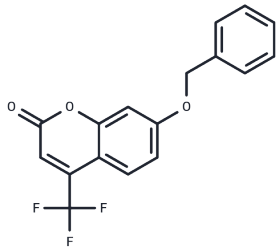
Data Sheet (Cat.No.T117521)

TargetMol

7-BFC

Chemical Properties



CAS No. : 220001-53-6

Formula: C17H11F3O3

Molecular Weight: 320.26

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	7-BFC (7-Benzyloxy-4-(trifluoromethyl)coumarin) is a coumarin-like fluorescent substrate that serves as a biomarker for cytochrome P 450 and can be used to study CYP isoforms and cytochrome P 450 metabolism.
Targets(IC50)	Cytochromes P450
In vitro	I. CYP activity detection 1. Material preparation: 1) 7-BFC solution: usually prepared as a 1-10 μM solution, dissolved in an appropriate solvent (such as DMSO or PBS). 2) Enzyme source: CYP subtype (such as CYP3A4, CYP2D6, etc.) expression system, or use human liver microsomes. 3) Reaction buffer: usually use phosphate buffer (pH 7.4) containing NADPH to simulate the in vivo metabolic environment. 4) Fluorescence detection equipment: such as fluorescence spectrophotometer, excitation wavelength 405 nm, emission wavelength 460 nm (specific wavelength depends on the experimental setting). 2. Steps: 1) Prepare the reaction system: mix the 7-BFC solution with CYP subtypes or liver microsomes, and add NADPH as an electron donor. 2) Reaction incubation: Incubate the reaction system at 37°C for 15-30 minutes to allow 7-BFC to undergo metabolic reactions and produce fluorescence. 3) Fluorescence detection: Use a fluorescence spectrophotometer to detect the fluorescence intensity of the product, usually setting the excitation wavelength to 405 nm and the emission wavelength to 460 nm. 4) Data analysis: By measuring the changes in fluorescence intensity, the activity of cytochrome P450 and its metabolic efficiency on 7-BFC can be evaluated. II. CYP subtype-specific detection 1. Material preparation: 1) CYP subtype inhibitors: such as ketoconazole (an inhibitor of CYP3A4), or inhibitors of specific subtypes. 2) Metabolite analysis: Metabolites can be further analyzed by techniques such as high-performance liquid chromatography (HPLC). 3. Steps: 1) Set up experimental groups: Add different CYP inhibitors to identify the metabolic effects of specific CYP subtypes on 7-BFC. 2) Fluorescence detection and data analysis:

In vitro	Compare the fluorescence signal intensity of different inhibitors and untreated samples to further confirm the metabolic characteristics of specific CYP subtypes. Notes: 1) Reaction conditions: The choice of temperature, pH and buffer will affect the efficiency of the reaction and should be optimized according to the experimental requirements. 2) Solvent effect: When dissolving 7-BFC, a solvent that has no effect on the experimental system should be selected to avoid inhibition of CYP activity. 3) Fluorescence stability: The fluorescence signal of 7-BFC is relatively stable, but long-term exposure to strong light should be avoided. The above information is based on published literature. Experimental procedures should be appropriately modified to meet specific research demands.

Solubility Information

Solubility	DMSO: 55 mg/mL (171.74 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.1225 mL	15.6123 mL	31.2246 mL
5 mM	0.6245 mL	3.1225 mL	6.2449 mL
10 mM	0.3122 mL	1.5612 mL	3.1225 mL
50 mM	0.0624 mL	0.3122 mL	0.6245 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Mooiman KD, et al. The effect of complementary and alternative medicines on CYP3A4-mediated metabolism of three different substrates: 7-benzyloxy-4-trifluoromethyl-coumarin, midazolam and docetaxel. J Pharm Pharmacol. 2014 Jun;66(6):865-74.

Davydov DR,et al. Pivotal role of P450-P450 interactions in CYP3A4 allostery: the case of α-naphthoflavone. Biochem J. 2013 Jul 15;453(2):219-30.

Kumar S, Liu H, Halpert JR. Engineering of cytochrome P450 3A4 for enhanced peroxide-mediated substrate oxidation using directed evolution and site-directed mutagenesis. Drug Metab Dispos. 2006 Dec;34(12):1958-65.