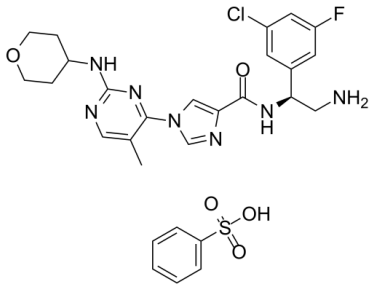
Data Sheet

Product Name:	ERK-IN-3 (benzenesulfonate)
Cat. No.:	CS-0146258
CAS No.:	2055597-39-0
Molecular Formula:	$C_{28}H_{31}ClFN_7O_5S$
Molecular Weight:	632.11
Target:	ERK
Pathway:	MAPK/ERK Pathway; Stem Cell/Wnt
Solubility:	DMSO : 320 mg/mL (506.24 mM; Need ultrasonic); H2O : 100 mg/mL (158.20 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

ERK-IN-3 benzenesulfonate is a potent and orally active inhibitor of **ERK**. ERK-IN-3 benzenesulfonate inhibits **ERK1/2** with low single-digit nM **IC_{50}** values. ERK-IN-3 benzenesulfonate can be used for the research of cancers driven by RAS mutations[1]. IC50 & Target: ERK[1] **In Vitro:** ERK-IN-3 inhibits the phosphorylation of ERK1/2 substrates such as RSK1, FRA1, and Elk1 in various cell lines[1].

ERK-IN-3 showes single-digit nanomolar antiproliferative activity that is selective for MAPK-pathway dependent cancer cell lines[1]. **In Vivo:** ERK-IN-3 (daily p.o.) inhibits tumor growth in multiple BRAF and KRAS mutant xenograft models in mice and was well tolerated at efficacious doses[1].

References:

[1]. Sanjeeva PR, et, al. Abstract B150: ASN007, a novel oral ERK inhibitor, shows robust antitumor activity in RAS mutant cancer models. Molecular Cancer Therapeutics. 2018 Jan; 17(1).

CAIndexNames:

1H-Imidazole-4-carboxamide, N-[(1S)-2-amino-1-(3-chloro-5-fluorophenyl)ethyl]-1-[5-methyl-2-[(tetrahydro-2H-pyran-4-yl)amino]-4-pyrimidinyl]-, compd. with benzenesulfonate (1:1)

SMILES:

O=C(C1=CN(C2=NC(NC3CCOCC3)=NC=C2C)C=N1)N[C@@H](C4=CC(F)=CC(Cl)=C4)CN.O=S(C5=CC=CC=C5)(O)=O

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

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