

Product Name: BAY 876

Catalog No.: 6199

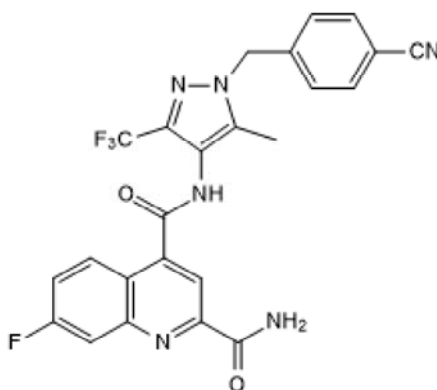
Batch No.: 1

CAS Number: 1799753-84-6

IUPAC Name: *N*4-[1-[(4-Cyanophenyl)methyl]-5-methyl-3-(trifluoromethyl)-1*H*-pyrazol-4-yl]-7-fluoro-2,4-quinolinedicarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₁₆F₄N₆O₂
Batch Molecular Weight: 496.42
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.48 (Dichloromethane:Methanol [9:1])
HPLC: Shows 99.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.07	3.25	16.93
Found	57.76	3.37	17.08

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Description:

BAY 876 is a potent and selective GLUT1 inhibitor ($IC_{50} = 2 \text{ nM}$) that displays selectivity for GLUT1 over GLUT2/3/4 (IC_{50} values are 10.8, 1.67 and 0.29 μM , respectively). BAY 876 induces cell death in hypoxic conditions in vitro and inhibits glucose uptake by HeLa-MaTu cells. In ovarian cancer, BAY 876 reduces glycolysis rates and ATP production and inhibits proliferation in vitro and in vivo. This compound is cell permeable and orally bioavailable.

Physical and Chemical Properties:

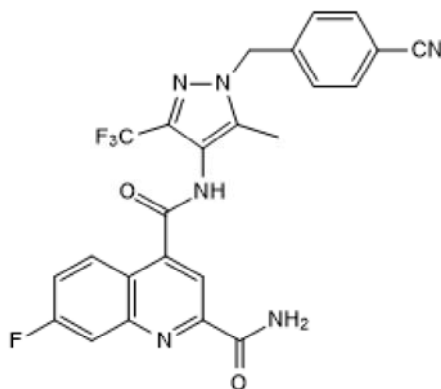
Batch Molecular Formula: $C_{24}H_{16}F_4N_6O_2$

Batch Molecular Weight: 496.42

Physical Appearance: Off-white solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Ma et al (2018) Ovarian cancer relies on glucose transporter 1 to fuel glycolysis and growth: anti-tumor activity of BAY-876. *Cancers (Basel)* **11** 33. PMID: 30602670.

Siebeneicher et al (2016) Identification and optimization of the first highly selective GLUT1 inhibitor BAY-876. *ChemMedChem.* **11** 2261. PMID: 27552707 .

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956