DATA SHEET

Jena Bioscience

Frag Xtal Screen

Fragment Screen for Crystallographic Screening

Cat. No.	Amount
X-FS-101	96 fragments (2x 50 nmol each)

For *in vitro* use only!

Shipping: shipped at ambient temperature

Storage Conditions: store in aluminum bag at -20 °C

Shelf Life: 12 months

Applications:
Fragment-based lead discovery (FBLD) by crystallographic screening
Protein surface mapping by crystallographic screening

Description:
The Frag Xtal Screen provides 96 different fragments spotted onto the protein wells of a crystallization plate (MRC 3 Well Plate, #CPL-149). Two protein wells are spotted with 50 nmol fragment each while the third one is kept free. This allows to vary the stabilizing solution, e.g. the DMSO content.
Crystallographic screening and the structural data collected are the only reliable information to verify fragment binding for structure-based drug design. It was shown that the biochemical and biophysical assays routinely performed as prescreens show distinct hits with minimal overlap eliminating promising candidates and maybe focussing on the poor ones [1-3]. The Frag Xtal Screen is designed to directly collect structural data of protein crystals soaked with 96 different fragments.

Short Fragment Soaking Protocol:
1) Remove foil carefully
2) Add 30 µl crystallization buffer to the reservoir (manually or by robot)
3) Add 0.5 µl crystallization buffer on dried fragments (manually or by robot)
4) Add 1-2 crystals per drop
5) Seal the plate & incubate 1-48 h
6) Fish & cryo-cool at least one crystal per condition

The fragment screen was developed in cooperation with the HZB MX-group at BESSY II (AG Weiss) and the Institute of Pharmaceutical Chemistry, University of Marburg (AG Klebe).

Selected References:
[1] Huschmann *et al.* (2016) Structures of endothiapepsin-fragment complexes from crystallographic fragment screening using a novel, diverse and affordable 96-compound fragment library. *Acta Cryst F* **72**:346.
[2] Schiebel *et al.* (2016) Six Biophysical Screening Methods Miss a Large Proportion of Crystallographic Discovered Fragment Hits: A Case Study. *ACS Chem. Biol.* **11**:1693.
[3] Schiebel *et al.* (2015) One Question, Multiple Answers: Biochemical and Biophysical Screening Methods Retrieve Deviating Fragment Hit Lists. *ChemMedChem* **10**:1511.