Certificate of Analysis

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: $C_{27}H_{22}N_2O_5.C_2HF_3O_2$

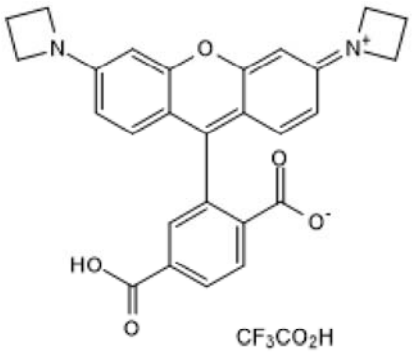
Batch Molecular Weight: 568.5

Physical Appearance: Dark grey solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 94.1% purity

^{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:

Janelia Fluor® 549, free acid is a yellow fluorescent dye; supplied as a free acid. Used in protocol (2017 Grimm et al - see references below) for the synthesis of Janelia Fluor® HaloTag® and SNAP-Tag® ligands, for use in live cell imaging experiments. Also suitable for flow cytometry. Excitation maximum = 549 nm; emission maximum = 571 nm; Quantum yield = 0.88; Extinction coefficient = 101,000 $M^{-1}cm^{-1}$.

Physical and Chemical Properties:

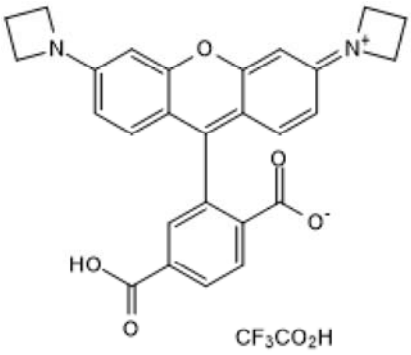
Batch Molecular Formula: $C_{27}H_{22}N_2O_5.C_2HF_3O_2$

Batch Molecular Weight: 568.5

Physical Appearance: Dark grey solid

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. 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 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 .