1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** $C_{22}H_{21}N_3O_3S.\frac{1}{2}H_2O$
- **Batch Molecular Weight:** 416.5
- **Physical Appearance:** White solid
- **Solubility:** DMSO to 20 mM
- **Storage:** Store at +4°C
- **Batch Molecular Structure:**

![Molecular Structure Image]

2. ANALYTICAL DATA

- **HPLC:** Shows 100% purity
- **$^1H$ NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:** Carbon Hydrogen Nitrogen
  - Theoretical: 63.44 5.32 10.09
  - Found: 63.11 5.05 10
Product Name: ANA 12
Catalog No.: 4781
Batch No.: 2

CAS Number: 219766-25-3
IUPAC Name: \( N \)-[2-[[Hexahydro-2-oxo-1\(H\)-azepin-3-yl]amino]carbonyl]phenyl]benzo[b]thiophene-2-carboxamide

Description:
TrkB receptor antagonist. Demonstrates a 2-site mode of action, preventing activation by BDNF non-competitively (IC\(_{50}\) values are 45.6 nM and 41.1 \( \mu \)M for the high and low affinity sites respectively). Displays no effect on TrkA and TrkC in an assay of neurite outgrowth. Demonstrates antidepressant properties. Also exhibits anti-seizure effects in an ischemia-induced neonatal seizure model by blocking down-regulation of KCC2.

Physical and Chemical Properties:
Batch Molecular Formula: C\(_{22}\)H\(_{24}\)N\(_2\)O\(_2\)S.\( \frac{1}{2} \)H\(_2\)O
Batch Molecular Weight: 416.5
Physical Appearance: White solid
Minimum Purity: >99%

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 20 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: