

Product Name: BOP

Catalog No.: 6047

Batch No.: 2

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·¼H₂O

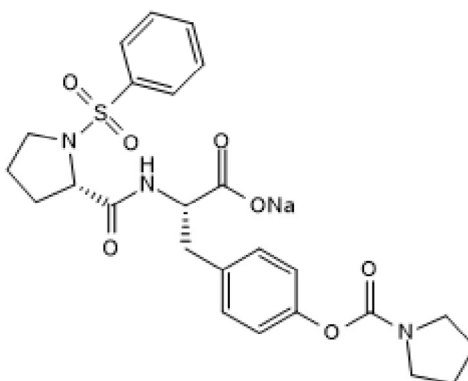
Batch Molecular Weight: 542.06

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.0% purity at 220 nm

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.39	5.3	7.75
Found	55.05	4.91	7.48

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Description:

BOP is a 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:

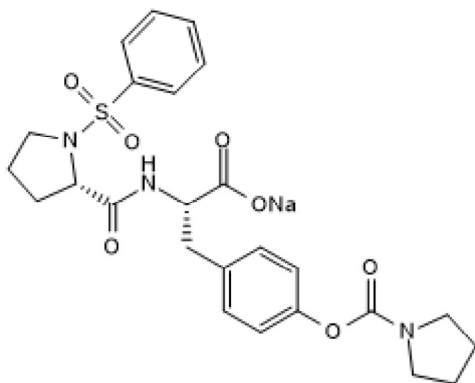
Batch Molecular Formula: $C_{25}H_{28}N_3O_7SNa \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 542.06

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$. This product is packaged under an inert atmosphere.

Solubility & Usage Info:

water to 100 mM

DMSO to 100 mM

This product is supplied in lyophilized form. It may appear as a solid, gel or film and 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 $45-60^{\circ}C$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *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 $-20^{\circ}C$ 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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