

Certificate of Analysis

Axon Catalogue ID: 1621 Batch Number: 2

Product Name: XMD 8-92 trifluoroacetate

Alternative Name(s): N.A.

IUPAC Name: 2-(2-Ethoxy-4-(4-hydroxypiperidin-1-yl)phenylamino)-5,11-dimethyl-5H-benzo[e]pyrimido[5,4-b][1,4]diazepin-6(11H)-

one 2,2,2-trifluoroacetate

Structure: Amount:

N N N HO C

CAS number: 1234480-50-2 **MW:** 588.58

 Batch Molecular Formula:
 C26H30N6O3.C2HF3O2
 Batch MW:
 588.58

Appearance: Off-white solid **Observed mp:** $146.1 - 147.5 ^{\circ}$ C

TLC (R_f): 0.35 DCM/MeOH (9:1)

Chemical Purity: 99.1%

Optical Purity (ee):

1H-NMR (300 MHz): Analytical data confirm chemical structure

Mass Spec: Analytical data confirm chemical structure

Microanalysis: Not available

Storage Conditions: Desiccate at +4 °C

Solubility Data: Solvent Solubility Solubility Remarks

 (mg/ml)
 (mM)

 Water
 0.1
 0.2
 Poorly soluble, DMSO improves solubility.

 0.1N NaOH (aq)
 Not Tested

 0.1N HCl (aq)
 Not Tested

 DMSO
 46.0
 78.2

EtOH Not Tested

Remarks:

QC Date: 12-04-2012

The purity of Axon products is confirmed by HPLC, MS, NMR and/or microanalysis. Analytical data are available upon request. Request can be submitted by e-mail to info@axonmedchem.com indicating Axon Catalogue ID and Batch number.

Caution: Not fully tested. For research purposes only