Certificate of Analysis

Product Name: **PARPi-FL** **Catalog No.: 6461** **Batch No.: 2**

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: $C_{34}H_{32}BF_3N_6O_3$

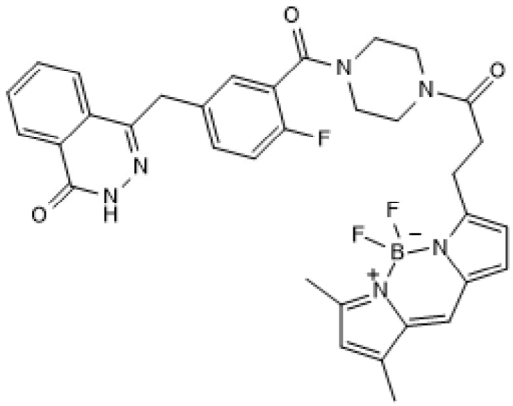
Batch Molecular Weight: 640.46

Physical Appearance: Orange solid

Solubility: DMSO to 10 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 96.5% purity at 502 nm

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

UV Spectrum: Consistent with structure

λ_{max}: 505 nm (Ethanol)

λ_{ex}: 505 nm (Ethanol)

λ_{em}: 511 nm (Ethanol)

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

PARPi-FL is a fluorescent potent PARP inhibitor (IC_{50} = 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:

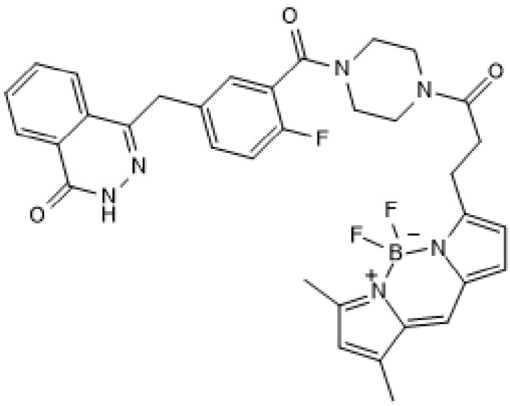
Batch Molecular Formula: $C_{34}H_{32}BF_3N_6O_3$

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.Commun. ***4*** 1504. PMID: 23422672.