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Print Date: Jun 2nd 2016

Product Name: AC 4 Catalog No.: 5464 Batch No.: 1

CAS Number: 1459809-09-6

IUPAC Name: 1,3,4,5-Tetrahydro-7,8-dihydro-*N*-[2-[4-[2-[4-(trifluoromethyl)phenyl]diazenyl]phenyl]ethyl]-2*H*-2-benzazepine-2-

carbothioamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{25}F_3N_4O_2S$

Batch Molecular Weight: 514.56

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM

water to 20 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.4$ (Chloroform:Methanol [19:1])

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 60.69 4.9 10.89 Found 60.62 4.9 10.76

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



Product Information

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Description:

Photoswitchable TRPV1 channel blocker (IC $_{50}$ = 3.1 μ M). Acts as an antagonist in trans conformation during voltage gated activation. Also acts as an antagonist in the cis formation during capsaicin-induced TRPV1 currents. Switches conformation from cis to trans at 440 nm and trans to cis at 360 nm. Allows photoswitchable antagonist and an agonist to be applied at the same time.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₆H₂₅F₃N₄O₂S Batch Molecular Weight: 514.56

Physical Appearance: Orange solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM

water to 20 mM with gentle warming

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:

Stein et al (2013) Optical control of TRPV1 channels. Angew.Chem.Int.Ed.Engl. 52 9845. PMID: 23873837.