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TOCRIS

Print Date: Oct 21st 2024

Certificate of Analysis

www.tocris.com

Product Name: **Janelia Fluor® 549, free acid** **Catalog No.: 6503** **Batch No.: 2**

CAS Number: 2245946-45-4

IUPAC Name: 3,6-Di-1-azetidinyl-9-(2,5-dicarboxyphenyl)xanthylium, inner salt trifluoroacetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{22}N_2O_5.C_2HF_3O_2$

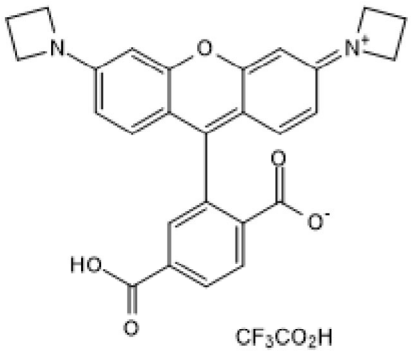
Batch Molecular Weight: 568.5

Physical Appearance: Dark grey solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 93.9% purity at 550 nm

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

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IUPAC Name: 3,6-Di-1-azetidinyl-9-(2,5-dicarboxyphenyl)xanthylium, inner salt trifluoroacetate

Description:

Key Information: Janelia Fluor® 549, free acid is a yellow fluorescent dye; supplied with a free acid reactive group. Suitable for live cell imaging. Application: Suitable for flow cytometry, confocal microscopy, super resolution microscopy (SRM) including dSTORM (in both live and fixed cells) and STED. Used in protocol (2017 Grimm et al - see references below) for the synthesis of Janelia Fluor® HaloTag® and SNAP-Tag® ligands. Cell permeable. Properties and Photophysical Data: Excitation and emission maxima (λ) are 549 nm and 571 nm, respectively; quantum yield = 0.88; extinction coefficient = 101,000 $M^{-1}cm^{-1}$, A280 co... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

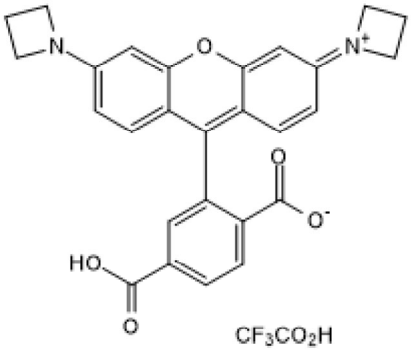
Batch Molecular Formula: $C_{27}H_{22}N_2O_5.C_2HF_3O_2$

Batch Molecular Weight: 568.5

Physical Appearance: Dark grey solid

Minimum Purity: ≥90%

Batch Molecular Structure:



Storage: Store at -20°C. This product is packaged under an inert atmosphere.

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

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:

Sold under license from the Howard Hughes Medical Institute, Janelia Research Campus

References:

Grimm *et al* (2017) Synthesis of Janelia Fluor HaloTag and SNAP-Tag Ligands and Their Use in Cellular Imaging Experiments. Methods Mol.Biol. ***1663*** 179. PMID: 28924668 .

Grimm *et al* (2015) A general method to improve fluorophores for live-cell and single-molecule microscopy. Nat. Methods ***12*** 244. PMID: 25599551 .

Zheng *et al* Rational design of fluorogenic and spontaneously blinking labels for super-resolution imaging. ACS Cent.Sci. ***5*** 1602. PMID: 31572787.

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