

Product Name: R-BC154

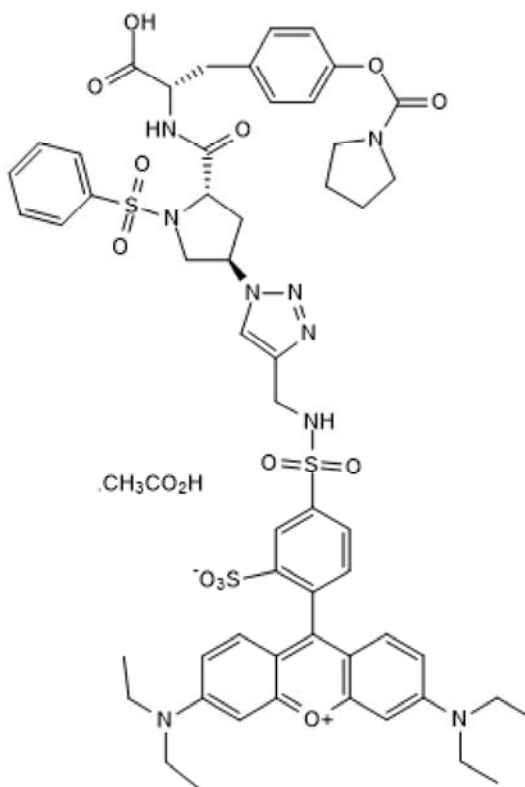
Catalog No.: 6048

Batch No.: 1

IUPAC Name: (4*R*)-4-[4-[[[4-[3,6-Bis(diethylamino)xanthylium-9-yl]-3-sulfophenyl]sulfonyl]amino]methyl]-1*H*-1,2,3-triazol-1-yl]-1-(phenylsulfonyl)-L-prolyl-O-(1-pyrrolidinyl)-L-tyrosine acetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₅₅ H ₆₁ N ₉ O ₁₃ S ₃ .CH ₃ CO ₂ H
Batch Molecular Weight:	1212.37
Physical Appearance:	Pink solid
Solubility:	DMSO to 5 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.22 (Chloroform/Methanol/Acetic acid 90:9.5:0.5)
HPLC:	Shows 97.6% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

High affinity fluorescent $\alpha 4\beta 1/\alpha 9\beta 1$ inhibitor (K_d values are 12.7 and 38 nM, respectively); fluorescent version of BOP (Cat.No. 6047). Rapidly and preferentially mobilizes HSCs and progenitors *in vivo*. Excitation maximum, 561 nm; emission maximum, 585 nm.

Physical and Chemical Properties:

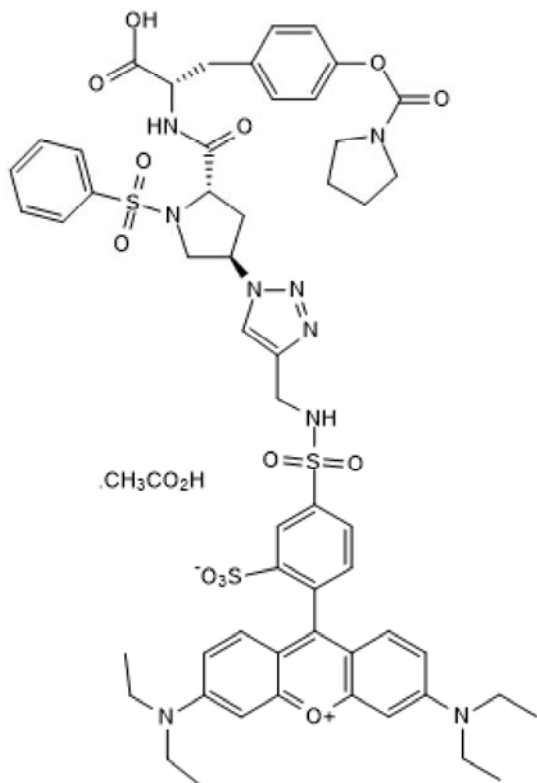
Batch Molecular Formula: $C_{55}H_{61}N_9O_{13}S_3 \cdot CH_3CO_2H$

Batch Molecular Weight: 1212.37

Physical Appearance: Pink solid

Minimum Purity: >97%

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 5 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Cao *et al* (2016) Therapeutic targeting and rapid mobilization of endosteal HSC using a small molecule integrin antagonist. *Nat. Commun.* **7** 11007. PMID: 26975966.

Cao *et al* (2014) Design, synthesis and binding properties of a fluorescent $\alpha 9\beta 1/\alpha 4\beta 1$ integrin antagonist and its application as an *in vivo* probe for bone marrow haemopoietic stem cells. *Org. Biomol. Chem.* **12** 965. PMID: 24363056.

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