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

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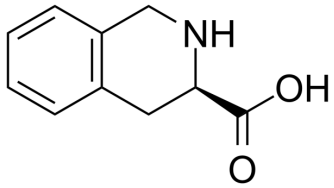
|---|---|
| **Cat. No.:** | HY-13987 |
| **CAS No.:** | 103733-65-9 |
| **Molecular Formula:** | $C_{10}H_{11}NO_2$ |
| **Molecular Weight:** | 177.2 |
| **Target:** | Others |
| **Pathway:** | Others |
| **Storage:** | Powder -20°C 3 years<br>4°C 2 years<br>In solvent -80°C 2 years<br>-20°C 1 year |




## SOLVENT & SOLUBILITY

**In Vitro**

$H_2O$ : 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 | Mass / Solvent / 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-Tic- sequences 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

[1]. Valle G, et al. Constrained phenylalanine analogues. Preferred conformation of the 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid (Tic) residue. Int J Pept Protein Res. 1992 Sep-Oct;40(3-4):222-32.



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