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# DATASHEET

JHU37152 (DREADD ligand)

## Product overview

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|---|---|
| **Name** | JHU37152 (DREADD ligand) |
| **Cat No** | HB6252 |
| **Description** | Novel DREADD agonist with high affinity and potency for hM3Dq and hM4Di. Active in vivo. Freebase. |
| **Alternative names** | J52 |
| **Purity** | >98% |

## Biological Data

**Biological description**

**Overview**

JHU37152 is reported to be a novel DREADD agonist with high in vivo DREADD potency for CNS applications.

It has high affinity in vitro for hM3Dq and hM4Di ($K_i$ values are 1.8 nM (hM3Dq) and 8.7 nM (hM4Di).

It selectively displaces [$^3$H]clozapine from DREADDs and not from other clozapine-binding sites at concentrations up to 10 nM when tested for in situ [3H]clozapine displacement in brain tissue from WT and $D_1$-DREADD mice.

JHU37152 activates hM3Dq and hM4Di with high potency and efficacy in fluorescent and BRET-based assays in HEK-293 cells ($EC_{50}$ values are 5 and 0.5 nM at hM3Dq and hM4Di respectively.

**Occupancy**

JHU37152 exhibits high in vivo DREADD occupancy and was not reported to be a P-gp substrate.

**In vivo application**

JHU37152 is reported to be a potent in vivo DREADD agonist, which selectively inhibits locomotor activity in $D_1$-hM3Dq and $D_1$-hM4Di mice without any significant locomotor effects observed in wild type (WT) mice (at doses ranging 0.01 - 1 mg/kg).

It also produces robust and selective increases in hM3Dq-stimulated locomotion in rats expressing hM3Dq in tyrosine hydroxylase expressing neurons (at doses ranging 0.01 – 0.3 mg/kg).

While its selectivity is not ideal (i.e. comparable to clozapine), its high in vivo potency allows for dose adjustments with minimal off-target effects. The compound exhibits promising characteristics for DREADD use in monkeys.

Water soluble version also available.

Sold under license from the NIH, US patent pending 62/627,527

## Solubility & Handling

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|---|---|
| **Storage instructions** | Room temperature |

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| **Solubility overview** | Soluble in DMSO (100 mM) |
| **Important** | This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not for human or veterinary use |

## Chemical Data

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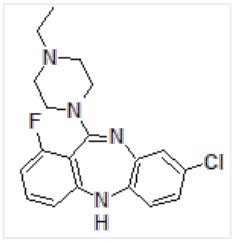
|---|---|
| **Chemical name** | 8-chloro-11-(4-ethylpiperazin-1-yl)-1-fluoro-5H-dibenzo[b,e][1,4]diazepine |
| **Molecular Weight** | 358.84 |
| **Chemical structure** |  |
| **Molecular Formula** | $C_{19}H_{20}ClFN_4$ |
| **CAS Number** | 2369979-67-7 |
| **PubChem identifier** | 0 |
| **SMILES** | CCN1CCN(CC1)C2=Nc4cc(Cl)ccc4Nc3cccc(F)c23 |
| **Source** | Synthetic |
| **InChi** | InChI=1S/C19H20ClFN4/c1-2-24-8-10-25(11-9-24)19-18-14(21)4-3-5-16(18)22-15-7-6-13(20)12-17(15)23-19/h3-7,12,22H,2,8-11H2,1H3 |
| **InChiKey** | NZMZJNNWMSYDNX-UHFFFAOYSA-N |
| **Appearance** | Yellow solid |
| **Licensing details** | Sold under license from the NIH, US patent pending 62/627,527 |

## References


**Chemogenetic ligands for translational neurotheranostics**

Bonaventura et al (2018) bioRxiv doi: https://doi.org/10.1101/487

**High-potency ligands for DREADD imaging and activation in rodents and monkeys.**

Bonaventura et al (2019) Nat Commun. 10(1)
**PubMedID** 31604917

**0067 Humanized Chemogenetic Approach to Treat Sleep Apnea**

Curado et al (2019) Sleep (42)

**OP-01-02 Graft-host synaptic connectivity can be chemogenetically inhibited with clinically relevant activators to eliminate graft-induced dyskinesias (GID) without loosing anti-parkinsonian benefits of dopaminergic grafts**

Subramanian et al (2019) World Congress On Parkinson's Disease And Related Disorders 2019 Poster abstract

**DREADDs: The Power of the Lock, the Weakness of the Key. Favoring the Pursuit of Specific Conditions Rather than Specific Ligands.**

Goutaudier et al (2019) eNeuro 6
**PubMedID** 31562177