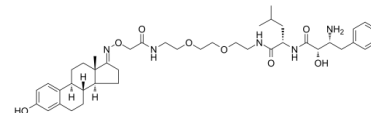


Data Sheet

Product Name:	PROTAC ER α Degradator-2
Cat. No.:	CS-0093244
CAS No.:	1351169-29-3
Molecular Formula:	C ₄₂ H ₆₁ N ₅ O ₈
Molecular Weight:	763.96
Target:	Estrogen Receptor/ERR; PROTACs; SNIPERS
Pathway:	Others; PROTAC
Solubility:	DMSO : 200 mg/mL (261.79 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

PROTAC ER α Degradator-2 comprises a **IAP** ligand binding group, a linker and an **estrogen receptor α (ER α)** binding group. PROTAC ER α Degradator-2 is an **ER α** degrader. Maximal ER α degradation at 30 μ M concentration in human mammary tumor MCF7 cells. Degradation inducers based on cIAP1 are called specific and non-genetic IAP-dependent protein erasers (**SNIPERS**)^[1].

References:

[1]. Scheepstra M, et al. Bivalent Ligands for Protein Degradation in Drug Discovery. Comput Struct Biotechnol J. 2019 Jan 25;17:160-176.

CAIndexNames:

Benzenebutanamide, β -amino- α -hydroxy-N-[(1S)-14-[[[E)-(3-hydroxyestra-1,3,5(10)-trien-17-ylidene)amino]oxy]-1-(2-methylpropyl)-2,13-dioxo-6,9-dioxo-3,12-diazatetradec-1-yl]-, (α S, β R)-

SMILES:

C[C@@]12[C@](CC/C2=N\OCC(NCCOCCOCCNC([C@H](CC(C)C)NC([C@@H](O)[C@H](N)CC3=CC=CC=C3)=O)=O)([H])[C@@]4([H])[C@](C5=C=C(O)C=C5CC4)([H])CC1

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

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