

Product Name: BAY 876

Catalog No.: 6199

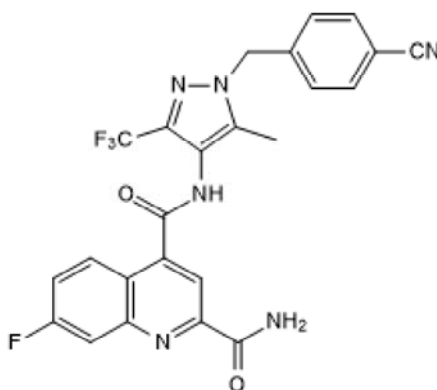
Batch No.: 1

CAS Number: 1799753-84-6

IUPAC Name: N4-[1-[(4-Cyanophenyl)methyl]-5-methyl-3-(trifluoromethyl)-1H-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. This compound is cell permeable and orally bioavailable.

Physical and Chemical Properties:

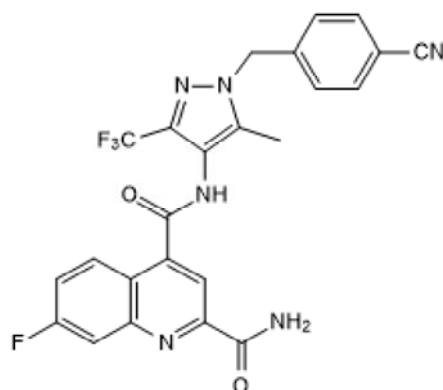
Batch Molecular Formula: $C_{24}H_{16}F_4N_6O_2$

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:

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