1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** \( \text{C}_{18}\text{H}_{16}\text{F}_{3}\text{IN}_{2}\text{O}_{2} \)
- **Batch Molecular Weight:** 476.23
- **Physical Appearance:** White solid
- **Solubility:** DMSO to 100 mM, ethanol to 100 mM
- **Storage:** Store at +4°C
- **Batch Molecular Structure:**

![Molecular Structure](image)

2. ANALYTICAL DATA

- **TLC:** \( R_f = 0.43 \) (Ethyl acetate:Petroleum ether [1:3])
- **Melting Point:** Between 140 - 141°C
- **HPLC:** Shows >98.8% purity
- **\(^{1}\text{H NMR:}\)** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  - Theoretical: 45.4 3.39 5.88
  - Found: 45.37 3.29 5.8

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: PD 198306
Catalog No.: 2605  Batch No.: 1

CAS Number: 212631-61-3
IUPAC Name: N-(Cyclopropylmethoxy)-3,4,5-trifluoro-2-[(4-iodo-2-methylphenyl)amino]-benzamide

Description:
Potent inhibitor of MEK1/2. Inhibits isolated enzyme at a concentration of 8 nM and inhibits MEK activity in synovial fibroblasts at concentrations of 30 - 100 nM. Highly selective for MEK; IC₅₀ values are > 1, > 4, > 4 and > 10 μM for ERK, c-Src, cdks and PI 3-kinase γ respectively. Antihyperalgesic; blocks static allodynia in the streptozocin model of neuropathic pain following i.t. administration.

Physical and Chemical Properties:
- Batch Molecular Formula: C₂₁H₁₇F₅IN₂O₂
- Batch Molecular Weight: 476.23
- Physical Appearance: White solid
- Minimum Purity: >98%

Storage: Store at +4°C
CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:
DMSO to 100 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).

Reference: