

Product Name: BOP

Catalog No.: 6047

Batch No.: 1

CAS Number: 1947348-42-6

IUPAC Name: *N*-(Benzenesulfonyl)-L-prolyl-L-O-(1-pyrrolidinylcarbonyl)tyrosine sodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₈N₃O₇SNa.H₂O

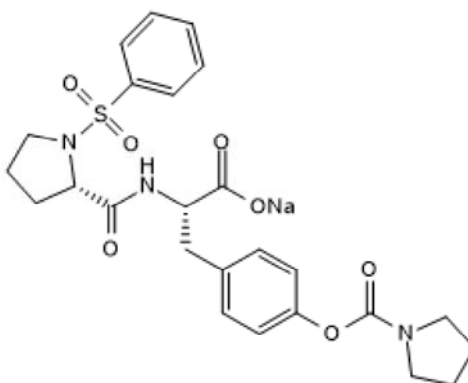
Batch Molecular Weight: 555.58

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.27 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.05	5.44	7.56
Found	53.71	5.66	7.47

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Description:

Dual $\alpha 9\beta 1/\alpha 4\beta 1$ integrin inhibitor; rapidly and preferentially mobilizes HSCs and progenitors. Augments HSC mobilization in combination with AMD3100 (Cat. No. 3299). Fluorogenic, bright and photostable Fluorescent Conjugate BOP-JF646 (Cat. No. 6997) also available. High affinity fluorescent derivative R-BC154 (Cat. No. 6048) also available.

Physical and Chemical Properties:

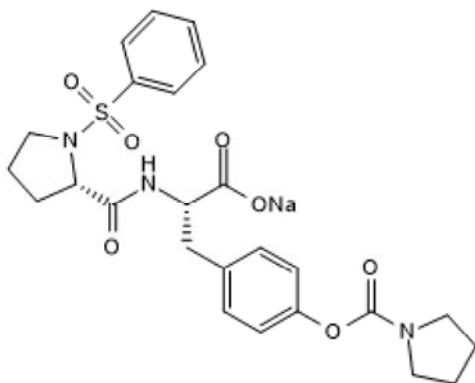
Batch Molecular Formula: $C_{25}H_{28}N_3O_7SNa.H_2O$

Batch Molecular Weight: 555.58

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

Solubility & Usage Info:

water to 100 mM
DMSO to 100 mM
ethanol 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 $45-60^{\circ}C$ 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 $-20^{\circ}C$ 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.

Pepinsky et al (2002) Comparative assessment of the ligand and metal ion binding properties of integrins $\alpha 9\beta 1$ and $\alpha 4\beta 1$. *Biochemistry* **41** 7125. PMID: 12033947.

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