

Product Name: ITE

Catalog No.: 1803

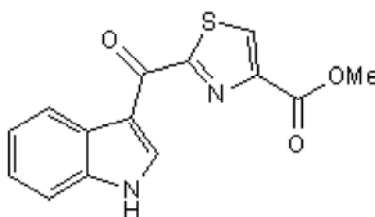
Batch No.: 12

CAS Number: 448906-42-1

IUPAC Name: 2-(1*H*-Indol-3-ylcarbonyl)-4-thiazolecarboxylic acid methyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₁₀N₂O₃S
Batch Molecular Weight: 286.3
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol [95:5])
HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.73	3.52	9.78
Found	58.51	3.46	9.58

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

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Description:

Endogenous aryl hydrocarbon receptor (AhR) agonist ($K_i = 3$ nM). Decreases Oct4 levels in U87 glioblastoma cells. Induces stem-like cancer cell differentiation in U87 tumor spheres and inhibits ovarian cancer cell proliferation in vitro. Suppresses tumor growth in U87 and OVCAR-3 cell xenografts in mice. Also inhibits TGF- β -induced human myofibroblast differentiation.

Physical and Chemical Properties:

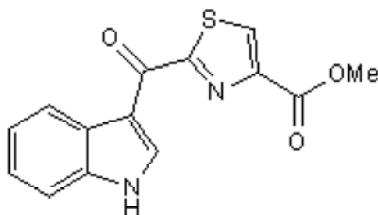
Batch Molecular Formula: C₁₄H₁₀N₂O₃S

Batch Molecular Weight: 286.3

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Cheng et al (2015) Tryptophan derivatives regulate the transcription of Oct4 in stem-like cancer cells. *Nat.Commun.* **6** 7209. PMID: 26059097.

Wang et al (2013) An endogenous aryl hydrocarbon receptor ligand inhibits proliferation and migration of human ovarian cancer cells. *Cancer Lett.* **340** 63. PMID: 23851185.

Lehmann et al (2011) The aryl hydrocarbon receptor ligand ITE inhibits TGF β 1-induced human myofibroblast differentiation. *Am.J.Pathol.* **178** 1556. PMID: 21406171.

Song et al (2002) A ligand for the aryl hydrocarbon receptor isolated from lung. *Proc.Natl.Acad.Sci.U.S.A.* **99** 14694. PMID: 12409613.

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.

Licensing Information:

Sold under license, US Patent Application 2002183524

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