

## Certificate of Analysis

[www.tocris.com](http://www.tocris.com)

**Product Name:** TC-E 5001

**Catalog No.:** 5049

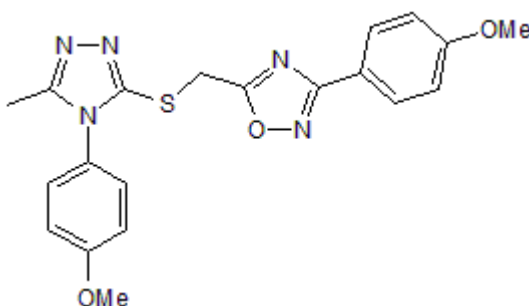
**Batch No.:** 1

**CAS Number:** 865565-29-3

**IUPAC Name:** 3-(4-Methoxyphenyl)-5-[[[4-(4-methoxyphenyl)-5-methyl-4*H*-1,2,4-triazol-3-yl]thio]methyl]-1,2,4-oxadiazole

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>20</sub>H<sub>19</sub>N<sub>5</sub>O<sub>3</sub>S  
**Batch Molecular Weight:** 409.46  
**Physical Appearance:** Beige solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows 99.3% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	58.67	4.68	17.1
Found	58.48	4.6	17.03

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

## Product Information

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### Description:

Dual tankyrase (TNKS) inhibitor ( $K_d$  values are 79 and 28 nM for TNKS1 and TNKS2 respectively,  $IC_{50}$  = 33 nM for TNKS2) that is devoid of activity at PARP1 and PARP2 ( $IC_{50}$  >19  $\mu$ M). Inhibits Wnt signaling and stabilizes Axin2 levels.

### Physical and Chemical Properties:

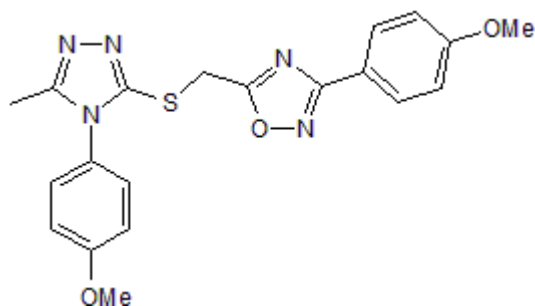
Batch Molecular Formula:  $C_{20}H_{19}N_5O_3S$

Batch Molecular Weight: 409.46

Physical Appearance: Beige solid

**Minimum Purity:** >98%

### Batch Molecular Structure:



**Storage:** Store at +4°C

**CAUTION** - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

### Solubility & Usage Info:

DMSO to 100 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:

**Shultz *et al*** (2012) [1,2,4]Triazole-3-ylsulfanylmethyl-3-phenyl-[1,2,4]oxadiazoles: antagonists of the wnt pathway that inhibit tankyrases 1 and 2 via novel adenosine pocket binding. *J.Med.Chem.* **55** 1127. PMID: 22260203.

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