Certificate of Analysis

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Print Date: Apr 1st 2021

ML 210 Product Name:

Catalog No.: 6429

Batch No.: 2

CAS Number: IUPAC Name: 1360705-96-9

[4-[Bis(4-chlorophenyl)methyl]-1-piperazinyl](5-methyl-4-nitro-3-isoxazolyl)methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight:

Physical Appearance: Solubility:

Storage:

Batch Molecular Structure:

 $C_{22}H_{20}CI_2N_4O_4.$ 475.32 Beige solid DMSO to 50 mM Store at -20°C



2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 99.8% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitrogen					
Theoretical	55.59	4.24	11.79			
Found	55.59	4.22	11.79			

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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IUPAC Name: [4-[Bis(4-chlorophenyl)methyl]-1-piperazinyl](5-methyl-4-nitro-3-isoxazolyl)methanone

Description:

Glutathione peroxidase (GPX4) inhibitor. Kills mutant RASexpressing cell lines (IC_{50} values are 71 and 272 nM for HRAS G12v mutant expressing cell lines BJeLR and BJeH-LT, respectively). Exhibits 4-fold selectivity for HRAS mutantexpressing cell lines. Induces ferroptosis in tumor initiation "persister" cells and drug-resistant tumor cells.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{22}H_{20}CI_2N_4O_4$. Batch Molecular Weight: 475.32 Physical Appearance: Beige solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info: DMSO to 50 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

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Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Hangauer et al (2017) Drug-tolerant persister cancer cells are vulnerable to GPX4 inhibition. Nature 551 247. PMID: 29088702.

Yang et al (2014) Regulation of ferroptotic cancer cell death by GPX4. Cell 156 317. PMID: 24439385.

Weïwer et al (2012) Development of small-molecule probes that selectively kill cells induced to express mutant RAS. Bioorg.Med.Chem.Lett. 22 1822. PMID: 22297109.

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