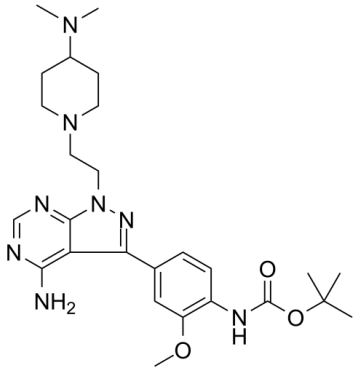
Data Sheet

Product Name:	eCF506
Cat. No.:	CS-0043341
CAS No.:	1914078-41-3
Molecular Formula:	C26H38N8O3
Molecular Weight:	510.63
Target:	Src
Pathway:	Protein Tyrosine Kinase/RTK
Solubility:	H2O : < 0.1 mg/mL (insoluble); DMSO : 62.5 mg/mL (122.40 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

eCF506 is a highly potent and orally bioavailable inhibitor of the non-receptor tyrosine kinase **Src** with an **IC_{50}** of less than 0.5 nM. IC50 & Target: IC50: less than 0.5 nM (Src)[1] **In Vitro:** eCF506 induces a very potent antiproliferative effect in both MCF7 and MDA-MB-231 cells. eCF506 inhibits phosphorylation of SRC and FAK at low nanomolar levels, with complete inhibition observed at 100 nM. eCF506 significantly reduces cell motility at 10 nM as early as 6 h into the study, with equivalent efficacy to dasatinib. eCF506 exclusively inhibits SFK, with subnanomolar IC_{50} values against SRC and YES (IC_{50}=0.5, 2.1 nM). It is important to highlight that eCF506 displays a vast difference in activity (>950-fold difference) between ABL and its primary target SRC[1]. **In Vivo:** eCF506 shows a moderate oral bioavailability (25.3%). A significant reduction of phospho-SRC^{Y416} is observed in the xenograft sections from mice treated with eCF506 relative to the untreated animal controls[1].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: eCF506 is prepared in 0.1% (v/v) DMSO[1].[1]**MDA-MB-231 cells** are treated with **eCF506 or dasatinib (10 nM),** and cell migration compared with untreated cell control (DMSO, 0.1%, v/v) at 6, 12, and 24 h. Cells are imaged and analyzed using an IncuCyte-ZOOM microscope with integrated scratch-wound migration software module[1]. **Animal Administration:** eCF506 is prepared in nanopure water[1].[1]Mice[1]

In vivo PD study is performed in a xenograft model of **HCT116 cells in mice.** HCT116 cells are injected subcutaneously, and tumors are allowed to grow up to 3-mm in diameter. Subsequently, mice are dosed daily for 3 d with **eCF506 (50 mg/kg, in nanopure water) or vehicle (nanopure water) by oral gavage** and culled 3 h after the last dose (n=4). Tumors are excised, fixed, and sections labeled for phospho-SRCY416 and stained with hematoxylin[1].

References:

[1]. Fraser C, et al. Rapid Discovery and Structure-Activity Relationships of Pyrazolopyrimidines That Potently Suppress Breast Cancer Cell Growth via SRC Kinase Inhibition with Exceptional Selectivity over ABL Kinase. J Med Chem. 2016 May 26;59(10):4697-710.

CAIndexNames:

tert-butyl (4-(4-amino-1-(2-(4-(dimethylamino)piperidin-1-yl)ethyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl)-2-methoxyphenyl)carbamate

SMILES:

NC1=C2C(C3=CC(OC)=C(NC(OC(C)(C)C)=O)C=C3)=NN(CCN4CCC(N(C)C)CC4)C2=NC=N1

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

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA