Epelsiban

Cat. No.: HY-105018

CAS No.: 872599-83-2

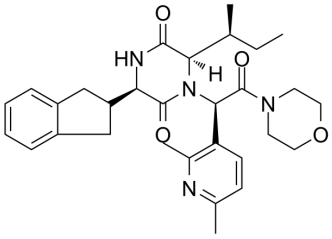
Molecular Formula: $C_{30}H_{38}N_4O_4$

Molecular Weight: 518.65

Target: Oxytocin Receptor

Pathway: GPCR/G Protein

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Epelsiban (GSK 557296) is a potent, selective and orally bioavailable oxytocin receptor antagonist, with a pK_i of 9.9 for human oxytocin receptor.
IC_{50} & Target	pKi: 9.9 (human oxytocin receptor)[1] IC50: 192 nM (human oxytocin receptor)[1]
In Vitro	Epelsiban is a potent oxytocin receptor, with a pK_i of 9.9 for human oxytocin receptor, >31000-fold selectivity over all three human vasopressin receptors hV1aR (pK_i, <5.2), hV2R (pK_i, <5.1), and hV1bR (pK_i, 5.4), and shows no significant P450 inhibition[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Epelsiban shows an IC_{50} of 192 nM for oxytocin receptor in rats. Epelsiban has low levels of intrinsic clearance against the microsomes of rat, dog, and cynomolgus monkey, good bioavailability (55%), but is negative in the genotoxicity screens with a satisfactory oral safety profile in female rats[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Borthwick AD, et al. Pyridyl-2,5-diketopiperazines as potent, selective, and orally bioavailable oxytocin antagonists: synthesis, pharmacokinetics, and in vivo potency. J Med Chem. 2012 Jan 26;55(2):783-96.

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