Certificate of Analysis

Product Name: **Lu AA 47070** **Catalog No.: 4783** **Batch No.: 1**

CAS Number: 913842-25-8

IUPAC Name: 4-[(3,3-Dimethyl-1-oxobutyl)amino]-3,5-difluoro-*N*-[3-[(phosphonooxy)methyl]-2(3*H*)-thiazolylidene]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{20}F_2N_3O_6PS.¾H_2O$

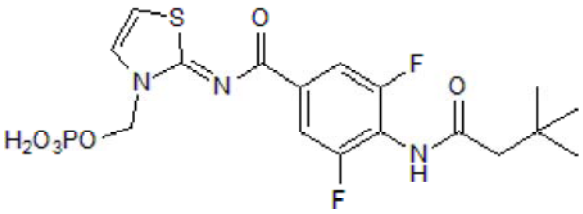
Batch Molecular Weight: 476.9

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.05 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	42.82	4.54	8.81
Found	42.78	4.48	8.85

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Product Information

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Description:

Prodrug of a potent and selective adenosine A_{2A} receptor antagonist (K_i values are 5.9, 260, 410 and <10,000 nM for A_{2A}, A_{2B}, A_1 and A_3 receptors respectively. Reverses parkinsonian motor impairment and motivational effects produced by dopamine D_2 receptor blockade in rats. Orally bioavailable.

Physical and Chemical Properties:

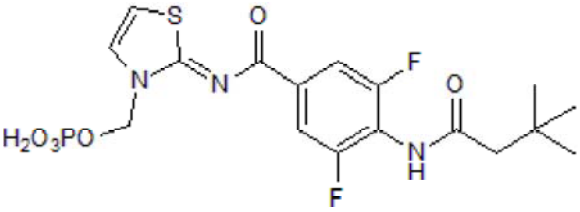
Batch Molecular Formula: $C_{17}H_{20}F_2N_3O_6PS.¾H_2O$

Batch Molecular Weight: 476.9

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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:

Collins *et al* (2012) The novel adenosine A_{2A} antagonist Lu AA47070 reverses the motor and motivational effects produced by DA D_2 receptor blockade. Pharmacol.Biochem.Behav. ***100*** 498. PMID: 22037410.

Sams *et al* (2011) Discovery of phosphoric acid mono-{2-[(*E/Z*)-4-(3,3-dimethyl-butyrylamino)-3,5-difluoro-benzoylimino]-thiazol-3-ylmethyl} ester (Lu AA47070): a phosphonooxymethylene prodrug of a potent and selective hA_{2A} receptor antagonist. J.Med.Chem. ***54*** 751. PMID: 21210664.

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