

## Certificate of Analysis

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**Product Name:** RWJ 52353

**Catalog No.:** 3935

**Batch No.:** 1

CAS Number: 245744-10-9

IUPAC Name: 5-(6,7-Dihydrobenzo[*b*]thien-4-yl-1*H*-imidazole hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>11</sub>H<sub>10</sub>N<sub>2</sub>S·¼H<sub>2</sub>O

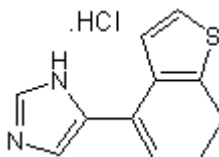
**Batch Molecular Weight:** 206.78

**Physical Appearance:** Yellow solid

**Solubility:** DMSO to 50 mM  
ethanol to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.18 (Dichloromethane:Methanol [92:8])

**HPLC:** Shows 98.2% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	54.32	4.77	11.52
Found	54.18	4.48	11.34

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**Description:**

Agonist of the  $\alpha_{2D}$  adrenergic receptor ( $K_i$  values are 1.5, 254, 443 and 621 nM for  $\alpha_{2D}$ ,  $\alpha_{2A}$ ,  $\alpha_1$  and  $\alpha_{2B}$  adrenergic receptors respectively).

**Physical and Chemical Properties:**

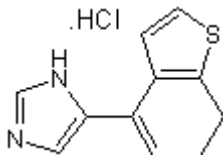
Batch Molecular Formula:  $C_{11}H_{10}N_2S \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 206.78

Physical Appearance: Yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 50 mM

ethanol 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:**

**Ross et al** (2000)  $\alpha_2$  adrenoceptor agonists as potential analgesic agents. 2. Discovery of 4-(4-imidazo)-1,3-dimethyl-6,7-dihydrothianaphthene as a high-affinity ligand for the  $\alpha_{2D}$  adrenergic receptor. *J.Med.Chem.* **43** 765. PMID: 10753480.

**Amphoux et al** (2010) Inhibitory and facilitatory actions of isocyanine derivatives at human and rat organic cation transporters 1, 2 and 3: a comparison to human  $\alpha_1$ - and  $\alpha_2$ -adrenoceptor subtypes. *Eur.J.Pharmacol.* **634** 1. PMID: 20170649.

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