

Certificate of Analysis

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Product Name: ITH 12575

Catalog No.: 5692

Batch No.: 1

CAS Number: 1802013-08-6

IUPAC Name: 7-Chloro-1,5-dihydro-5-[2-(1-methylethyl)phenyl]-4,1-benzothiazepin-2(3H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₈ClNOS.¼H₂O

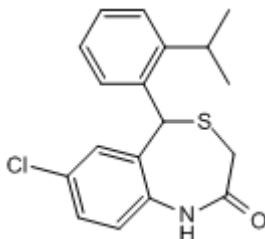
Batch Molecular Weight: 336.36

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.28	5.54	4.16
Found	64.55	5.32	4.1

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

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Description:

Mitochondrial Na⁺/Ca²⁺ exchange (mNCX) inhibitor. Reduces Ca²⁺ efflux from the mitochondria to the cytosol in HeLa cells (EC₅₀ = 0.69 μM). Protects against glutamate-induced excitotoxicity in rat hippocampal slices and oligomycin A/rotenone induced oxidative stress in neuroblastoma cells in vitro.

Physical and Chemical Properties:

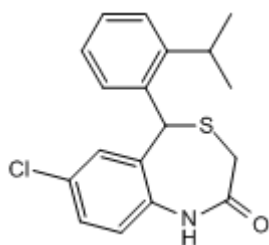
Batch Molecular Formula: C₁₈H₁₈ClNOS.¼H₂O

Batch Molecular Weight: 336.36

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Martínez-Sanz et al (2015) Benzothiazepine CGP37157 analogues exert cytoprotection in various *in vitro* models of neurodegeneration. ACS Chem.Neurosci. **6** 1626. PMID: 26192029.

Moreno-Ortega et al (2015) Benzothiazepine CGP37157 and its 2'-isopropyl analogue modulate Ca²⁺ entry through CALHM1. Neuropharmacology **95** 503. PMID: 25908402.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 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).

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.

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