

Certificate of Analysis

Product Name: LU AA33810

Catalog No.: 3562

Batch No.: 2

CAS Number: 304008-29-5

IUPAC Name: *N*-[[*trans*-4-[(4,5-Dihydro[1]benzothiepi[5,4-*d*]thiazol-2-yl)amino]cyclohexyl]methyl]methanesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₂₅N₃O₂S₃·½H₂O

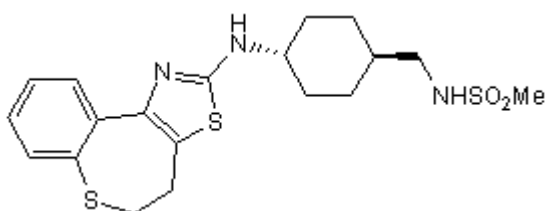
Batch Molecular Weight: 432.63

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.59 (Chloroform:Methanol [9:1])

HPLC: Shows 98.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.75	6.06	9.71
Found	52.89	5.8	9.7

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Description:

Potent neuropeptide Y (NPY) Y₅ receptor antagonist (K_i = 1.5 nM in vitro). Displays ≥ 3300-fold affinity for Y₅ over Y₁, Y₂ and Y₄ receptors. Also binds human 5-HT_{2B} and 5-HT_{1A} receptors (K_i values are 247 and 478 nM respectively). Exerts anxiolytic- and antidepressant-like effects in rat models of stress sensitivity.

Physical and Chemical Properties:

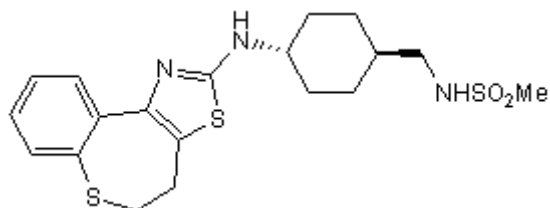
Batch Molecular Formula: C₁₉H₂₅N₃O₂S₃·½H₂O

Batch Molecular Weight: 432.63

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Walker et al (2009) The novel neuropeptide Y Y₅ receptor antagonist Lu AA33810 [*N*-[[*trans*-4-[(4,5-dihydro[1]benzothiepi[5,4-*d*]thiazol-2-yl)amino]cyclohexyl]methyl]-methanesulfonamide] exerts anxiolytic- and antidepressant-like effects in rat models of stress anxiety. *J.Pharmacol.Exp.Ther.* **328** 900. PMID: 19098165.

Storage: Store at RT

Solubility & Usage Info:

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.

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