

**Product Name:** BI 4394

**Catalog No.:** 8842

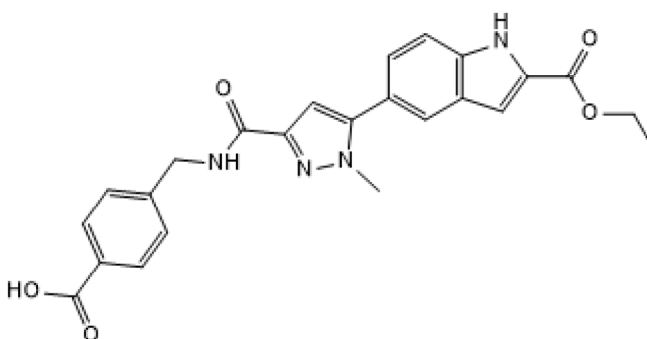
**Batch No.:** 1

CAS Number: 1222173-37-6

IUPAC Name: 2-Ethyl 5-[3-[[[(4-carboxyphenyl)methyl]amino]carbonyl]-1-methyl-1*H*-pyrazol-5-yl]-1*H*-indole-2-carboxylate

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>24</sub>H<sub>22</sub>N<sub>4</sub>O<sub>5</sub>  
**Batch Molecular Weight:** 446.46  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.1% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	64.57	4.97	12.55
Found	64.13	4.9	12.46

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

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**Description:**

BI 4394 is a highly potent and selective MMP-13 inhibitor (IC<sub>50</sub> = 1 nM). BI 4394 inhibits the degradation of isolated bovine nasal cartilage explants (IC<sub>50</sub> = 31 nM). It shows high selectivity (>1000 fold) for MMP-13 over other MMPs. In vivo, BI 4394 decreases the mean arthritic score vs control in a murine model of rheumatoid arthritis, when administered at a dose of 100 mg/kg over a 14-day period. BI 4394 is orally bioavailable.

**Physical and Chemical Properties:**

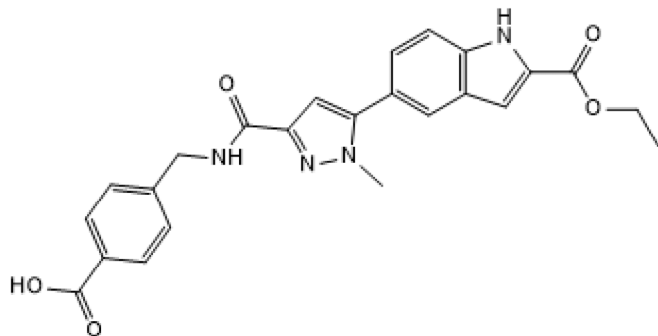
Batch Molecular Formula: C<sub>24</sub>H<sub>22</sub>N<sub>4</sub>O<sub>5</sub>.

Batch Molecular Weight: 446.46

Physical Appearance: White solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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 BI 4394 page on the SGC website.

**References:**

**Taylor et al** (2021 ) Indole inhibitors of MMP-13 for arthritic disorders. ACS Omega **6** 18635. PMID: 34337203.

**Taylor et al** (2011) Fragment-based discovery of indole inhibitors of matrix metalloproteinase-13. J.Med.Chem. **54** 8174. PMID: 22017539.

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