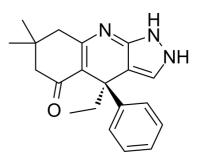


# **Data Sheet**

Product Name:	BRD5648
Cat. No.:	CS-0114013
CAS No.:	2056261-42-6
Molecular Formula:	C <sub>20</sub> H <sub>23</sub> N <sub>3</sub> O
Molecular Weight:	321.42
Target:	GSK-3
Pathway:	PI3K/Akt/mTOR; Stem Cell/Wnt
Solubility:	DMSO : 300 mg/mL (933.36 mM; Need ultrasonic)



### **BIOLOGICAL ACTIVITY:**

BRD5648 ((R)-BRD0705) is a negative control of BRD0705. BRD0705 is a potent, paralog selective and orally active GSK3 $\alpha$  inhibitor with an IC<sub>50</sub> of 66 nM and a K<sub>d</sub> of 4.8  $\mu$ M. BRD0705 displays increased selectivity for GSK3 $\alpha$  (8-fold) versus GSK3 $\beta$  (IC<sub>50</sub> of 515 nM). BRD0705 can be used for acute myeloid leukemia (AML)<sup>[1][2]</sup>. **In Vitro:** BRD5648, the inactive enantiomer of BRD0705, does not induce changes in enzyme phosphorylation or total  $\beta$ -catenin protein stabilization<sup>[1]</sup>.

#### **References:**

[1]. Wagner FF, et al. Exploiting an Asp-Glu "switch" in glycogen synthase kinase 3 to design paralog-selective inhibitors for use in acute myeloid leukemia. Sci Transl Med. 2018 Mar 7;10(431). pii: eaam8460.

[2]. Wagner FF, et al. Exploiting an Asp-Glu "switch" in glycogen synthase kinase 3 to design paralog-selective inhibitors for use in acute myeloid leukemia. Sci Transl Med. 2018 Mar 7;10(431). pii: eaam8460.

#### **CAIndexNames:**

5H-Pyrazolo[3,4-b]quinolin-5-one, 4-ethyl-1,2,4,6,7,8-hexahydro-7,7-dimethyl-4-phenyl-, (4R)-

## SMILES:

O=C1C2=C(N=C3C([C@@]2(CC)C4=CC=CC=C4)=CNN3)CC(C)(C)C1

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

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