

Certificate of Analysis

Product Name: ER 50891

Catalog No.: 3823

Batch No.: 1

CAS Number: 187400-85-7

IUPAC Name: 4-[5-[8-(1-Methylethyl)-4-phenyl-2-quinolinyl]-1*H*-pyrrolo-2-benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{24}N_2O_2 \cdot \frac{1}{4}H_2O$

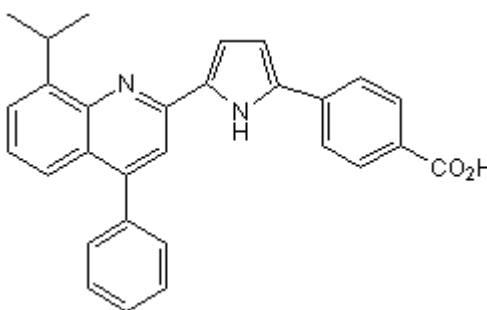
Batch Molecular Weight: 437.01

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.39$ (Dichloromethane:Methanol [95:5])

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	79.7	5.65	6.41
Found	79.77	5.57	6.58

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Description:

Antagonist of RAR α receptors (IC₅₀ = 31.2 nM). Displays selective affinity for RAR α (relative IC₅₀ values are 1.8, 432 and 535 nM for RAR α , RAR γ and RAR β respectively).

Physical and Chemical Properties:

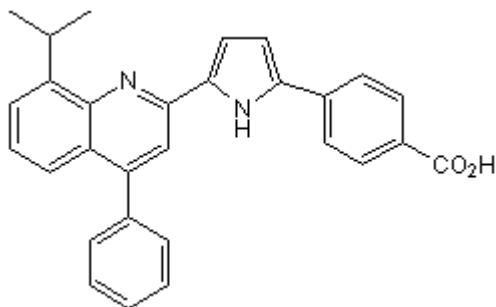
Batch Molecular Formula: C₂₉H₂₄N₂O₂·¼H₂O

Batch Molecular Weight: 437.01

Physical Appearance: Orange solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 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:

Kikuchi et al (2001) Syntheses and evaluation of quinoline derivatives as novel retinoic acid receptor α antagonists. *Bioorg.Med.Chem.Lett.* **11** 1215. PMID: 11354380.

Ren et al (2005) Impaired retinoic acid (RA) signal leads to RAR β 2 epigenetic silencing and RA resistance. *Mol.Cell.Biol.* **25** 10591. PMID: 16287870.

Somenzi et al (2007) Disruption of retinoic acid receptor alpha reveals the growth promoter face of retinoic acid. *PLoS ONE* **9** e836. PMID: 17786207.

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