Product Name: Pyr3  
Catalog No.: 3751  
Batch No.: 1

CAS Number: 1160514-60-2  
IUPAC Name: 1-[(2,3,3-Trichloro-1-oxo-2-propen-1-yl)amino]phenyl]-5-(trifluoromethyl)-1H-pyrazole-4-carboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{16}H_{11}Cl_3F_3N_3O_3 \)
Batch Molecular Weight: 456.63
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.35 \) (Ethyl acetate:Petroleum ether [2:8])
HPLC: Shows 98.1% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>42.08</td>
<td>42.04</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>2.43</td>
<td>2.43</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>9.20</td>
<td>9.07</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
**Product Name:** Pyr3

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**Batch No.:** 1

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**CAS Number:** 1160514-60-2  
**IUPAC Name:** 1-[[4-[[2,3,3-Trichloro-1-oxo-2-propen-1-yl]amino]phenyl]-5-(trifluoromethyl)-1H-pyrazole-4-carboxylic acid

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**Description:**
Selective antagonist of the canonical transient receptor potential channel 3 (TRPC3). Inhibits TRPC3-mediated Ca$^{2+}$ influx ($IC_{50} = 0.7 \mu M$) and suppresses activation of nuclear factor of activated T cells (NFAT). Inhibits hypertrophic responses in cardiomyocytes.

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**Physical and Chemical Properties:**

**Batch Molecular Formula:** C$_{16}$H$_{11}$Cl$_3$F$_3$N$_3$O$_3$

**Batch Molecular Weight:** 456.63

**Physical Appearance:** White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**

![Molecular Structure](image)

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**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM

This product may degrade over time when stored in solution and we therefore recommend that solutions are routinely prepared, aliquoted and used as quickly as possible.

**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.

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**References:**