# Product data sheet

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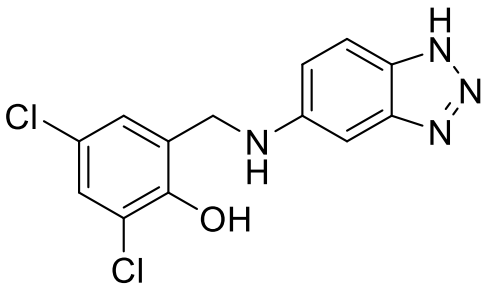
|---|---|
| MedKoo Cat#: 526932<br>Name: IC87201<br>CAS: 866927-10-8<br>Chemical Formula: $C_{13}H_{10}Cl_2N_4O$<br>Exact Mass: 308.0232<br>Molecular Weight: 309.15 |  |
| Product supplied as: | Powder |
| Purity (by HPLC): | ≥ 98% |
| Shipping conditions | Ambient temperature |
| Storage conditions: | Powder: -20°C 3 years; 4°C 2 years. |
| | In solvent: -80°C 3 months; -20°C 2 weeks. |

**1. Product description:**
IC87201 is a nNOS-PDZ/PSD-95-PDZ inhibitor. IC87201 showed great promise in cellular experiments and animal models of ischemic stroke and pain. IC87201 inhibited the in vitro binding of nNOS with PSD95, without inhibiting nNOS catalytic activity. nNOS-PSD95 interaction is important in maintaining hypersensitivity in acute and chronic pain. Disruption of the nNOS-PSD95 interaction provides a novel approach to obtain selective anti-hyperalgesic compounds.

**2. CoA, QC data, SDS, and handling instruction**
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

**3. Solubility data**

| Solvent | Max Conc. mg/mL | Max Conc. mM |
|---|---|---|
| DMF | 30.0 | 97.04 |
| DMSO | 29.0 | 93.81 |
| DMSO:PBS (pH 7.2) (1:3) | 0.25 | 0.81 |
| Ethanol | 1.0 | 3.23 |

**4. Stock solution preparation table:**

| **Concentration / Solvent Volume / Mass** | **1 mg** | **5 mg** | **10 mg** |
|---|---|---|---|
| 1 mM | 3.23 mL | 16.17 mL | 32.35 mL |
| 5 mM | 0.65 mL | 3.23 mL | 6.47 mL |
| 10 mM | 0.32 mL | 1.62 mL | 3.23 mL |
| 50 mM | 0.07 mL | 0.32 mL | 0.65 mL |

**5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator**
Please refer the product web page under section of "Calculator"

**6. Recommended literature which reported protocols for in vitro and in vivo study**
In vitro study

1. Florio SK, Loh C, Huang SM, Iwamaye AE, Kitto KF, Fowler KW, Treiberg JA, Hayflick JS, Walker JM, Fairbanks CA, Lai Y. Disruption of nNOS-PSD95 protein-protein interaction inhibits acute thermal hyperalgesia and chronic mechanical allodynia in rodents. Br J Pharmacol. 2009 Sep;158(2):494-506. doi: 10.1111/j.1476-5381.2009.00300.x. PMID: 19732061; PMCID: PMC2757689.

In vivo study

1. Carey LM, Lee WH, Gutierrez T, Kulkarni PM, Thakur GA, Lai YY, Hohmann AG. Small molecule inhibitors of PSD95-nNOS protein-protein interactions suppress formalin-evoked Fos protein expression and nociceptive behavior in rats. Neuroscience. 2017 May 4;349:303-317. doi: 10.1016/j.neuroscience.2017.02.055. Epub 2017 Mar 8. PMID: 28285942; PMCID: PMC5518314.

2. Smith AE, Xu Z, Lai YY, Kulkarni PM, Thakur GA, Hohmann AG, Crystal JD. Source memory in rats is impaired by an NMDA receptor antagonist but not by PSD95-nNOS protein-protein interaction inhibitors. Behav Brain Res. 2016 May 15;305:23-9. doi: 10.1016/j.bbr.2016.02.021. Epub 2016 Feb 22. PMID: 26909849; PMCID: PMC4808404.

**7. Bioactivity**

Biological target:

IC87201, an inhibitor of PSD95-nNOS protein-protein interactions, suppresses NMDAR-dependent NO and cGMP formation.

In vitro activity

The resulting compound, IC87201, 2-[(1H-benzotriazol-5-ylamino)-methyl]-4,6-dichloro-phenol (Figure 1A), showed dose-dependent inhibition of nNOS–PSD95 binding (Figure 1B) with an IC50 of 31 µM (95% confidence interval 25–38 µM, n= 5).

Reference: Br J Pharmacol. 2009 Sep;158(2):494-506. https://pubmed.ncbi.nlm.nih.gov/19732061/

In vivo activity

IC87201 and ZL006, but not ZL007, suppressed phase 2 of formalin-evoked pain behavior and decreased the number of formalin-induced Fos-like immunoreactive cells in spinal dorsal horn regions associated with nociceptive processing.

Reference: Neuroscience. 2017 May 4;349:303-317. https://pubmed.ncbi.nlm.nih.gov/28285942/

*Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.*