

Product Name: NTRC 824

Catalog No.: 5438

Batch No.: 1

CAS Number: 1623002-61-8

IUPAC Name: *N*-[2-[5-[[4-Methylphenyl)sulfonyl]amino]-3-(2,2,2-trifluoroacetyl)-1*H*-indol-1-yl]acetyl]-*L*-leucine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₆F₃N₃O₆S.H₂O

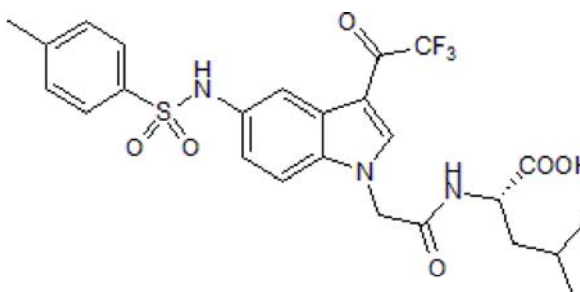
Batch Molecular Weight: 571.57

Physical Appearance: Cream solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.18 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.2% purity

Chiral HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -26.8 (Concentration = 0.62, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.54	4.94	7.35
Found	52.63	4.85	7.32

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Description:

Potent and selective non-peptide neurotensin (NTS) type-2 receptor antagonist (IC₅₀ = 38 nM). Exhibits >150-fold selectivity for NTS₂ over NTS₁.

Physical and Chemical Properties:

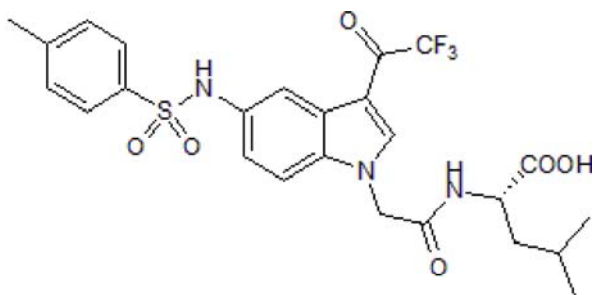
Batch Molecular Formula: C₂₅H₂₆F₃N₃O₆S.H₂O

Batch Molecular Weight: 571.57

Physical Appearance: Cream solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

Thomas *et al* (2014) Identification of *N*-[5-[[4-methylphenyl)sulfonyl]amino]-3-(trifluoroacetyl)-1*H*-indol-1-yl]acetyl]-*L*-leucine (NTRC-824), a neurotensin-like nonpeptide compound selective for the neurotensin receptor type 2. *J.Med.Chem.* **57** 7472. PMID: 25157640.

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