

# **Certificate of Analysis**

Print Date: Feb 7th 2022

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Product Name: CBR-470-1 Catalog No.: 7018 Batch No.: 1

CAS Number: 2416095-06-0

IUPAC Name: (3R,4S)-rel-4-[(4-Chlorophenyl)sulfonyl]tetrahydro-N-(2-methylpropyl)-3-thiophenamine-1,1-dioxide

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{14}H_{20}CINO_4S_2$ .

**Batch Molecular Weight:** 365.89 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 20 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

(and enantiomer)

### 2. ANALYTICAL DATA

**HPLC:** Shows 99.6% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 45.96 5.51 3.83 Found 46.17 5.53 3.82

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

www.tocris.com/distributors Tel:+1 612 379 2956



## **Product Information**

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#### **Description:**

CBR-470-1 is a phosphoglycerate kinase 1 (PGK1) inhibitor. CBR-470-1 promotes accumulation of the reactive metabolites methylglyoxal (MGO) resulting in KEAP1 modification and dimerization, which in turn leads to activation of the Nrf2 transcriptional program. CBR-470-1 protects SH-SY5Y neuroblastoma cells from MPP+-induced cytotoxicity via the Keap1-Nrf2 cascade.

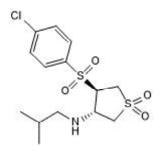
#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>14</sub>H<sub>20</sub>CINO<sub>4</sub>S<sub>2</sub>.

Batch Molecular Weight: 365.89 Physical Appearance: White solid

Minimum Purity: ≥98%

#### **Batch Molecular Structure:**



(and enantiomer)

Storage: Store at -20°C

#### 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.

#### References:

**Zheng** *et al* (2020) PGK1 inhibitor CBR-470-1 protects neuronal cells from MPP+. Aging (Albany NY) *12* 13388. PMID: 32649311. **Bollong** *et al* (2018) A metabolite-derived protein modification integrates glycolysis with KEAP1-NRF2 signalling. Nature *562* 600. PMID: 30323285.

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