

Product Name: PSEM 89S

Catalog No.: 6426

Batch No.: 1

CAS Number: 1336913-03-1

IUPAC Name: *N*-(3*S*)-1-Azabicyclo[2.2.2]oct-3-yl-2,5-dimethoxybenzamide trifluoroacetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₂₂N₂O₃.CF₃CO₂H.½H₂O

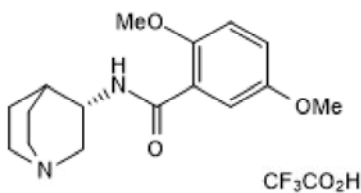
Batch Molecular Weight: 413.39

Physical Appearance: White solid

Solubility: DMSO to 100 mM
water to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (10% MeOH/DCM (with NH₄OH))

HPLC: Shows 99.6% purity

Chiral HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.3	5.85	6.78
Found	52.43	5.9	6.8

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Description:

PSAM^{L141F}-GlyR and PSAM^{L141F,Y115F}-5-HT₃ chimeric ion channel agonist (EC₅₀ values are 3.4 and 2.2 μM, respectively). Activates cortical neurons expressing PSAM^{L141F,Y115F}-5-HT₃ chimeric ion channels and inhibits activity of neurons expressing PSAM^{L141F}-GlyR in vitro. Silences hypothalamic AGRP neurons transfected with PSAM^{L141F}-GlyR chimeric ion channels in mice in vivo, leading to suppression of feeding. Brain penetrant. Plasmid vectors for the transfection of cells with PSAM^{L141F}-GlyR and PSAM^{L141F,Y115F}-5-HT₃ are available from Addgene. Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

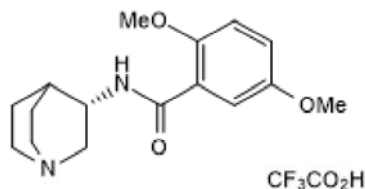
Batch Molecular Formula: C₁₆H₂₂N₂O₃.CF₃CO₂H.½H₂O

Batch Molecular Weight: 413.39

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

water 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.

Licensing Information:

Sold under license from the Howard Hughes Medical Institute, Janelia Research Campus.

For scientific research use only. This product may not be used to research, develop, make, use, offer to sell, sell, or import any products for human therapeutic uses.

References:

Cerritelli et al (2016) Activation of brainstem pro-opiomelanocortin neurons produces opioidergic analgesia, bradycardia and bradypnoea. *PLoS One* **11** e0153187. PMID: 27077912.

Magnus et al (2011) Chemical and genetic engineering of selective ion channel-ligand interactions. *Science* **333** 1292. PMID: 21885782 .

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