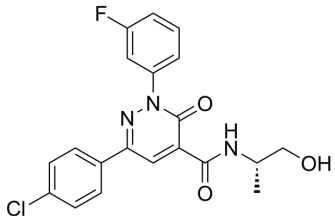
BAY-218

Cat. No.:	HY-111449
CAS No.:	2162982-11-6
Molecular Formula:	$C_{20}H_{17}ClFN_3O_3$
Molecular Weight:	401.82
Target:	Aryl Hydrocarbon Receptor
Pathway:	Immunology/Inflammation
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 250 mg/mL (622.17 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4887 mL	12.4434 mL	24.8868 mL
	5 mM	0.4977 mL	2.4887 mL	4.9774 mL
	10 mM	0.2489 mL	1.2443 mL	2.4887 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 (5.18 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.18 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-218 (AHR antagonist 1) is an aryl hydrocarbon receptor (AHR) antagonist. BAY-218 has AHR inhibitory activity with an IC_{50} of 39.9 nM in in U87 glioblastoma cells. BAY-218 can be used for the research of cancer or conditions with dysregulated immune responses[1].

IC_{50} & Target

IC50: 39.9 nM (AHR in human cell line)[1]

In Vitro

BAY-218 (example 23) (72 pM-20 μM) has AHR inhibitory activity with an IC_{50} of 39.9 μM in in U87 glioblastoma cells[1].
?BAY-218 (1 nM-3 μM) has CYP1A1 inhibitory activity with an IC_{50} of 70.7 μM in human monocytic U937 cell line[1].
?BAY-218 (1 μM) reverses KA-induced inhibition of TNFα production by LPS stimulated human monocytes[1].

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

RT-PCR[1]

Cell Line:	human monocytic U937 cells
Concentration:	1 nM-3 μM
Incubation Time:	
Result:	Regulated antagonise ligand-induced AHR gene in a dose-dependent manner.

In Vivo

BAY-218 (example 23) (p.o; 30 mg/kg; bid) has good anti-tumor effect combinated with aPD-L1[1].

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

Animal Model:	Balb/c mice (subcutaneously CT26 cells)[1]
Dosage:	30 mg/kg
Administration:	p.o, bid
Result:	Significantly decreased tumors size combinated with aPD-L1.

REFERENCES

[1]. Norbert Schmees, et al. 3-oxo-2,6-diphenyl-2,3-dihydropyridazine-4-carboxamides. WO2017202816A1.

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