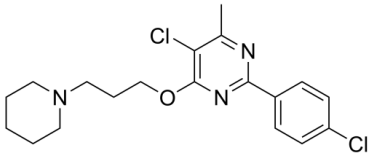
Data Sheet

Product Name:	Sigma-1 receptor antagonist 1
Cat. No.:	CS-0100225
CAS No.:	1639220-19-1
Molecular Formula:	$C_{19}H_{23}Cl_2N_3O$
Molecular Weight:	380.31
Target:	Sigma Receptor
Pathway:	Neuronal Signaling
Solubility:	DMSO : 6.25 mg/mL (16.43 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Sigma-1 receptor antagonist 1 (compound 137) is a potent and selective **sigma-1 receptor (σ1R)** antagonist, with a high binding affinity to σ1R receptor (**K_i** = 1.06 nM). Sigma-1 receptor antagonist 1 exhibits antineuropathic pain activity and acts as a promising agent for the treatment of neuropathic pain[1]. IC50 & Target:Ki: 1.06 nM (σ1R)[1] ***In Vitro:*** Sigma?1 receptor antagonist 1 exhibits a high binding affinity to σ1R receptor (K_i = 1.06 nM) and good σ-1/2 selectivity (1344-fold)[1].
In Vivo: Sigma?1 receptor antagonist 1 exerts dose-dependent antinociceptive effects in mice formalin model and rats CCI models of neuropathic pain[1].

References:

[1]. Lan Y, et al. Synthesis and biological evaluation of novel sigma-1 receptor antagonists based on pyrimidine scaffold as agents for treating neuropathic pain. J Med Chem. 2014 Dec 26;57(24):10404-23.

CAIndexNames:

Pyrimidine, 5-chloro-2-(4-chlorophenyl)-4-methyl-6-[3-(1-piperidinyl)propoxy]-

SMILES:

CC1=NC(C2=CC=C(Cl)C=C2)=NC(OCCCN3CCCCC3)=C1Cl

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