Screening Libraries

DUPA(OtBu)-OH

Cat. No.: HY-103591 CAS No.: 1026987-94-9 Molecular Formula: $C_{23}H_{40}N_{2}O_{9}$ Molecular Weight: 488.57 **PSMA** Target:

Pathway: Immunology/Inflammation

Powder -20°C Storage: 3 years

2 years

-80°C In solvent 2 years

> -20°C 1 year

Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

DMSO: 125 mg/mL (255.85 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.0468 mL	10.2339 mL	20.4679 mL
	5 mM	0.4094 mL	2.0468 mL	4.0936 mL
	10 mM	0.2047 mL	1.0234 mL	2.0468 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.08 mg/mL (4.26 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.08 mg/mL (4.26 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (4.26 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

DUPA(OtBu)-OH is a DUPA precursor. DUPA is used as the targeting moiety to actively deliver Docetaxel (DTX) for treatment of Prostate-Specific Membrane Antigen (PSMA) expressing prostate cancer.

In Vitro

 $DUPA(OtBu)-OH\ (DUPA\ precursor\ 17)\ is\ a\ 2-[3-(1,3-dicarboxypropyl)] ureido]\ pentanedioic\ acid\ (DUPA)\ reagent \ [1].$ The targeting ligand DUPA enhances the transport capability and selectivity of Paclitaxel (PTX) to tumor cells via prostatespecific membrane antigen (PSMA) mediated endocytosis. Besides, DUPA is conjugated with PTX via a disulfide bond, which facilitates the rapid and differential drug release in tumor cells^[2].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	DUPA-targeted Docetaxel (DTX) conjugate with longer spacer has no toxicity in major organs of treated mice ^[3] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

• Research Square Preprint. 2021 Jun.

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REFERENCES

[1]. Roy J, et al. DUPA conjugation of a cytotoxic indenoisoquinoline topoisomerase I inhibitor for selective prostate cancer cell targeting. J Med Chem. 2015 Apr 9;58(7):3094-103.

[2]. Lv Q, et al. Prostate-Specific Membrane Antigen Targeted Therapy of Prostate Cancer Using a DUPA-Paclitaxel Conjugate. Mol Pharm. 2018 May 7;15(5):1842-1852.

[3]. Peng ZH, et al. Spacer length impacts the efficacy of targeted docetaxel conjugates in prostate-specificmembrane antigen expressing prostate cancer. J Drug Target. 2013 Dec;21(10):968-80.

Caution: Product has not been fully validated for medical applications. For research use only.

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