

**Product Name:** (S)-HexylHIBO

**Catalog No.:** 1750

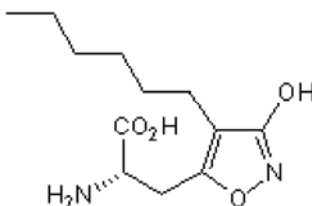
**Batch No.:** 1

CAS Number: 334887-48-8

IUPAC Name: (*αS*)-*α*-Amino-4-hexyl-2,3-dihydro-3-oxo-5-isoxazolepropanoic acid

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>12</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>·½H<sub>2</sub>O  
**Batch Molecular Weight:** 265.31  
**Physical Appearance:** Cream solid  
**Solubility:** 1eq. NaOH to 20 mM  
**Storage:** Store at RT  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.5 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])  
**Melting Point:** Between 219 - 222°C(dec)  
**Chiral HPLC:** Shows >99.8% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**<sup>13</sup>C NMR:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = +19 (Concentration = 0.2, Solvent = 1N HCl)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	54.33	7.98	10.56
Found	54.57	7.74	10.54

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

Group I mGlu receptor antagonist ( $K_b$  values are 30 and 61  $\mu$ M at mGlu<sub>1a</sub> and mGlu<sub>5a</sub> receptors respectively). Racemate also available.

**Physical and Chemical Properties:**

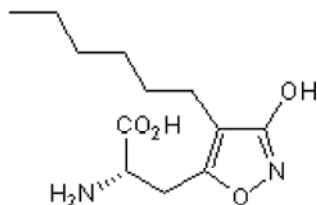
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Batch Molecular Weight: 265.31

Physical Appearance: Cream solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**Madsen *et al*** (2001) Synthesis and pharmacology of 3-isoxazolol amino acids as selective antagonists at group I metabotropic glutamic acid receptors *J.Med.Chem.* **44** 1051. PMID: 11297452.

**Storage:** Store at RT

**Solubility & Usage Info:**

1eq. NaOH 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.

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**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel:+1 612 379 2956