Print Date: Nov 13th 2019

Certificate of Analysis

www.tocris.com

Product Name: **G-1** **Catalog No.: 3577** **Batch No.: 7**

CAS Number: 881639-98-1

IUPAC Name: (±)-1-[(3a*R**,4*S**,9b*S**)-4-(6-Bromo-1,3-benzodioxol-5-yl)-3a,4,5,9b-tetrahydro-3*H*-cyclopenta[*c*]quinolin-8-yl]-ethanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{18}BrNO_3$

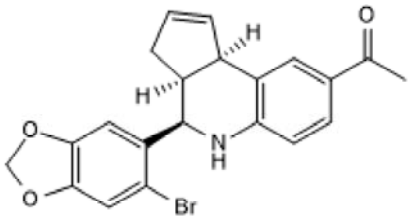
Batch Molecular Weight: 412.28

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



(and enantiomer)

2. ANALYTICAL DATA

TLC: R_f = 0.5 (Ethyl acetate:Petroleum ether [3:7])

HPLC: Shows 98.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.18	4.4	3.4
Found	60.95	4.39	3.27

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Description:

Potent and selective GPER agonist (K_i = 11 nM, EC_{50} = 2 nM); displays no activity at ERα and ERβ at concentrations up to 10 μM. Increases cytosolic Ca^{2+} and inhibits migration of SKBr3 cells and MCF-7 cells in response to chemoattractants (IC_{50} values are 0.7 and 1.6 nM respectively) in vitro. Blocks MCF-1 cell cycle progression at the G_1 phase. Displays therapeutic effects in the mouse EAE model of multiple sclerosis. Also inhibits glutamate-induced autophagy and neuronal loss in cultured primary cortical neurons.

Physical and Chemical Properties:

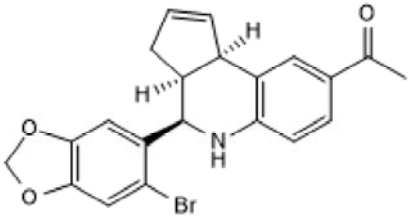
Batch Molecular Formula: $C_{21}H_{18}BrNO_3$

Batch Molecular Weight: 412.28

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



(and enantiomer)

Storage: Store at -20°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.

References:

Yue *et al* (2019) Activation of G-protein-coupled receptor 30 protects neurons against excitotoxicity through inhibiting excessive autophagy induced by glutamate. ACS Chem.Neurosci ***10*** 4227. PMID: 31545891.

Ariazi *et al* (2010) The G protein-coupled receptor GPR30 inhibits proliferation of estrogen receptor-positive breast cancer cells. Cancer Res. ***70*** 1184. PMID: 20086172.

Blasko *et al* (2009) Beneficial role of the GPR30 agonist G-1 in an animal model of multiple sclerosis. J.Neuroimmunol. ***214*** 67. PMID: 19664827.

Albanito *et al* (2007) G protein-coupled receptor 30 (GPR30) mediates gene expression changes and growth response to 17β-OE and selective GPR30 ligand G-1 in ovarian cancer cells. Cancer Res. ***67*** 1859. PMID: 17308128.

Bologa *et al* (2006) Virtual and biomolecular screening converge on a selective agonist for GPR30. Nature Chem.Biol. ***2*** 207.

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