Product Data Sheet

Product Name: MS37452
Cat. No.: GC12630

Chemical Properties

Cas. No.	423748-02-1		
Chemical Name	1-[4-(2,3-dimethoxybenzoyl)-1-piperazinyl]-2-(3-methylphenoxy)-ethanone		
SMILES	COC1=CC=CC(C(N2CCN(C(COC3=CC(C)=CC=C3)=O)CC2)=O)=C1OC		
Formula	$C_{22}H_{26}N_2O_5$	M.Wt	398.5
Solubility	≤30mg/ml in ethanol;30mg/ml in DMSO;30mg/ml in dimethyl formamide	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	MS37452		

Background

Ki = 43 μM

MS37452 is a competitive inhibitor of CBX7 chromodomain binding to H3K27me3.

Chromobox homolog 7 (CBX7) functions via its N-terminal chromodomain, which recognizes histone 3 trimethyl lysine 27 (H3K27me3), to repress gene transcription. Chromobox homolog 7 plays a critical role in gene transcription in cellular processes associated with stem cell differentiation and self-renewal, as well as tumor progression.

In vitro: In a previous study, the crystal structures revealed the binding modes of MS37452 and its close analogs that competed against H3K27me3 binding via interactions with key residues in the methyl-lysine binding pocket of CBX7ChD. It was further found that MS37452 as the lead compound was able to derepress the transcription of Polycomb repressive complex target gene p16/CDKN2A through

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA

displacing CBX7 binding to the INK4A/ARF locus in prostate cancer cells. These findings showed that MS37452 and its close analogs had the potential to be developed into high-potency chemical modulators targeting CBX7 functions in gene transcription in various disease pathways [1].

In vivo: Up to now, there is no animal in vivo data reported.

Clinical trial: So far, no clinical study has been conducted.

Reference:
[1] Ren, C. ,Morohashi, K.,Plotnikov, A.N., et al. Small-molecule modulators of methyl-lysine binding for the CBX7 chromodomain. Chemistry & Biology 22, 161-168 (2015).