

## Certificate of Analysis

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**Product Name:** TTP 22

**Catalog No.:** 4432

**Batch No.:** 1

CAS Number: 329907-28-0

IUPAC Name: 3-[[5-(4-Methylphenyl)thieno[2,3-d]pyrimidin-4-yl]thio]propanoic acid

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>

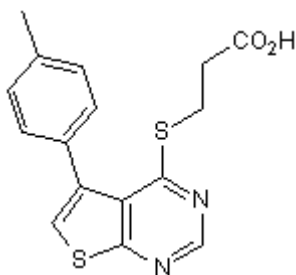
**Batch Molecular Weight:** 330.42

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 20 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**Melting Point:** Between 182 - 183°C

**HPLC:** Shows 99% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	58.16	4.27	8.48
Found	58.22	4.42	8.39

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

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**Description:**

High affinity, ATP-competitive casein kinase 2 (CK2) inhibitor ( $IC_{50} = 0.1 \mu\text{M}$ ,  $K_i = 40 \text{ nM}$ ). Displays selectivity for CK2 over JNK3, ROCK1 and MET (no inhibitory effects at  $10 \mu\text{M}$ ).

**Physical and Chemical Properties:**

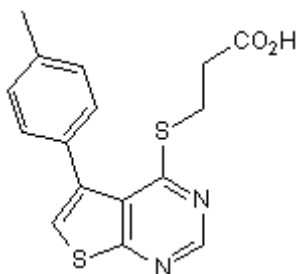
Batch Molecular Formula:  $C_{16}H_{14}N_2O_2S_2$

Batch Molecular Weight: 330.42

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°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:**

**Golub et al** (2011) Synthesis and biological evaluation of substituted (thieno[2,3-d]pyrimidin-4-ylthio)carboxylic acids as inhibitors of human protein kinase CK2. *Eur.J.Med.Chem.* **46** 870. PMID: 21276643.

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