

Molecules of the Month

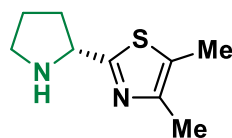
Experimental Kinetic Solubility for Ro3 Compliant Fragments

Liverpool ChiroChem Ltd. (LCC) is a chemical technology innovator that produces chiral small molecules for biotech and pharmaceutical R&D, and knows that solubility of fragments is an important property that limits their use in various screening techniques. LCC has a unique library of fragments; not only are they **Ro3 compliant**, but also **3D-rich**, mainly based on **sp³-rich N-heterocyclic cores** and most uniquely, available as **single enantiomers**. In all cases, good aqueous solubilities were predicted, however, LCC decided to take a step forward and get **experimental solubility data** for fragments available from stock.

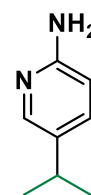
Ro3 compliant LCC's Fragments

Key criteria:

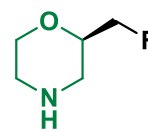
- Mw < 300 g.mol⁻¹
- HBA ≤ 3
- HBD ≤ 3
- Rot. B ≤ 3
- **Kinetic solubility > 850 μM¹**
- *in vitro assessment* -



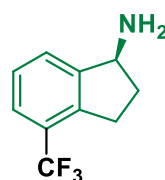
A0508



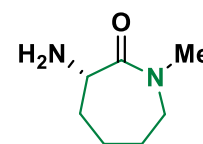
A4539



A6846



A6597



A6370

With **85% of the tested fragments** exhibiting a **kinetic solubility > 850 μM**, the measured solubility results validated the initially predicted high solubility. Thus, LCC is delighted to have, in stock, fragments with such essential physicochemical properties. The kinetic solubility measurements for a second sample of compounds representative of LCC's fragment library are underway.

Should you require any further information, do not hesitate to get in touch with us at info@liverpoolchirochem.com.

Thanks to the University of Liverpool and XenoGesis Ltd. for supporting this project.

¹ Average kinetic solubility measured *in vitro* for 46 fragments, kinetic aqueous solubility in PBS pH 7.4 containing 1% DMSO determined by UV plate-reader or LC-MS, min = 643 μM (1 compound) – max = > 1000 μM (33 compounds).

