

Product Name: Bay 59-3074

Catalog No.: 2500

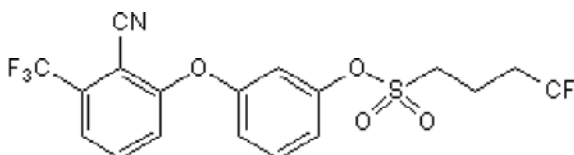
Batch No.: 2

CAS Number: 406205-74-1

IUPAC Name: 3-[2-Cyano-3-(trifluoromethyl)phenoxy]phenyl 4,4,4-trifluoro-1-butananesulfonic acid ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₃F₆NO₄S
Batch Molecular Weight: 453.35
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.32 (Diethyl ether:Petroleum ether [1:1])
HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

	Carbon Hydrogen Nitrogen		
	Carbon	Hydrogen	Nitrogen
Theoretical	47.69	2.89	3.09
Found	47.89	2.9	3.07

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

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Description:

Novel CB₁/CB₂ receptor partial agonist (K_i values are 48.3 and 45.5 nM at human CB₁ and CB₂ receptors respectively). Orally active CB₁ agonist in vivo. Displays anti-hyperalgesic and antiallodynic properties in rat models of chronic neuropathic and inflammatory pain.

Physical and Chemical Properties:

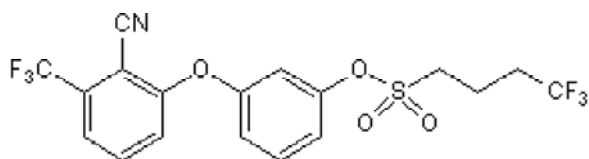
Batch Molecular Formula: C₁₈H₁₃F₆NO₄S

Batch Molecular Weight: 453.35

Physical Appearance: Off-white solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at +4°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.

Licensing Information:

Sold for research purposes under agreement from Bayer

References:

De Vry et al (2004) 3-[2-Cyano-3-(trifluoromethyl)phenoxy]phenyl-4,4,4-trifluoro-1-butan-1-sulfonate (BAY 59-3074): a novel cannabinoid CB₁/CB₂ receptor partial agonist with antihyperalgesic and antiallodynic effects. *J.Pharmacol.Exp.Ther.* **310** 620. PMID: 15140913.

De Vry et al (2004) Discriminative stimulus effects of the structurally novel cannabinoid CB₁/CB₂ receptor partial agonist BAY 59-3074 in the rat. *Eur J Pharmacol.* **505** 127. PMID: 15556145.

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