bio-techne
TOCRIS

Print Date: Apr 4th 2024

Certificate of Analysis

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Product Name: **10-Cl-BBQ** **Catalog No.: 6321** **Batch No.: 3**

CAS Number: 23982-76-5

IUPAC Name: 10-Chloro-7*H*-benzimidazo[2,1-*a*]benz[de]isoquinolin-7-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_9ClN_2O$.

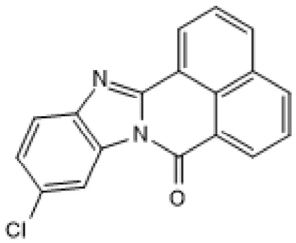
Batch Molecular Weight: 304.73

Physical Appearance: Yellow solid

Solubility: DMSO to 1 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.95	2.98	9.19
Found	70.88	2.84	9.17

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Description:

10-Cl-BBQ is a potent aryl hydrocarbon receptor (AhR) agonist, discovered as a screening hit (IC_{50} = 2.6 nM). Directly binds $CD4^+$ T cells to induce AhR-dependent Tregs. Suppresses IL-17 production and prevents insulitis in NOD mice. In vivo half llife ~ 2 hours, orally bioavailable.

Physical and Chemical Properties:

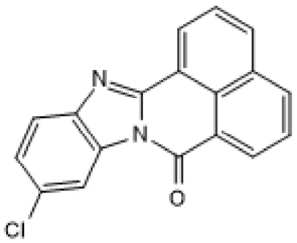
Batch Molecular Formula: $C_{18}H_9ClN_2O$.

Batch Molecular Weight: 304.73

Physical Appearance: Yellow solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 1 mM with gentle warming

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Ehrlich *et al* (2016) Activation of the aryl hydrocarbon receptor by 10-Cl-BBQ prevents insulitis and effector T cell development independently of Foxp3+ regulatory T Cells in nonobese diabetic mice. J.Immunol. ***196*** 264. PMID: 26573835.

Punj *et al* (2014) Benzimidazoisoquinolines: a new class of rapidly metabolized aryl hydrocarbon receptor (AhR) ligands that induce AhR-dependent Tregs and prevent murine graft-versus-host disease. PLoS One ***9*** e88726. PMID: 24586378.