

Bioactive Molecules, Building Blocks, Intermediates

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Product Name:	Myclobutanil	
Cat. No.:	CS-8015	CI
CAS No.:	88671-89-0	\rightarrow
Molecular Formula:	C15H17CIN4	
Molecular Weight:	288.78	N N
Target:	Fungal	
Pathway:	Anti-infection	
Solubility:	DMSO : 103 mg/mL (356.67 mM; Need ultrasonic and warming)	

Data Sheet

BIOLOGICAL ACTIVITY:

Myclobutanil is a conazole class fungicide widely used as an agrichemical. **In Vitro**: Myclobutanil reduces cell viability to <50% at 100 ppm and to <10% at 500 ppm. Myclobutanil promotes a slight, but significant, increase in fatty acid (FA)-induced steatotosis at doses from 1 to 100 ppm. Anti-apoptotic biomarkers are significantly reduced by Myclobutanil^[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: ^[1]To further evaluate apoptosis, cell extracts are collected after 24 h of exposure to Myclobutanil, centrifuged, and analyzed with a multiplex biometric ELISA-based immunoassay containing dyed microspheres conjugated to a monoclonal antibody specific for the target protein. Apoptosis biomarkers are BCL-xL/Bak dimer and Mcl-1/Bak dimer, quantified using RBM Apoptosis Panel 3. Each experiment is performed in triplicate and apoptosis biomarker levels determined using the Bio-Plex Array Reader. The analytic concentrations are calculated using a standard curve, according to the manufacturer's instructions^[1]. **Cell Assay:** Myclobutanil is solubilized in 100% DMSO and diluted to 0.5% in serum-free Eagle's Minimum Essential Medium (EMEM).^[1]The hepatoma cell line HepG2 is used in this study. The cells are grown on tissue culture plates in an incubator with a humidified atmosphere (95% air/5% CO $_2$ v/v) at 37°C. Steatosis is induced by incubating the hepatocytes with 6 mM of a 1:1 v/v mixture of oleic (18:1) and linoleic (18:2) fatty acids (Fas) for 24 h. After a wash with PBS, cells are exposed for an additional 24 h to Myclobutanil at 0.1, 1, 10, 100 or 500 ppm. Cytotoxicity is assessed in HepG2 cells (1.0×10⁵ cells/well in 24-well plates) by measuring the reduction of the tetrazolium dye 3-(4, 5-dimethylthiazol-2-yl)-5-(3carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium (MTT)^[1].

References:

[1]. Stellavato A, et al. Myclobutanil worsens nonalcoholic fatty liver disease: An in vitro study of toxicity and apoptosis on HepG2 cells. Toxicol Lett. 2016 Nov 16;262:100-104.

CAIndexNames:

1H-1,2,4-Triazole-1-propanenitrile, α -butyl- α -(4-chlorophenyl)-

SMILES:

N#CC(C1=CC=C(Cl)C=C1)(CCCC)CN2N=CN=C2

Caution: Product has not been fully validated for medical applications. For research use only.

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