# **Product data sheet**



| MedKoo Cat#: 532313   |  |     |
|---|--|-----|
| Name: NCX-4016  |  |     |
| CAS: 175033-36-0  |  | 0 . |
|   |  |     |
| Chemical Formula: C <sub>16</sub> H <sub>13</sub> NO <sub>7</sub> |  |     |
| Exact Mass: 331.0692  |  |     |
| Molecular Weight: 331.28  |  |     |
| 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:

NCX-4016 is a nitroderivative of aspirin that combines cyclooxygenase inhibitor with an NO donor. NCX 4016 improves postischemic ventricular dysfunction and to reduce myocardial infarct size in rabbit. NCX-4016 is an NO-NSAID type compound.

## 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 |
|---------|-----------------|--------------|
| TBD     | TBD             | TBD          |

4. Stock solution preparation table:

| Concentration / Solvent Volume / Mass | 1 mg    | 5 mg     | 10 mg    |
|---------------------------------------|---------|----------|----------|
| 1 mM                                  | 3.02 mL | 15.09 mL | 30.19 mL |
| 5 mM                                  | 0.60 mL | 3.02 mL  | 6.04 mL  |
| 10 mM                                 | 0.30 mL | 1.51 mL  | 3.02 mL  |
| 50 mM                                 | 0.06 mL | 0.30 mL  | 0.60 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. Selvendiran K, Bratasz A, Tong L, Ignarro LJ, Kuppusamy P. NCX-4016, a nitro-derivative of aspirin, inhibits EGFR and STAT3 signaling and modulates Bcl-2 proteins in cisplatin-resistant human ovarian cancer cells and xenografts. Cell Cycle. 2008 Jan 1;7(1):81-8. doi: 10.4161/cc.7.1.5103. Epub 2007 Sep 28. PMID: 18196976; PMCID: PMC2890223.
- 2. Corazzi T, Leone M, Maucci R, Corazzi L, Gresele P. Direct and irreversible inhibition of cyclooxygenase-1 by nitroaspirin (NCX 4016). J Pharmacol Exp Ther. 2005 Dec;315(3):1331-7. doi: 10.1124/jpet.105.089896. Epub 2005 Sep 6. PMID: 16144976.

#### In vivo study

- 1. Rambotti MG, Mariucci G, Tantucci M, Ambrosini MV. Ultracytochemical demonstration of soluble guanylate cyclase activation in rat aorta by NCX4016, a NO-releasing aspirin derivative. J Submicrosc Cytol Pathol. 2006 Jun-Sep;38(2-3):149-54. PMID: 17784643.
- 2. Bertuglia S, Giusti A, Del Soldato P. Antioxidant activity of nitro derivative of aspirin against ischemia-reperfusion in hamster cheek pouch microcirculation. Am J Physiol Gastrointest Liver Physiol. 2004 Mar;286(3):G437-43. doi: 10.1152/ajpgi.00339.2003. Epub 2003 Oct 16. PMID: 14563672.

#### 7. Bioactivity

Biological target:

NCX-4016 is a nitroderivative of aspirin that combines cyclooxygenase inhibitor with an NO donor.

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### In vitro activity

Dialysis experiments showed that oCOX-1 inhibition by NCX 4016, similar to aspirin, is irreversible. Reversible COX inhibitors (indomethacin) or salicylic acid incubated with the enzyme before NCX 4016 prevent the irreversible inhibition of oCOX-1 by NCX 4016 as well as by aspirin. In conclusion, these data show that NCX 4016 acts as a direct and irreversible inhibitor of COX-1 and that the presence of a spacer and NO-donating moiety in the molecule slows the kinetics of COX-1 inhibition by NCX 4016, compared with aspirin.

Reference: J Pharmacol Exp Ther. 2005 Dec;315(3):1331-7. https://pubmed.ncbi.nlm.nih.gov/16144976/

#### In vivo activity

Hamsters were treated with NCX-4016 (100 mg/kg or 30 mg.kg(-1).day(-1) for 5 days po) or DETA-NO (0.5 mg/kg). Mean arterial blood pressure increased slightly but significantly after NCX-4016 treatment. During 5- and 15-min reperfusion, lipid peroxides in the systemic blood increased by 72 and 89% vs. baseline, respectively, and were still higher than in basal conditions after 30-min reperfusion in the I/R group. Pretreatment with NCX-4016 maintained ROS at normal levels; increased arteriolar diameter, blood flow, and PCL; and decreased leukocyte adhesion (P < 0.05).

Reference: Am J Physiol Gastrointest Liver Physiol. 2004 Mar;286(3):G437-43. https://pubmed.ncbi.nlm.nih.gov/14563672/

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.