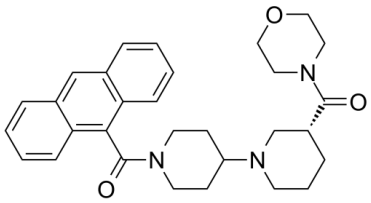
Data Sheet

Product Name:	CP-640186 (hydrochloride)
Cat. No.:	CS-3135
CAS No.:	591778-70-0
Molecular Formula:	C30H36ClN3O3
Molecular Weight:	522.08
Target:	Acetyl-CoA Carboxylase
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 48 mg/mL (91.94 mM); H2O : 50 mg/mL (95.77 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

CP-640186 Hcl is an isozyme-nonselective acetyl-CoA carboxylase (ACC) inhibitor with IC50s of 53 nM and 61 nM for rat liver ACC1 and rat skeletal muscle ACC2 respectively; with improved metabolic stability vs CP-610431. IC50 value: 53 nM/61 nM (rat liver ACC1/skeletal muscle ACC2) [1] Target: acetyl-CoA carboxylase in vitro: CP-640186, also inhibited both isozymes with IC50s of ~55 nM but was 2–3 times more potent than CP-610431 in inhibiting HepG2 cell fatty acid and TG synthesis. CP-640186 also stimulated fatty acid oxidation in C2C12 cells (ACC2) and in rat epitrochlearis muscle strips with EC50s of 57 nM and 1.3 uM [1]. in vivo: In rats, CP-640186 lowered hepatic, soleus muscle, quadriceps muscle, and cardiac muscle malonyl-CoA with ED50s of 55, 6, 15, and 8 mg/kg. Consequently, CP-640186 inhibited fatty acid synthesis in rats, CD1 mice, and ob/ob mice with ED50s of 13, 11, and 4 mg/kg, and stimulated rat whole body fatty acid oxidation with an ED50 of ~30 mg/kg [1].

References:

[1]. Harwood HJ Jr, et al. Isozyme-nonselective N-substituted bipiperidylcarboxamide acetyl-CoA carboxylase inhibitors reduce tissue malonyl-CoA concentrations, inhibit fatty acid synthesis, and increase fatty acid oxidation in cultured cells and in experimental animals. J Biol Chem. 2003 Sep 26;278(39):37099-111.

[2]. Yamashita T, et al. Design, synthesis, and structure-activity relationships of spirolactones bearing 2-ureidobenzothiophene as acetyl-CoA carboxylases inhibitors. Bioorg Med Chem Lett. 2011 Nov 1;21(21):6314-8.

CAIndexNames:

Morpholine, 4-[[(3R)-1'-(9-anthracenylcarbonyl)[1,4'-bipiperidin]-3-yl]carbonyl]-, monohydrochloride (9CI)

SMILES:

O=C([C@H]1CN(C2CCN(C(C3=C(C=CC=C4)C4=CC5=C3C=CC=C5)=O)CC2)CCC1)N6CCOCC6.Cl

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