Sorafenib-d_3

Cat. No.: HY-10201S

CAS No.: 1130115-44-4

Molecular Formula: $C_{21}H_{13}D_3ClF_3N_4O_3$

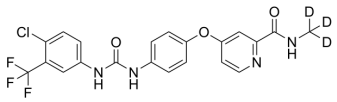
Molecular Weight: 467.84

Target: Raf; Ferroptosis; VEGFR; FLT3; Autophagy; Apoptosis

Pathway: MAPK/ERK Pathway; Apoptosis; Protein Tyrosine Kinase/RTK; 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 : 100 mg/mL (213.75 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1375 mL	10.6874 mL	21.3748 mL
	5 mM	0.4275 mL	2.1375 mL	4.2750 mL
	10 mM	0.2137 mL	1.0687 mL	2.1375 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: ≥ 2.5 mg/mL (5.34 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.34 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.34 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Sorafenib-d_3 (Donafenib), a deuterated compound of Sorafenib, is the first deuterium-generation tumor suppressor small molecule. Sorafenib is a multikinase inhibitor IC_{50}s of 6 nM, 20 nM, and 22 nM for Raf-1, B-Raf, and VEGFR-3, respectively[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]. Wilhelm SM, et al. BAY 43-9006 exhibits broad spectrum oral antitumor activity and targets the RAF/MEK/ERK pathway and receptor tyrosine kinases involved in tumor progression and angiogenesis. Cancer Res. 2004 Oct 1;64(19):7099-109.

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