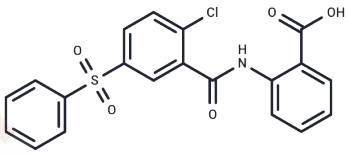
Data Sheet (Cat.No.T5208)

TargetMol

BAY-8002

Chemical Properties



CAS No. : 724440-27-1

Formula: C20H14ClNO5S

Molecular Weight: 415.85

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	BAY-8002 is a potent dual MCT1/2 inhibitor (IC50 values are 3, 8, and 12 nM at rat (C6), human (DLD-1) and mouse (4T1) MCT1 respectively).
Targets(IC50)	Monocarboxylate transporter
In vitro	BAY-8002 inhibited cellular SNARF-5 fluorescence change with an IC50 of 85 nM in MCT1-expressing DLD-1 cells and displayed excellent selectivity against MCT4 (IC50 >50 μmol/L in EVSA-T cells).
In vivo	Raji tumor-bearing mice were treated twice daily per os with 80 and 160 mg/kg BAY-8002. BAY-8002 showed significant inhibition of tumor growth, however, no tumor regression was observed. Daudi Burkitt's lymphoma model showed some response to MCT1 inhibition, albeit not significant for BAY-8002.
Cell Research	Cells were seeded at 3000- 6000 cells per well in a 90 μl volume in 96-well plates. Triplicates were treated in a dose range of 0-10 μmol/L. Cells were continuously exposed to the drug at 37°C and 5 % CO2. After 72 h, cell viability was measured using the CellTiter Glo cell viability assay. For the generation of resistant cell lines, cells were treated at IC50 and upon regrowth treated with increasing concentrations of the drug.
Animal Research	For in vivo studies, tumor cells were subcutaneously (s.c.) injected in 0.1 ml suspension to the left flank of 7-10 weeks old immunocompromised female mice (3 x 10^6 Raji cells in 10% Matrigel) to NOD SCID mice, 2 x 10^6 Colo320DM cells in 50% MatrigelTM to NMRI nu/nu mice, 3 x 10^6 WSU-DLCL2 cells or 1 x 10^7 Daudi cells in 50% MatrigelTM to CB17 SCID mice. Tumor area (length x width) and body weight was determined at least twice weekly. Tumors were allowed to establish before mice were allocated to different treatment and control groups by stratified randomization based on their primary tumor size. Oral treatments (p.o.) via gavage were performed as indicated. Final tumor weights were determined at the end of each study. For statistical analysis of tumor area as well as final tumor weights, data were analyzed using one-way ANOVA followed by Tukey's multiple comparisons test.

Solubility Information

Solubility	DMSO: 120 mg/mL (288.57 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (4.81 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.4047 mL	12.0236 mL	24.0471 mL
5 mM	0.4809 mL	2.4047 mL	4.8094 mL
10 mM	0.2405 mL	1.2024 mL	2.4047 mL
50 mM	0.0481 mL	0.2405 mL	0.4809 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

Quanz M, et al. Preclinical Efficacy of the Novel Monocarboxylate Transporter 1 Inhibitor BAY-8002 and Associated Markers of Resistance. Mol Cancer Ther. 2018 Nov;17(11):2285-2296.