Print Date: Mar 1st 2021

Certificate of Analysis

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Product Name: **cis-22a** **Catalog No.: 7118** **Batch No.: 1**

CAS Number: 1819366-84-1

IUPAC Name: 1-[*cis*-4-(3-Methylphenyl)cyclohexyl]-4-(3-pyridinyl)piperazine ditrifluoroacetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{29}N_3.2CF_3CO_2H.½H_2O$

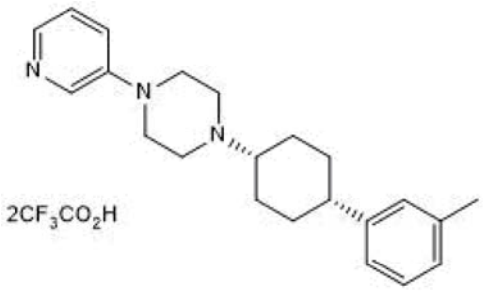
Batch Molecular Weight: 572.55

Physical Appearance: Off White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.54	5.63	7.34
Found	51.43	4.95	6.45

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

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Description:

cis-22a is a TRPV6 inhibitor (IC_{50} = 0.32 µM), which exhibits selectivity against related TRPV channels and calcium channels. cis-22a displays antiproliferative effects on T47D human breast cancer cells.

Physical and Chemical Properties:

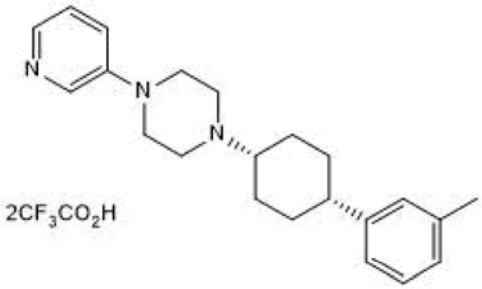
Batch Molecular Formula: $C_{22}H_{29}N_3.2CF_3CO_2H.½H_2O$

Batch Molecular Weight: 572.55

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM
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:

Cunha *et al* (2019) Photoswitchable inhibitor of the calcium channel TRPV6. ACS Med.Chem.Lett. ***10*** 1341. PMID: 31531207.

Simonin *et al* (2015) Optimization of TRPV6 calcium channel inhibitors using a 3D ligand-based virtual screening method. Angew.Chem.Int.Ed.Engl. ***54*** 14748. PMID: 26457814.

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