

Product Name: MSC 4381

Catalog No.: 8008

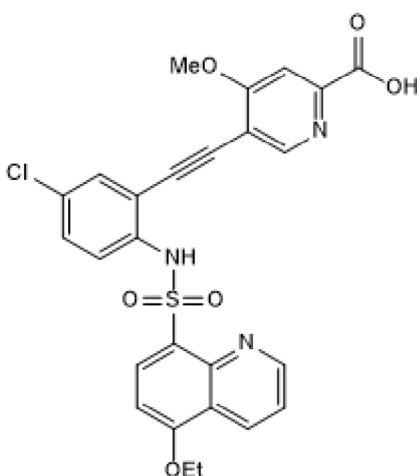
Batch No.: 1

CAS Number: 2445185-57-7

IUPAC Name: 5-[2-[5-Chloro-2-[[[(5-ethoxy-8-quinolinyl)sulfonyl]amino]phenyl]ethynyl]-4-methoxy-2-pyridinecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₂₀ClN₃O₆S
Batch Molecular Weight: 537.97
Physical Appearance: Beige solid
Solubility: DMSO to 50 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.05	3.75	7.81
Found	57.16	3.52	7.6

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Description:

MSC 4381 is a potent and selective monocarboxylate transporter 4 (MCT4) inhibitor ($IC_{50} = 77$ nM; $K_i = 11$ nM). Inhibits lactate efflux in MDA-MB-231 cells ($IC_{50} = 1$ nM) and reduces viability of cells expressing high levels of MCT4.

Physical and Chemical Properties:

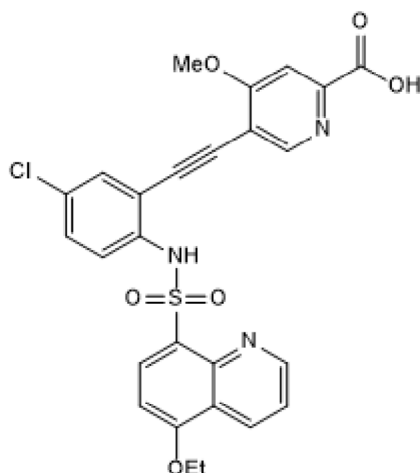
Batch Molecular Formula: $C_{26}H_{20}ClN_3O_6S$

Batch Molecular Weight: 537.97

Physical Appearance: Beige solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

Solubility & Usage Info:

DMSO to 50 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 $45-60^{\circ}C$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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 $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the MSC 4381 probe summary on the SGC website.

References:

Heinrich *et al* (2021) Discovery of 5-{2-[5-Chloro-2-(5-ethoxyquinoline-8-sulfonamido)phenyl]ethynyl}-4-methoxypyridine-2-carboxylic acid, a highly selective in vivo measurable chemical probe to dissect MCT4 biology. *J.Med.Chem.* **64** 11904. PMID: 34382802.

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