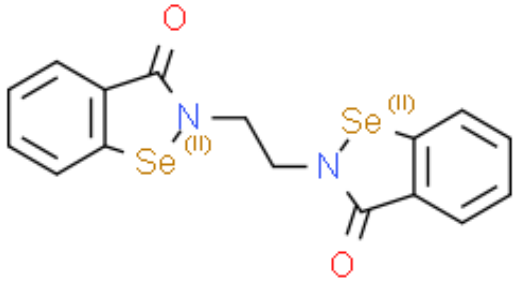
Product Data Sheet

Cas No.:	217798-39-5	Cat. No:	PL12476
Product Name:	Ethaselen		
Product synonym:	-		
Chemical name:	Ethaselen		
MF:	C16H12N2O2SE2	FW:	422.19868183136
Purity:	≥98%	Batch No.:	-
Storage:			
Structural formula:			
λmax:	-	Formulation:	-
Solubility :			
SMILES :	[Se]1C2C=CC=CC=2C(N1CCN1C(C2C=CC=CC=2[Se]1)=O)=O		
InChI Code:	-		
InChI Key:			
WARNING This product is not for human or veterinary use.			

Product Description

Ethaselen (BBSKE) 是具有口服活性的，选择性的硫氧还蛋白还原酶 (TrxR) 抑制剂，对野生型人 TrxR1 和大鼠 TrxR1 的 IC_{50} 分别为 0.5 和 0.35 μM。Ethaselen 特异性结合哺乳动物 TrxR1 C 端活性位点中独特的硒代半胱氨酸-半胱氨酸氧化还原对。Ethaselen 是一种有机硒化合物，一种有效的抗肿瘤候选药物，可通过靶向 TrxR 对非小细胞肺癌 (NSCLC) 发挥有效抑制作用。

生物活性	Ethaselen (BBSKE) is an orally active, selective thioredoxin reductase (TrxR) inhibitor with IC 50 s of 0.5 and 0.35 μM for the wild-type human TrxR1 and rat TrxR1, respectively. Ethaselen specifically binds to the unique selenocysteine-cysteine redox pair in the C-terminal active site of mammalian TrxR1. Ethaselen, an organoselenium compound, is a potent antitumor candidate that exerts potent inhibition on non-small cell lung cancer (NSCLC) by targeting TrxR.
IC50 & Target[1][2]	TrxR

体外研究(In Vitro)	Ethaselen (2.5-10 μM; 12, 24 hours) suppresses A549 cell viability in a both concentration- and time-dependent manner. H1666, which has considerably lower TrxR1 expression level, is less susceptible to 24 h treatment with Ethaselen. Ethaselen inhibits the intracellular TrxR1 activity in a concentration- and time-dependent manner, with IC50 values of 4.2 and 2 μM for 12- and 24-h treatments, respectively. Ethaselen (2.5-10 μM; 12, 24 hours) has no effect on the protein amounts of TrxR1 and Trx. The mRNA level of TrxR1 does not show significant alteration in Ethaselen-treated A549 cells. Ethaselen (2.5-50 μM; 1-24 hours) causes intracellular Trx oxidation in A549 cells. Ethaselen (5-10 μM; 12, 24 hours) causes a clear concentration-dependent increase in ROS levels in A549 cells. The inhibition constants for Ethaselen binding to free enzyme (K
体内研究(In Vivo)	Ethaselen (BBSKE; 36-108 mg/kg/day; PO; for 10 days) shows increased inhibition of tumor growth in a dose-independent manner. has not independently confirmed the accuracy of these methods. They are for reference only. Animal Model: Five
包装储存	Powder -20°C 3 years；4°C 2 years
溶解度数据	In Vitro: DMSO : 12.5 mg/mL (29.61 mM; ultrasonic and warming and heat to 60°C)配制储备液