

Product Name: LE 135

Catalog No.: 2021

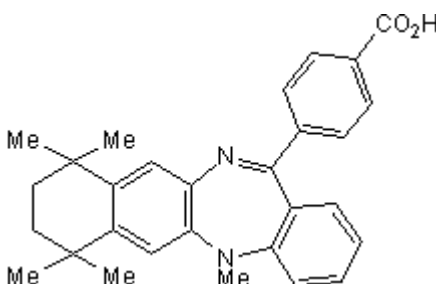
Batch No.: 2

CAS Number: 155877-83-1

IUPAC Name: 4-(7,8,9,10-Tetrahydro-5,7,7,10,10-pentamethyl-5H-benzo[e]naphtho[2,3-b][1,4]diazepin-13-yl)benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₃₀N₂O₂
Batch Molecular Weight: 438.56
Physical Appearance: Orange solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.1 (Ethyl acetate:Petroleum ether [9:1])
HPLC: Shows 97.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	79.42	6.89	6.39
Found	79.41	6.89	6.43

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

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Description:

Retinoic acid antagonist; displays moderate selectivity for RAR β over RAR α (K_i values are 0.22 and 1.4 μ M respectively). Highly selective over RAR γ and RXR α . Inhibits human HL-60 leukemia cell differentiation induced by Am80 (IC₅₀ = 150 nM).

Physical and Chemical Properties:

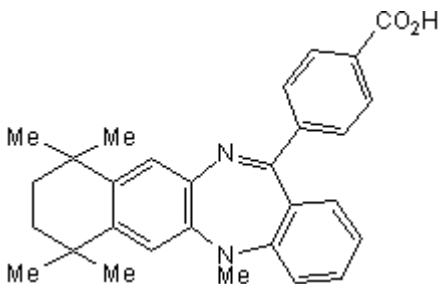
Batch Molecular Formula: C₂₉H₃₀N₂O₂

Batch Molecular Weight: 438.56

Physical Appearance: Orange solid

Minimum Purity: >97%

Batch Molecular Structure:



References:

Eyrolles et al (1994) Retinobenzoic acids. 6. Retinoid antagonists with heterocyclic ring. *J.Med.Chem.* **37** 1508. PMID: 8182710.

Umemiya et al (1997) Regulation of retinoidal actions by diazepinylbenzoic acids. Retinoid synergists which activate the RXR-RAR heterodimers. *J.Med.Chem.* **40** 4222. PMID: 9435893.

Li et al (1999) Identification of a novel class of retinoic acid receptor β -selective retinoid antagonists and their inhibitory effects on AP-1 activity and retinoic acid-induced apoptosis in human breast cancer cells. *J.Biol.Chem.* **274** 15360. PMID: 10336422.

Storage: Store at +4°C

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.

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