

Product data sheet



MedKoo Cat#: 531120 Name: DAA1106 CAS#: 220551-92-8 Chemical Formula: C ₂₃ H ₂₂ FNO ₄ Exact Mass: 395.1533 Molecular Weight: 395.4304		
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:

DAA1106 is a potent and selective ligand for peripheral benzodiazepine receptor (PBR), as a potent and selective agonist at the peripheral benzodiazepine receptor.

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
DMSO	56.0	141.62

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.53 mL	12.64 mL	25.29 mL
5 mM	0.51 mL	2.53 mL	5.06 mL
10 mM	0.25 mL	1.26 mL	2.53 mL
50 mM	0.05 mL	0.25 mL	0.51 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

- Venneti S, Wagner AK, Wang G, Slagel SL, Chen X, Lopresti BJ, Mathis CA, Wiley CA. The high affinity peripheral benzodiazepine receptor ligand DAA1106 binds specifically to microglia in a rat model of traumatic brain injury: implications for PET imaging. *Exp Neurol*. 2007 Sep;207(1):118-27. doi: 10.1016/j.expneurol.2007.06.003. Epub 2007 Jun 19. PMID: 17658516; PMCID: PMC2042945.
- Venneti S, Wang G, Wiley CA. The high affinity peripheral benzodiazepine receptor ligand DAA1106 binds to activated and infected brain macrophages in areas of synaptic degeneration: implications for PET imaging of neuroinflammation in lentiviral encephalitis. *Neurobiol Dis*. 2008 Feb;29(2):232-41. doi: 10.1016/j.nbd.2007.08.016. Epub 2007 Sep 7. PMID: 17920902; PMCID: PMC2258458.

In vivo study

- Zhang MR, Kida T, Noguchi J, Furutsuka K, Maeda J, Suhara T, Suzuki K. [(11C)DAA1106: radiosynthesis and in vivo binding to peripheral benzodiazepine receptors in mouse brain. *Nucl Med Biol*. 2003 Jul;30(5):513-9. doi: 10.1016/s0969-8051(03)00016-7. PMID: 12831989.

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7. Bioactivity

Biological target:

DAA1106 is a potent and selective ligand for peripheral benzodiazepine receptor (PBR) and is a potent and selective agonist at the peripheral benzodiazepine receptor.

In vitro activity

This study wanted to determine the relative contributions of astrocytes and activated brain macrophages to [3H]DAA1106 binding. Since macrophages are the predominant infected cells in the brain in lentiviral encephalitis (Ellis et al., 2007), the association between infected macrophages and [3H]DAA1106 binding in the brain was also determined. Immunostaining for astrocytes (GFAP), activated brain macrophages (CD68) and the SIV envelope protein gp110 with [3H]DAA1106 autoradiography were combined on frozen brain sections obtained from the frontal cortex of SIVE macaques. [3H]DAA1106 binding overlapped with CD68 labeled activated macrophages (Figure 4A) and SIV-infected macrophages (Figure 4C), but not with GFAP labeled astrocytes (Figure 4B). Similar results including colocalization of HIV infected cells with [3H]DAA1106 autoradiography were seen in HIVE brain tissues (Figure 4D). Next, it was tested whether [3H]DAA1106 binding in homogenized brain tissue correlated with the abundance of astrocytes or activated macrophages or SIV-infected macrophages labeled with GFAP, CD68 and SIV gp110 respectively. Each cell-type was quantified using confocal microscopy and correlated with [3H]DAA1106 Bmax values obtained from the same brain regions in the same macaques. [3H]DAA1106 binding correlated significantly with the abundance of SIV-infected macrophages ($r=0.9646$; $p=0.0084$) and activated macrophages ($r=0.8308$; $p=0.0160$) but weakly with the abundance of GFAP-stained astrocytes ($r=0.6755$; $p=0.0958$) (Table 2).

Reference: Neurobiol Dis. 2008 Feb; 29(2): 232–241. <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2258458/>

In vivo activity

DAA1106 (N-(2,5-Dimethoxybenzyl)-N-(5-fluoro-2-phenoxyphenyl)acetamide), is a potent and selective ligand for peripheral benzodiazepine receptors (PBR) in mitochondrial fractions of rat ($K(i)=0.043$ nM) and monkey ($K(i)=0.188$ nM) brains. After iv injection of [(11)C]DAA1106 into mice, high accumulations of radioactivity were found in the olfactory bulb and cerebellum, the high PBR density regions in the brain. Coinjection of [(11)C]DAA1106 with unlabeled DAA1106 and PBR-selective PK11195 displayed a significant reduction of radioactivity, suggesting a high specific binding of [(11)C]DAA1106 to PBR. Although this tracer was rapidly metabolized in the plasma, only [(11)C]DAA1106 was detected in the brain tissues, suggesting the specific binding in the brain due to the tracer itself. These findings revealed that [(11)C]DAA1106 is a potential and selective positron emitting radioligand for PBR.

Reference: Nucl Med Biol. 2003 Jul;30(5):513-9. <https://pubmed.ncbi.nlm.nih.gov/12831989/>

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.