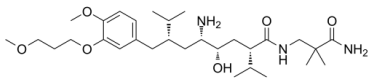
Data Sheet

Product Name:	Aliskiren
Cat. No.:	CS-0443
CAS No.:	173334-57-1
Molecular Formula:	C30H53N3O6
Molecular Weight:	551.76
Target:	Autophagy; Renin
Pathway:	Autophagy; Metabolic Enzyme/Protease
Solubility:	DMSO : 100 mg/mL (181.24 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Aliskiren(CGP 60536) is a direct renin inhibitor with IC50 of 1.5 nM. IC50 value: 1.5 nM [1] Target: renin in vitro: Aliskiren hemifumarate appears to bind to both the hydrophobic S1/S3-binding pocket and to a large, distinct subpocket that extends from the S3-binding site towards the hydrophobic core of renin. Oral bioavailability of Aliskiren hemifumarate is 2.4% in rats, 16% in marmosets and about 2.5% in humans [2]. in vivo: Aliskiren hemifumarate (< 10 mg/kg, oral) inhibits plasma renin activity and lowers blood pressure in sodium-depleted marmosets[3].Once-daily oral treatment with Aliskiren hemifumarate lowers blood pressure effectively, with a safety and tolerability profile, in patients with mild-to-moderate hypertension[4].

References:

[1]. Yuji Nakamura, et al. Discovery of DS-8108b, a Novel Orally Bioavailable Renin Inhibitor. ACS Med. Chem. Lett., 2012, 3 (9), pp 754–758

[2]. Buczko W, et al. Pharmacokinetics and pharmacodynamics of aliskiren, an oral direct renin inhibitor. Pharmacol Rep. 2008 Sep-Oct;60(5):623-31.

[3]. Wood JM, et al. Structure-based design of aliskiren, a novel orally effective renin inhibitor.Biochem Biophys Res Commun, 2003, 308(4), 698-705.

[4]. Gradman AH, et al.Aliskiren, a novel orally effective renin inhibitor, provides dose-dependent antihypertensive efficacy and placebo-like tolerability in hypertensive patients. Circulation, 2005, 111(8), 1012-1018.

[5]. Chang AY, et al. Interplay between brain stem angiotensins and monocyte chemoattractant protein-1 as a novel mechanism for pressor response after ischemic stroke. Neurobiol Dis. 2014 Nov;71:292-304.

CAIndexNames:

Benzeneoctanamide, .delta.-amino-N-(3-amino-2,2-dimethyl-3-oxopropyl)-.gamma.-hydroxy-4-methoxy-3-(3-methoxypropoxy)-.alpha.,.zeta.-bis(1-methylethyl)-, (.alpha.S,.gamma.S,.delta.S,.zeta.S)-

SMILES:

COCCCOC1=CC(C[C@@H](C[C@@H]([C@H](C[C@H](C(NCC(C)(C(N)=O)C)=O)C(C)C)O)N)C(C)C)=CC=C1OC

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

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