

Product Name: BAY-u 3405

Catalog No.: 2732

Batch No.: 2

CAS Number: 116649-85-5

IUPAC Name: (3*R*)-3-[[[4-Fluorophenyl)sulfonyl]amino]-1,2,3,4-tetrahydro-9*H*-carbazole-9-propanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₁FN₂O₄S

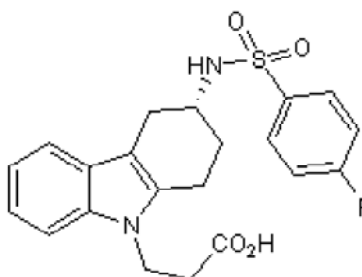
Batch Molecular Weight: 416.47

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +69.1 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.56	5.08	6.73
Found	60.52	5.1	6.62

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

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Description:

Potent dual antagonist of TP/DP₂ (CRTH2) prostanoid receptors (K_i values are 4.3, 4.5 and > 10000 nM for hDP₂, hTP and hDP₁ receptors respectively). Suppresses PGD₂-induced migration of human eosinophils (IC₅₀ = 170 nM).

Physical and Chemical Properties:

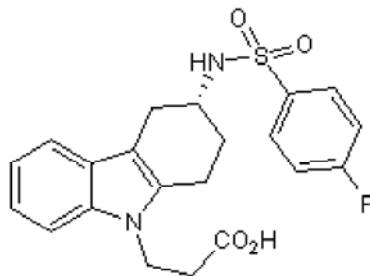
Batch Molecular Formula: C₂₁H₂₁FN₂O₄S

Batch Molecular Weight: 416.47

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Desiccate at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Ulven and Kostenis (2005) Minor structural modifications convert the dual TP/CRTH2 antagonist ramatroban into a highly selective and potent CRTH2 antagonist. *J.Med.Chem.* **48** 897. PMID: 15715457.

Ishizuka et al (2004) Ramatroban (BAY u3405): a novel dual antagonist of TXA₂ receptor and CRTh2, a newly identified prostaglandin D₂ receptor. *Cardiovasc.Drug Rev.* **22** 71. PMID: 15179446.

Sundstrom et al (2003) Interactions among three classes of mediators explain antigen-induced bronchoconstriction in the isolated perfused and ventilated guinea pig lung. *J.Pharmacol.Exp.Ther.* **307** 408. PMID: 12954791.

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