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Technical Note

Acequinocyl Summary

Summary of Use

Acequinocyl, also known as Kanemite, is a miticide that can undergo deacetylation (the removal of an acetyl group) to produce the metabolite hydroxyacequinocyl. The deacetylation is known to occur quickly in aqueous solution at neutral or basic pH but appears to be more stable at acidic pH. Exposure of solutions to sunlight also promotes deacetylation.

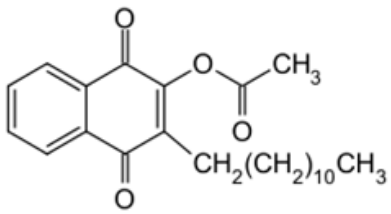
It has been observed that deacetylation can occur in certain products containing protic solvents as well as the other proton-containing compounds. In some cases, the majority of acequinocyl may have converted to the hydroxy metabolite. These standards should be stored in the freezer upon receipt and when not in use. Direct exposure of the standards to sunlight should be avoided. Follow all instructions for use, preparation and storage found on the product certificate.

Quantitation of acequinocyl is recommended as a sum of the acequinocyl and the hydroxyacequinocyl. The reported quantitation ion of acequinocyl in positive mode (LC/MS) (ESI) is 385 (M). One may also detect the ions at 386 (M+H) or 387 (M+2H) for acequinocyl and 343 for hydroxyacequinocyl. Masses 357 and 411 correspond to unknown analogs that have been detected in positive mode (TIC) and may be included in the quantitation.

Note: the following parts contain acequinocyl: STPS01040, STPS01040B, STPS01038, STPS01038B, STPS01031, STPS01058, STPS01053, STPS01036, STPS01019, LCS-6394, SPXPR-9, SS-SPXPR-9, LC-NES-509, SS-LC-NEA-509 BAL, CAN-CAN-5, CAN-CAN-5A.

Background

Common Name:	Acequinocyl
Empirical Formula:	$C_{24}H_{32}O_4$
Molecular Weight:	384.50 g/mol
Chemical Name:	3-Dodecyl-2-hydroxy-1,4-naphthoquinone acetate; 2-(Acetyloxy)-3-dodecyl-1,4-naphthalenedione
IUPAC Name:	(3-dodecyl-1,4-dioxonaphthalen-2-yl) acetate
CAS #:	57960-19-7
Brand Name:	Kanemite
Pests Controlled:	Mites including spider mites, spruce spider mite and red palm mite; ticks
Structure:	



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Information: Acequinocyl is an acaricide that is currently being evaluated for EU use. It is practically insoluble in water, but it is highly soluble in most organic solvents. Acequinocyl is not mobile and is not expected to leach to groundwater or persist in soil or aquatic systems. It has a low mammalian toxicity, but there is some concern regarding its potential for bioaccumulation. Acequinocyl is moderately toxic to birds, fish, honeybees, and earthworms and highly toxic to aquatic invertebrates.

Chemistry

Chemical Properties:

Table 1. Chemical Properties of pure acequinocyl

Property	Value
Color	Yellow solid
Physical State	Crystals
Odor	Faintly earthy
Storage Stability	Neat material is stable for 2 years in HDPE at ambient temperature. **Standards must be stored in freezer when not in use to maintain stability until expiration date.**
Viscosity	Solid at room temperature
Density	1.15 g/cm^3 at 25 °C
Melting Point	59.6 °C
Solubility @ 20 °C Water Methanol n-Hexane Acetone Toluene	 6.69 x 10-3 mg/L 7,800 mg/L 44,000 mg/L 220,000 mg/L 450,000 mg/L
Hydrolytic Stability (DT50) @ 25 °C pH 4 pH 7 pH 9	 74 days 53 hours 76 minutes

Degradation:

Solid acequinocyl is stable under normal conditions for up to two years. In soil, it has a half-life of 2 days. In solution, acequinocyl has a half-life of 74 days at pH4 (25 °C), 53 hours at pH 7 (25 °C), and 76 minutes at pH 9 (25 °C). In the presence of light, acequinocyl has a half-life of 19 days at pH 1.2 (37 °C). In all cases, the major degradant is hydroxyacequinocyl. Hydroxyacequinocyl is the major metabolite of acequinocyl and is a powerful inhibitor of the ubiquinol oxidation site in Complex III in mitochondrial mite cells. It blocks cellular respiration.

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Common Name: Hydroxyacequinocyl

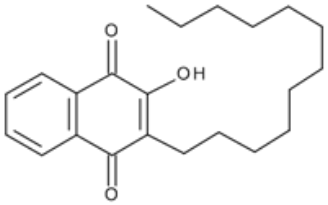
Empirical Formula: $C_{17}H_{20}O_3$

Molecular Weight: 342.47 g/mol

Chemical Name: 3-dodecyl-4-hydroxynaphthalene-1,2-dione

CAS #: 57960-31-3

Structure:



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