

Certificate of Analysis

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Product Name: FERb 033

Catalog No.: 3523

Batch No.: 1

CAS Number: 1111084-78-6

IUPAC Name: 2-Chloro-3'-fluoro-3,4'-dihydroxy-[1,1'-biphenyl]-4-carboxaldehyde oxime

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₉ClFNO₃·½H₂O

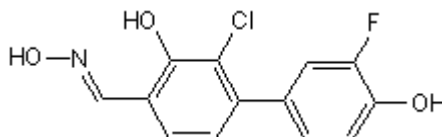
Batch Molecular Weight: 290.68

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 53.72 3.47 4.78

Found 53.74 3.18 4.78

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

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Description:

Potent and selective ER β receptor agonist (K_i = 7.1 nM, EC_{50} = 4.8 nM). Displays 62-fold selectivity over ER α .

Physical and Chemical Properties:

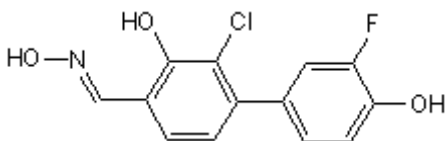
Batch Molecular Formula: C₁₃H₉ClFNO₃. $\frac{1}{2}$ H₂O

Batch Molecular Weight: 290.68

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

Minutolo et al (2009) Structural evolutions of salicylaldoximes as selective agonists for estrogen receptor β . *J.Med.Chem.* **52** 858. PMID: 19128016.

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