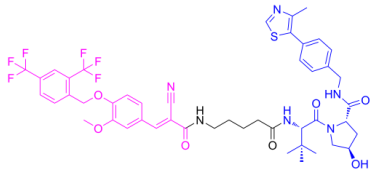
Data Sheet

Product Name:	PROTAC ERRα Degrader-3
Cat. No.:	CS-0181524
CAS No.:	2306388-65-6
Molecular Formula:	$C_{47}H_{50}F_6N_6O_7S$
Molecular Weight:	956.99
Target:	Estrogen Receptor/ERR; PROTACs
Pathway:	PROTAC; Vitamin D Related/Nuclear Receptor
Solubility:	DMSO : 80 mg/mL (ultrasonic)



BIOLOGICAL ACTIVITY:

PROTAC ERRα Degrader-3 is a potent and selective **ERRα** degrader based on **von Hippel-Lindau** ligand. PROTAC ERRα Degrader-3 is capable of specifically degrading ERRα protein by >80% at a concentration of 30 nM. PROTAC ERRα Degrader-3 is inactive against ERRβ and ERRγ proteins[1]. ***In Vitro:*** PROTAC ERRα Degrader-3 (compound 6c; 0.3 nM-10 μM; 4 hours) dose-dependently induces ERRα degradation with an efficacious dose as low as 3.0 nM at 4.0 h. PROTAC ERRα Degrader-3 potently decreases protein levels of ERRα downstream target genes, e.g., ATP5B, medium-chain acyl CoA dehydrogenase (MCAD), and pyruvate dehydrogenase kinase 4 (PDK4) in the MDA-MB-231 cells after a 24 h treatment[1].
PROTAC ERRα Degrader-3 exhibits an IC_{50} value of 12.67 nM to block the protein-protein interaction of ERRα with PGC-1α peptide and induces approximately 96% protein degradation at 100 nM (D100 nM) after 4.0 h treatment[1].

References:

[1]. Lijie Peng, et al. Identification of New Small-Molecule Inducers of Estrogen-related Receptor α (ERRα) Degradation. ACS Med Chem Lett. 2019 Apr 12;10(5):767-772.

CAIndexNames:

(2S,4R)-1-((S)-2-(5-((E)-3-(4-((2,4-Bis(trifluoromethyl)benzyl)oxy)-3-methoxyphenyl)-2-cyanoacrylamido)pentanamido)-3,3-dimethylbutanoyl)-4-hydroxy-N-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide

SMILES:

COC(C=C1/C=C(C#N)/C(NCCCCC(N[C@@H](C(C)(C)C)C(N2[C@@H](C[C@H](C2)O)C(NCC3=CC=C(C4=C(C)N=CS4)C=C3)=O)=O)=O)=O)=C(C=C1)OCC5=C(C=C(C=C5)C(F)(F)F)C(F)(F)F

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

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