Product Name: SR 2211
Catalog No.: 4869
Batch No.: 2
CAS Number: 1359164-11-6
IUPAC Name: 2-Fluoro-4’-[4-(4-pyridinylmethyl)-1-piperazinyl]methyl]-a,a-bis(trifluoromethyl)-[1,1’-biphenyl]-4-methanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{26}\text{H}_{24}\text{F}_{7}\text{N}_{3}\text{O} \)
Batch Molecular Weight: 527.48
Physical Appearance: Off White solid
Solubility:
- DMSO to 100 mM
- 1eq. HCl to 50 mM
Storage:
- Store at -20°C

2. ANALYTICAL DATA

TLC:
- \( R_f = 0.42 \) (Chloroform:Methanol [9:1])
HPLC:
- Shows 99.9% purity
\(^1\text{H NMR:}\)
- Consistent with structure
Mass Spectrum:
- Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
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<tr>
<td>Carbon</td>
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<tr>
<td>Hydrogen</td>
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<td>Nitrogen</td>
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Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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Catalog No.: 4869 Batch No.: 2

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Description:
Selective inverse agonist of retinoic acid receptor-related orphan receptor γ (RORγ) (Kᵢ = 105 nM; IC₅₀ ~320 nM). Exhibits weak activity at liver X receptor α (LXRα); does not affect the transcriptional activity of farnesoid X receptors (FXR), and has no impact on the transcriptional activity of RORα.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₀H₂₂F₇N₄O
Batch Molecular Weight: 527.48
Physical Appearance: Off White solid
Minimum Purity: >98%

Storage: Store at -20°C

Solubility & Usage Info:
DMSO to 100 mM
1eq. HCl 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: