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**Product Data Sheet**

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Product Name: BACE1-IN-4

Cat. No.: GC35455

**Chemical Properties**

Cas. No. 2361157-92-6

SMILES NC1=N[C@@](C2=CC(NC(C3=NC=C(OCF)N=C3)=O)=CC=C2F)(C)C4(CCS(CC4)(=O)=O)CS1Formula C<sub>21</sub>H<sub>23</sub>F<sub>2</sub>N<sub>5</sub>O<sub>4</sub>S<sub>2</sub>

M.Wt

511.57

Solubility Soluble in DMSO

Storage

Store at -20°C

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure **Background**

BACE1-IN-4 is a potent and highly selective BACE1 inhibitor, with an IC<sub>50</sub> of 3.8 nM and a K<sub>i</sub> of 1.9 nM, more selective at BACE1 over BACE2. Anti-Alzheimer's disease[1]. IC<sub>50</sub>: 3.8 nM (BACE1), 2090 nM (BACE2)[1] K<sub>i</sub>: 1.9 nM (BACE1), 1740 nM (BACE2)[1]

BACE1-IN-4 (Compound 22) is a potent and highly selective BACE1 inhibitor, with an IC<sub>50</sub> of 3.8 nM and a K<sub>i</sub> of 1.9 nM, more selective at BACE1 over BACE2 (IC<sub>50</sub>, 2090 nM; K<sub>i</sub>, 1740 nM)[1].

[1]. Fujimoto K, et al. Structure-Based Design of Selective  $\beta$ -Site Amyloid Precursor Protein Cleaving Enzyme 1 (BACE1) Inhibitors: Targeting the Flap to Gain Selectivity over BACE2. J Med Chem. 2019 May 23;62(10):5080-5095.

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

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