TOCRIS
a bio-techne brand

Print Date: Jan 15th 2016

Certificate of Analysis

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Product Name: **A 841720** **Catalog No.: 3060** **Batch No.: 1**

CAS Number: 869802-58-4

IUPAC Name: 9-(Dimethylamino)-3-(hexahydro-1*H*-azepin-1-yl)pyrido[3',2':4,5]thieno[3,2-*d*]pyrimidin-4(3*H*)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{21}N_5OS$

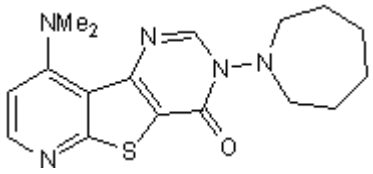
Batch Molecular Weight: 343.45

Physical Appearance: White solid

Solubility: DMSO to 50 mM
ethanol to 50 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Sulfur
Theoretical	53.75	5.84	18.43	8.44
Found	54.02	5.87	18.33	8.58

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Description:

Potent, non-competitive $mGlu_1$ receptor antagonist that displays 34-fold selectivity over $mGlu_5$ (IC_{50} values are 10 and 342 nM respectively). Displays no significant activity at a range of other GPCRs, ion channels and transporters. Exhibits analgesic effects; decreases mechanical allodynia in models of neuropathic pain. Also impairs cognitive function.

Physical and Chemical Properties:

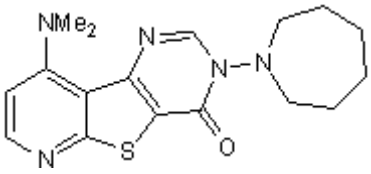
Batch Molecular Formula: $C_{17}H_{21}N_5OS$

Batch Molecular Weight: 343.45

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 50 mM
ethanol to 50 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:

Zheng *et al* (2005) Structure-activity relationship of triazafluorenone derivatives as potent and selective mGluR1 antagonists. J.Med.Chem. ***48*** 7374. PMID: 16279797.

El-Kouhen *et al* (2006) Blockade of mGluR1 receptor results in analgesia and disruption of motor and cognitive performances: effects of A-841720, a novel non-competitive mGluR1 receptor antagonist. Br.J.Pharmacol. ***149*** 761. PMID: 17016515.

More *et al* (2007) Comparison of the mGluR1 antagonist A-841720 in rats models of pain and cognition. Behav.Pharmacol. ***18*** 273. PMID: 17551319.