

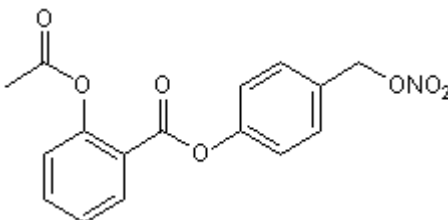
Certificate of Analysis

Product Name: NCX 4040
CAS Number: 287118-97-2
IUPAC Name: 2-(Acetyloxy)benzoic acid 4-[(nitrooxy)methyl]phenyl ester

Catalog No.: 4531 **Batch No.:** 1

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₃NO₇
Batch Molecular Weight: 331.28
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 5 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

Melting Point: Between 90 - 92°C
HPLC: Shows 99.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.01	3.96	4.23
Found	57.96	3.94	4.19

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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IUPAC Name: 2-(Acetyloxy)benzoic acid 4-[(nitrooxy)methyl]phenyl ester

Description:

NO-donating aspirin; anti-inflammatory. Blocks inflammatory mediator production in isolated human monocytes (IC₅₀ values are 0.07, 0.13, 0.15 and 0.18 μM for IL-1β, PGE₂, IL-10 and TNF-α respectively). Decreases COX-2 expression (IC₅₀ = 0.13 μM); disrupts proteasome-mediated degradation of IκB-α. Antiproliferative in HCT116 colon cancer cells; sensitizes drug-resistant ovarian tumor cells to cisplatin (Cat. No. 2251).

Physical and Chemical Properties:

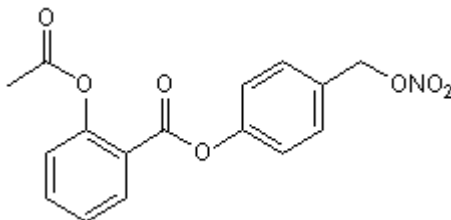
Batch Molecular Formula: C₁₆H₁₃NO₇

Batch Molecular Weight: 331.28

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Yamakawa et al (2008) Growth inhibition of human colon cancer cell line HCT116 by bis[2-(acetylamino)phenyl] disulfide and its action mechanism. *Biol.Pharm.Bull.* **31** 916. PMID: 18451518.

Bratasz et al (2008) NCX-4040, a nitric oxide-releasing aspirin, sensitizes drug-resistant human ovarian xenograft tumors to cisplatin by depletion of cellular thiols. *J.Transl.Med.* **6** 9. PMID: 18302761.

Gao et al (2008) Immunomodulatory activity of synthetic triterpenoids: inhibition of lymphocyte proliferation, cell-mediated cytotoxicity, and cytokine gene expression through suppression of NF-κB. *Immunopharmacol.Immunotoxicol.* **30** 581. PMID: 18608528.

Ricciotti et al (2010) NCX 4040, a nitric oxide-donating aspirin, exerts anti-inflammatory effects through inhibition of I kappa B-alpha degradation in human monocytes. *J.Immunol.* **184** 2140. PMID: 20065114.

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 5 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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