

Certificate of Analysis

Print Date: Nov 25th 2019

www.tocris.com

Product Name: Mirabegron Catalog No.: 7070 Batch No.: 1

CAS Number: 223673-61-8

IUPAC Name: 2-Amino-*N*-[4-[2-[[(2*R*)-2-hydroxy-2-phenylethyl]amino]ethyl]phenyl]-4-thiazoleacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{24}N_4O_2S$

Batch Molecular Weight: 396.51

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = -22$ (Concentration = 0.5, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 63.61 6.1 14.13 Found 63.44 6.11 14.17



Product Information

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Description:

Potent and selective β_3 -adrenoceptor agonist (EC $_{50}$ = 22.4 nM). Displays >440-fold selectivity for β_3 over β_1 and β_2 adrenoceptors. Increases cAMP concentration in CHO cells expressing human β_3 -adrenoceptor. Displays relaxant effect in ex vivo rat bladder muscle preparation precontracted with carbachol (Cat. No. 2810). Decreases frequency of bladder contraction in rats. Also promotes browning of white adipose tissue, reduces body weight, and improves glucose tolerance and insulin sensitivity in mice fed a high fat diet. Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₂₄N₄O₂S Batch Molecular Weight: 396.51 Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:

NH2

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM ethanol to 20 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:

Hao et al (2019) Beneficial metabolic effects of mirabegron in vitro and in high-fat diet-induced obese mice. J.Pharmacol.Exp.Ther. **369** 419. PMID: 30940691.

Sui et al (2019) Bladder drug mirabegron exacerbates atherosclerosis through activation of brown fat-mediated lipolysis. Proc.Natl.Acad.Sci.U.S.A. **116** 10937. PMID: 31085638.

Takasu et al (2007) Effect of (R)-2-(2-aminothiazol-4-yl)-4'-{2-[(2-hydroxy-2-phenylethyl)amino]ethyl} acetanilide (YM178), a novel selective β_3 -adrenoceptor agonist, on bladder function. J.Pharmacol.Exp.Ther. **321** 642. PMID: 17293563.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use