bio-techne
TOCRIS

Print Date: Jun 28th 2023

Certificate of Analysis

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Product Name: (*R*,*R*)-THC **Catalog No.: 1990** **Batch No.: 6**

CAS Number: 138090-06-9

IUPAC Name: (*R*,*R*)-5,11-Diethyl-5,6,11,12-tetrahydro-2,8-chrysenediol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{24}O_2.¼H_2O$

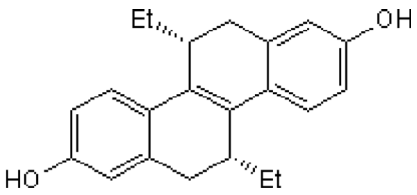
Batch Molecular Weight: 324.92

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Ethyl acetate:Petroleum ether [1:3])

HPLC: Shows 99.1% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	81.32	7.6	
Found	81.53	7.44	

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CAS Number: 138090-06-9

IUPAC Name: (*R*,*R*)-5,11-Diethyl-5,6,11,12-tetrahydro-2,8-chrysenediol

Description:

(R,R)-THC is a non-steroidal, selective estrogen receptor ligand. (R,R)-THC is an agonist at ERα receptor (K_i = 9.0 nM) and antagonist at ERβ receptor (K_i = 3.6 nM).

Physical and Chemical Properties:

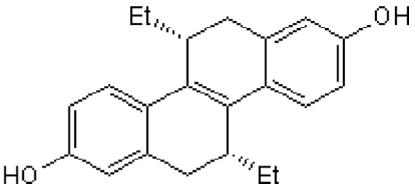
Batch Molecular Formula: $C_{22}H_{24}O_2.¼H_2O$

Batch Molecular Weight: 324.92

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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°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:

Kraichely *et al* (2000) Conformational changes and coactivator recruitment by novel ligands for estrogen receptor-α and estrogen receptor-β: correlations with biological character and distinct differences among SRC coactivator family members. Endocrinology ***141*** 3534. PMID: 11014206.

Meyers *et al* (1999) Estrogen receptor subtype-selective ligands: asymmetric synthesis and biological evaluation of *cis*- and *trans*-5,11-dialkyl- 5,6,11, 12-tetrahydrochrysenes. J.Med.Chem. ***42*** 2456. PMID: 10395487.

Sun *et al* (1999) Novel ligands that function as selective estrogens or antiestrogens for estrogen receptor-α or estrogen receptor-β. Endocrinology ***140*** 800. PMID: 9927308.