

Product Name: TAN 452

Catalog No.: 6729

Batch No.: 1

CAS Number: 892039-23-5

IUPAC Name: Ethyl (4*b*S,8*R*,8*a*S,14*b*R)-7-(cyclopropylmethyl)-5,6,7,8,8*a*,9,14,14*b*-octahydro-1,8*a*-dihydroxy-4,8-methanobenzofuro[2,3-*a*]pyrido[4,3-*b*]carbazole-12-carboxylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₃₀N₂O₅·1/4H₂O

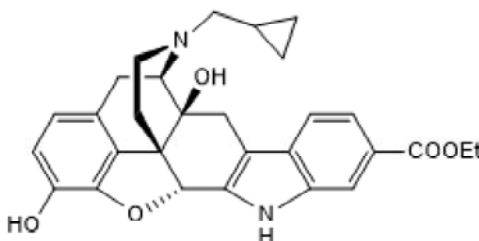
Batch Molecular Weight: 491.06

Physical Appearance: Beige solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.68 (Dichloromethane:Methanol [4:1])

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.93	6.26	5.7
Found	70.68	6.22	5.79

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

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Description:

Potent and selective peripherally acting δ opioid antagonist; K_i values are 0.47, 5.31 and 36.56 nM at hDOR, hKOR, and hMOR, respectively. K_b values are 0.21, 7.18 and 9.43 nM, respectively. Attenuates morphine-induced side effects in vivo. Antianalgesic.

Physical and Chemical Properties:

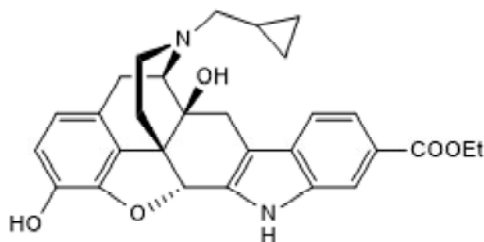
Batch Molecular Formula: $C_{29}H_{30}N_2O_5 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 491.06

Physical Appearance: Beige solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



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

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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 $45-60^{\circ}C$ 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.

References:

Lattanzi *et al* (2018) *In vitro* and *in vivo* pharmacological activities of 14-O-phenylpropyloxymorphone, a potent mixed $\mu/\delta/\kappa$ -opioid receptor agonist with reduced constipation in mice. *Front.Pharmacol.* **9** 10.3389/fphar.2018.0. PMID: 30233377.

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