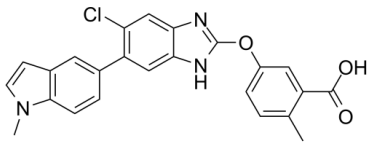
Data Sheet

Product Name:	EX229
Cat. No.:	CS-0063368
CAS No.:	1219739-36-2
Molecular Formula:	C24H18ClN3O3
Molecular Weight:	431.87
Target:	AMPK
Pathway:	Epigenetics; PI3K/Akt/mTOR
Solubility:	DMSO : 13 mg/mL (30.10 mM; Need ultrasonic and warming)



BIOLOGICAL ACTIVITY:

EX229, a Benzimidazole derivative, is a potent and allosteric activator of AMP-activated protein kinase **(AMPK)**, with **K_ds** of 0.06 μM, 0.06 μM and 0.51 μM for α1β1γ1, α2β1γ1 and α1β2γ1 in biolayer interferometry, respectively. IC50 & Target: Kd: 0.06 μM (α1β1γ1), 0.06 μM (α2β1γ1), 0.51 μM (α1β2γ1)[1]. **In Vitro:** EX229 is a potent and allosteric activator of AMP-activated protein kinase (AMPK), with K_ds of 0.06 μM, 0.06 μM and 0.51 μM for α1β1γ1, α2β1γ1 and α1β2γ1, respectively.[1]. Treatment of hepatocytes with EX229 (991) alone results in a slight increase in the phosphorylation of AMPK and RAPTOR only at 0.3 μM, whereas a robust increase in ACC phosphorylation is readily observed and saturated at a concentration of 0.03 μM EX229. AICAR or C13 alone robustly increases T172 phosphorylation of AMPKα, and when EX229 is coincubated, there is a modest additional dose-dependent increase in AMPKα phosphorylation. RAPTOR phosphorylation is modestly increased by AICAR or C13 alone, and it is dose dependently increased when coincubations are carried out with EX229. EX229 also dose dependently (0.01 and 0.1 μM) inhibits lipogenesis (34% and 63%, respectively), which is further reduced when it is coincubated with a low dose of AICAR (0.03 mM) or C13 (1 μM). Treatment with EX229 promotes dose-dependent increases in ACC and RAPTOR phosphorylation. Similar to the observations in hepatocytes[2].

References:

[1]. Xiao B, et al. Structural basis of AMPK regulation by small molecule activators. Nat Commun. 2013;4:3017.

[2]. Bultot L, et al. Benzimidazole derivative small-molecule 991 enhances AMPK activity and glucose uptake induced by AICAR or contraction in skeletal muscle. Am J Physiol Endocrinol Metab. 2016 Oct 1;311(4):E706-E719.

CAIndexNames:

Benzoic acid,5-[[6-chloro-5-(1-methyl-1H-indol-5-yl)-1H-benzimidazol-2-yl]oxy]-2-methyl-

SMILES:

O=C(O)C1=CC(OC2=NC3=CC(Cl)=C(C4=CC5=C(N(C)C=C5)C=C4)C=C3N2)=CC=C1C

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