Product Name: Kenpaullone
CAS Number: 142273-20-9
IUPAC Name: 9-Bromo-7,12-dihydro-indolo[3,2-d][1]benzazepin-6(5H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{11}BrN_{2}O\cdot\frac{1}{4}H_{2}O$
Batch Molecular Weight: 331.68
Physical Appearance: Tan solid
Solubility: DMSO to 100 mM
ethanol to 5 mM with gentle warming
Storage: Store at RT

2. ANALYTICAL DATA

TLC: $R_f = 0.5$ (Dichloromethane:Methanol [9:1])
Melting Point: Greater than 300°C (dec)
HPLC: Shows 98.9% purity
$^1$H NMR: Consistent with structure
Microanalysis:

<table>
<thead>
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<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
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</table>
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Description:
Potent inhibitor of CDK1/cyclin B and GSK-3β (IC$_{50}$ values are 0.4 and 0.23 μM respectively). Also inhibits CDK2/cyclin A, CDK2/cyclin E and CDK5/cyclin/p35 (IC$_{50}$ values are 0.68, 7.5 and 0.85 μM respectively). Selective over c-src (IC$_{50}$ = 15 μM), casein kinase 2 (IC$_{50}$ = 20 μM), ERK1 (IC$_{50}$ = 20 μM), ERK2 (IC$_{50}$ = 9 μM) and a range of other protein kinases (IC$_{50}$ values > 35 μM). Generates induced pluripotent stem cells (iPSCs) from somatic cells when used in combination with reprogramming factors; can replace Klf4.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{16}$H$_{13}$BrN$_2$O.1/4H$_2$O
Batch Molecular Weight: 331.68
Physical Appearance: Tan solid
Minimum Purity: >98%

References: