



Certificate of Analysis

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Product Name: BINA Catalog No.: 4048 Batch No.: 2

CAS Number: 866823-73-6

IUPAC Name: 3'-[[(2-Cyclopentyl-2,3-dihydro-6,7-dimethyl-1-oxo-1*H*-inden-5-yl)oxy]methyl]-[1,1'-biphenyl]-4-carboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{30}H_{30}O_4$ Batch Molecular Weight: 454.56

Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.39$ (Dichloromethane:Methanol [9:1])

HPLC: Shows 100% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 79.27 6.65 Found 78.81 6.63



Product Information

Print Date: Jan 14th 2016

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Description:

Selective positive allosteric modulator of $mGlu_2$ (EC₅₀ = 33.2 nM in CHO cells expressing human $mGlu_2$). Displays no effect on glutamate-induced activation of other mGlu receptor subtypes. Exhibits antipsychotic and anxiolytic properties in mice.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₀H₃₀O₄ Batch Molecular Weight: 454.56 Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Desiccate 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.

References:

Bonnefous *et al* (2005) Biphenyl-indanones: allosteric potentiators of the metabotropic glutamate subtype 2 receptor. Bioorg.Med.Chem.Lett. *15* 4354. PMID: 16046122.

Galici *et al* (2006) Biphenyl-indanone A, a positive allosteric modulator of the metabotropic glutamate receptor subtype 2, has antipsychotic- and anxiolytic-like effects in mice. J.Pharmacol.Exp.Ther. *318* 173. PMID: 16608916.

Benneyworth et al (2007) A selective positive allosteric modulator of metabotropic glutamate receptor subtype 2 blocks a hallucinogenic drug model of psychosis. Mol.Pharmacol. 72 477. PMID: 17526600.