Certificate of Analysis

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: $C_{26}H_{37}N_3O_3.¼H_2O$

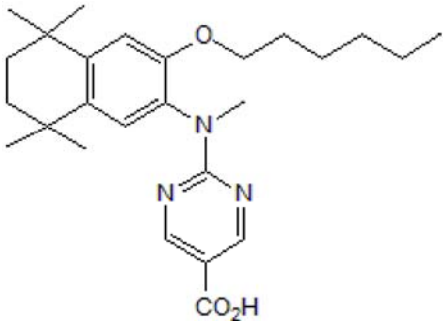
Batch Molecular Weight: 444.09

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

^{1}H 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:

PA 452 is an 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:

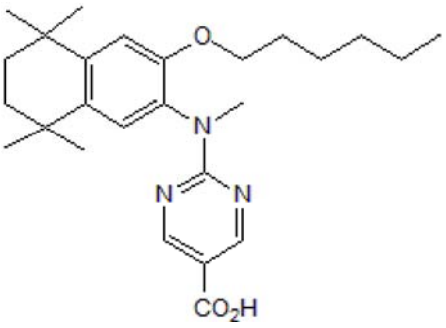
Batch Molecular Formula: $C_{26}H_{37}N_3O_3.¼H_2O$

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:

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.

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.

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.