

Product Data Sheet

Product Name: TD-5471 hydrochloride

Cat. No.: GC31453

Chemical Properties

Cas. No. 530084-35-6

SMILES O=C1NC2=C(C([C@@H](O)CNCCC3=CC=C(NC4=CC(C5=CC=CC=C5)=C(OC)C=C4)C=C3)=CC=C2O)C=C1.[H]Cl

Formula $C_{32}H_{32}ClN_3O_4$ M.Wt 558.07

Solubility Soluble in DMSO Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure

Background

TD-5471 hydrochloride is a potent and selective full agonist of the human β_2 -adrenoceptor.

TD-5471 is potent, with slow onset in an in vitro guinea pig trachea model. TD-5471 has potency with pEC₅₀ of 8.7 in the guinea pig tracheal ring assay. TD-5471 is structurally differentiated from Milveterol and its long duration of action is consistent with a correlation with hydrophobicity observed in other long-acting β_2 -agonist discovery programs[1].

TD-5471 shows a dose-dependent and long duration of action in an in vivo guinea pig model of bronchoprotection. In a guinea pig model of in vivo bronchoprotection, TD-5471 shows excellent potency (measured 1.5 h after nebulized dosing). Because a high dose of Salmeterol (300 μ g/mL) provides bronchoprotection lasting \geq 24 h in this model, a 72 h time point is selected to provide confidence that TD-5471 will be suitable for once-daily dosing in man. TD-5471-mediated bronchoprotection at 72 h is dose-dependent and is significantly greater than that of Salmeterol at nebulizer concentrations of \geq 30 μ g/mL[1].

[1]. Jacobsen JR, et al. Multivalent design of long-acting $\beta(2)$ -adrenoceptor agonists incorporating biaryl amines. Bioorg Med Chem Lett. 2014 Jun 15;24(12):2625-30.

Caution: Product has not been fully validated for medical applications. For research use only.

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