

Certificate of Analysis

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Product Name: PHTPP

Catalog No.: 2662

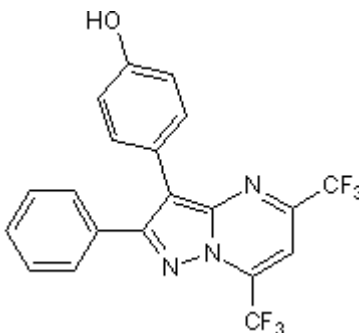
Batch No.: 2

CAS Number: 805239-56-9

IUPAC Name: 4-[2-Phenyl-5,7-bis(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-3-yl]phenol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₁F₆N₃O
Batch Molecular Weight: 423.31
Physical Appearance: Yellow solid
Solubility: DMSO to 33 mM
ethanol to 100 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.33 (Diethyl ether:Petroleum ether [2:1])
HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.75	2.62	9.93
Found	56.97	2.6	9.81

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

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Description:

Selective estrogen ER β receptor antagonist that displays 36-fold selectivity over ER α . Exhibits full antagonism at ER β in a cotransfection assay in human endometrial cancer cells (HEC-1), with minimal effects on ER α .

Physical and Chemical Properties:

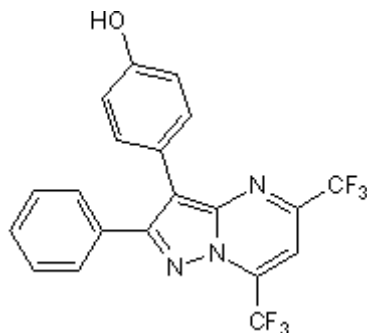
Batch Molecular Formula: C₂₀H₁₁F₆N₃O

Batch Molecular Weight: 423.31

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 33 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. 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:

Compton et al (2004) Pyrazolo[1,5-a]pyrimidines: estrogen receptor ligands possessing estrogen receptor β antagonist activity. *J.Med.Chem.* **47** 5872. PMID: 15537344.

Compton et al (2005) Erratum. *J.Med.Chem.* **48** 2724.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956