# Data Sheet

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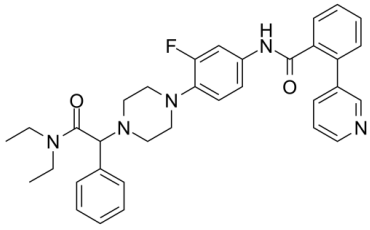
| **Product Name:** | JNJ-31020028 |
| **Cat. No.:** | CS-3499 |
| **CAS No.:** | 1094873-14-9 |
| **Molecular Formula:** | C34H36FN5O2 |
| **Molecular Weight:** | 565.68 |
| **Target:** | Neuropeptide Y Receptor |
| **Pathway:** | GPCR/G Protein; Neuronal Signaling |
| **Solubility:** | DMSO : 21.5 mg/mL (38.01 mM; Need ultrasonic and warming) |



## BIOLOGICAL ACTIVITY:

JNJ-31020028 is a selective brain penetrant antagonist of neuropeptide Y2 receptor with high affinity(pIC50=8.07, human; pIC50=8.22 rat); >100-fold selective versus human Y1/Y4/Y5 receptors. IC50 value: 8.07/8.22(human/rat pIC50) [1] Target: Y2 receptor antagonist in vitro: JNJ-31020028 was demonstrated to be an antagonist (pK(B) = 8.04 +/- 0.13) in functional assays [1]. in vivo: JNJ-31020028 occupied Y(2) receptor binding sites (approximately 90% at 10 mg/kg) after subcutaneous administration in rats [1]. Neither systemic (0, 15, 30, and 40 mg/kg, subcutaneously [s.c.]) nor intracerebroventricular (0.0, 0.3, and 1.0 nmol/rat) administration of JNJ-31020028 affected alcohol-reinforced lever pressing or relapse to alcohol seeking behavior following stress exposure. JNJ-31020028 (15 mg/kg, s.c.) did reverse the anxiogenic effects of withdrawal from a single bolus dose of alcohol on the elevated plus-maze, confirming the anxiolytic-like properties of NPY Y2 antagonism [2]. Chronic administration of JNJ-31020028 induced a decrease in immobility time in the forced swim test in OBX while had no effect in control animals [3].

## PROTOCOL (Extracted from published papers and Only for reference)

Radioligands binding assays [1]: Cells used in the radioligand binding experiments with NPY receptor subtypes were SK-N-MC endogenously expressing Y1 receptors, KAN-Ts endogenously expressing Y2 receptors, Chinese hamster ovary (CHO) cells transfected with human Y4 cDNA for Y4 receptors, and HEK-293 transfected with human Y5 cDNA for Y5 receptors. Membranes from rat and mouse hippocampus were also prepared and assayed for [125I]PYY binding. IC50 values (i.e., concentration of unlabeled antagonist required to compete for 50% of specific binding to the radioligand) were calculated using the GraphPad Prism software with a fit to a sigmoidal dose-response curve. Data were expressed as pIC50 values where pIC50= -log IC50. Animal adminstration(Ex vivo receptor occupancy) [1]: Male Sprague-Dawley rats (300-350 g) were treated by s.c. administration of vehicle or JNJ-31020028 (three animals per dose and three animals per time point). JNJ-31020028 was formulated at 1-15 mg/ml in 40% 2-hydroxypropyl-beta-cyclodextrin or 5% pharmasolve, 19% 2-hydroxypropyl-beta-cyclodextrin, and delivered in a volume of 1 or 2 ml/kg. The animals were euthanized at various time points after drug administration using carbon dioxide and brain tissues were collected.

## References:

[1]. Shoblock JR, et al. In vitro and in vivo characterization of JNJ-31020028 (N-(4-<4-[2-(diethylamino)-2-oxo-1-phenylethyl]piperazin-1-yl>-3-fluorophenyl)-2-pyridin-3-ylbenzamide), a selective brain penetrant small molecule antagonist of the neuropeptide Y Y(2) receptor. Psychopharmacology (Berl). 2010 Feb;208(2):265-77.

[2]. Cippitelli A, et al. The novel, selective, brain-penetrant neuropeptide Y Y2 receptor antagonist, JNJ-31020028, tested in animal models of alcohol consumption, relapse, and anxiety. Alcohol. 2011 Sep;45(6):567-76.

[3]. Morales-Medina JC, et al. Chronic administration of the Y2 receptor antagonist, JNJ-31020028, induced anti-depressant like-behaviors in olfactory bulbectomized rat. Neuropeptides. 2012 Dec;46(6):329-34.

## CAIndexNames:

1-Piperazineacetamide, N,N-diethyl-4-[2-fluoro-4-[[2-(3-pyridinyl)benzoyl]amino]phenyl]- -phenyl-

## SMILES:

O=C(N(CC)CC)C(N1CCN(C2=CC=C(NC(C3=C(C4=CC=CN=C4)C=CC=C3)=O)C=C2F)CC1)C5=CC=CC=C5



Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA