Certificate of Analysis

Product Name: **FNIR-Tag, NHS ester** **Catalog No.: 7373** **Batch No.: 2**

CAS Number: 2365033-54-9

IUPAC Name: 2-((*E*)-2-((*E*)-2-(3-((4-((2,5-dioxopyrrolidin-1-yl)oxy)-4-oxobutyl)dimethylammonio)propoxy)-3-(2-((*E*)-1-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,3-dimethyl-5-sulfonatoindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,3-dimethyl-3*H*-indol-1-ium-5-sulfonate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{57}H_{80}N_4O_{17}S_2$

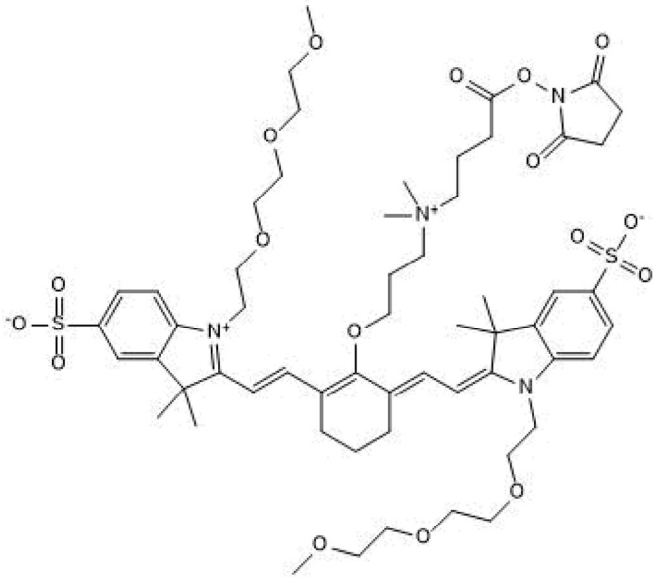
Batch Molecular Weight: 1157.4

Physical Appearance: Dark green solid

Solubility: DMSO to 10 mM
DMF to 10 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 87.6% purity at 770 nm

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

UV Spectrum: Consistent with structure

λ_{max}: 770 nm (0.01M PBS)

λ_{ex}: 768 nm (0.01M PBS)

λ_{em}: 788 nm (0.01M PBS)

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Product Name: **FNIR-Tag, NHS ester** **Catalog No.: 7373** **Batch No.: 2**

CAS Number: 2365033-54-9

IUPAC Name: 2-((*E*)-2-((*E*)-2-(3-((4-((2,5-dioxopyrrolidin-1-yl)oxy)-4-oxobutyl)dimethylammonio)propoxy)-3-(2-((*E*)-1-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,3-dimethyl-5-sulfonatoindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,3-dimethyl-3*H*-indol-1-ium-5-sulfonate

Description:

Key information: FNIR-Tag, NHS ester is a near-infrared fluorescent dye; supplied with an NHS ester reactive group for the labeling of primary amines with a high degree of labeling (DOL). Application: Designed for in vivo imaging. Also suitable for flow cytometry. Properties and Photophysical Data: FNIR-Tag, NHS ester provides a higher degree of labeling (DOL) with less aggregation than a leading competitor product when used for antibody conjugation. FNIR-Tag, NHS ester- antibody conjugates exhibit reduced liver uptake in vivo compared with leading competitor conjugates. In addition, FNIR-Tag, NHS ester conjugates are significantly brighter... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

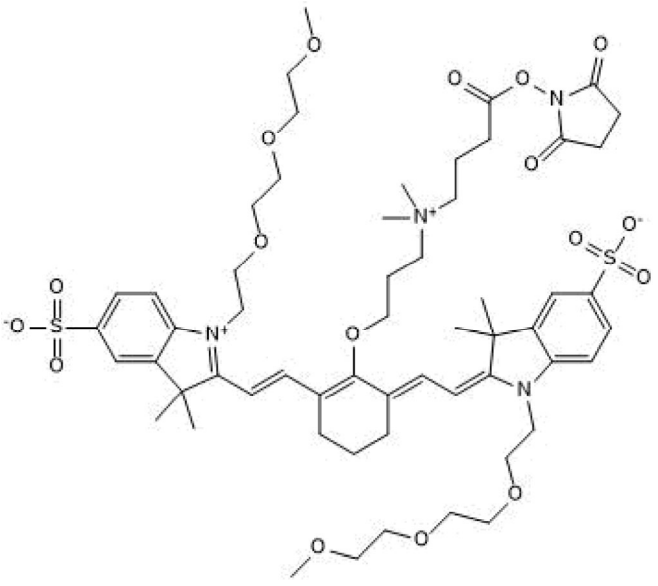
Batch Molecular Formula: $C_{57}H_{80}N_4O_{17}S_2$

Batch Molecular Weight: 1157.4

Physical Appearance: Dark green solid

Minimum Purity: ≥85%

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 10 mM
DMF to 10 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 National Institute of Health

References:

Luciano *et al* (2019) A nonaggregating heptamethine cyanine for building brighter labeled biomolecules. ACS Chem.Biol. ***14*** 934. PMID: 31030512.