

Certificate of Analysis

Axon Catalogue ID: 1851 Batch Number: 1

Product Name: Rolofylline metabolite M1-trans

Alternative Name(s): Compound 3

IUPAC Name: 8-(Hexahydro-7-hydroxy-2,5-methanopentalen-3a(1H)-yl)-3,9-dihydro-1,3-dipropyl-1H-Purine-2,6-dione

Structure: O Amount:

ОН

CAS number: 160943-06-6

Batch Molecular Formula:C20H28N4O3Batch MW:372.46

Appearance: White Solid Observed m.p.: 226.2-227.3°C

TLC (R_f): 0.5 19:1 DCM/Methanol

Chemical Purity: >99.5% Wavelength for purity check: 278 nm

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) Insoluble Water 1eq. NaOH Not tested 1eq. HCI Not tested DMSO 20.00 53.70 Soluble

EtOH Soluble

Remarks:

Quality controller: M. Brandsma, MSc. **Date:** 18-4-2012

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