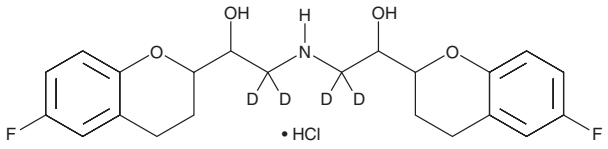
PRODUCT INFORMATION

(±)-Nebivolol-d_4 (hydrochloride)

Item No. 26659

CAS Registry No.: 2701283-32-9
Formal Name: 2,2'-azanediylbis(1-(6-fluorochroman-2-yl) ethan-2,2-d_2-1-ol), monohydrochloride
MF: $C_{22}H_{21}D_4F_2NO_4$ • HCl
FW: 445.9
Chemical Purity: ≥98% (mixture of diastereomers; Nebivolol)
Deuterium Incorporation: ≥99% deuterated forms (d_1-d_4); ≤1% d_0
Supplied as: A solid
Storage: -20°C
Stability: ≥4 years



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

Laboratory Procedures

(±)-Nebivolol-d_4 (hydrochloride) is intended for use as an internal standard for the quantification of nebivolol (Item No. 23660) 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).

(±)-Nebivolol-d_4 (hydrochloride) is supplied as a solid. A stock solution may be made by dissolving the (±)-nebivolol-d_4 (hydrochloride) in the solvent of choice, which should be purged with an inert gas. (±)-Nebivolol-d_4 (hydrochloride) is soluble in DMSO.

Description

(±)-Nebivolol-d_4 is intended for use as an internal standard for the quantification of nebivolol (Item No. 23660) by GC- or LC-MS. Nebivolol is an antagonist of the β_1-adrenergic receptor (β_1-AR; IC_{50} = 7.41 nM).[1] It is selective for β_1- over β_2-ARs (IC_{50} = 251 nM), as well as the serotonin (5-HT) receptor subtypes 5-HT_{1A} and 5-HT_2 and the α_1- and α_2-adrenergic, histamine H_1, and dopamine D_2 receptors (IC_{50}s = 27.5, 2,239, 3,162, >10,000, 5,623, and 10,000 nM, respectively). Nebivolol induces vasodilation in isolated mouse renal arteries (EC_{50} = 11.36 µM) and decreases contraction of isolated human left ventricular trabeculae induced by isoproterenol (Item No. 15592; IC_{50} = 7 µM).[2,3] Nebivolol inhibits proliferation of primary human coronary artery smooth muscle cells (HCASMCs) in the presence and absence of growth factors (IC_{50}s = 6.1, 6.8, 6.4, and 7.7 µM for HCASMCs grown in media containing no growth factor, PDGF-BB, basic FGF, and TGF-β1, respectively).[4] It is also an inhibitor of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) main protease (M^{pro}), also known as 3C-like protease ($3CL^{pro}$; IC_{50} = 60.2 µg/ml), and inhibits SARS-CoV-2 pathogenicity *in vitro* (IC_{50} = 0.03 µg/ml).[5] Formulations containing nebivolol have been used in the treatment of hypertension.

References

1. Pauwels, P.J., Gommeren, W., Van Lommen, G., *et al. Mol. Pharmacol.* **34(6)**, 843-851 (1988).
2. Georgescu, A., Pluteanu, F., Flonta, M.L., *et al. Pharmacology* **81(2)**, 110-117 (2008).
3. Brixius, K., Bundkirchen, A., Bölck, B., *et al. Br. J. Pharmacol.* **133(8)**, 1330-1338 (2001).
4. Brehm, B.R., Wolf, S.C., Bertsch, D., *et al. Cardiovasc. Res.* **49(2)**, 430-439 (2001).
5. Hamed, M.I.A., Darwish, K.M., Soltane, R., *et al. RSC Adv.* **11(56)**, 35536-35558 (2021).

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