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Print Date: Jan 16th 2016

Certificate of Analysis

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Product Name: **TDFA** **Catalog No.: 5482** **Batch No.: 1**
CAS Number: 1345019-64-8

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	$C_{17}H_{29}FN_6O_7$
Batch Molecular Weight:	448.45
Physical Appearance:	White lyophilised solid
Net Peptide Content:	78%
Counter Ion:	TFA
Solubility:	Soluble to 2 mg/ml in water
Storage:	Store at -20°C
Peptide Sequence:	Ac-Thr-Asp-[N^5-(2-fluoro-1-iminoethyl)]-Orn-NH_2

2. ANALYTICAL DATA

HPLC:	Shows 98% purity
Mass Spectrum:	Consistent with structure

3. AMINO ACID ANALYSIS DATA

Amino Acid	Theoretical	Actual	Amino Acid	Theoretical	Actual
Ala			Lys		
Arg			Met		
Asx	1.00	1.03	Phe		
Cys			Pro		
Glx			Ser		
Gly			Thr	1.00	0.97
His			Trp		
Ile			Tyr		
Leu			Val		

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Product Name: **TDFA** **Catalog No.: 5482** **Batch No.: 1**

CAS Number: 1345019-64-8

Description:

Protein arginine deiminase 4 (PAD4) inhibitor (IC_{50} values are 2.3, 8.5, 26 and 71 µM for PAD4, PAD1, PAD3 and PAD2, respectively).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{17}H_{29}FN_6O_7$

Batch Molecular Weight: 448.45

Physical Appearance: White lyophilised solid

Peptide Sequence:

Ac-Thr-Asp-[N^5-(2-fluoro-1-iminoethyl)]-Orn-NH_2

Storage: Store at -20°C

Solubility & Usage Info:

Soluble to 2 mg/ml in water

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

Net Peptide Content: 78% (Remaining weight made up of counterions and residual water).

Counter Ion: TFA

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).

Peptides in solution are much less stable than in lyophilized form. This is especially true for peptides whose sequences contain amino acids such Cys, Met,Trp, Asn, Gln, and N-terminal Glu.

Therefore we recommend storing peptides in solution for as short a time as possible. Avoid repeated freeze thaw cycles by dividing the peptide solution into aliquots and storing the aliquots at -20°C. Any portion of an aliquot unused after thawing should be discarded.

Peptides stored in solution can occasionally be susceptible to bacterial degradation. We recommend using sterile solutions or passing the peptide solution through a 0.2 µm filter to remove potential bacterial contamination whenever possible.

References:

Jones *et al* (2012) Synthesis and screening of a haloacetamidine containing library to identify PAD4 selective inhibitors. ACS Chem.Biol. ***7*** 160. PMID: 22004374.