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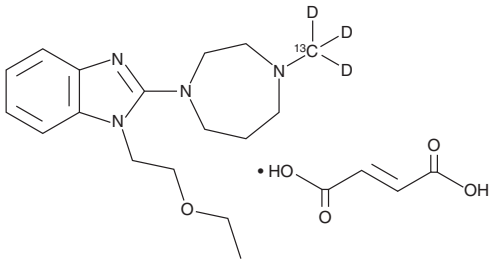
PRODUCT INFORMATION

Emedastine-^{13}C-d$_3$ (fumarate)

Item No. 33378

Formal Name: 1-(2-ethoxyethyl)-2-(hexahydro-4-methyl-^{13}C-d$_3$-1H-1,4-diazepin-1-yl)-1H-benzimidazole, 2E-butenedioate
MF: $C_{16}[^{13}C]H_{23}D_3N_4O \bullet C_4H_4O_4$
FW: 422.5
Chemical Purity: ≥95% (Emedastine)
Deuterium Incorporation: ≥99% deuterated forms (d$_1$-d$_3$); ≤1% d$_0$
Supplied as: A solid
Storage: -20°C
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Emedastine-^{13}C-d$_3$ (fumarate) is intended for use as an internal standard for the quantification of emedastine (Item No. 23946) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated *versus* unlabeled).

Emedastine-^{13}C-d$_3$ (fumarate) is supplied as a solid. A stock solution may be made by dissolving the emedastine-^{13}C-d$_3$ (fumarate) in the solvent of choice, which should be purged with an inert gas. Emedastine-^{13}C-d$_3$ (fumarate) is soluble in organic solvents such as methanol, DMSO, and acetonitrile.

Description

Emedastine is a histamine H$_1$ receptor antagonist (K$_i$ = 1.3 nM).[1] It is selective for histamine H$_1$ over H$_2$ and H$_3$ receptors (K$_i$s = 49 and 12.43 µM, respectively), as well as α$_1$-, α$_2$-, and β$_1$-adrenergic and dopamine D$_1$ and D$_2$ receptors, and the serotonin (5-HT) receptor subtypes 5-HT$_1$ and 5-HT$_2$ at 10 µM.[1,2] Emedastine inhibits histamine-induced phosphoinositide turnover and intracellular calcium mobilization in primary human conjunctival epithelial cells (HCECs; IC$_{50}$s = 1.6 and 2.9 nM, respectively).[3] It also inhibits histamine-stimulated secretion of IL-6, IL-8, and GM-CSF by primary HCECs (IC$_{50}$s = 2.23, 3.42, and 1.50 nM, respectively).[4] Ocular application of emedastine prior to histamine challenge inhibits vascular permeability in guinea pigs.[2] Formulations containing emedastine have been used in the treatment of allergic conjunctivitis.

References

1. Sharif, N.A., Su, S.X., and Yanni, J.M. Emedastine: A potent, high affinity histamine H$_1$-receptor-selective antagonist for ocular use: Receptor binding and second messenger studies. *J. Ocul. Pharmacol.* **10(4)**, 653-664 (1994).
2. Yanni, J.M., Stephens, D.J., Parnell, D.W., *et al.* Preclinical efficacy of emedastine, a potent, selective histamine H$_1$ antagonist for topical ocular use. *J. Ocul. Pharmacol.* **10(4)**, 665-675 (1994).
3. Sharif, N.A., Xu, S.X., Magnino, P.E., *et al.* Human conjunctival epithelial cells express histamine-1 receptors coupled to phosphoinositide turnover and intracellular calcium mobilization: Role in ocular allergic and inflammatory diseases. *Exp. Eye Res.* **63(2)**, 169-178 (1996).
4. Weimer, L.K., Gamache, D.A., and Yanni, J.M. Histamine-stimulated cytokine secretion from human conjunctival epithelial cells: Inhibition by the histamine H$_1$ antagonist emedastine. *Int. Arch. Allergy. Immunol.* **115(4)**, 288-293 (1998).

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