

**Product Name:** SMBA 1

**Catalog No.:** 5314

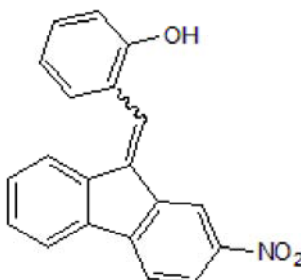
**Batch No.:** 1

CAS Number: 906440-37-7

IUPAC Name: 2-[(2-Nitro-9H-fluorene-9-ylidene)methyl]phenol

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>20</sub>H<sub>13</sub>NO<sub>3</sub>·¼H<sub>2</sub>O  
**Batch Molecular Weight:** 319.82  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 100 mM  
ethanol to 10 mM with gentle warming  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.5 (Dichloromethane:Petrol Ether [4:1])  
**HPLC:** Shows 99.7% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

Microanalysis:	Carbon Hydrogen Nitrogen		
	Carbon	Hydrogen	Nitrogen
Theoretical	75.11	4.25	4.38
Found	75.28	4.15	4.43

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

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**Description:**

High affinity and selective activator of Bax ( $K_i = 43.3$  nM). Binds to the S184 binding pocket to block Bax phosphorylation. Does not bind to other Bcl-2 family members, including Bcl-2, Bak and Bid. Facilitates Bax insertion into the mitochondrial membrane and promotes Bax-dependent cytochrome c release. Induces apoptosis in lung cancer cell lines expressing high levels of Bax selectively over normal cells expressing low levels of Bax. Represses tumor growth of A549 lung cancer xenografts in mice.

**Physical and Chemical Properties:**

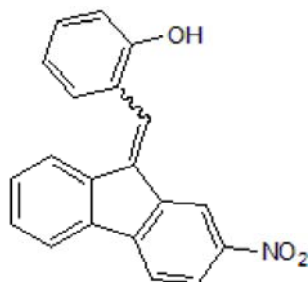
Batch Molecular Formula:  $C_{20}H_{13}NO_3 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 319.82

Physical Appearance: Yellow solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**References:**

Xin *et al* (2014) Small-molecule Bax agonists for cancer therapy. *Nat. Commun.* **5** 4935. PMID: 25230299.

**Storage:** Store at  $-20^{\circ}C$

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 10 mM with gentle warming

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a  $45-60^{\circ}C$  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  $-20^{\circ}C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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