TOCRIS
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Print Date: Jun 6th 2019

Certificate of Analysis

www.tocris.com

Product Name: **UBP 310** **Catalog No.: 3621** **Batch No.: 4**

CAS Number: 902464-46-4

IUPAC Name: (*S*)-1-(2-Amino-2-carboxyethyl)-3-(2-carboxy-thiophene-3-yl-methyl)-5-methylpyrimidine-2,4-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{14}H_{15}N_3O_6S.¼H_2O$

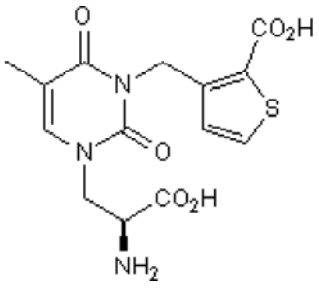
Batch Molecular Weight: 357.85

Physical Appearance: White solid

Solubility: DMSO to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (PAW/BuOH 2/3)

HPLC: Shows >99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -6.3 (Concentration = 0.35, Solvent = 6N HCl)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	46.99	4.37	11.74
Found	46.93	4.33	11.55

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Product Information

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Description:

GluK1 (formerly GLU_{K5}) kainate receptor antagonist (IC_{50} = 130 nM); also blocks recombinant homomeric GluK3 (forrmerly GLU_{K7}) receptors. Displays 12,700-fold selectivity for GluK1 (formerly GLU_{K5}) over GluK2 (formerly GLU_{K6}). Exhibits no activity at mGlu group I or NMDA receptors at concentrations of up to 10 µM. Apparent K_D value is 18 ± 4 nM for depression of kainate responses on the dorsal root. Please refer to IUPHAR Guide to Pharmacology for the most recent naming conventions. Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

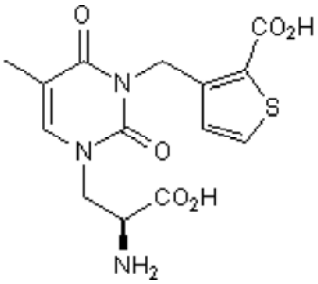
Batch Molecular Formula: $C_{14}H_{15}N_3O_6S.¼H_2O$

Batch Molecular Weight: 357.85

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 20 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:

Perrais *et al* (2009) Antagonism of recombinant and native GluK3-containing kainate receptors. Neuropharmacology ***56*** 131. PMID: 18761361.

Dolman *et al* (2007) Synthesis and pharmacological characterization of N^3-substituted willardiine derivatives: Role of the substituent at the 5-position of the uracil ring in development of highly potent and selective GLU_{K5} kainate receptor antagonists. J.Med.Chem. ***50*** 1558. PMID: 17348638.

Mayer *et al* (2006) Crystal structures of the kainate receptor GluR5 ligand binding core dimer with novel GluR5-selective antagonists. J.Neurosci. ***26*** 2852. PMID: 16540562.

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