

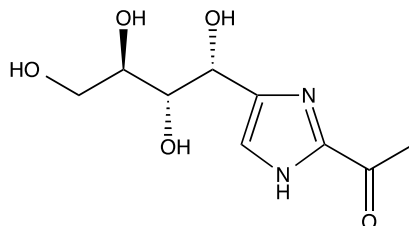
Catalog #10-2477

THI

CAS# 94944-70-4

2-Acetyl-4-tetrahydroxybutyl Imidazole; 1-[5-[(1R,2S,3R)-1,2,3,4-tetrahydroxybutyl]-1H-imidazol-2-yl]-ethanone

Lot # X106422



THI was identified as a biologically active impurity in caramel food coloring.¹ It is a potent inhibitor of sphingosine-1-phosphate (S1P) lyase.² It disrupts lymphocyte egress from lymphoid tissue by interfering with S1P gradients.^{3,4} The novel immunomodulatory activity of THI and its biochemical mechanism may represent a new target for the development of new generation of immunosuppressants.⁵

- 1) MacKenzie *et al.* (1992), *Toxicity Studies of Caramel Colour III and 2-Acetyl-4(5)-Tetrahydroxybutylimidazole in F344 rats*; Food Chem.Toxicol. **30** 417
- 2) Ohtoyo *et al.* (2015), *Sphingosine 1-phosphate lyase inhibition by 2-acetyl-4-(tetrahydroxybutyl)imidazole (THI) under conditions of vitamin B6 deficiency*; Mol.Cell Biochem. **400** 125
- 3) Gugasyan *et al.* (1998), *Emigration of mature T cells from the thymus is inhibited by the imidazole-based compound 2-acetyl-4-tetrahydroxybutylimidazole*; Immunology **93** 398
- 4) Schwab *et al.* (2005), *Lymphocyte sequestration through S1P lyase inhibition and disruption of S1P gradients*; Science **309** 1735
- 5) Bradbury *et al.* (1997), *The immunomodulatory compound 2-acetyl-4-tetrahydroxybutyl imidazole causes sequestration of lymphocytes in non-lymphoid tissue*; Immunol.Cell Biol. **75** 497

PHYSICAL DATA

Molecular Weight:	230.22
Molecular Formula:	C ₉ H ₁₄ N ₂ O ₅
Purity:	>98% (TLC)
	NMR: (Conforms)
Solubility:	Water (10 mg/mL)
Physical Description:	White solid
Storage and Stability:	Store as supplied at -20°C for up to 1 year from the date of purchase. Solutions in distilled water may be stored at -20°C for up to 3 months.

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