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## Product Data Sheet

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Product Name: BX 513 hydrochloride

Cat. No.: GC13299

### Chemical Properties

Cas. No. 1216540-18-9

Chemical Name 5-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)-2,2-diphenylpentanenitrile hydrochloride

SMILES C1C=CC=C(C(CC2)(O)CCN2CCCC(C3=CC=CC=C3)(C4=CC=CC=C4)C#N)C=C1.Cl

Formula  $C_{28}H_{29}ClN_2O.HCl$  M.Wt 481.46

Solubility <48.15mg/ml in DMSO; <24.07mg/ml in ethanol 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

Ligands for the CCR1 receptor (MIP-1 $\alpha$  and RANTES) have been implicated in plenty of chronic inflammatory diseases, most notably multiple sclerosis and rheumatoid arthritis. BX 513 is a novel non-peptide CCR1 receptor antagonists.

In vitro: BX 513 has been shown to have at least 200-fold selectivity for CCR1 inhibition over other human 7-TM receptors, including other chemokine receptors. In addition, data obtained from in-vitro functional assays demonstrated the functional antagonism of BX 513 and structurally related analogues against the CCR1 receptor in a dose-dependent manner [1]. BX 513 also showed concentration-dependent inhibition of MIP-1 $\alpha$ -induced extracellular acidification and Ca<sup>2+</sup> mobilization demonstrating functional antagonism. When given alone, the compound did not elicit any responses, suggesting the absence of intrinsic agonist activity. BX 513 inhibited MIP-1 $\alpha$ - and RANTES-induced migration in peripheral blood cells in a dose-responsive manner. Selectivity testing against a panel of

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

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7 transmembrane domain receptors indicated that BX 513 is inactive on a number of receptors at concentrations up to 10  $\mu$ M [2].

In vivo: Currently, there is no animal in-vivo data available.

Clinical trial: Up to now, BX 513 is still in the preclinical development stage.

### Reference:

[1] Ng HP, May K, Bauman JG, Ghannam A, Islam I, Liang M, Horuk R, Hesselgesser J, Snider RM, Perez HD, Morrissey MM. Discovery of novel non-peptide CCR1 receptor antagonists. J Med Chem. 1999 Nov 4;42(22):4680-94.

[2] Hesselgesser J, Ng HP, Liang M, Zheng W, May K, Bauman JG, Monahan S, Islam I, Wei GP, Ghannam A, Taub DD, Rosser M, Snider RM, Morrissey MM, Perez HD, Horuk R. Identification and characterization of small molecule functional antagonists of the CCR1 chemokine receptor. J Biol Chem. 1998 Jun 19;273(25):15687-92.

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