

Product Name: DDR1-IN-1

Catalog No.: 5077

Batch No.: 2

CAS Number: 1780303-76-5

IUPAC Name: *N*-[3-[(2,3-Dihydro-2-oxo-1*H*-indol-5-yl)oxy]-4-methylphenyl]-4-[(4-ethyl-1-piperazinyl)methyl]-3-(trifluoromethyl)benzamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₀H₃₁F₃N₄O₃·2HCl·½H₂O

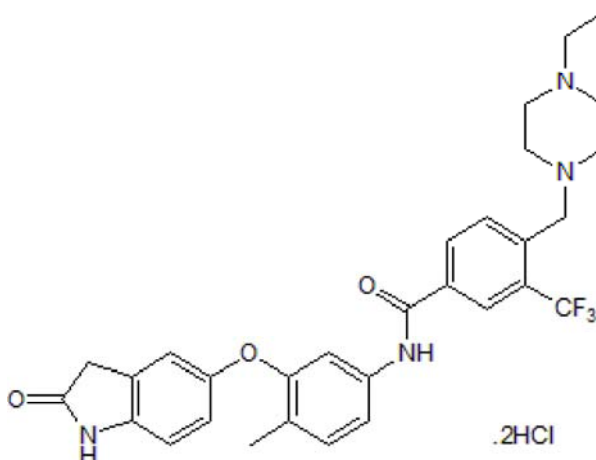
Batch Molecular Weight: 634.52

Physical Appearance: Cream solid

Solubility: water to 100 mM
DMSO to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.17 (Dichloromethane:Methanol [4:1])

HPLC: Shows 98.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.79	5.4	8.83
Found	56.64	5.26	8.75

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

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Description:

Selective discoidin domain receptor 1 (DDR1) tyrosine kinase inhibitor (IC₅₀ values are 105 and 413 nM for DDR1 and DDR2 respectively). Inhibits integrin-induced DDR1 autophosphorylation in an osteosarcoma cell line.

Physical and Chemical Properties:

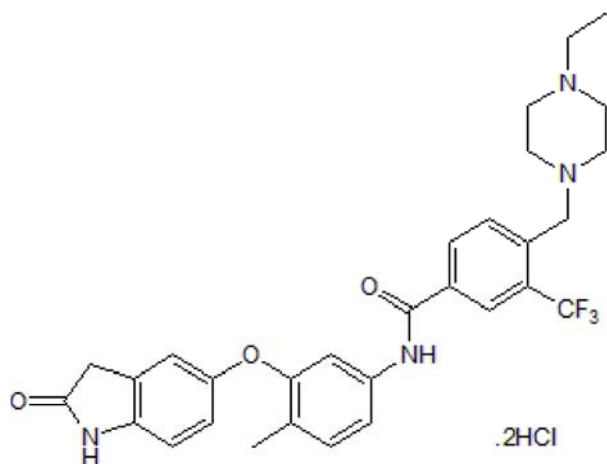
Batch Molecular Formula: C₃₀H₃₁F₃N₄O₃·2HCl·½H₂O

Batch Molecular Weight: 634.52

Physical Appearance: Cream solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM

DMSO 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:

Canning *et al* (2014) Structural Mechanisms Determining Inhibition of the Collagen Receptor DDR1 by Selective and Multi-Targeted Type II Kinase Inhibitors. *J.Mol.Biol.* **426** 2457. PMID: 24768818.

Kim *et al* (2013) Discovery of a potent and selective DDR1 receptor tyrosine kinase inhibitor. *ACS.Chem.Biol.* **8** 2145. PMID: 23899692.

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