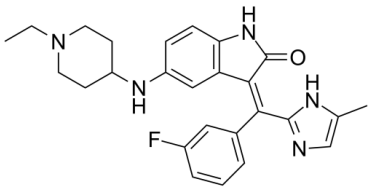
Data Sheet

Product Name:	Tyrosine kinase-IN-1
Cat. No.:	CS-0018466
CAS No.:	705946-27-6
Molecular Formula:	C26H28FN5O
Molecular Weight:	445.53
Target:	FGFR; PDGFR; VEGFR
Pathway:	Protein Tyrosine Kinase/RTK
Solubility:	DMSO : ≥ 62.5 mg/mL (140.28 mM)



BIOLOGICAL ACTIVITY:

Tyrosine kinase-IN-1 is a multi-targeted tyrosine kinase inhibitor with **IC_{50}**s of 4, 20, 4, 2 nM for **KDR**, **Flt-1**, **FGFR1** and **PDGFRα**, respectively. IC50 & Target: IC50: 4 nM (KDR), 20 nM (Flt-1), 4 nM (FGFR1), 2 nM (PDGFRα)[1] **In Vitro:** Tyrosine kinase-IN-1 is from reference (compound 8K)[1]. **In Vivo:** Tyrosine kinase-IN-1 shows a reasonable PK profile ($AUC_{(0-\infty)}$=1.9, $t_{1/2}$=4.6 h). It has a favorable oral bioavailability (F=63%) in rats[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]Kinase Inhibition Assays Kinase activities of KDR and PDGFRα are measured as the percent of ATP consumed following the kinase reaction using luciferaseluciferin-coupled chemiluminescence. Kinase reactions are initiated by combining test compound (Tyrosine kinase-IN-1), ATP, kinases and substrates in a 20 mL volume using 384-well microtiter plates. For KDR, the final reaction mixture contained 3 mM ATP, 1.6 mM poly(Glu, Tyr) 4:1 and 1.5 nM KDR of residues D807-V1356 with an N-terminal GST tag. For PDGFRα, the final reaction mixture contained 2 mM ATP, 10 mM MBP and 14 nM PDGFRα of residues Q551-L1089 with an N-terminal GST tag. The reaction mixture is incubated at room temperature for 4 h (KDR) or 2 h PDGFRα before a 20 mL aliquot of Kinase Glo is added and luminescence signal is measured using a Victor2 plate reader. Total ATP consumption is limited below 50%[1].

References:

[1]. Moon K, et al. The design, synthesis, and biological evaluation of potent receptor tyrosine kinase inhibitors. Bioorganic & Medicinal Chemistry Letters 22 (2012) 4979–4985

CAIndexNames:

2H-Indol-2-one, 5-[(1-ethyl-4-piperidinyl)amino]-3-[(3-fluorophenyl)(5-methyl-1H-imidazol-2-yl)methylene]-1,3-dihydro-, (3Z)-

SMILES:

O=C1NC2=C(C=C(NC3CCN(CC)CC3)C=C2)/C1=C(C4=CC=CC(F)=C4)/C5=NC=C(C)N5

Caution: Product has not been fully validated for medical applications. For research use only.

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