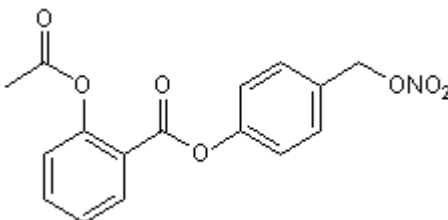


**Product Name:** NCX 4040  
**CAS Number:** 287118-97-2  
**IUPAC Name:** 2-(Acetyloxy)benzoic acid 4-[(nitrooxy)methyl]phenyl ester

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

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>16</sub>H<sub>13</sub>NO<sub>7</sub>  
**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  
**<sup>1</sup>H 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

**Product Name:** NCX 4040

**Catalog No.:** 4531

**Batch No.:** 1

CAS Number: 287118-97-2

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 (IC<sub>50</sub> values are 0.07, 0.13, 0.15 and 0.18 μM for IL-1β, PGE<sub>2</sub>, IL-10 and TNF-α respectively). Decreases COX-2 expression (IC<sub>50</sub> = 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:**

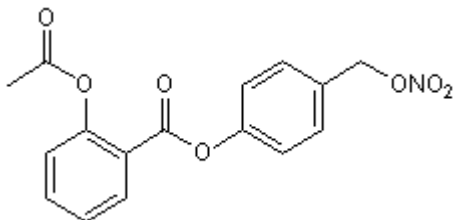
Batch Molecular Formula: C<sub>16</sub>H<sub>13</sub>NO<sub>7</sub>

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.

**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.

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

Tocris Bioscience is an R&D Systems company

USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373

[www.RnDSystems.com](http://www.RnDSystems.com)