Certificate of Analysis

Product Name: **BDY TR-X, SE** **Catalog No.: 5467** **Batch No.: 1**

CAS Number: 197306-80-2

IUPAC Name: (*T*-4)-[*N*-[6-[(2,5-Dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-2-[4-[5-[[5-(2-thienyl)-2*H*-pyrrol-2-ylidene-κ*N*]methyl]-1*H*-pyrrol-2-yl-κ*N*]phenoxy]acetamidato]difluoroboron

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{31}H_{29}BF_2N_4O_6S$

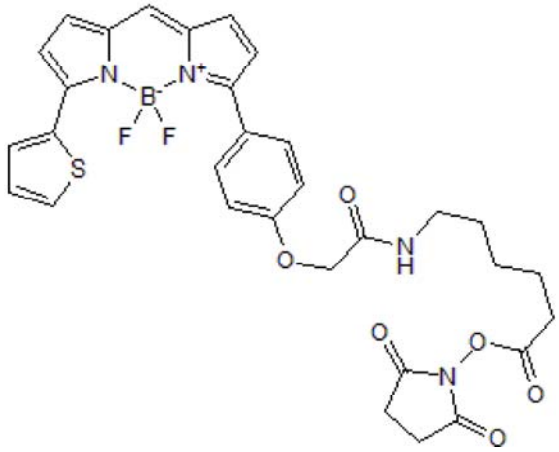
Batch Molecular Weight: 634.46

Physical Appearance: Purple solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

Mass Spectrum: Consistent with structure

λ_{max}: 589 nm (Methanol)

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Product Name: **BDY TR-X, SE** **Catalog No.: 5467** **Batch No.: 1**

CAS Number: 197306-80-2

IUPAC Name: (*T*-4)-[*N*-[6-[(2,5-Dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-2-[4-[5-[[5-(2-thienyl)-2*H*-pyrrol-2-ylidene-κ*N*]methyl]-1*H*-pyrrol-2-yl-κ*N*]phenoxy]acetamidato]difluoroboron

Description:

BDY TR-X, SE is a fluorescent orange BDY (BODIPY® or boron-dipyrromethene) dye for the labeling of amines. Exhibits similar excitation and emission spectra to dye Texas Red®. Displays high fluorescence quantum yield and high extinction coefficient and is relatively insensitive to pH change. This dye contains a seven-atom aminohexanoyl ("X") spacer between the fluorophore and the NHS ester group, reducing the potential for interactions between the fluorophore and conjugated biomolecule. The hydrophobic nature of BDY TR-X makes it ideal for labeling lipids and cell membranes. BDY TR-X also exhibits narrow emission bandwidths a... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

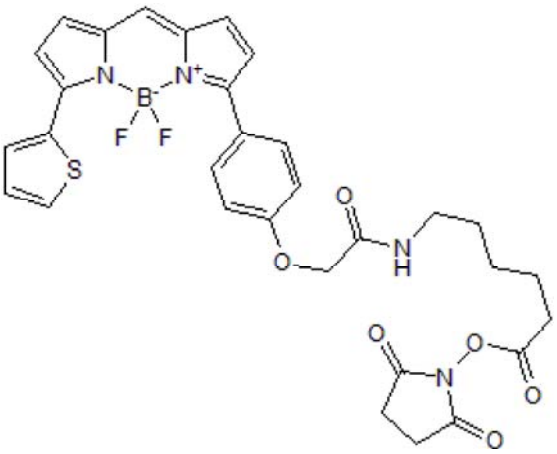
Batch Molecular Formula: $C_{31}H_{29}BF_2N_4O_6S$

Batch Molecular Weight: 634.46

Physical Appearance: Purple solid

Minimum Purity: ≥95%

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

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:

Vernall *et al* (2012) Highly potent and selective fluorescent antagonists of the human adenosine A_3 receptor based on the 1,2,4-triazolo [4,3-*a*]quinoxalin-1-one scaffold. J.Med.Chem. ***55*** 1771. PMID: 22277057.