

Product Name: AT 56

Catalog No.: 3531

Batch No.: 2

CAS Number: 162640-98-4

IUPAC Name: 4-(5*H*-Dibenzo[*a,d*]cyclohepten-5-ylidene)-1-[4-(2*H*-tetrazol-5-yl)butyl]-piperidine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₇N₅·½H₂O

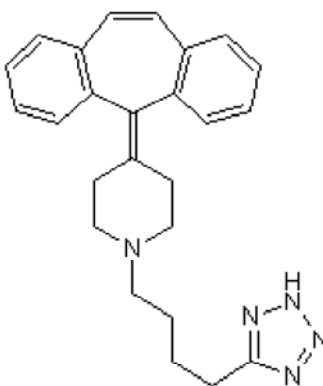
Batch Molecular Weight: 406.53

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.1 (Chloroform:Methanol [9:1])

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	73.86	6.94	17.23
Found	73.49	6.84	17.17

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Description:

Orally active inhibitor of lipocalin-type prostaglandin D synthase (L-PGDS) ($K_i = 75 \mu\text{M}$, $\text{IC}_{50} = 95 \mu\text{M}$). Inhibits the production of PGD_2 from PGH_2 in vitro, with no effect on PGE_2 or $\text{PGF}_{2\alpha}$ production.

Physical and Chemical Properties:

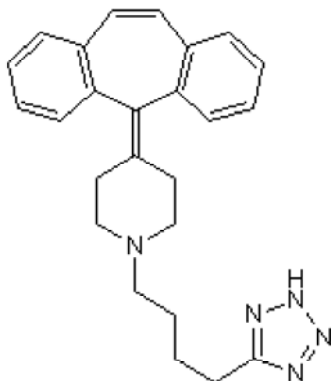
Batch Molecular Formula: $\text{C}_{25}\text{H}_{27}\text{N}_5 \cdot \frac{1}{2}\text{H}_2\text{O}$

Batch Molecular Weight: 406.53

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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 $45\text{-}60^\circ\text{C}$ 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:

Irikura *et al* (2009) Biochemical, functional and pharmacological characterization of AT-56, an orally active and selective inhibitor of lipocalin-type prostaglandin D synthase. *J.Biol.Chem.* **284** 7623. PMID: 19131342.

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