

Certificate of Analysis

Product Name: WAY 200070

Catalog No.: 3366

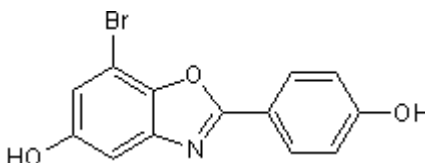
Batch No.: 1

CAS Number: 440122-66-7

IUPAC Name: 7-Bromo-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₈BrNO₃
Batch Molecular Weight: 306.11
Physical Appearance: Beige solid
Solubility: DMSO to 100 mM
ethanol to 50 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.01	2.63	4.58
Found	51.25	2.58	4.55

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

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IUPAC Name: 7-Bromo-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol

Description:

Selective ER β receptor agonist that displays 68-fold selectivity over ER α (EC₅₀ values are 2 and 155 nM for ER β and ER α respectively). Displays anxiolytic and antidepressive effects in vivo.

Physical and Chemical Properties:

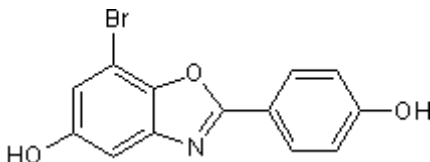
Batch Molecular Formula: C₁₃H₈BrNO₃

Batch Molecular Weight: 306.11

Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Malamas et al (2004) Design and synthesis of aryl diphenolic azoles as potent and selective estrogen receptor- β ligands. *J. Med. Chem.* **47** 5021. PMID: 15456246.

Hughes et al (2008) WAY-200070, a selective agonist of estrogen receptor beta as a potential novel anxiolytic/antidepressant agent. *Neuropharmacology* **54** 1136. PMID: 18423777.

Clipperton et al (2008) Differential effects of estrogen receptor alpha and beta specific agonists on social learning of food preferences in female mice. *Neuropsychopharmacology* **33** 2362. PMID: 18004284.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 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.

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