1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** \( \text{C}_{22}\text{H}_{27}\text{NO}_5\cdot \text{HCl} \cdot \text{H}_2\text{O} \)
- **Batch Molecular Weight:** 439.93
- **Physical Appearance:** Off-white solid
- **Solubility:** DMSO to 100 mM, ethanol to 50 mM
- **Storage:** Desiccate at RT

2. ANALYTICAL DATA

- **TLC:** \( R_f = 0.42 \) (Chloroform:Methanol [4:1])
- **HPLC:** Shows 99.3% purity
- **\(^1\text{H NMR:}\)** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  - Theoretical: 60.06  6.87  3.18
  - Found: 60.17  6.55  3.07
Product Name: LY 2365109 hydrochloride
Catalog No.: 3397
Batch No.: 3

CAS Number: 1779796-27-8
IUPAC Name: \(N\)-[2-[4-(1,3-Benzodioxol-5-yl)-2-(1,1-dimethylethyl)phenoxy]ethyl]-\(N\)-methylglycine hydrochloride

Description:
Potent and selective glycine transporter 1 (GlyT1) inhibitor (IC\(_{50}\) values are 15.8 and > 30 000 nM at GlyT1 and GlyT2 respectively). Induces a dose-dependent elevation in CSF levels of glycine, and enhances acetylcholine and dopamine release in the striatum and prefrontal cortex respectively. Produces profound locomotor and respiratory impairments at higher doses.

Physical and Chemical Properties:
Batch Molecular Formula: \(C_{22}H_{27}NO_5\cdot HCl\cdot H_2O\)
Batch Molecular Weight: 439.93
Physical Appearance: Off-white solid
Minimum Purity: >98%

Storage: Desiccate at RT

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 50 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: