

# Product data sheet



MedKoo Cat#: 563653 Name: NS3861 CAS: 216853-60-0 Chemical Formula: C <sub>16</sub> H <sub>18</sub> BrNO <sub>4</sub> S Exact Mass: 399.014 Molecular Weight: 400.287		
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:

NS3861 is an  $\alpha 3\beta 2$  full agonist and an  $\alpha 3\beta 4$  partial agonist.

## 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	70.02	174.91
Water	20.01	49.99

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.50 mL	12.49 mL	24.98 mL
5 mM	0.50 mL	2.50 mL	5.00 mL
10 mM	0.25 mL	1.25 mL	2.50 mL
50 mM	0.05 mL	0.25 mL	0.50 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. Harpsøe K, Hald H, Timmermann DB, Jensen ML, Dyhring T, Nielsen EØ, Peters D, Balle T, Gajhede M, Kastrup JS, Ahring PK. Molecular determinants of subtype-selective efficacies of cytisine and the novel compound NS3861 at heteromeric nicotinic acetylcholine receptors. *J Biol Chem.* 2013 Jan 25;288(4):2559-70. doi: 10.1074/jbc.M112.436337. Epub 2012 Dec 10. PMID: 23229547; PMCID: PMC3554923.

### In vivo study

1. Gade AR, Kang M, Khan F, Grider JR, Damaj MI, Dewey WL, Akbarali HI. Enhanced Sensitivity of  $\alpha 3\beta 4$  Nicotinic Receptors in Enteric Neurons after Long-Term Morphine: Implication for Opioid-Induced Constipation. *J Pharmacol Exp Ther.* 2016 Jun;357(3):520-8. doi: 10.1124/jpet.116.233304. Epub 2016 Apr 11. PMID: 27068812; PMCID: PMC4885510.

## 7. Bioactivity

### Biological target:

NS3861 fumarate is an agonist of nicotinic acetylcholine receptors (nAChRs) and binds with high affinity to heteromeric  $\alpha 3\beta 4$  nAChR.

### In vitro activity

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The novel compound NS3861 and cytosine are agonists of nicotinic acetylcholine receptors (nAChRs) and both bind with high affinity to heteromeric  $\alpha 3\beta 4$  and  $\alpha 4\beta 2$  nAChRs. The maximal efficacy of NS3861 appeared solely dependent on the nature of the ligand-binding domain, whereas efficacy of cytosine was additionally affected by the nature of the  $\beta$ -subunit transmembrane domain.

Reference: J Biol Chem. 2013 Jan 25;288(4):2559-70. <https://pubmed.ncbi.nlm.nih.gov/23229547/>

## In vivo activity

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The present study examined whether the increased sensitivity to nicotine could be observed in single enteric neurons after long-term morphine exposure, determined the subunits in mouse enteric neurons, and examined the effect of nicotine in reversing opioid-induced constipation. NS3861, a partial agonist at  $\alpha 3\beta 4$  nAChR, enhanced fecal pellet expulsion in a dose-dependent manner in mice that received long-term, but not short-term, morphine treatment.

Reference: J Pharmacol Exp Ther. 2016 Jun;357(3):520-8. <https://pubmed.ncbi.nlm.nih.gov/27068812/>

*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.*