1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** $C_{23}H_{25}F_4N_3O_3S.HCl.\frac{3}{4}H_2O$
- **Batch Molecular Weight:** 549.49
- **Physical Appearance:** White solid
- **Solubility:** DMSO to 100 mM, ethanol to 20 mM with sonication
- **Storage:** Store at $-20^\circ C$

2. ANALYTICAL DATA

- **TLC:** $R_f = 0.33$ (Chloroform:Methanol [9:1])
- **HPLC:** Shows 99.7% purity
- **Chiral HPLC:** Shows 100% 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>50.27</td>
<td>50.16</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.04</td>
<td>4.86</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>7.65</td>
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</tr>
</tbody>
</table>

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

**Product Name:** (R)-PFI 2 hydrochloride

**CAS Number:** 1627607-87-7

**IUPAC Name:** (1R)-1-[3-(Trifluoromethyl)phenyl]methyl]-2-oxo-2-(1-pyrrolidinyl)ethyl]-1,2,3,4-tetrahydro-6-isooquinolinesulfonamide hydrochloride

**Description:**
Potent and selective SETD7 histone lysine methyltransferase inhibitor (IC₅₀ = 2 nM). Exhibits >1000-fold selectivity over DNMT1 and a panel of 18 other methyltransferases. Inhibits YAP nuclear translocation and function following activation of the Hippo signaling pathway in MCF7 cells. Negative Control also available.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C₂₂H₂₆F₃N₁₀O₅S.HCl.¾H₂O
- **Batch Molecular Weight:** 549.49
- **Physical Appearance:** White solid
- **Minimum Purity:** >97%

**Storage:** Store at -20°C. This product is packaged under an inert atmosphere.

**Solubility & Usage Info:**
- DMSO to 100 mM ethanol to 20 mM with sonication
- This product has been packed under inert atmosphere, and should be stored under inert atmosphere after use.

**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.

**Licensing Information:**
This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the (R)-PFI 2 probe summary on the SGC website.

**References:**