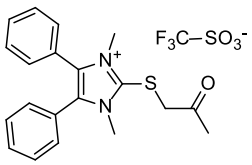
Product Data Sheet

Product Number	**D004**
Revision Number	RN3.0

Product Name	1,3-Dimethyl-4,5-diphenyl-2-[(2-oxopropyl)thio]imidazolium trifluorosulfonic acid salt
Synonym	“L-683.685”; 1,3-Dimethyl-2-(2-oxopropylthio)-4,5-diphenyl-1H-imidazol-3-ium trifluoromethanesulfonate
Quantity	10 mg
Application	Inhibitior for transglutaminase
Efficacy	The molecule was developed to block coagulation factor XIIIa, however the compound inhibits tissue transglutaminase as well. Both enzymes are inhibited with an IC_{50} of about 0.35 µM.
Molecular Formula	$C_{21}H_{21}F_3N_2O_4S_2$ (free cation: $C_{20}H_{21}N_2OS^+$)
Molecular Weight	486.53 (free cation: 337.46)
Chemical Structure	
Purity by HPLC	>90 % (214 nm)
Solubility	Pre-dissolve e.g. 2.02 mg in 207.6 µl DMSO to obtain a 20 mM stock solution - dilute 20 µl of that stock solution with 980 µl buffer (e.g. 50 mM TRIS-HCl, pH 7.5) to obtain a 400 µM solution
Appearance	Off white solid
Storage	Store at -20°C, desiccate
Related Products	A101 Abz-NE(CAD-DNP)EQVSPLTLLK-OH A102 Abz-APE(CAD-DNP)QEA-OH T006 Guinea pig liver transglutaminase T002 Human tissue transglutaminase (hTG2, recombinant in *E. coli*) T007 Coagulation factor XIII purified from human plasma (pFXIII, A_2B_2) T027 Human blood coagulation Factor XIII, recombinant
Reference(s)	[1] Lorand L. *et al. Exp. Eye Res.* **1998**, *66*, 531. [2] Barsigian C. *et al. J. Biol. Chem.* **1991**, *266*, 22501.
Release date	02 December 2021
NOTE	INTENDED FOR RESEARCH USE ONLY, NOT FOR USE IN HUMAN, THERAPEUTIC OR DIAGNOSTIC APPLICATIONS.

APPLICATION

INHIBITION OF PURIFIED TISSUE-TGase (HIS$_6$-rhTG2)

1,3-Dimethyl-4,5-diphenyl-2-[(2-oxopropyl)thio]imidazolium, trifluorosulfonic acid salt is a potent, active site directed inhibitor. The reaction results in an acetonylation of active site cysteine. The inhibition parameters were obtained by progress curve analysis using a continuous assay after preincuabation with the inhibitor (Fig. 1a and 1b).

Inhibition of His$_6$-rhTG2 by preincubation with 1,3-Dimethyl-4,5-diphenyl-2-[(2-oxopropyl)thio]imidazolium, trifluorosulfonicacid salt.

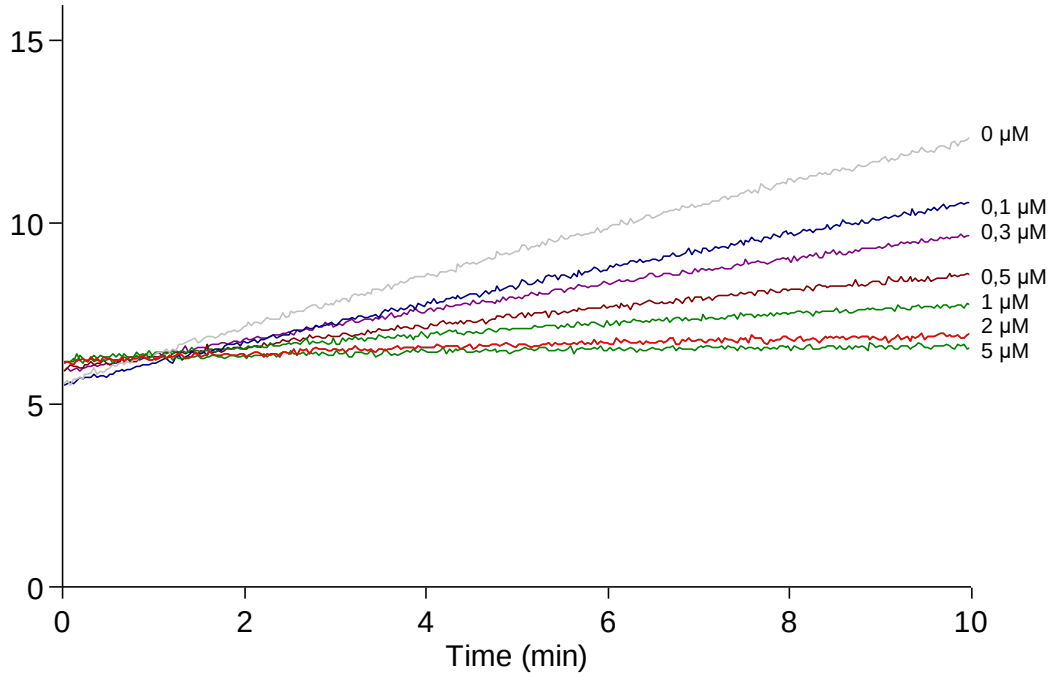


Fig.1a: 10 µg His$_6$-rhTG2 were preincubated with 0.1-5 µM 1,3-Dimethyl-4,5-diphenyl-2-[(2-oxopropyl)thio]imidazolium, trifluorosulfonic acid salt, containing 10 mM $CaCl_2$. After 5 min at 37°C, remaining activity was measured continuously using Abz-APE(CAD-DNP)QEA-OH as substrate. The substrate carries a fluorescent dye and a suitable quencher. The fluorescence increases upon transglutaminase-catalysed removal of the quencher molecule and can be measured online (37°C, ex. wavelength = 313 nm, em. wavelength = 418 nm). The activity is determined by the difference of fluorescence intensity between 5 and 10 min.

Inhibition of His_6-hTG2 by preincubation with 1,3-Dimethyl-4,5-diphenyl-2-[(2-oxopropyl)thio]imidazolium, trifluorosulfonicacid salt.

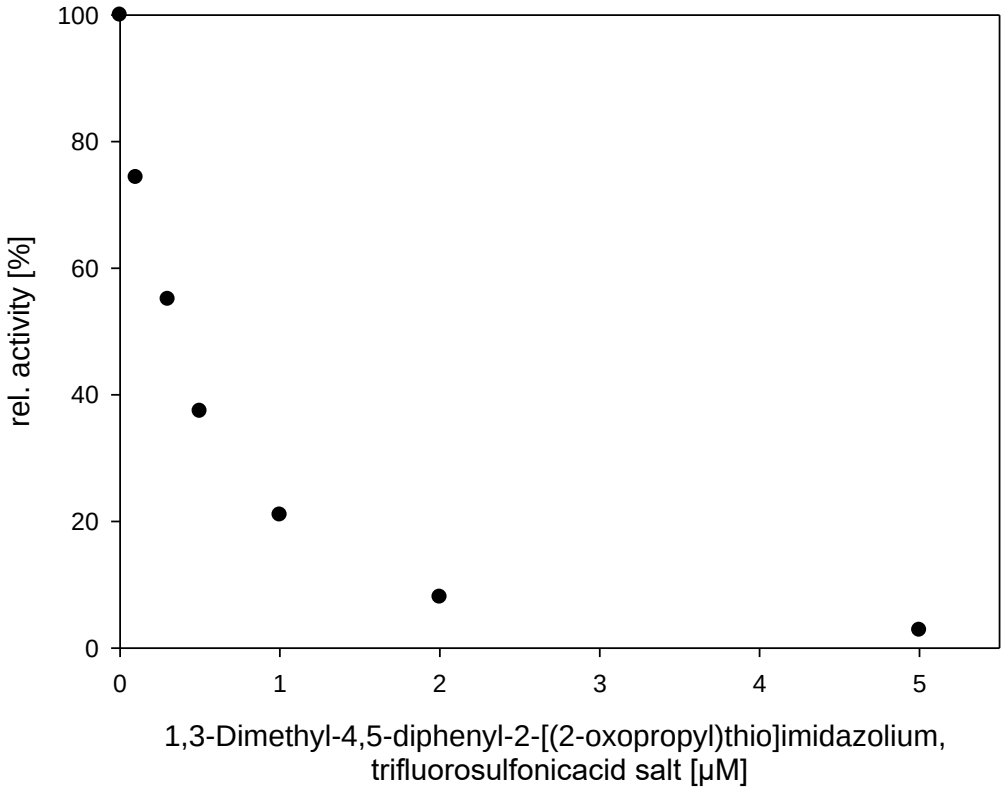


Fig.1b: Transglutaminase activity vs. inhibitor concentration. Illustration results from online-measurements, displayed in Fig.1a. Activity of sample in the absence of inhibitor was taken as 100%, the other values were compared with this value.