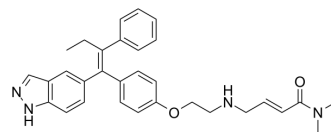


H3B-5942

Cat. No.:	HY-112611		
CAS No.:	2052128-15-9		
Molecular Formula:	C ₃₁ H ₃₄ N ₄ O ₂		
Molecular Weight:	494.63		
Target:	Estrogen Receptor/ERR		
Pathway:	Others		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro	DMSO : 83.33 mg/mL (168.47 mM; Need ultrasonic)				
		Solvent Concentration	Mass 1 mg	5 mg	10 mg
	Preparing Stock Solutions	1 mM	2.0217 mL	10.1086 mL	20.2171 mL
		5 mM	0.4043 mL	2.0217 mL	4.0434 mL
10 mM		0.2022 mL	1.0109 mL	2.0217 mL	
Please refer to the solubility information to select the appropriate solvent.					
In Vivo	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.08 mg/mL (4.21 mM); Clear solution				
	2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (4.21 mM); Clear solution				

BIOLOGICAL ACTIVITY

Description	H3B-5942 is a selective, irreversible and orally active estrogen receptor covalent antagonist, inactivates both wild-type and mutant ERα by targeting Cys530, with K _i s of 1 nM and 0.41 nM, respectively. H3B-5942 reduces ERα target gene GREB1, shows potent antitumor activity both in multiple cell lines or animals bearing ERα ^{WT} or ERα mutations ^[1] .	
IC ₅₀ & Target	ERα ^{Y537S} 0.41 nM (K _i)	ERα ^{WT} 1 nM (K _i)
In Vitro	H3B-5942 is a selective and irreversible estrogen receptor covalent antagonist, inactivates both wild-type and mutant ERα by targeting Cys530, with K _i s of 1 nM and 0.41 nM, respectively ^[1] . H3B-5942 elevates ERα protein level distinct from SERMs/SERD, blocks ERα-dependent transcription in breast cancer cells.	

H3B-5942 (0.01-10 μ M) reduces ER α target gene GREB1 in MCF7-ER α^{WT} , various MCF7-ER α MUT lines, and the PDX-ER α^{Y537S} /WT line^[1].

H3B-5942 also decreases proliferation of MCF7-Parental, MCF7-LTED-ER α^{WT} , and MCF7-LTED-ER α^{Y537C} lines with GI₅₀s of 0.5, 2, and 30 nM, respectively. H3B-5942 (10-25 nM) in combination with CDK4/6 inhibitors (\geq 25 pM) has synergic inhibitory effect on multiple cell lines bearing ER α^{WT} or clinically frequent ER α mutations^[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

H3B-5942 (1, 3, 10, or 30 mg/kg, p.o, q.d. for 17 days) dose-dependently inhibits tumor growth in MCF7 xenograft model in athymic female nude mice^[1].

H3B-5942 (3, 10, 30, 100, and 200 mg/kg, p.o, q.d.) exhibits similar anti-tumor activity in the ER $\alpha^{Y537S/WT}$ ST941 model in athymic female nude mice^[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	MCF7 xenograft model in athymic female nude mice ^[1]
Dosage:	1, 3, 10, or 30 mg/kg
Administration:	P.O. once a day (q.d. \times 1) for 17 days
Result:	Exhibited tumor growth inhibition (TGI) on day 17 of 19%, 41%, 68%, and 83%, respectively.

REFERENCES

[1]. Puyang X, et al. Discovery of Selective Estrogen Receptor Covalent Antagonists for the Treatment of ER α WT and ER α MUT Breast Cancer. Cancer Discov. 2018 Sep;8(9):1176-1193.

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

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