

Certificate of Analysis

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Product Name: CDPBB

Catalog No.: 3235

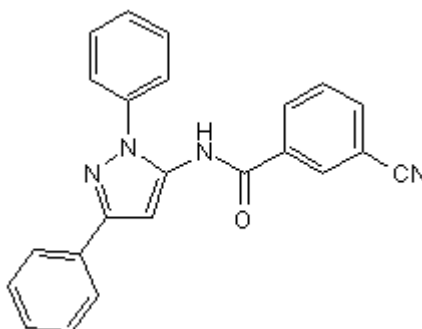
Batch No.: 5

CAS Number: 781652-57-1

IUPAC Name: 3-Cyano-*N*-(1,3-diphenyl-1*H*-pyrazol-5-yl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₁₆N₄O
Batch Molecular Weight: 364.4
Physical Appearance: White solid
Solubility: DMSO to 75 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.23 (Dichloromethane)
HPLC: Shows 98.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	75.81	4.43	15.38
Found	75.46	4.37	15.08

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

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Description:

Brain penetrant, selective positive allosteric modulator at the mGlu₅ receptor (EC₅₀ values are 10 and 20 nM for human and rat receptors respectively). Antipsychotic; reverses amphetamine-induced locomotor activity and amphetamine-induced deficits in prepulse inhibition in rats.

Physical and Chemical Properties:

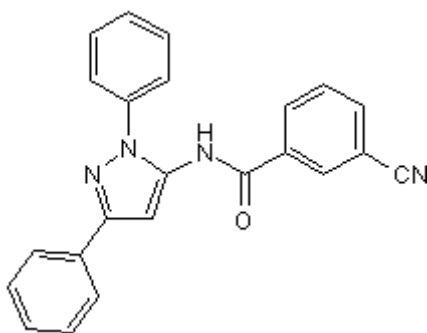
Batch Molecular Formula: C₂₃H₁₆N₄O

Batch Molecular Weight: 364.4

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 75 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:

Lindsley et al (2004) Discovery of positive allosteric modulators for the metabotropic glutamate receptor subtype 5 from a series of *N*-(1,3-diphenyl-1*H*-pyrazol-5-yl)benzamides that potentiate receptor function in vivo. *J.Med.Chem.* **47** 5825. PMID: 15537338.

Kinney et al (2005) A novel selective positive allosteric modulator of metabotropic glutamate receptor subtype 5 has in vivo activity and antipsychotic-like effects in rats behavioral models. *J.Pharmacol.Exp.Ther.* **313** 199. PMID: 15608073.

Chen et al (2007) Interaction of novel positive allosteric modulators of metabotropic glutamate receptor 5 with the negative allosteric antagonist site is required for potentiation of receptor responses. *Mol.Pharmacol.* **71** 1389. PMID: 17303702.

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