BAY-876

Cat. No.: HY-100017

CAS No.: 1799753-84-6

Molecular Formula: $C_{24}H_{16}F_4N_6O_2$

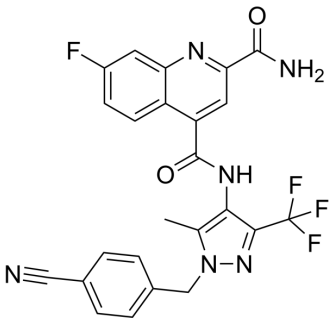
Molecular Weight: 496.42

Target: GLUT

Pathway: Membrane Transporter/Ion Channel

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 (201.44 mM)

Methanol : 1 mg/mL (2.01 mM; ultrasonic and warming and heat to 60°C)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.0144 mL	10.0721 mL	20.1442 mL
5 mM	0.4029 mL	2.0144 mL	4.0288 mL
10 mM	0.2014 mL	1.0072 mL	2.0144 mL

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

In Vivo

1. Add each solvent one by one: 50% PEG300 >> 50% saline
   Solubility: 5 mg/mL (10.07 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.04 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-876 is an orally active and selective glucose transporter 1 (GLUT1) inhibitor with an IC_{50} of 2 nM. BAY-876 is >130-fold more selective for GLUT1 than GLUT2, GLUT3, and GLUT4[1]. BAY-876 is also a potent blocker of glycolytic metabolism and ovarian cancer growth[2].

IC_{50} & Target

GLUT1	GLUT2	GLUT3	GLUT4
2 nM (IC_{50})	10.08 μM (IC_{50})	1.67 μM (IC_{50})	0.29 μM (IC_{50})

In Vitro

BAY-876 (25-75 nM; 24 and 72 hours) has the growth-inhibitory effect and leads to a dose-dependent decrease in numbers of

SKOV-3 and OVCAR-3 cells[2].

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

Cell Proliferation Assay[2]

Cell Line:	SKOV-3 and OVCAR-3 cells
Concentration:	25, 50, 75 nM
Incubation Time:	24 and 72 hours
Result:	Led to a dose-dependent decrease in numbers of SKOV-3 and OVCAR-3 cells.

In Vivo

BAY-876 (oral administration; 1.5-4.5 mg/kg/day for 28 days) causes a clear dose-dependent inhibition of tumorigenicity in mice[2].

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

Animal Model:	Female NOD-scid IL2rg^{null} (NSG) mice carrying SKOV-3 subcutaneous (s.c.) xenografts[2]
Dosage:	1.5, 3, 4.5 mg/kg
Administration:	Oral administration; daily; for 28 days
Result:	Caused a clear dose-dependent inhibition of tumorigenicity.

CUSTOMER VALIDATION

- Small. 2021 Aug 4;e2102695.
- Redox Biol. 2021 Jul 26;46:102082.
- J Hazard Mater. 16 October 2021, 127512.
- Expert Opin Ther Pat. 2022 Jan 9.
- Cancers (Basel). 2022, 14(2), 345.

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REFERENCES

[1]. Siebeneicher H et al. Identification and Optimization of the First Highly Selective GLUT1 Inhibitor BAY-876. ChemMedChem. 2016 Aug 23.

[2]. Ma Y, et al. Ovarian Cancer Relies on Glucose Transporter 1 to Fuel Glycolysis and Growth: Anti-Tumor Activity of BAY-876. Cancers (Basel). 2018 Dec 31;11(1).

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