

**Product Name:** XCT 790

**Catalog No.:** 3928

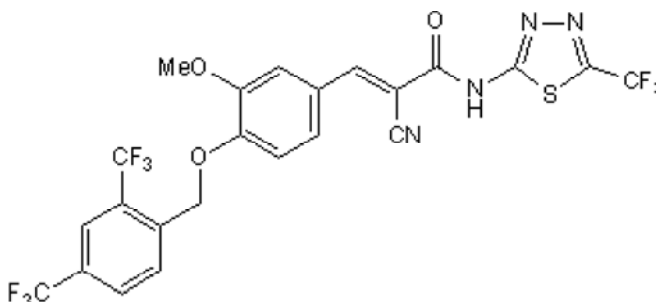
**Batch No.:** 1

CAS Number: 725247-18-7

IUPAC Name: 3-[4-(2,4-Bis-trifluoromethylbenzyloxy)-3-methoxyphenyl]-2-cyano-N-(5-trifluoromethyl-1,3,4-thiadiazol-2-yl)acrylamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>23</sub>H<sub>13</sub>F<sub>9</sub>N<sub>4</sub>O<sub>3</sub>S  
**Batch Molecular Weight:** 596.42  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 10 mM with gentle warming  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.36 (Chloroform:Methanol [9:1])  
**HPLC:** Shows 99% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	46.32	2.2	9.39
Found	46.39	2.17	9.4

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

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**Description:**

XCT 790 is a selective ERR $\alpha$  inverse agonist (IC<sub>50</sub> = ~400 nM). Displays no antagonist activity at ERR $\gamma$  or ER $\alpha$  at concentrations below 10  $\mu$ M. Interferes with PPAR $\gamma$  coactivator-1 $\alpha$  (PGC-1 $\alpha$ )/ERR $\alpha$ -dependent signaling; inhibits PGC-1 $\alpha$  induction of ERR $\alpha$  and MAO-B gene expression and downregulates the constitutive transcriptional activity of ERR $\alpha$  in numerous cell lines.

**Physical and Chemical Properties:**

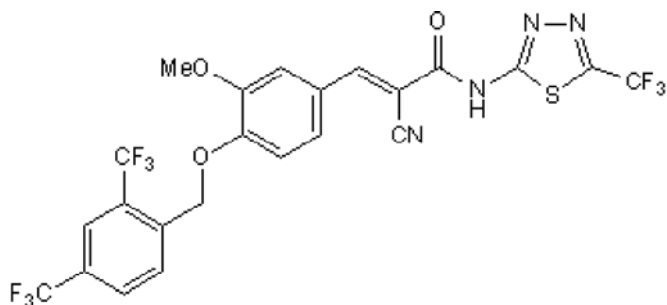
Batch Molecular Formula: C<sub>23</sub>H<sub>13</sub>F<sub>9</sub>N<sub>4</sub>O<sub>3</sub>S

Batch Molecular Weight: 596.42

Physical Appearance: Yellow solid

**Minimum Purity:**  $\geq$ 99%

**Batch Molecular Structure:**



**References:**

**Theodoris et al** (2021) Network-based screen in iPSC-derived cells reveals therapeutic candidate for heart valve disease. *Science*. **371**. PMID: 33303684.

**Kong et al** (2009) Peroxisome proliferator-activated receptor  $\gamma$  coactivator-1 $\alpha$  enhances antiproliferative activity of 5'-deoxy-5-fluorouridine in cancer cells through induction of uridine phosphorylase. *Mol.Pharmacol.* **76** 854. PMID: 19602572.

**Lanvin et al** (2007) Potentiation of ICI182,780 (Fulvestrant)-induced estrogen receptor- $\alpha$  degradation by the estrogen receptor-related receptor- $\alpha$  inverse agonist XCT790. *J.Biol.Chem.* **282** 28328. PMID: 17631492.

**Storage:** Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

DMSO to 10 mM with gentle warming

**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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