1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: \( \text{C}_{31}\text{H}_{29}\text{ClN}_{6}\text{O}_{3}\text{S}.\text{HCl}.1\frac{1}{2}\text{H}_{2}\text{O} \)

   Batch Molecular Weight: 664.6

   Physical Appearance: Pale beige solid

   Solubility: water to 100 mM
              DMSO to 100 mM

   Storage: Store at -20°C

   Batch Molecular Structure:

2. ANALYTICAL DATA

   TLC: \( R_f = 0.35 \) (10% 7M methanolic ammonia/DCM)

   HPLC: Shows 99.6% purity

   Chiral HPLC: Shows 100% purity

   \(^1\text{H NMR:}\) Consistent with structure

   Mass Spectrum: Consistent with structure

   Microanalysis:

   Carbon   Hydrogen   Nitrogen
   Theoretical 56.02  5  12.65
   Found       55.9  4.62  12.42
Product Name: AMG 18 hydrochloride
Catalog No.: 6166 Batch No.: 1

IUPAC Name: 2-Chloro-N-[6-methyl-5-[[3-[2-[(3S)-3-piperidinylamino]-4-pyrimidinyl]-2-pyridinyl]oxy]-1-naphthalenyl]benzenesulfonamide hydrochloride

Description:
Potent and selective IRE1α inhibitor (IC\textsubscript{50} values are 13 and 99 nM for recombinant and cellular IRE1α, respectively). Exhibits selectivity for IRE1α in a panel of over 100 other kinases.

Physical and Chemical Properties:
Batch Molecular Formula: C\textsubscript{31}H\textsubscript{30}ClN\textsubscript{8}O\textsubscript{5}S.HCl.1½H\textsubscript{2}O
Batch Molecular Weight: 664.6
Physical Appearance: Pale beige solid
Minimum Purity: >98%

Storage: Store at -20°C

Solubility & Usage Info:
water to 100 mM
DMSO 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).

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.

References: