

Product Name: PA 452

Catalog No.: 5086

Batch No.: 1

CAS Number: 457657-34-0

IUPAC Name: 2-[[3-(Hexyloxy)-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl]methylamino]-5-pyrimidinecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{37}N_3O_3 \cdot \frac{1}{4}H_2O$

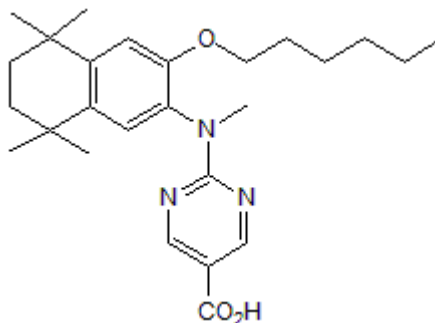
Batch Molecular Weight: 444.09

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 10 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.32$ (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows >99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 70.32 | 8.51 | 9.46 |
| Found | 70.38 | 8.3 | 9.58 |

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Description:

RXR antagonist ($pA_2 = 7.11$). Triggers dissociation of RXR tetramers. Attenuates cell proliferation and induces apoptosis in MCF-7 breast cancer cells.

Physical and Chemical Properties:

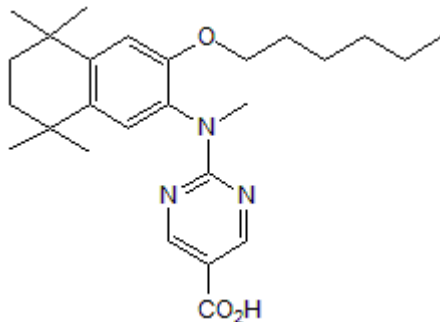
Batch Molecular Formula: $C_{26}H_{37}N_3O_3 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 444.09

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 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.

References:

Takahashi et al (2002) Novel retinoid X receptor antagonists: specific inhibition of retinoid synergism in RXR-RAR heterodimer actions. *J.Med.Chem.* **45** 3327. PMID: 12139443.

Yasmin et al (2010) Inhibition of mammary carcinoma cell growth by RXR is mediated by the receptor's oligomeric switch. *J.Mol.Biol.* **397** 1121. PMID: 20188110.

Nakayama et al (2011) Discovery of a potent retinoid X receptor antagonist structurally closely related to RXR agonist NEt-3IBIB. *J.Med.Chem.Lett* **2** 896. PMID: 24900278.

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