reported. <sup>1</sup>					
Simazine	0.10	5						
D	0.01 (LOQ)	5						
Propazine	0.10	5						
	Confirmation Ion							
Duomoturu	0.01 (LOQ)	5						
Prometryn	0.10	5						
A 4	0.01 (LOQ)	5						
Atrazine	0.10	5						
g: -:	0.01 (LOQ)	5						
Simazine	0.10	5						
D	0.01 (LOQ)	5						
Propazine	0.10	5						

<sup>1</sup> Recovery results presented in Tables 2-3 of the ECM study report are data generated by Primera Analytical Solutions Corp. for the ILV (pp. 24-25 of MRID 49537101; Tables 1-8, pp. 26-33 of MRID 49570102).

Table 3. Independent Validation Method Recoveries for Prometryn, Atrazine, Simazine, and

Propazine in Sandy Loam Soil<sup>1</sup>

Analyte	Fortification	Number	Recovery	Mean	Standard	Relative Standard	
Analyte	Level (mg/kg)	of Tests	Range (%)	Recovery (%)	<b>Deviation</b> (%)	Deviation (%)	
	Quantitation Ion						
Duomonturu	0.01 (LOQ)	5	105.00-110.00	107.80	2.17	2.01	
Prometryn	0.10	5	89.00-94.60	91.84	2.43	2.64	
Atrazine	0.01 (LOQ)	5	83.20-95.00	89.86	4.24	4.72	
Atrazine	0.10	5	84.50-90.70	88.26	2.28	2.58	
G:i	0.01 (LOQ)	5	94.00-99.40	96.06	2.16	2.24	
Simazine	0.10	5	89.90-97.60	93.20	2.85	3.06	
D	0.01 (LOQ)	5	96.60-99.90	97.88	1.48	1.51	
Propazine	0.10	5	84.80-92.70	89.30	3.00	3.36	
	Confirmation Ion						
Prometryn	0.01 (LOQ)	5	96.70-101.00	99.28	1.66	1.67	
	0.10	5	87.40-92.00	90.46	1.78	1.97	
	0.01 (LOQ)	5	83.60-98.90	90.76	5.55	6.12	
Atrazine	0.10	5	83.10-89.90	86.82	2.82	3.24	
G:i	0.01 (LOQ)	5	86.70-110.00	97.94	8.93	9.12	
Simazine	0.10	5	88.60-96.20	93.36	3.55	3.80	
D	0.01 (LOQ)	5	87.90-103.00	95.46	6.32	6.62	
Propazine	0.10	5	83.90-90.40	87.78	2.48	2.82	

Data (recovery results) were obtained from Tables 1-8, pp. 26-33 of MRID 49537102. Example equations allow for correction of recovery results, and residues were detected in the provided matrix control sample chromatograms, but the data tables do not indicate the recoveries are corrected (Tables 1-8, pp. 26-33; Figure 1, p. 38; Figure 2, p. 44; Figure 3, p. 50; Figure 4, p. 56; Figure 5, p. 62; Figure 6, p. 68; Figure 7, p. 74; Figure 8, p. 80; Appendix 3, p. 150). 1 The soil matrix, supplied by Syngenta, was characterized, but source location was not reported (p. 13 of MRID 49537102; Table 1, p. 24 of MRID 49537101).

### **III. Method Characteristics**

In the ECM, the LOO for prometryn, atrazine, simazine and propazine in soil was 0.01 mg/kg (ppm, 10 ppb; pp. 10, 20 of MRID 49537101). The ECM defined the LOQ as the lowest analyte concentration at which the methodology has been validated and a mean recovery of 70-110% and RSD of ≤20% has been obtained. For all four analytes, the ECM determined a LOD of 1.0 pg injected on the column and equivalent to 0.10 pg/µL (ng/mL) for a 10-µL injection volume. The ECM defined the LOD as the lowest analyte concentration detectable above the mean amplitude of the background noise in an untreated matrix control sample at the corresponding retention time, and an estimate of the LOD can be taken as three times the background noise. The ILV reported the same LOQ as the ECM, but did not specify the LOD (pp. 8, 10 of MRID 49537102).

Table 4. Method Characteristics for Prometryn, Atrazine, Simazine, and Propazine in Soil

		Prometryn	Atrazine	Simazine	Propazine			
Limit of Quantitation (LOQ)		0.01 mg/kg (ppm, 10 ppb)						
Limit of Detection (LOD)		1.0 pg on column, equivalent to 0.10 pg/μL (ng/mL) for a 10-μL injection volume.						
Linearity (calibration	ECM:	Q ion: $r^2 = 0.9928$ C ion: $r^2 = NR^2$	Q ion: $r^2 = 0.9984$ C ion: $r^2 = NR$	Q ion: $r^2 = 0.9992$ C ion: $r^2 = NR$	Q ion: $r^2 = 0.9992$ C ion: $r^2 = NR$			
curve r <sup>2</sup> and concentration range	II V·	Q ion: $r^2 = 0.9932$ C ion: $r^2 = 0.9984$	Q ion: $r^2 = 0.9956$ C ion: $r^2 = 0.9960$	Q ion: $r^2 = 0.9980$ C ion: $r^2 = 0.9956$	Q ion: $r^2 = 0.9950$ C ion: $r^2 = 0.9966$			
	Range:	0.10-10.0 pg/μL (ng/mL, ppb)						
D 4-1-1-	ECM:	Method recovery data were not reported. Recovery results presented in Tables 2-3 (pp. 24-25) of the study report are data generated by Primera Analytical Solutions Corp. for the ILV						
Repeatable	ILV:	[sand	Yes at LOQ and 10x LOQ. [sandy loam (17% clay, 4.4% organic carbon) soil matrix] <sup>3</sup>		atrix] <sup>3</sup>			
Reproducible	·	Yes. However, the registrant did not verify that the ILV was conducted with a soil of the most difficult analytical sample condition.						
Е	CM: <sup>3</sup>	Yes. For Q ion for all four analytes, interferences (based on peak height) were $\leq ca$ . 30% of LOD (0.10 pg/ $\mu$ L calibrant) at analyte retention times in matrix control. C ion chromatograms were not provided.						
Specific	V:	Yes. For Q and C ions for all four analytes, interferences (based on peak height) were <5% of LOQ at analyte retention times in matrix control.						
	<b>.</b> V .	Matrix effects were not "significant" (p. 23, quantitative data were not reported). Matrix matched standards were not required.						

Data were obtained from pp. 10, 20; Figure 5, p. 31; Figures 8-9, pp. 32-33; Figure 11, p. 34; Figures 14-15, pp. 35-36; Figure 17, p. 37; Figures 20-21, pp. 38-39; Figure 23, p. 40; Figures 26-27, pp. 41-42 of MRID 49537101; pp. 8, 10, 23; Tables 1-8, pp. 26-33; Figure 1, pp. 38-40; Figure 2, pp. 44-46; Figure 3, pp. 50-52; Figure 4, pp. 56-58; Figure 5, pp. 62-64; Figure 6, pp. 68-70; Figure 7, pp. 74-76; Figure 8, pp. 80-82 of MRID 49537102; DER Attachment 2. Linearity is satisfactory when  $r^2 \ge 0.995$ .

<sup>1</sup> Linear regression with no weighting for ECM calibration curves and 1/x weighting for ILV (pp. 17-18; Figure 8, p. 32; Figure 14, p. 35; Figure 20, p. 38; Figure 26, p. 41 of MRID 49537101; Figure 1, p. 40; Figure 2, p. 46; Figure 3, p. 52; Figure 4, p. 58; Figure 5, p. 64; Figure 6, p. 70; Figure 7, p. 76; Figure 8, p. 82 of MRID 49537102). Coefficient of determination (r²) values are reviewer-generated from reported correlation coefficient (r) values (DER Attachment 2).

<sup>2</sup> NR = Not Reported.

<sup>3</sup> Soil characterization was provided, but source location was not reported (p. Table 1, p. 24 of MRID 49537101; p. 13 of MRID 49537102). Soil matrix for ILV was supplied by Syngenta.

#### IV. Method Deficiencies and Reviewer's Comments

- 1. Two sets of performance data were not submitted for the method. For the ECM validation, no quantitative method recovery data were reported. All of the recovery results presented in the tables of the ECM study report (Tables 2-3, pp. 24-25 of MRID 49537101) are the data generated by Primera Analytical Solutions Corp. for the ILV (pp. 19-22; Tables 1-8, pp. 26-33 of MRID 49537102). The chromatograms provided with the ECM study report were generated by Syngenta, but do not provide any quantitative recovery results (Figures 5-28, pp. 31-42 of MRID 49537101; Appendix 1, Appendix A, Figures 5-28, pp. 128-139 of MRID 49537102). The author, Louis C. Mayer, of the ECM study report was the study monitor for the ILV (p. 1 of MRID 49537101; p. 5 of MRID 49537102). Additionally, the PASC Study No. 141-1030 was reported for both the ECM and ILV documents.
- 2. The determination of the LOQ and LOD were not based on scientifically acceptable procedures as defined in 40 CFR Part 136, Appendix B. The ECM defined the LOQ as the lowest analyte concentration at which the methodology has been validated and a mean recovery of 70-110% and RSD of ≤20% has been obtained (p. 20 of MRID 45937101). The ECM defined the LOD as the lowest analyte concentration detectable above the mean amplitude of the background noise in an untreated matrix control sample at the corresponding retention time, and an estimate of the LOD can be taken as three times the background noise. The ILV reported the same LOQ as the ECM, but did not specify the LOD (pp. 8, 10 of MRID 49537102). Detection limits should not be based on the arbitrarily selected lowest concentration in the spiked samples. Additionally, the lowest toxicological level of concern in soil was not reported. A LOQ above toxicological levels of concern results in an unacceptable method classification.
- 3. For both the ECM study report and ILV, linearity of the prometryn quantitation ion analysis calibration curve was not satisfactory ( $r^2 \ge 0.995$ ; DER Attachment 2).
- 4. For the ILV, chromatograms for reagent blanks and 10× LOQ sample analyses were not provided (Figures 1-8, pp. 35-82 of MRID 49537102). Standard curve plots with regression curve analyses were provided, but the individual calibration standard data were not provided.
- 5. For the ECM study report, chromatograms for reagent blanks,  $10 \times \text{LOQ}$  sample analyses, and confirmation ion analyses were not provided (Figures 5-28, pp. 31-42 of MRID 49537101). Standard curve plots (quantitation ion only) with correlation coefficients (r values) were provided, but the regression curve equation and individual calibration standard data were not provided. In section **5.1 Multi Point Calibration Procedure**, the ECM specifies that "R-Squared" values should be included in the raw data; only r values were provided with the calibration curves (p. 18; Figure 8, p. 32; Figure 14, p. 35; Figure 20, p. 38; Figure 26, p. 41).
- 6. For the ILV, the source location for the soil matrix was not reported (p. 13 of MRID 49537102; Table 1, p. 24 of MRID 49537102). The registrant did not verify that the ILV was conducted with a soil of the most difficult analytical sample condition.
- 7. For the ILV, it was unclear whether or not recoveries were corrected. Example equations allow for correction of recovery results, and residues were detected in the provided matrix

- control sample chromatograms, but the data tables do not indicate the recoveries are corrected (Tables 1-8, pp. 26-33; Figure 1, p. 38; Figure 2, p. 44; Figure 3, p. 50; Figure 4, p. 56; Figure 5, p. 62; Figure 6, p. 68; Figure 7, p. 74; Figure 8, p. 80; Appendix 3, p. 150 of MRID 49537102).
- 8. For the ECM, the soil used for the method development/validation was not characterized (Figures 9-10, p. 33; Figures 15-16, p. 36; Figures 21-22, p. 39; Figures 27-28, p. 42 of MRID 49537101).
- 9. For the ILV, the purity of the prometryn test compound was reported as "NA" in section **3.1 Test/Reference Substance** of the study report, but the Certificate of Analysis listed the purity as  $99.7 \pm 0.5\%$  (p. 11; Appendix 2, p. 146 of MRID 49537102).
- 10. The equipment substitutions and method modifications implemented by the independent laboratory (see section **I. Principle of the Method**, <u>ILV</u>: above for details) are not considered substantial changes to the ECM.
- 11. It was reported for the ILV that one analyst completed a set of thirteen samples (one reagent blank, two matrix controls, and ten fortified samples) in one working day, with LC/MS/MS analysis performed overnight (p. 23 of MRID 49537102).

#### 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**

## Prometryn (G34161, G-34-161)

**IUPAC Name:** N<sup>2</sup>,N<sup>4</sup>-diisopropyl-6-methylthio-1,3,5-triazine-2,4-diamine

CAS Name: N,N'-bis(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine.

N,N'-Diisopropyl-6-(methylsulfanyl)1,3,5-triazine-2,4-diamine. 1,3,5-Triazine-2,4-diamine, N,N'-bis(1-methylethyl-6-(methylthio)-.

**Chemical Name:** 2,4-Bis(isopropylamino)-6-methylthio-s-triazine

**CAS Number:** 7287-19-6

**SMILES String:** CSc1nc(NC(C)C)nc(NC(C)C)n1

$$H_3$$
C  $S$   $N$   $N$   $C$   $H_3$   $C$   $H_3$   $C$   $H_3$ 

# Atrazine (G30027)

**IUPAC Name:** 6-Chloro-N<sup>2</sup>-ethyl-N<sup>4</sup>-isopropyl-1,3,5-triazine-2,4-diamine 6-Chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine.

6-Chloro-N-ethyl-N'-isopropyl-1,3,5-triazine-2,4-diamine.

1,3,5-Triazine-2,4-diamine, 6-chloro-N-ethyl-N'-(1-methylethyl)-.

**Chemical Name:** 2-Chloro-4-ethylamino-6-isopropylamino-s-triazine.

CAS Number: 1912-24-9 SMILES String: Not available.

# **Simazine (G27692)**

**IUPAC Name:** 6-Chloro-N<sup>2</sup>,N<sup>4</sup>-diethyl-1,3,5-triazine-2,4-diamine 6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine.

1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-diethyl-.

**Chemical name:** 2-Chloro-4,6-bis(ethylamino)-s-triazine

CAS Number: 122-34-9 SMILES String: Not available.

# Propazine (G30028)

**IUPAC Name:** 6-Chloro-N<sup>2</sup>,N<sup>4</sup>-diisopropyl-1,3,5-triazine-2,4-diamine

**CAS Name:** 6-Chloro-N,N'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine.

6-Chloro-N,N'-diisopropyl-1,3,5-triazine-2,4-diamine.

1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-bis(1-methylethyl)-.

**Chemical Name:** 2-Chloro-4,6-bis(isopropylamino)-s-triazine.

CAS Number: 139-40-2 SMILES String: Not available.

ÇH₃ N ÇH₃