spex certiprep

Technical Note

Spiromesifen Summary

Summary of Use

Spiromesifen, under normal laboratory use and some conditions (including the presence of acid), can transform from the major product to the major metabolite, Spiromesifen-enol, and additional minor metabolites. Spiromesifen containing standards should be stored in a freezer upon receipt and while not in use. Follow all instructions for use and preparation found on the product certificate. Quantitation of the Spiromesifen is recommended as a sum of both the Spiromesifen product and the enol form. The reported quantitation ions of Spiromesifen and its enol by positive mode LC-MS (ESI) are (M+1) @ 371 m/z (product) and 273 m/z (enol). **NOTE: the following parts contain Spiromesifen: STPS01036, STPS01019, STPS01030, STPS01045, STPS01047, STPS01051, STPS01058, STPS01040B, STPS01038B, CAN-CAN-6, CAN-CAN-6A, SPXPR-8, LCS-6035, S-5296**.

Background

Common Name: Spiromesifen

Empirical Formula: $C_{23}H_{30}O_4$

Molecular Weight: 370.49 g/mol

Chemical Name: 2-oxo-3-(2,4,6-trimethylphenyl)-1-oxaspiro[4,4]non-3-en-4-yl 3,3-dimethylbutanoate

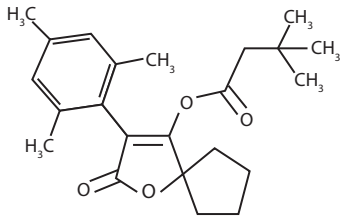
IUPAC Name: 3-mesityl-2-oxo-1-oxaspiro[4,4]non-3-en-4-yl 3,3-dimethylbutyrate

CAS #: 283594-90-1

Brand Name: Spiromesifen Technical, BSN 2060, Forbid 4 F, and Oberon 2 SC

Pests Controlled: Whiteflies, Spider Mites and other mites

Structure:



Information: Spiromesifen was developed by Bayer CropScience in 2006 and registered by the EPA in 2008. The pesticide is part of a newer class of pesticides called keto-enols. These pesticides are derivatives of spirocyclic phenyl substituted tetronic acids and are grouped under Group 23 pesticides being lipid synthesis inhibitors. These pesticides act upon all stages of mites and juvenile whiteflies. Spiromesifen is toxic to fish and other insects but has low human acute toxicity from inhalation or contact.

Chemistry

Chemical Properties:

Table 1. Chemical Properties of Spiromesifen

Property	Value
Color	Colorless
Physical State	Crystals
Odor	Intense
Storage Stability	Stable for 2 years in HDPE at ambient temperature
Viscosity	Solid at room temperature
Density	0.13 g/cm^3 at 21 °C
Density Partition Coefficient	log Pow = 4.55 at 20 °C
Solubility @ 20 °C Water n-Heptane Acetone, Xylene & Ethyl Acetate	 0.13 mg/L 23,000 mg/L 250,000 mg/L
Hydrolyic Stability (DT50) @ 50 °C pH 4 pH 7 pH 9	 2.2 days 1.7 days 2.6 hours
Hydrolytic Stability (DT50) @ 25 °C pH 4 pH 7 pH 9	 53.3 days 24.8 days 4.3 days

Chemistry

Degradation

Spiromesifen has low mobility in soil. Hydrolysis studies conducted in water at pH 4, 7 and 9 for 30 days at 25 °C. Under basic conditions, spiromesifen hydrolyzes with a half-life of 4.3 days. In neutral water, the pesticide is stable in the presence of sunlight and has a half-life of almost 87 days. In acidic water, spiromesifen degrades with a half-life of less than 2 days. (1) In another study of aqueous photolysis, spiromesifen had a half-life of 40.53 hours with major transformation products of the spiromesifen-enol product and secondary products. The residue definition has been cited by research as the sum of the spiromesifen and the spiromesifen-enol metabolite.

spex® certiprep

Technical Note

Spiromesifen & Metabolite Chemistry

Spiromesifen degrades within days to weeks under appropriate conditions to the major metabolite, spiromesifen-enol and additional minor metabolites (M02, M03, M04, M09, M16, and M17). The raw material has been noted as having a common known impurity of N,N-dimethylacetamide (MW: 87.12 g/mol) up to 4 g/kg (2).

Common Name: Spiromesifen enol metabolite (M01)

Empirical Formula: $C_{17}H_{20}O_3$

Molecular Weight: 272.34 g/mol

Chemical Name: 4-hydroxy-3-(2,4,6-trimethylphenyl) 1-Oxaspiro[4,4]non-3-en-2-one

CAS #: 148476-30-6

Structure:

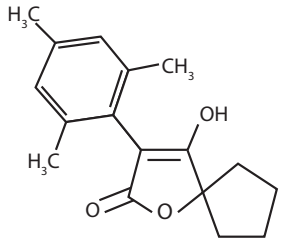


Table 2. Spiromesifen Impurity and Metabolites.

Metabolite Designation	Compound	Common Name	Degradation Site
-	N,N-dimethylacetamide	N,N-dimethylacetamide	Impurity
M01	4-hydroxy-3-(2,4,6-trimethylphenyl) 1-oxaspiro[4,4]non-3-en-2-one	BSN 2060-enol, BSN 0546	Soil, Sediment, Water, Crops
M02	4-hydroxy-3-[4-(hydroxymethyl)-2,6-dimethylphenyl)]-1-oxaspiro[4,4]non-3-en-2-one	4-hydroxymethyl-BSN 0546	Crops
M03	4-hydroxy-3-[4-(hydroxymethyl)-2,6-dimethylphenyl]-1-oxaspiro[4,4]non-3-en-2-one glucoside	4-hydroxymethyl-glucoside-BSN 0546	Crops
M04	4,x,y-trihydroxy-3-mesityl-1-oxaspiro[4,4]non-3-en-2-one (The exact position of the OH groups is undetermined)	dihydroxy-BSN 0546	Crops
M09	4-(4-hydroxy-2-oxo-1-oxaspiro[4,4]non-3-en-3-yl)-3,5-dimethylbenzoic acid	4-carboxy-BSN 0546	Soil, Sediment, Groundwater
M16	3,5-dimethyl-5'-oxodispiro[bicyclo[4.2.0]octa-1,3,5-triene-7,4'-furan-2',1"-cyclopentan]-3'-yl 3,3-dimethylbutanoate	BSN 2060-cyclobutyl photoisomer	Surface Water Photolysis Study
M17	8'-hydroxy-4',6'-dimethyl-8'-8a'-dihydrospiro[cyclopentane-1,1'-indeno[1,2-c]furan-3'(3a'H)-one	BSN 0546 photoisomer	Surface Water Photolysis Study

spex.com

Phone: +1.732.549.7144 • +1.800.LAB.SPEX
Fax: +1.732.603.9647
spexsales@antylia.com

Connect with us