# Certificate of Analysis



**Product Name:** **UBP 302** **Catalog No.: 2079** **Batch No.: 6**

CAS Number: 745055-91-8

IUPAC Name: (*S*)-1-(2-Amino-2-carboxyethyl)-3-(2-carboxybenzyl)pyrimidine-2,4-dione

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{15}H_{15}N_3O_6.½H_2O$

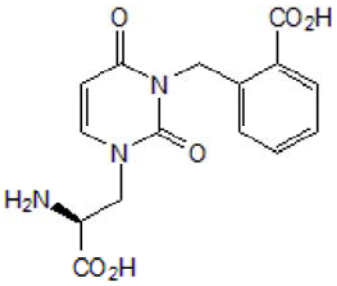
**Batch Molecular Weight:** 342.31

**Physical Appearance:** White solid

**Solubility:** 1eq. NaOH to 25 mM
DMSO to 20 mM with gentle warming

**Storage:** Store at RT

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.3 (2-Propanol:Acetic acid. [7:3])

**HPLC:** Shows 99.9% purity

**Chiral HPLC:** Shows 98.3% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** $[\alpha]_D$ = -13.2 (Concentration = 1, Solvent = 6N HCl)

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 52.63 | 4.71 | 12.28 |
| Found | 52.57 | 4.92 | 12.23 |



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**Description:**

Potent and selective GluK1 (formally GluR5)-subunit containing kainate receptor antagonist (apparent $K_D$ = 402 nM); active enantiomer of UBP 296 (Cat. No. 2078). Displays ~ 260-fold selectivity over AMPA receptors, ~ 90-fold selectivity over recombinant human GluK2 (formally GluR6) and GluK5 (formally KA2)-containing kainate receptors and has little or no action at NMDA or group I mGlu receptors. Selectively blocks kainate receptor-mediated LTP induction in rat hippocampal mossy fibers. Also protects against soman-induced seizures and neuronal degeneration for up to 30 days when administered one hour after soman exposure. Please refer to IU... Please see product datasheet on www.tocris.com for full description.

**Physical and Chemical Properties:**

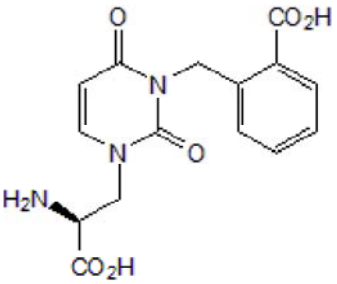
Batch Molecular Formula: $C_{15}H_{15}N_3O_6.½H_2O$

Batch Molecular Weight: 342.31

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Store at RT

**Solubility & Usage Info:**

1eq. NaOH to 25 mM
DMSO to 20 mM with gentle warming

Solubility analysis of this compound has determined that while this compound is soluble in 1eq. NaOH, it may decompose rapidly once in solution. Therefore we recommend that solutions that are made up in 1eq. NaOH are used as soon as possible on the day of preparation and are then discarded.

**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:**

**Apland** *et al* (2014) The Limitations of Diazepam as a Treatment for Nerve Agent-Induced Seizures and Neuropathology in Rats: Comparison with UBP302. J.Pharmacol.Exp.Ther. ***351*** 359. PMID: 25157087.

**Dolman** *et al* (2005) Synthesis and pharmacology of willardiine derivatives acting as antagonists of kainate receptors. J.Med.Chem. ***48*** 7867. PMID: 16302825.

**More** *et al* (2004) Characterisation of UBP296: a novel, potent and selective kainate receptor antagonist. Neuropharmacology ***47*** 46. PMID: 15165833.