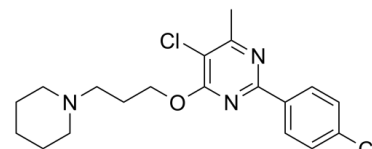


## Data Sheet

<b>Product Name:</b>	Sigma-1 receptor antagonist 1
<b>Cat. No.:</b>	CS-0100225
<b>CAS No.:</b>	1639220-19-1
<b>Molecular Formula:</b>	C <sub>19</sub> H <sub>23</sub> Cl <sub>2</sub> N <sub>3</sub> O
<b>Molecular Weight:</b>	380.31
<b>Target:</b>	Sigma Receptor
<b>Pathway:</b>	GPCR/G Protein; Neuronal Signaling
<b>Solubility:</b>	DMSO : 6.25 mg/mL (16.43 mM; Need ultrasonic)



### BIOLOGICAL ACTIVITY:

Sigma $\square$ 1 receptor antagonist 1 (compound 137) is a potent and selective **sigma-1 receptor ( $\sigma$ 1R)** antagonist, with a high binding affinity to  $\sigma$ 1R receptor ( $K_i = 1.06$  nM). Sigma $\square$ 1 receptor antagonist 1 exhibits antineuropathic pain activity and acts as a promising agent for the treatment of neuropathic pain<sup>[1]</sup>. IC<sub>50</sub> & Target:  $K_i$ : 1.06 nM ( $\sigma$ 1R)<sup>[1]</sup> **In Vitro:** Sigma $\square$ 1 receptor antagonist 1 exhibits a high binding affinity to  $\sigma$ 1R receptor ( $K_i = 1.06$  nM) and good  $\sigma$ -1/2 selectivity (1344-fold)<sup>[1]</sup>.

**In Vivo:** Sigma $\square$ 1 receptor antagonist 1 exerts dose-dependent antinociceptive effects in mice formalin model and rats CCI models of neuropathic pain<sup>[1]</sup>.

### 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

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

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