Test Material:	Azoxystrobin
MRID:	49112204
Title:	Azoxystrobin: Azoxystrobin – Residue Method (GRM057.04A) for the Determination of Azoxystrobin and Z-Isomer R230310 in Water by LC-MS/MS – Analytical Method
MRID:	49112202
Title:	Azoxystrobin: Azoxystrobin – Independent Laboratory Validation (ILV) of Residue Method (GRM057.04A) for the Determination of Azoxystrobin and Z-Isomer R230310 in Water by LC-MS/MS – Analytical Method
EPA PC Code:	128810
OCSPP Guideline:	850.6100

For CDM Smith

Primary Reviewer: Lisa Muto **Signature:** 

Date: 10/6/14

Secondary Reviewer: Lynne Binari **Signature:** 

Date: 10/6/14

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

Date: 10/6/14

Analytical method for azoxystrobin and its Z-isomer R230310 in water

Reports:	ECM: EPA MRID No.: 49112204. Mayer, L.C. 2012. Azoxystrobin: Azoxystrobin – Residue Method (GRM057.04A) for the Determination of Azoxystrobin and Z-Isomer R230310 in Water by LC-MS/MS – Analytical Method. Report No.: GRM057.04A. Task No.: TK0048239. Report prepared, sponsored and submitted by Syngenta Crop Protection, Inc., Greensboro, North Carolina; 58 pages. Final report issued June 12, 2012. ILV: EPA MRID No. 49112202. Smith, R.J. 2012. Azoxystrobin: Azoxystrobin – Independent Laboratory Validation (ILV) of Residue Method (GRM057.04A) for the Determination of Azoxystrobin and Z-Isomer R230310 in Water by LC-MS/MS – Analytical Method. Report and Study No: 1781.6873. Task No.: TK0048240. Report prepared by Smithers Viscient, Wareham, Massachusetts, sponsored and submitted by Syngenta Crop Protection, Inc., Greensboro, North Carolina; 160 pages. Final report issued October 26, 2012.
Document No.:	MRIDs 49112204 & 49112202
Guideline:	850.6100
Statements:	ECM: The study was conducted with no claim of compliance with USEPA or OECD Good Laboratory Practice (GLP) standards (p. 3 of MRID 49112204). Signed and dated No Data Confidentiality and GLP statements were provided (pp. 2-3). Quality Assurance and Authenticity statements were not provided. ILV: The study was conducted in compliance with USEPA GLP standards (p. 3 of MRID 49112202). Signed and dated No Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-4). A statement of the authenticity of the study report was included as part of the Quality Assurance Statement.
Classification:	This analytical method is classified as supplemental. The determinations of the LOQ and LOD were not shown to be based on scientifically acceptable procedures.
PC Code:	128810
Reviewer:	Michelle Colletti, Chemist U.S. EPA **Signature:** Michelle Colletti **Date:** 05/19/2015
Secondary Reviewer:	William Eckel, Ph.D., Senior Advisor U.S. EPA **Signature:** **Date:** 05/19/2015 William P. Eckel

Executive Summary

This analytical method, Syngenta Residue Method (GRM057.04A), is designed for the quantitative determination of azoxystrobin and its Z-isomer R230310 in ground water and surface water using HPLC/MS/MS. The method is quantitative for the analytes at the stated LOQ of 0.10 µg/L. The LOQ is less than the lowest toxicological level of concern in water. The independent laboratory validated the method after one trial with only two minor modifications.

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						
Azoxystrobin R230310 (Z-isomer of azoxystrobin)	49112204	49112202		Ground water & Surface water	12/06/2012	Syngenta	HPLC/MS/MS	0.10 µg/L

I. Principle of the Method

Samples (1.0 mL) of water were fortified, as necessary, and diluted to a final volume of 10 mL with acetonitrile:ultra-pure water (50:50, v:v) in a 15-mL or 50-mL polypropylene falcon tube (pp. 15-16; Appendix 1, p. 55; Appendix 4, p. 58 of MRID 49112204). An aliquot was transferred to an autosampler vial and analyzed directly using an Applied Biosystems API 5500 QTRAP LC/MS/MS.

Samples were analyzed for azoxystrobin and its Z-isomer R230310 by HPLC (ACE 5 C18, 3.0 mm x 50 mm column (or 3.0 mm x 150 mm column), 40°C; column particle size not reported) using a mobile phase of (A) OPTIMA Grade water in 0.1% acetic acid and (B) OPTIMA Grade acetonitrile in 0.1% acetic acid [percent A:B at 0.0-3.0 min. 50:50, isocratic flow] with MS/MS (turboionspray ionization, positive ion mode) detection and multiple reaction monitoring (MRM; pp. 16-18; Appendix 1, p. 55 of MRID 49112204). Injection volume was 30 µL. Azoxystrobin and its Z-isomer were identified and quantified using two ion transitions, primary and confirmatory. Ion transitions monitored were as follows: *m/z* 404→372 (primary) and *m/z* 404→329 (confirmatory) for azoxystrobin and R230310. The retention times for azoxystrobin and R230310 were 1.28 and 1.02 minutes, respectively.

The ILV was performed exactly as above using an AB MDS Sciex 5000 Turbo V ESI LC/MS/MS (pp. 19-21 of MRID 49112202). An additional confirmatory ion transition was monitored for each analyte. Ion transitions monitored were as follows: *m/z* 404.38→372.10 (primary), *m/z* 404.38→329.00 (confirmatory 1) and *m/z* 404.38→344.10 (confirmatory 2) for azoxystrobin; and *m/z* 404.39→372.00 (primary), *m/z* 404.39→329.00 (confirmatory 1) and *m/z* 404.39→344.10 (confirmatory 2) for R230310. The retention times for azoxystrobin and R230310 were *ca*. 1.47 and *ca*. 1.18 minutes, respectively. The modifications are not considered substantial changes to the ECM.

The LOQ for azoxystrobin and its Z-isomer R230310 was the same in the ECM and ILV at 0.1 µg/L and 0.100 µg/L, respectively (ppb; pp. 11, 22 of MRID 49112204; p. 13 of MRID 49112202). The LOD for both analytes was reported as 0.005 µg/L in the ECM and 0.00500 µg/L in the ILV (Figures 3-4, p. 33; Figures 15-16, p. 39 of MRID 49112204; and Figures 1-2, p. 36; Figures 15-16, p. 43; Figures 29-30, p. 50; Figures 49-50, p. 60; Figures 63-64, p. 67; Figures 77-78, p. 74 of MRID 49112202).

II. Recovery Findings

ECM (MRID 49112204): Mean recoveries and relative standard deviations (RSDs) were within guideline requirements (mean 70-120%; RSD ≤20%) for analysis of azoxystrobin and its Z-isomer R230310 in ground water and surface water at fortification levels of 0.10 µg/L (LOQ) and 1.0 µg/L (10×LOQ; Tables 2-5, pp. 27-28). Analytes were identified and quantified using two ion transitions, one primary and one confirmatory. The ground water and surface water matrices were characterized (Table 1, p. 26).

ILV (MRID 49112202): Mean recoveries and relative standard deviations (RSDs) were within guideline requirements (mean 70-120%; RSD ≤20%) for analysis of azoxystrobin and its Z-isomer R230310 in ground water and surface water at fortification levels of 0.10 µg/L (LOQ) and 1.0 µg/L (10×LOQ; pp. 22-23; Tables 3-8, pp. 29-34). Analytes were identified and quantified using three ion transitions, one primary and two confirmatory. The method was validated for the analytes at both fortification levels in both matrices after one trial, with minor instrument and method modifications (pp. 13, 18-19). The water matrices were characterized (p. 16; Table 1, p. 27).

Table 2. Initial Validation Method Recoveries for Azoxystrobin and its Z isomer R230310 in Water[1]

Analyte	Fortification Level (µg/L)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%)[2]	Relative Standard Deviation (%)
Surface Water						
Primary ion transition (*m/z* 404→372)						
Azoxystrobin	0.1 (LOQ)	5	77-92	82	6	7.9
	1.0	5	94-100	96	3	2.4
R230310	0.1 (LOQ)	5	81-96	89	7	7.5
	1.0	5	93-104	98	4	4.3
Confirmatory ion transition (*m/z* 404→329)						
Azoxystrobin	0.1 (LOQ)	5	72-105	84	13	15.8
	1.0	5	95-107	101	4	4.4
R230310	0.1 (LOQ)	5	73-100	87	10	11.3
	1.0	5	98-107	101	4	3.7
Ground Water						
Primary ion transition (*m/z* 404→372)						
Azoxystrobin	0.1 (LOQ)	5	91-100	96	4	3.9
	1.0	5	90-98	93	3	3.7
R230310	0.1 (LOQ)	5	99-114	107	6	5.4
	1.0	5	87-109	98	9	9.1
Confirmatory ion transition (*m/z* 404→329)						
Azoxystrobin	0.1 (LOQ)	5	74-103	92	11	12.3
	1.0	5	87-97	92	5	5.2
R230310	0.1 (LOQ)	5	83-105	97	11	11.2
	1.0	5	91-103	95	5	4.9

Data (uncorrected recovery results) were obtained from Tables 2-5, pp. 27-28 of MRID 49112204.

1 Ground water from Summerfield, North Carolina, and surface water from Greensboro, North Carolina, were characterized by Agvise Laboratories, Inc., Northwood, North Dakota (Table 1, p. 26 of MRID 49112204). The water sources were not further specified.

2 Standard deviations were reviewer-calculated from the data in the study report since the study author only reported means and RSDs (see DER Attachment 2).

Table 3. Independent Validation Method Recoveries for Azoxystrobin and its Z isomer R230310 in Water[1]

Analyte	Fortification Level (µg/L)	Number of Tests	Recovery Range (%)	Mean Recovery (%)	Standard Deviation (%)	Relative Standard Deviation (%)
Surface Water						
Primary ion transition[2]						
Azoxystrobin	0.100 (LOQ)	5	98.7-105	102	3.09	3.03
	1.00	5	91.4-96.3	94.6	1.95	2.06
R230310	0.100 (LOQ)	5	94.8-98.7	96.7	1.61	1.67
	1.00	5	94.3-96.6	95.6	0.921	0.964
Confirmatory #1 ion transition[2]						
Azoxystrobin	0.100 (LOQ)	5	96.3-110	104	5.93	5.73
	1.00	5	94.7-97.2	96.1	0.963	1.00
R230310	0.100 (LOQ)	5	95.8-109	104	5.16	4.96
	1.00	5	92.8-97.3	94.7	1.82	1.92
Confirmatory #2 ion transition[2]						
Azoxystrobin	0.100 (LOQ)	5	94.5-107	101	5.13	5.08
	1.00	5	95.2-99.8	97.2	1.95	2.00
R230310	0.100 (LOQ)	5	84.0-110	98.1	10.3[3]	10.5
	1.00	5	95.9-99.1	97.0	1.26	1.29
Ground Water						
Primary ion transition[2]						
Azoxystrobin	0.100 (LOQ)	5	100-104	102	1.56	1.53
	1.00	5	92.7-96.5	94.6	1.61	1.70
R230310	0.100 (LOQ)	5	94.8-102	98.3	3.10	3.15
	1.00	5	93.1-97.4	94.7	1.65	1.74
Confirmatory #1 ion transition[2]						
Azoxystrobin	0.100 (LOQ)	5	94.8-108	103	5.07	4.93
	1.00	5	93.4-99.6	97.4	2.36	2.42
R230310	0.100 (LOQ)	5	95.9-109	103	5.38	5.21
	1.00	5	95.1-98.5	96.5	1.71	1.77
Confirmatory #2 ion transition[2]						
Azoxystrobin	0.100 (LOQ)	5	92.9-106	99.1	6.03	6.08
	1.00	5	91.4-97.2	94.2	2.03	2.16
R230310	0.100 (LOQ)	5	89.5-97.8	94.8	3.36	3.54
	1.00	5	91.9-99.3	95.5	2.96	3.10

Data (uncorrected recovery results) were obtained from pp. 22-23; Tables 3-8, pp. 29-34 of MRID 49112202.

1 Ground water and surface water were characterized by Agvise Laboratories, Inc., Northwood, North Dakota (p. 16; Table 1, p. 27 of MRID 49112202). The specific sources of the water samples were not reported, only that they were provided by the Sponsor.

2 Ion transitions monitored were as follows: *m/z* 404.38→372.10 (primary), *m/z* 404.38→329.00 (confirmatory 1) and *m/z* 404.38→344.10 (confirmatory 2) for azoxystrobin; and *m/z* 404.39→372.00 (primary), *m/z* 404.39→329.00 (confirmatory 1) and *m/z* 404.39→344.10 (confirmatory 2) for R230310.

3 Value was reported as 10.5% on p. 23 and 0.0103 ppb (10.3%) in Table 8, p. 34. The reviewer chose to report 10.3% since this value seemed more accurate based on reviewer-calculations; however, the reviewer calculated s.d. value was 10.4% (see DER Attachment 2).

III. Method Characteristics

In the ECM, the LOQ for azoxystrobin and its Z-isomer R230310 was 0.1 µg/L (ppb); the ILV reported the same, but more exact value, 0.100 µg/L (pp. 11, 22 of MRID 49112204; p. 13 of MRID 49112202). In the ECM, the LOQ was defined as the lowest analyte concentration in a sample at which the method has been validated. The ECM study author also advised that the response for the analyte peak should be no less than four times the mean amplitude of the background noise at the analyte retention time in the control sample. The LOD for both analytes was reported as 0.005 µg/L in the ECM and the same, but more exact, value of 0.00500 µg/L in the ILV (Figures 3-4, p. 33; Figures 15-16, p. 39 of MRID 49112204; and Figures 1-2, p. 36; Figures 15-16, p. 43; Figures 29-30, p. 50; Figures 49-50, p. 60; Figures 63-64, p. 67; Figures 77-78, p. 74 of MRID 49112202). This value corresponded to the lowest calibration standard. The LOD was discussed in the ECM and ILV (p. 22 of MRID 49112204; p. 23 of MRID 49112202). In the ECM, the LOD was defined as the lowest analyte concentration which can be detected above the mean amplitude of the background noise at the analyte retention time in the control sample. The ECM study author also noted that the LOD can be estimated as three times the background noise and will vary between instruments and analytical runs. In the ILV, the LOD was referenced as a measure of matrix and instrument interferences, where interferences at ≤50% of the LOD were considered negligible. No calculations of the LOQ and LOD were reported in the ECM and ILV.

Table 4. Method Characteristics for Azoxystrobin and its Z isomer R230310 in Ground Water and Surface Water

	Azoxystrobin		R230310	
	Surface water	Ground water	Surface water	Ground water
Limit of Quantitation (LOQ)	0.1 µg/L			
Limit of Detection (LOD)	0.005 µg/L[1]			
Linearity (calibration curve r^2 and concentration range)[2,3]	r^2 = 0.99872 (primary) r^2 = 0.99861 (confirmatory #1) r^2 = **0.99064** (confirmatory #2)	r^2 = 0.99846 (primary) r^2 = 0.99916 (confirmatory #1) r^2 = 0.99894 (confirmatory #2)	r^2 = 0.99866 (primary) r^2 = 0.99847 (confirmatory #1) r^2 = 0.99840 (confirmatory #2)	r^2 = 0.99857 (primary) r^2 = 0.99815 (confirmatory #1) r^2 = 0.99837 (confirmatory #2)
	(0.00500-2.00 ppb)			
Repeatable	Yes			
Reproducible	Yes			
Specific	Yes			

Data were obtained from pp. 11, 22; Tables 2-5, pp. 27-28; Figures 3-4, p. 33; Figures 15-16, p. 39; Figures 43-48, pp. 57-59; Figures 91-96, pp. 81-83 of MRID 49112202; and pp. 13, 22-23; Figures 1-2, p. 36; Figures 15-16, p. 43; Figures 29-30, p. 50; Figures 49-50, p. 60; Figures 63-64, p. 67; Figures 77-78, p. 74 of MRID 49112204.

1 Reported in the Figures of the ECM and ILV in the chromatograms of the lowest calibration standard.

2 Linearity of the ILV calibration curves could not be fully verified by the reviewer since all of the raw data were not provided; however, reviewer-calculated curves were generated from provided chromatograms of calibration standards (r^2 values of 1 for all provided matrix/analyte/ion data sets; only data from the 0.00500, 0.01 and 0.1 µg/L standards were provided; DER Attachment 2; Figures 1-6, pp. 36-38; Figures 15-20, pp. 43-45; Figures 29-34, pp. 50-52; Figures 49-54, pp. 60-62; Figures 63-68, pp. 67-69; and Figures 77-82, pp. 74-76 of MRID 49112202). ECM reported r values were 0.9984-0.9993 for ground water (Figures 27-30, pp. 45-46 of MRID 49112204); linearity of those curves could not be fully verified by the reviewer since all of the raw data were not provided; however, reviewer-calculated curves were generated from provided chromatograms of calibration standards (r^2 values of 1 for all provided matrix/analyte/ion data sets; only data from the 0.00500, 0.01 and 0.1 µg/L standards were provided; DER Attachment 2; Figures 3-8, pp. 33-35 and Figures 15-20, pp. 39-41 of MRID 49112204).

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

IV. Method Deficiencies and Reviewer's Comments

1. The reviewer could not determine if the LOQ was based on scientifically acceptable procedures. The LOQ (0.1 µg/L, ppb) was defined as the lowest analyte concentration in a sample at which the method has been validated (pp. 11, 22 of MRID 49112204; p. 13 of MRID 49112202). The ECM study author also advised that the response for the analyte peak should be no less than four times the mean amplitude of the background noise at the analyte retention time in the control sample, but no calculations or background values were provided. In the ILV, the equation for the calculation of the LOQ was shown in general, but not with specific values (Appendix 4, p. 156 of MRID 49112204). The LOD was reported as the lowest calibration standard in the ECM and ILV (Figures 3-4, p. 33; Figures 15-16, p. 39 of MRID 49112204; and Figures 1-2, p. 36; Figures 15-16, p. 43; Figures 29-30, p. 50; Figures 49-50, p. 60; Figures 63-64, p. 67; Figures 77-78, p. 74 of MRID 49112202). The ECM study author discussed acceptable means for calculating the LOD; however, those calculations were not provided (p. 22 of MRID 49112204; p. 23 of MRID 49112202).

   Detection limits should not be based on the arbitrarily selected lowest concentration in the spiked samples. Additionally, the lowest toxicological level of concern in water was not

reported. An LOQ above toxicological levels of concern results in an unacceptable method classification.

2. The ECM report MRID 49112204 was a summary of the original report with all raw data (Mayer, L. 2012. Azoxystrobin – Validation of Residue Method (GRM057.04A) for the Determination of Azoxystrobin and Z-Isomer R230310 in Water by LC-MS/MS. TK0120502) which was written by the same author in the same year (p. 24).

   The reviewer noted a minor discrepancy in the ECM analytical procedure regarding the size of poly tube used , 15 mL versus 50 mL (p. 15; Appendix 4, p. 58). Another discrepancy in the ECM analytical procedure was noted: the HPLC column was reported as an ACE 5 C18, 3.0 mm x 50 mm column on p. 16 and an ACE 5 C18, 3.0 mm x 150 mm column in Appendix 1, p. 55. An ACE 5 C18, 3.0 mm x 50 mm column was used by the ILV. Also, the reviewer noted one typographical error in the ECM: the calibration range for R230310 was listed as 0.005 ppb – 5 ppb, as opposed to 0.005 ppb – 2 ppb (Figure 28, p. 45). The method flow diagram and equipment list of the ECM should be corrected.

3. The ECM study author reported that LC/MS/MS chromatograms were similar for water types other than surface and ground water (pp. 18, 23, 30 of MRID 49112204). Additionally, the ECM author assumed that the method could be applied to other water types and that the stability results would be similar in other water types. No chromatograms or data from water types other than surface and ground were included in the report.

4. The ECM residue calculations specify correcting recovery results for any residues detected in the matrix control samples (p. 19 of MRID 49112204). However, it could not be determined if residues were actually corrected since recoveries in the controls were not provided. Some raw data of the controls were included in the form of chromatograms (Figures 9-10, p. 36; Figures 21-22, p. 42; Figures 31-32, p. 47; Figures 37-38, p. 50 of MRID 49112204). From that raw data, the reviewer concluded that recoveries were not corrected since no peak was found in those chromatograms. In the ILV, calculations did not show correction for control residues (Appendix 4, p. 156 of MRID 49112202). Also, the raw data of the controls were included in the form of chromatograms (Figures 9-10, p. 40; Figures 23-24, p. 47; Figures 37-38, p. 54; Figures 57-58, p. 64; Figures 71-72, p. 71; Figures 85-86, p. 78 of MRID 49112202). From that raw data, the reviewer concluded that recoveries were not corrected since no peak was found in those chromatograms.

5. For the ECM and ILV, the individual peak area count data used to generate the provided multi-point standard curves were not reported (Figures 43-48, pp. 57-59; Figures 91-96, pp. 81-83 of MRID 49112202; and Figures 27-30, pp. 45-46 of MRID 49112204). The reviewer generated three-point curves using peak area count data from provided chromatograms of calibration standards (see Table 4 above; DER Attachment 2). For the ECM, chromatograms of reagent blank samples were not included.

6. The summary of communications between the independent laboratory and Syngenta study monitors and study director was provided (p. 23; Appendix 5, pp. 157-160 of MRID 49112202). Most of the provided communication regarded the elimination of one or two of the ILV calibration standards from several calibration curves in order to achieve acceptable linearity results ($r^2 \geq 0.990$ according to the ILV laboratory standards). From the provided calibration curves, the reviewer observed that the ECM calibration curve contained eight

points, while the ILV calibration curve contained five to six points (Figures 43-48, pp. 57-59; Figures 91-96, pp. 81-83 of MRID 49112202; and Figures 27-30, pp. 45-46 of MRID 49112204). The ECM only specified that the calibration curve contain "at least five" concentration levels (p. 18 of MRID 49112204). The ILV procedure reported that six calibration standards were prepared (p. 18 of MRID 49112202). The reviewer could not see any evidence in the ILV calibration curves of the elimination of any calibration standard for the purpose of achieving better linearity. Based on the ILV report, only one calibration curve failed to meet OCSPP linearity standards: azoxystrobin in surface water, confirmatory transition #2 (r^2 = 0.99064; Figure 95, p. 83 of MRID 49112202). The raw data were not included in the ECM or ILV reports.

7. In the ECM, LC/MS/MS matrix effects were assessed and found to be insignificant for the water types tested (Table 6, p. 29).

8. It was reported for the ILV that one analyst could complete two batches of samples (36 samples total; 12 fortifications and 6 standards per batch) in 8 hours (one working day) with LC/MS/MS analysis performed overnight (p. 23 of MRID 49112202).

9. As part of the ECM, a supplemental experiment showed that azoxystrobin and R230310 were stable in the final extracts [acetonitrile:ultra-pure water (50:50, v:v)] when stored at 4°C for seven days (pp. 23, 30 of MRID 49112204). The study author reported that "stability in other water types is assumed to be similar" (p. 30). The results are shown in Table 5 below.

Table 5. Final extract stability data

Analyte	Matrix	Number of Tests	Recovery (%)		
			Range	Mean	RSD
Azoxystrobin	Surface water	5	74-100	88	11.0
	Ground water	5	75-94	82	8.8
R230310	Surface water	5	90-105	97	5.7
	Ground water	5	85-98	90	5.7

Data were obtained from Tables 7-8, p. 30 of MRID 49112204. Samples were fortified at the LOQ, 0.1 µgL.

V. References

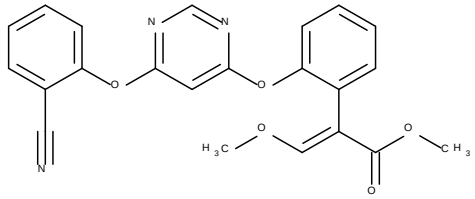
U.S. Environmental Protection Agency. 2012. Ecological Effects Test Guidelines, OCSPP 850.6100, Environmental Chemistry Methods and Associated Independent Laboratory Validation. Office of Chemical Safety and Pollution Prevention, Washington, DC. EPA 712-C-001.

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

Azoxystrobin

IUPAC Name: Methyl (2E)-2-{2-[6-(2-cyanophenoxy)pyrimidin-4-yloxy]phenyl}-3-methoxyacrylate
CAS Name: Methyl (αE)-2-[[6-(2-cyanophenoxy)-4-pyrimidinyl]oxy]-α-(methoxymethylene)benzeneacetate
CAS Number: 131860-33-8
SMILES String: N#Cc1ccccc1Oc2ncnc(Oc3ccccc3C(C(=O)OC)=COC)c2



R230310 Z-Isomer (Figure 2, p. 32 of MRID 49112204)

IUPAC Name: Methyl (Z)-2-{2-[6-(2-cyanophenoxy)pyrimidin-4-yloxy]phenyl}-3-methoxyacrylate
CAS Name: Methyl ester 2-[[6-(2-cyanophenoxy)-4-pyrirnidinyl]oxy]-á-(methoxymethylene)-benzeneacetic acid
CAS Number: NA
SMILES String: CO/C=C(/c1ccccc1Oc2cc(ncn2)Oc3ccccc3C#N)\C(=O)OC