1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** C_{34}F_{43}F_5O_5S_{1/4}H_2O
- **Batch Molecular Weight:** 663.26
- **Physical Appearance:** Pale yellow solid
- **Solubility:** DMSO to 100 mM, ethanol to 100 mM
- **Storage:** Store at +4°C

2. ANALYTICAL DATA

- **HPLC:** Shows 95.4% purity
- **\(^1\)H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  - Theoretical: Carbon 61.57, Hydrogen 6.61, Nitrogen 6.61
  - Found: Carbon 61.32, Hydrogen 6.8, Nitrogen 6.8
Product Name: RU 58668
Catalog No.: 3224
Batch No.: 1

CAS Number: 151555-47-4
IUPAC Name: (11β,17β)-11-[4-[5-[(4,4,5,5,5-Pentafluoropentyl)sulfonyl]pentyl]oxy]phenylestra-1,3,5,(10)-triene-3,17-diol

Description:
Pure antiestrogen that downregulates estrogen receptor expression (IC₅₀ = 0.04 nM). Displays potent antiproliferative activity in vitro (IC₅₀ = 0.035 - 0.09 nM in MCF-7 cells) and causes long term regression of tamoxifen-resistant MCF-7 xenografts in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C₃₄F₄₅F₅O₅S.¼H₂O
Batch Molecular Weight: 663.26
Physical Appearance: Pale yellow solid
Minimum Purity: >95%

Storage: Store at +4°C

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).

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: