

Certificate of Analysis

Print Date: Jan 13th 2016 **WWW.tocris.com**

Product Name: RS 79948 hydrochloride Catalog No.: 0987 Batch No.: 2

CAS Number: 186002-54-0

IUPAC Name: (8aR,12aS,13aS)-5,8,8a,9,10,11,12,12a,13,13a-dechydro-3-methoxy-12-(ethylsulfonyl)-6*H*-isoquino[2,1-*g*][1,6]

naphthyridine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{28}N_2O_3S.HCl.\frac{1}{2}H_2O_3$

Batch Molecular Weight: 409.97

Physical Appearance: White solid

Solubility: water to 25 mM

DMSO to 50 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.47$ (Chloroform:Methanol:Ammonia soln. [95:4.5:0.5])

HPLC: Shows 99.5% purity
Chiral HPLC: Shows 99.2% purity

1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = +19.5$ (Concentration = 0.4, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.66 7.38 6.83 Found 55.78 7.27 6.87



Product Information

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naphthyridine hydrochloride

Description:

 α_2 -adrenoreceptor antagonist (K_d values are; 0.18, 0.19 and 0.42 nM for α_{2B} α_{2C} and α_{2A} , respectively in rat).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{19}H_{28}N_2O_3S.HCI.1/2H_2O$

Batch Molecular Weight: 409.97 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

water to 25 mM DMSO to 50 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:

Clark et al (1989) $(8a\alpha,12a\alpha,13a\alpha)$ -5,8,8a,9,10,11,12,12a,13,13a-Decahydro-3-methoxy-12-(ethylsulphonyl)-6H-isoquino[2,1-g][1,6]-naphthyridine, a potent and highly selective α_2 -adrenoceptor antagonist. J. Med. Chem. **32** 2034. PMID: 2570150.

Hume et al (1996) Evaluation in rat of RS-79948-197 as a potential PET ligand for central α_2 -adrenoceptors. Eur.J.Pharmacol. **317** 67. PMID: 8982721.

Uhlen *et al* (1998) [3 H]RS79948-197 binding to rat, guinea pig and pig α_{2A} -, α_{2B} and α_{2C} -adrenoceptors. Comparison with MK912, RX821002, rauwolscine and yohimbine. Eur. J. Pharmacol. **343** 93. PMID: 9551719.