

**Product Name:** XY 018

**Catalog No.:** 6223

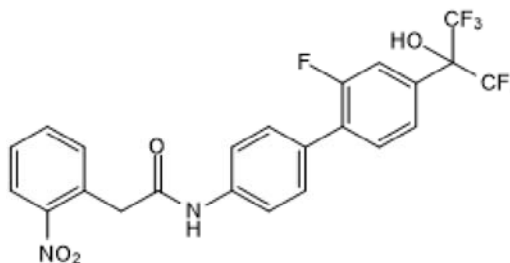
**Batch No.:** 1

CAS Number: 1873358-87-2

IUPAC Name: *N*-[2'-Fluoro-4'-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl][1,1'biphenyl]-4-yl]-2-nitrobenzeneacetamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>23</sub>H<sub>15</sub>F<sub>7</sub>N<sub>2</sub>O<sub>4</sub>  
**Batch Molecular Weight:** 516.36  
**Physical Appearance:** Off White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.21 (30% Ethyl acetate:Petroleum ether )  
**HPLC:** Shows 99.5% purity  
<sup>1</sup>H NMR: Consistent with structure  
 Mass Spectrum: Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	53.5	2.93	5.43
Found	53.67	2.79	5.51

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

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**Description:**

ROR $\gamma$  antagonist (EC<sub>50</sub> = 190 nM). Suppresses androgen receptor expression in prostate cancer cell lines. Also inhibits growth of tumors in androgen receptor-positive xenograft models.

**Physical and Chemical Properties:**

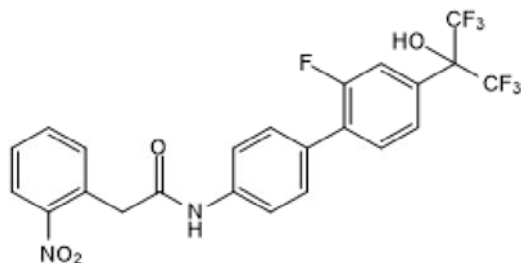
Batch Molecular Formula: C<sub>23</sub>H<sub>15</sub>F<sub>7</sub>N<sub>2</sub>O<sub>4</sub>

Batch Molecular Weight: 516.36

Physical Appearance: Off White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°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:**

**Ndagi *et al*** (2016) Re-emergence of an orphan therapeutic target for the treatment of resistant prostate cancer - a through conformational and binding analysis for ROR $\gamma$  protein. *J.Biomol.Struct.Dyn.* **36** 1.

**Wang *et al*** (2016) ROR- $\gamma$  drives androgen receptor expression and represents a therapeutic target in castration-resistant prostate cancer. *Nat.Med.* **22** 488. PMID: 27019329.

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