

# **Data Sheet**

Product Name: VU041

 $\begin{array}{lll} \textbf{Cat. No.:} & \textbf{CS-0067612} \\ \textbf{CAS No.:} & 332943-64-3 \\ \textbf{Molecular Formula:} & \textbf{C}_{19}\textbf{H}_{20}\textbf{F}_3\textbf{N}_3\textbf{O} \\ \end{array}$ 

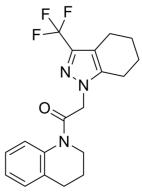
Molecular Weight: 363.38

Target: Parasite; Potassium Channel

Pathway: Anti-infection; Membrane Transporter/Ion Channel

Solubility: DMSO: 20 mg/mL (55.04 mM; ultrasonic and warming and heat

to 60°C)



### **BIOLOGICAL ACTIVITY:**

VU041 is a first submicromolar-affinity inhibitor of *Anopheles (An.) gambiae* and *Aedes (Ae.) aegypti* **inward rectifier potassium 1 (Kir1) channels** with **IC**<sub>50</sub> values of 2.5 μM and 1.7 μM, respectively. VU041 inhibits appreciably is mammalian **Kir2.1** (**IC**<sub>50</sub> of 12.7 μM), and has less inhibitory effect on mammalian Kir1.1, Kir4.1, Kir6.2/SUR1, and Kir7.1. VU041 also induces impaired Malpighian tubule function<sup>[1]</sup>. IC50 & Target: IC50: 2.5 μM (*Anopheles (An.) gambiae* Kir1 channels), 1.7 μM (*Aedes (Ae.) aegypti* Kir1 channels) and 12.7 μ M (Mammalian Kir2.1)<sup>[1]</sup> *In Vitro*: VU041 is only moderately metabolized by cytochrome P450 enzymes and does not appear to be metabolized by esterases. VU041 is the first small-molecule inhibitor of mosquito Kir1 channels that exhibits topical toxicity in both insecticide-susceptible and -resistant lines of mosquitoes<sup>[1]</sup>. *In Vivo*: Topical VU041 application to adult female mosquitoes of both species inhibits their fecundity. Importantly, VU041 is selective for mosquito Kir channels over mammalian Kir channel orthologs and non-lethal to adult honey bees (Apis mellifera). The in vivo experiments of blood meal processing and diuretic capacity suggest that one mechanism of action of VU041 is the disruption of excretory functions mediated by Malpighian tubules<sup>[1]</sup>.

#### References:

[1]. Swale DR, et al. An insecticide resistance-breaking mosquitocide targeting inward rectifier potassium channels in vectors of Zika virus and malaria. Sci Rep. 2016 Nov 16;6:36954.

#### **CAIndexNames:**

Ethanone, 1-(3,4-dihydro-1(2H)-quinolinyl)-2-[4,5,6,7-tetrahydro-3-(trifluoromethyl)-1H-indazol-1-yl]-

## SMILES:

FC(C1=NN(CC(N2CCCC3=C2C=CC=C3)=O)C4=C1CCCC4)(F)F

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

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