

Certificate of Analysis

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Product Name: ML 382

Catalog No.: 5738

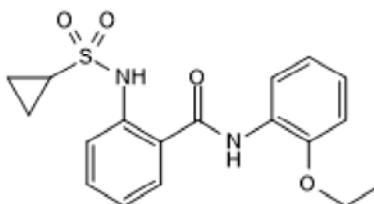
Batch No.: 1

CAS Number: 1646499-97-9

IUPAC Name: 2-[(Cyclopropylsulfonyl)amino]-N-(2-ethoxyphenyl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₀N₂O₄S
Batch Molecular Weight: 360.43
Physical Appearance: Orange solid
Solubility: DMSO to 100 mM
ethanol to 20 mM with gentle warming
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.98	5.59	7.77
Found	59.95	5.48	7.73

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Catalog No.: 5738

Batch No.: 1

CAS Number: 1646499-97-9

IUPAC Name: 2-[(Cyclopropylsulfonyl)amino]-N-(2-ethoxyphenyl)benzamide

Description:

Selective MRGPRX1 positive allosteric modulator (EC_{50} = 190 nM). Exhibits selectivity for MrgX1 over MrgX2, MrgC11 and a panel of 68 other GPCRs, ion channels and transporters. Enhances BAM (8-22) potency at MRGPRX1 by 7-fold.

Physical and Chemical Properties:

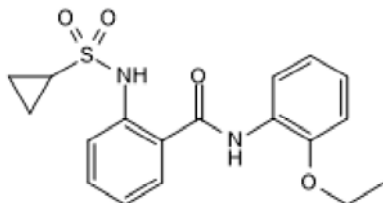
Batch Molecular Formula: $C_{18}H_{20}N_2O_4S$

Batch Molecular Weight: 360.43

Physical Appearance: Orange solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 mM with gentle warming

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:

Wen et al (2015) Discovery and characterization of 2-(cyclopropanesulfonamido)-N-(2-ethoxyphenyl)benzamide, ML382: a potent and selective positive allosteric modulator of MrgX1. *ChemMedChem* **10** 57. PMID: 25209672.

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