# Data Sheet

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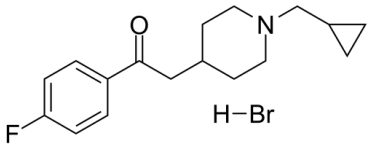
| **Product Name:** | DuP 734 |
| **Cat. No.:** | CS-0127541 |
| **CAS No.:** | 135135-87-4 |
| **Molecular Formula:** | $C_{17}H_{23}BrFNO$ |
| **Molecular Weight:** | 356.27 |
| **Target:** | Sigma Receptor |
| **Pathway:** | GPCR/G Protein; Neuronal Signaling |
| **Solubility:** | DMSO : 250 mg/mL (701.71 mM; Need ultrasonic) |




## BIOLOGICAL ACTIVITY:

DuP 734 is a **sigma receptor** antagonist. DuP 734 is a selective and potent sigma and 5-HT2 receptor ligand with weak affinity for D2 receptors. DuP 734 may have antipsychotic activity without the liability of motor side effects typical of neuroleptics[1][2][3]. IC50 & Target: Sigma receptor; 5-HT2 receptor; D2 receptor[1][2][3] **In Vivo:** DuP 734 potently blocks mescaline-induced scratching ($ED_{50}$ =0.35 mg/kg, p.o.) and aggressive activity ($ED_{50}$=1.9 mg/kg, p.o.) and is relatively much weaker as an apomorphine antagonist ($ED_{50}$ =12 mg/kg, p.o.)[1].

Administration of DuP 734 potently antagonizes the binding of [$^3$H]DuP 734 and [$^3$H](+)-SKF 10,047 to brain sigma receptors in vivo with $ID_{50}$ values of 0.02 and 0.07 mg/kg (0.07 and 0.25μmol/kg), respectively[2].

Following intravenous dosing, the disposition of DuP 734 in mice, rats, beagle dogs and cynomolgus monkeys is characterized by high total body systemic plasma clearance (46 to 87 mL/min/kg) and large steady-state volume of distribution (3.6 to 6.8 L/kg). The terminal elimination half-life ranged from 50 to 83 min. The gastrointestinal absorption from an aqueous solution is very rapid in mice and rats with peak DuP 734 plasma concentrations attain within 5 and 20 min following administration, respectively. The peak plasma concentrations in dogs and monkeys are attained within 45 and 130 min, respectively. The absolute bioavailability in mice ranges from 29 to 46% at doses of 3.1 to 30.1 mg/kg. The bioavailability increases from 4 to 10% and from 14 to 72% when doses are increased from 12.5 to 50 mg/kg and 1 to 3 mg/kg of DuP 734 in rats and dogs, respectively. The bioavailability in monkeys is 30.5% at 9.3 mg/kg DuP 734 dose. The dose dependent pharmacokinetics of DuP 734 is observed within narrow dose ranges in all animal species investigated[3].

## References:

[1]. L Cook, et al. DuP 734 [1-(cyclopropylmethyl)-4-(2'(4"-fluorophenyl)-2'- Oxoethyl)piperidine HBr], a Potential Antipsychotic Agent: Preclinical Behavioral Effects. J Pharmacol Exp Ther. 1992 Dec;263(3):1159-66.

[2]. M Watanabe, et al. [$^3$H]1-(cyclopropylmethyl)-4-(2-(4-fluorophenyl)-2-oxoethyl) Piperidine HBr (DuP 734). A Selective Ligand for Sigma Receptors in Mouse Brain in Vivo. J Pharmacol Exp Ther. 1993 Sep;266(3):1541-8.

[3]. R P Kapil, et al. Dose and Species Dependent Pharmacokinetics of a Novel Sigma Receptor Antagonist, DuP 734. Res Commun Mol Pathol Pharmacol. 1995 Apr;88(1):3-20.

## CAIndexNames:

Ethanone, 2-[1-(cyclopropylmethyl)-4-piperidinyl]-1-(4-fluorophenyl)-, hydrobromide (1:1)

## SMILES:

FC1=CC=C(C(CC2CCN(CC3CC3)CC2)=O)C=C1.[H]Br

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

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