

Product Name: PARPi-FL

Catalog No.: 6461

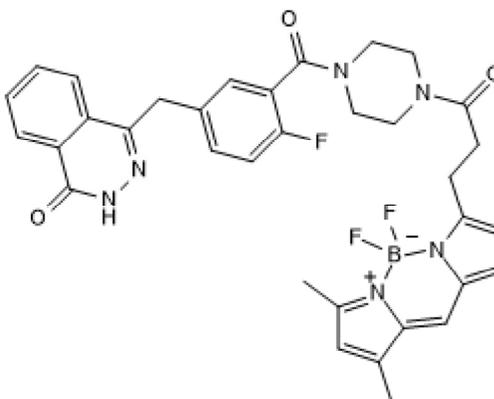
Batch No.: 3

CAS Number: 1380359-84-1

IUPAC Name: (T-4)-[4-[[3-[[4-[3-[5-[(3,5-Dimethyl-2*H*-pyrrol-2-ylidene- κ N)methyl]-1*H*-pyrrol-2-yl- κ N-1-oxopropyl]-1-piperazinyl]carbonyl]-4-fluorophenyl]methyl]-1(2*H*)-phthalazinonato]difluoroboron

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₃₄ H ₃₂ BF ₃ N ₆ O ₃
Batch Molecular Weight:	640.46
Physical Appearance:	Orange solid
Solubility:	DMSO to 10 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 99.6% purity at 210 nm
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
UV Spectrum:	Consistent with structure
λ_{max}:	505 nm (EtOH)
λ_{ex}:	505 nm (EtOH)
λ_{em}:	511 nm (EtOH)

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

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Description:

PARPi-FL is a fluorescent potent PARP inhibitor (IC₅₀ = 12 nM). Composed of a PARP inhibitor conjugated to BDY FL, SE (Cat. No. 5465). Colocalizes with PARP immunostaining in multiple cancer cell lines *in vivo* and accumulates in tumor cells and tumor associated macrophages. Enables high temporal and subcellular spatial resolution of drug distribution. Emission max = 525 nm. Cell permeable.

Physical and Chemical Properties:

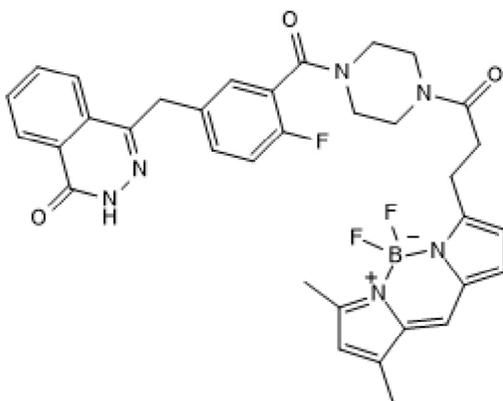
Batch Molecular Formula: C₃₄H₃₂BF₃N₆O₃

Batch Molecular Weight: 640.46

Physical Appearance: Orange solid

Minimum Purity: ≥90%

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 10 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°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.

References:

Dubach *et al* (2017) Quantitating drug-target engagement in single cells *in vitro* and *in vivo*. *Nat.Chem.Biol.* **13** 168. PMID: 27918558.

Thurber *et al* (2014) Effect of small-molecule modification on single-cell pharmacokinetics of PARP inhibitors. *Mol.Cancer Ther.* **13** 986. PMID: 24552776.

Thurber *et al* (2013) Single-cell and subcellular pharmacokinetic imaging allows insight into drug action *in vivo*. *Nat.Comm.* **4** 1504. PMID: 23422672.

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