Product Name: **Janelia Fluor® 669, NHS ester** **Catalog No.: 6420** **Batch No.: 4**

CAS Number: 2127150-20-1

IUPAC Name: 1-[7-(1-Azetidinyl)-10-[2-Carboxy-5-[(2-(2,5-dioxopyrrolidin-1-yl)oxy)-2-oxoethyl]thio-3,4,6-trifluorophenyl]-9,9-dimethyl-9-silaanthracen-2(9*H*)-ylidene]azetidinium, inner salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{34}H_{30}F_3N_3O_6SSi$

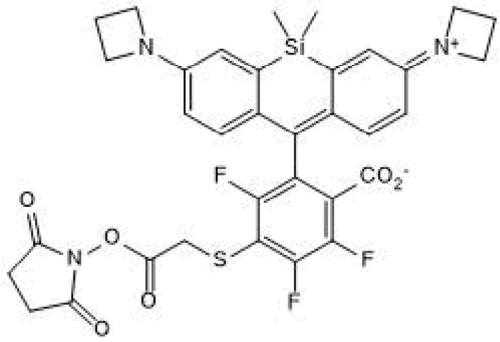
Batch Molecular Weight: 693.77

Physical Appearance: Green solid

Solubility: DMSO to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 91.7% purity at 672 nm

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

UV Spectrum: Consistent with structure

λ_{max}: 670 nm (EtOH + 0.1% TFA)

λ_{ex}: 673 nm (EtOH + 0.1% TFA)

λ_{em}: 688 nm (EtOH + 0.1% TFA)

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Description:

Key Information: Janelia Fluor® 669, NHS ester is a red fluorescent dye; supplied with an NHS ester reactive group for the labeling of primary amines. Suitable for live cell imaging. Application: Suitable for confocal microscopy, super resolution microscopy (SRM) techniques including dSTORM (in both live and fixed cells) and STED. Cell permeable.Properties and Photophysical Data: NHS ester can be converted to relevant substrate for use in self-labeling tag systems, e.g. HaloTag® and SNAP-tag®. Excitation and emission maxima (λ) are 669 nm and 682 nm, respectively; quantum yield = 0.37; extinction coefficient = 116,000 $M^{-1}cm$... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

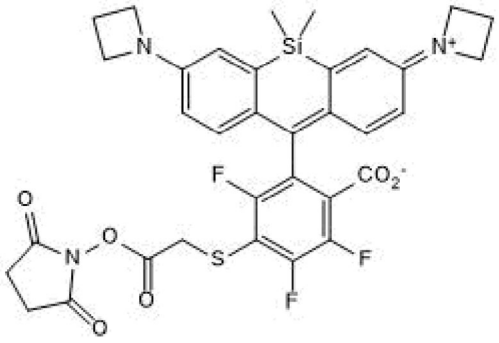
Batch Molecular Formula: $C_{34}H_{30}F_3N_3O_6SSi$

Batch Molecular Weight: 693.77

Physical Appearance: Green 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 20 mM

CAUTION - This product is chemically unstable in the presence of Trifluoroacetic acid (TFA).

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* (2020) A general method to optimize and functionalize red-shifted rhodamine dyes. Nat.Methods ***17*** 815. PMID: 32719532.

Grimm *et al* (2017) General synthetic method for Si-Fluoresceins and Si-Rhodamines. ACS Cent.Sci. ***3*** 975. PMID: 28979939.

Grimm *et al* (2017) A general method to fine-tune fluorophores for live-cell and *in vivo* imaging. Nat.Methods ***14*** 987. PMID: 28869757.

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