# **Product data sheet**



MedKoo Cat#: 540304				
Name: Myclobutanil				
CAS: 88671-89-0				
Chemical Formula: C <sub>15</sub> H <sub>17</sub> ClN <sub>4</sub>				
Exact Mass: 288.1142				
Molecular Weight: 288.779				
Product supplied as:	Powder			
Purity (by HPLC):	$\geq 98\%$			
Shipping conditions	Ambient temperature			
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.			
	In solvent: -80°C 3 months; -20°C 2 weeks.			



## 1. Product description:

Myclobutanil is a  $14-\alpha$  demethylase inhibitor that inhibits ergosterol synthesis and fungal cell wall formation. It also weakly inhibits testosterone production.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

#### 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	79.0	273.57

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.46 mL	17.31 mL	34.63 mL
5 mM	0.69 mL	3.46 mL	6.93 mL
10 mM	0.35 mL	1.73 mL	3.46 mL
50 mM	0.07 mL	0.35 mL	0.69 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

## 6. Recommended literature which reported protocols for in vitro and in vivo study

### In vitro study

1. Terpou A, Dimopoulou M, Belka A, Kallithraka S, Nychas GE, Papanikolaou S. Effect of Myclobutanil Pesticide on the Physiological Behavior of Two Newly Isolated Saccharomyces cerevisiae Strains during Very-High-Gravity Alcoholic Fermentation. Microorganisms. 2019 Dec 9;7(12):666. doi: 10.3390/microorganisms7120666. PMID: 31835377; PMCID: PMC6956295.

2. Stellavato A, Lamberti M, Pirozzi AVA, de Novellis F, Schiraldi C. 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. doi: 10.1016/j.toxlet.2016.09.013. Epub 2016 Sep 28. PMID: 27693777.

In vivo study

1. Taylor R, Armstrong L, Bhattacharya A, Henry Z, Brinker A, Buckley B, Kong B, Guo G. Myclobutanil-mediated alteration of liver-gut FXR signaling in mice. Toxicol Sci. 2023 Feb 17;191(2):387-399. doi: 10.1093/toxsci/kfac129. PMID: 36511616; PMCID: PMC9936201.

## 7. Bioactivity

Biological target:

Myclobutanil is a conazole class fungicide widely used as an agrichemical.

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In vitro activity

This study investigated myclobutanil's effects on the human liver cell line HepG2. This study found that myclobutanil increases the amount of fatty acids in these hepatic cells, as evaluated with Oil Red O staining, and progressively reduces cell viability from 1ppm to 500ppm. Analysis of biomarkers such as Bcl-xL/Bak and Mcl-1/Bak confirmed activation of cell death pathways at low doses.

Reference: Toxicol Lett. 2016 Nov 16;262:100-104. https://pubmed.ncbi.nlm.nih.gov/27693777/

## In vivo activity

In a diet-induced NAFLD study, low-fat diet (LFD) fed mice administered myclobutanil displayed decreased FXR activity in the liver and ileum, while high-fat-high-sugar-diet (HFHSD) fed mice showed an increase in hepatic FXR activity and an induction of target genes regulated by constitutive androstane receptor and/or pregnane X receptor.

Reference: Toxicol Sci. 2023 Feb 17;191(2):387-399. https://pubmed.ncbi.nlm.nih.gov/36511616/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.