## **Product** Data Sheet

# (R)-1,2,3,4-Tetrahydro-3-isoquinolinecarboxylic acid

Cat. No.: HY-13987 CAS No.: 103733-65-9 Molecular Formula: C<sub>10</sub>H<sub>11</sub>NO<sub>2</sub> Molecular Weight: 177.2 Target: Others

Others Storage: Powder -20°C 3 years

2 years

In solvent -80°C 2 years

> 1 year -20°C

### **SOLVENT & SOLUBILITY**

In Vitro

Pathway:

H<sub>2</sub>O: 1 mg/mL (5.64 mM; ultrasonic and warming and heat to 60°C) DMSO: < 1 mg/mL (ultrasonic; warming; heat to 60°C) (insoluble or slightly soluble)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	5.6433 mL	28.2167 mL	56.4334 mL
	5 mM	1.1287 mL	5.6433 mL	11.2867 mL
	10 mM			

Please refer to the solubility information to select the appropriate solvent.

### **BIOLOGICAL ACTIVITY**

Description

(R)-1,2,3,4-Tetrahydro-3-isoquinolinecarboxylic acid is a constrained Phe analogue which can fold into a beta-bend and a helical structure, and to adopt a preferred side-chain disposition in the peptide.IC50 value:Target: Three Tic-containing (Tic = 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid) model peptides were synthesized to assess the tendency of this constrained Phe analogue to fold into a beta-bend and a helical structure, and to adopt a preferred side-chain disposition. The results of the solution conformational analysis, performed by using Fourier transform infrared absorption and 1H nuclear magnetic resonance, indicate that in chloroform the -Aib-D-Tic-Aib-, -(Aib)2-D-Tic-(Aib)2-, and -L-Pro-D-Ticsequences fold into intramolecularly H-bonded forms to a great extent. An X-ray diffraction analysis on p-BrBz-(Aib)2-DL-Tic-(Aib)2-OMe monohydrate and p-BrBz-L-Pro-D-Tic-NHMe allows us to conclude that, while the pentapeptide methylester forms an incipient (distorted) 3(10)-helix, the dipeptide methylamide adopts a type-II beta-bend conformation. In both cases, the D-Tic side-chain conformation is D, gauche(-). The implications for the use of the Tic residue in designing conformationally restricted analogues of bioactive peptides are briefly discussed.

#### **REFERENCES**



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