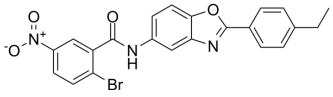
BAY-0069

Cat. No.:	HY-148351
CAS No.:	420826-65-9
Molecular Formula:	$C_{22}H_{16}BrN_3O_4$
Molecular Weight:	466.28
Target:	PPAR
Pathway:	Cell Cycle/DNA Damage; Vitamin D Related/Nuclear Receptor
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (214.46 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1446 mL	10.7232 mL	21.4463 mL
	5 mM	0.4289 mL	2.1446 mL	4.2893 mL
	10 mM	0.2145 mL	1.0723 mL	2.1446 mL

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

BIOLOGICAL ACTIVITY

Description

BAY-0069 is a potent and selective PPARγ inverse agonist with an IC_{50} value of 6.3 nM and 24 nM for human PPARγ and mouse PPARγ. BAY-0069 can be used to research cancer[1].

IC_{50} & Target

hPPARγ	mouse PPARγ
6.3 nM (IC_{50})	24 nM (IC_{50})

In Vitro

BAY-0069 inhibits CYP2C8 with an IC_{50} of 4.3 μM[1].

BAY-0069 (0.1 nM-1 μM; 7 days) leads to antiproliferative effects in the PPARγ-amplified cell line UM-UC-9[1].

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

Cell Proliferation Assay[1]

Cell Line:	PPARγ-amplified cell line UM-UC-9
Concentration:	0.0001, 0.001, 0.01, 0.01 and 1 μM
Incubation Time:	7 days

Result:	Inhibited PPARγ-amplified cell line UM-UC-9 with an IC_{50} of 2.54 nM.

In Vivo

BAY-0069 (1 μM; 1 h) exhibits excellent microsomal stability with $CL_{b,hmic}$ of 0.47 L/h/kg in human liver microsomes and $CL_{b,rhep}$ of 3.9 L/h/kg in rat liver hepatocytes[1].

Pharmacokinetic Parameters of BAY-0069 in female NMRI nu/nu mice[1].

Route	P.O. (100 mg/kg)	I.P.	S.C.
$AUC_{0\text{-}tlast}$ (mg/L·h)	0.074	0.26	0.045
C_{max} (nM)	35	59	4.4

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

REFERENCES

[1]. Orsi DL, Goldstein JT, et al. Discovery and Structure-Based Design of Potent Covalent PPARγ Inverse-Agonists BAY-4931 and BAY-0069. J Med Chem. 2022 Nov 10;65(21):14843-14863.

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