

Product Data Sheet

Deutenzalutamide-d₃

Cat. No.: HY-70002S

CAS No.: 1443331-82-5

Molecular Formula: C₂₁H₁₃D₃F₄N₄O₂S

Molecular Weight: 467.45

Target: Androgen Receptor; Autophagy

Pathway: Vitamin D Related/Nuclear Receptor; Autophagy

Storage: Powder -20°C 3 years

4°C 2 years

In solvent -80°C 6 months

-20°C 1 month

SOLVENT & SOLUBILITY

In Vitro

DMSO: 25 mg/mL (53.48 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.1393 mL	10.6963 mL	21.3927 mL
	5 mM	0.4279 mL	2.1393 mL	4.2785 mL
	10 mM	0.2139 mL	1.0696 mL	2.1393 mL

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

BIOLOGICAL ACTIVITY

Description

Deutenzalutamide (Enzalutamide- d_3) is a developed deuterium labeled Enzalutamide (MDV3100). Enzalutamide is an androgen receptor (AR) antagonist with an IC50 of 36 nM in LNCaP prostate cells^[1].

In Vitro

Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs^[1].

Potential advantages of deuterated compounds:

- (1) Extend the half-life in vivo. Deuterated compounds may be able to prolong the pharmacokinetic characteristics of the compound, that is, prolong the half-life in vivo. This can improve compound safety, efficacy and tolerability, and increase ease of administration.
- (2) Improve oral bioavailability. Deuterated compounds may reduce the degree of unwanted metabolism (first-pass metabolism) in the gut wall and liver, allowing a greater proportion of the unmetabolized drug to reach its target site of action. High bioavailability determines its activity at low doses and better tolerance.
- (3) Improve metabolic characteristics. Deuterated compounds may reduce the formation of toxic or reactive metabolites and improve drug metabolism.

- (4) Improve drug safety. Deuterated compounds may reduce or eliminate adverse side effects of pharmaceutical compounds and are safe.
- (5) Preserve the therapeutic properties. Deuterated compounds are expected to retain similar biochemical potency and selectivity to hydrogen analogs in previous studies.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Tran C, et al. Development of a second-generation antiandrogen for treatment of advanced prostate cancer. Science. 2009 May 8;324(5928):787-90.

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

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