

Product Name: LUF 5834

Catalog No.: 4603

Batch No.: 2

CAS Number: 333962-91-7

IUPAC Name: 2-Amino-4-(4-hydroxyphenyl)-6-[(1*H*-imidazol-2-ylmethyl)thio]-3,5-pyridinecarbonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₂N₆OS.0.2C₂H₅OH.¼H₂O

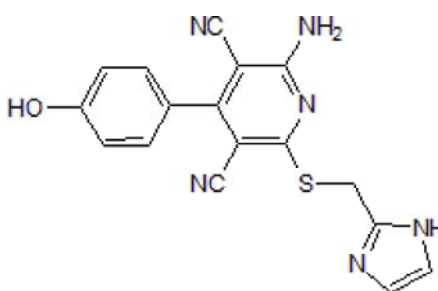
Batch Molecular Weight: 362.09

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.65 (Dichloromethane:Methanol:Ammonia soln. [80:19:1])

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.72	3.81	23.21
Found	57.89	3.74	23.22

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EC Number:

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Description:

LUF 5834 is a potent A_{2A} and A_{2B} adenosine receptor partial agonist (K_i = 2.6 nM and EC₅₀ = 12 nM respectively). Also exhibits selectivity for A₁ over A₃ (K_i values are 2.6 and 538 nM respectively).

Physical and Chemical Properties:

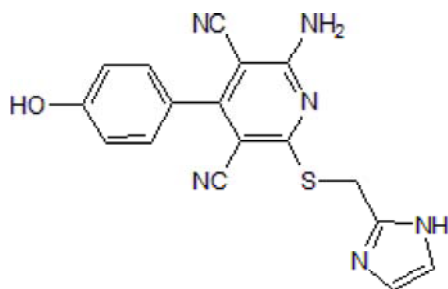
Batch Molecular Formula: C₁₇H₁₂N₆OS.0.2C₂H₅OH.¼H₂O

Batch Molecular Weight: 362.09

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

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.

References:

Lane *et al* (2012) A novel nonribose agonist, LUF5834, engages residues that are distinct from those of adenosine-like ligands to activate the adenosine A_{2a} receptor *Mol.Pharmacol.* **81** (3) 475. PMID: 22188926.

Beukers *et al* (2004) New, non-adenosine, high potency agonists for the human adenosine A_{2B} receptor with an improved selectivity profile compared to the reference agonist *N*-ethylcarboxamidoadenosine *J.Med.Chem* **47** (15) 3707. PMID: 15239649.

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