

**Product Name:** T 26c disodium salt

**Catalog No.:** 6134

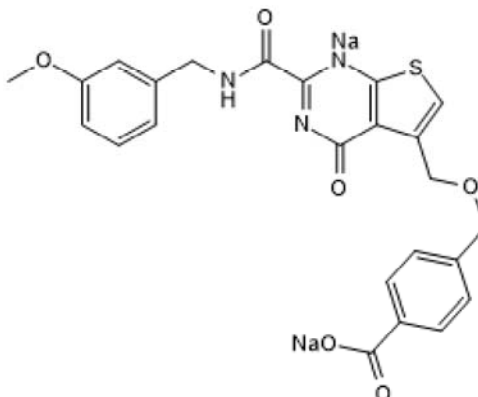
**Batch No.:** 1

CAS Number: 869298-22-6

IUPAC Name: Disodium 4-[[[2-[[[3-(Methoxy)phenyl]methyl]amino]carbonyl]-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-5-yl]methyl]oxy]methyl]benzoate

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>24</sub> H <sub>19</sub> N <sub>3</sub> Na <sub>2</sub> O <sub>6</sub> S.2½H <sub>2</sub> O
<b>Batch Molecular Weight:</b>	568.51
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	DMSO to 10 mM with gentle warming water to 1 mM
<b>Storage:</b>	Desiccate at RT
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>TLC:</b>	R <sub>f</sub> = 0.6 (Dichloromethane:Methanol [9:1])
<b>HPLC:</b>	Shows 99.6% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure

	Carbon	Hydrogen	Nitrogen	Sodium
Theoretical	50.71	4.25	7.39	8.09
Found	50.51	3.95	7.23	7.47

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

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**Description:**

Highly potent and selective MMP13 inhibitor (IC<sub>50</sub> = 6.9 pM). Exhibits >2600-fold selectivity for MMP13 over related MMPs. Inhibits degradation of bovine nasal septum cartilage explants in vitro. Orally bioavailable.

**Physical and Chemical Properties:**

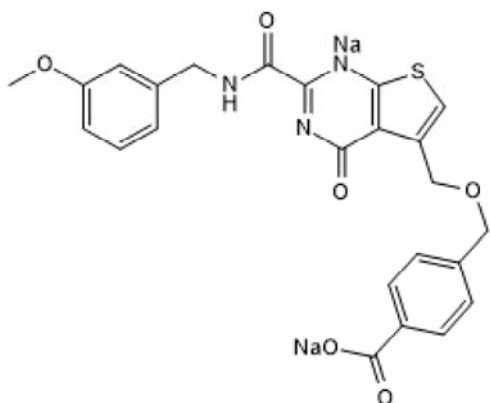
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Batch Molecular Weight: 568.51

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

DMSO to 10 mM with gentle warming  
water to 1 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.

**Licensing Information:**

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the T-26c probe summary on the SGC website.

**References:**

Nara *et al* (2014) Thieno[2,3-*d*]pyrimidine-2-carboxamides bearing a carboxybenzene group at 5-position: highly potent, selective, and orally available MMP-13 inhibitors interacting with the S1" binding site. *Bioorg.Med.Chem.* **22** 5487. PMID: 25192810.

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