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Print Date: Jan 13th 2016

Certificate of Analysis

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Product Name: **BMS 182874 hydrochloride** **Catalog No.: 1441** **Batch No.: 2**

CAS Number: 1215703-04-0

IUPAC Name: 5-(Dimethylamino)-*N*-(3,4-dimethyl-5-isoxazolyl)-1-naphthalenesulfonamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{19}N_3O_3S.HCl$

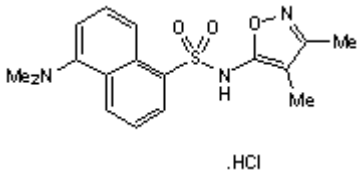
Batch Molecular Weight: 381.88

Physical Appearance: White crystalline solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Dichloromethane:Methanol:Ammonia soln. [85:15:5])

Melting Point: Between 195 - 200°C(Dec)

HPLC: Shows >98.9% purity

^{1}H NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	
Theoretical	53.47	5.28	11	0 0 0
Found	53.47	5.28	10.84	0 0 0

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Description:

Potent, selective and competitive non-peptide endothelin ET_A receptor antagonist (K_i = 48 nM). Displays > 1000-fold selectivity over ET_B receptors. Inhibits ET-1-induced pressor response following oral or intravenous administration in vivo. Inhibits ET-1-induced longitudinal muscle contraction in the mouse colon in vitro.

Physical and Chemical Properties:

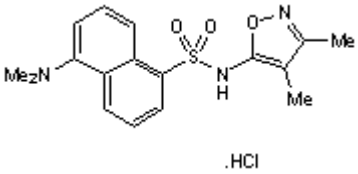
Batch Molecular Formula: $C_{17}H_{19}N_3O_3S.HCl$

Batch Molecular Weight: 381.88

Physical Appearance: White crystalline solid

Minimum Purity: >98%

Batch Molecular Structure:



.HCl

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Stein *et al* (1994) The discovery of sulfonamide endothelin antagonists and the development of the orally active ETA antagonist 5-(Dimethylamino)-*N*-(3,4-dimethyl-5-isoazolyl)-1-naphthalenesulfonamide. J.Med.Chem. ***37*** 329. PMID: 8308857.

Webb *et al* (1995) BMS-182874 is a selective, nonpeptide endothelin ET_A receptor antagonist. J.Pharmacol.Exp.Ther. ***272*** 1124. PMID: 7891325.

Khan *et al* (2006) Pharmacological characterization of endothelin receptors-mediated contraction in the mouse isolated proximal and distal colon. Br.J.Pharmacol. ***147*** 607. PMID: 16432510.

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