### Product Data Sheet

#### Chemical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Product Name:</strong></td>
<td>Aprepitant</td>
</tr>
<tr>
<td><strong>Cas No.:</strong></td>
<td>170729-80-3</td>
</tr>
<tr>
<td><strong>M.Wt:</strong></td>
<td>534.43</td>
</tr>
<tr>
<td><strong>Formula:</strong></td>
<td>C23H21F7N4O3</td>
</tr>
</tbody>
</table>

**Chemical Name:** 5-[[2R,3S]-2-[1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)morpholin-4-yl]methyl]-1,2-dihydro-1,2,4-triazol-3-one

**Canonical SMILES:** CC(C1=CC(=CC(CF)(F)F)C(F)F)OC2C(N(CCO2)CC3=NC(=O)NN3C4=CC=C(C=C4)F

**Solubility:** >26.7mg/mL in DMSO

**Storage:** Store at -20°C

**General tips:** For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

**Shopping Condition:** Evaluation sample solution: ship with blue ice
All other available size: ship with RT, or blue ice upon request

#### Biological Activity

**Targets:** Substance P/NK1 Receptor

**Pathways:** Neuroscience >> Substance P/NK1 Receptor

**Description:**

Aprepitant (also known as MK-0869) is a novel and highly selective Neurokinin-1 (NK-1) receptors that inhibits the activity of substance P (SP), an undecapeptide belonging to the tachykinin family of peptides, on the NK-1 receptor with the dissociation constant Kd of 86 pM for human NK-1.
receptor and the half maximal inhibition concentration IC50 of 0.1 nM, 4 nM and 0.7 nM for human, rat and ferret NK-1 receptors respectively [1,2].

Since SP has been demonstrated to induce cell proliferation in several human cancer cell lines with overexpressed NK-1 receptors, aprepitant has also been found to concentration-dependently induce growth inhibition in a variety of tumor cell lines, including glioma (GAMG), neuroblastoma (SKN-BE2, IMR-32 and KELLY), retinoblastoma (Y-79 and WERI-Rb-1), pancreas carcinoma (PA-TU-8902 and CAPAN-1), larynx carcinoma (HEp-2), gastric carcinoma (23132-87) and colon carcinoma (SW-403), with IC50 of 33.1 μM, 24.6 μM, 19.6 μM, 27.7 μM, 30.4 μM, 23 μM, 31.2 μM, 27.4 μM, 22.7 μM, 24.2 μM and 30.5 μM respectively [2].

Reference: