

Product Name: ML 179

Catalog No.: 4957

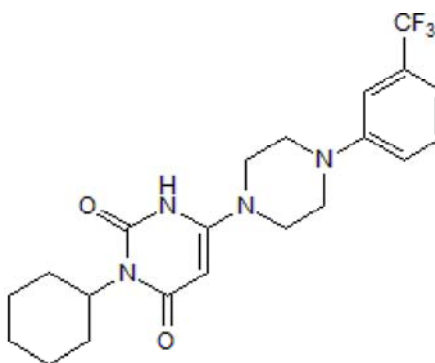
Batch No.: 1

CAS Number: 1883548-87-5

IUPAC Name: 3-Cyclohexyl-6-[4-[3-(trifluoromethyl)phenyl]piperazin-1-yl]-1*H*-pyrimidine-2,4-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₅F₃N₄O₂
Batch Molecular Weight: 422.44
Physical Appearance: White crystalline solid
Solubility: DMSO to 50 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.75 (Dichloromethane:Methanol [9:1])
HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.71	5.96	13.26
Found	60.02	5.97	13.25

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

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Description:

Selective liver receptor homolog 1 (LRH1, NR5A2) inverse agonist (IC₅₀ = 320 nM and maximum efficacy of 64% repression). Exhibits >31-fold selectivity over SF1.

Physical and Chemical Properties:

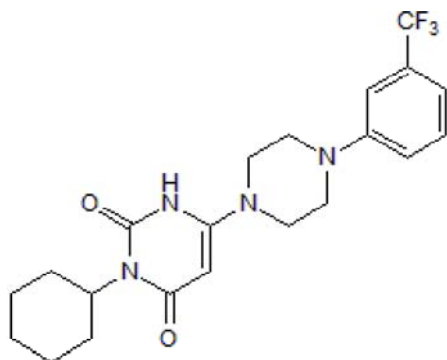
Batch Molecular Formula: C₂₁H₂₅F₃N₄O₂

Batch Molecular Weight: 422.44

Physical Appearance: White crystalline solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at +4°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°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:

Busby et al (2010) Discovery of inverse agonists for the liver receptor homologue-1 (LRH1; NR5A2). Probe Reports from the NIH Molecular Libraries Program . PMID: 23166964.

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