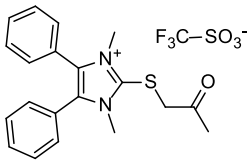
Product Data Sheet

Product Number	**D004**
Revision Number	RN3.1

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
Application	Inhibitior for transglutaminase, cell-permeable [3]
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. [3] Basso, M. et al. J. Neurosci. 2012, 32, 6561.
Release date	23 March 2022
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.

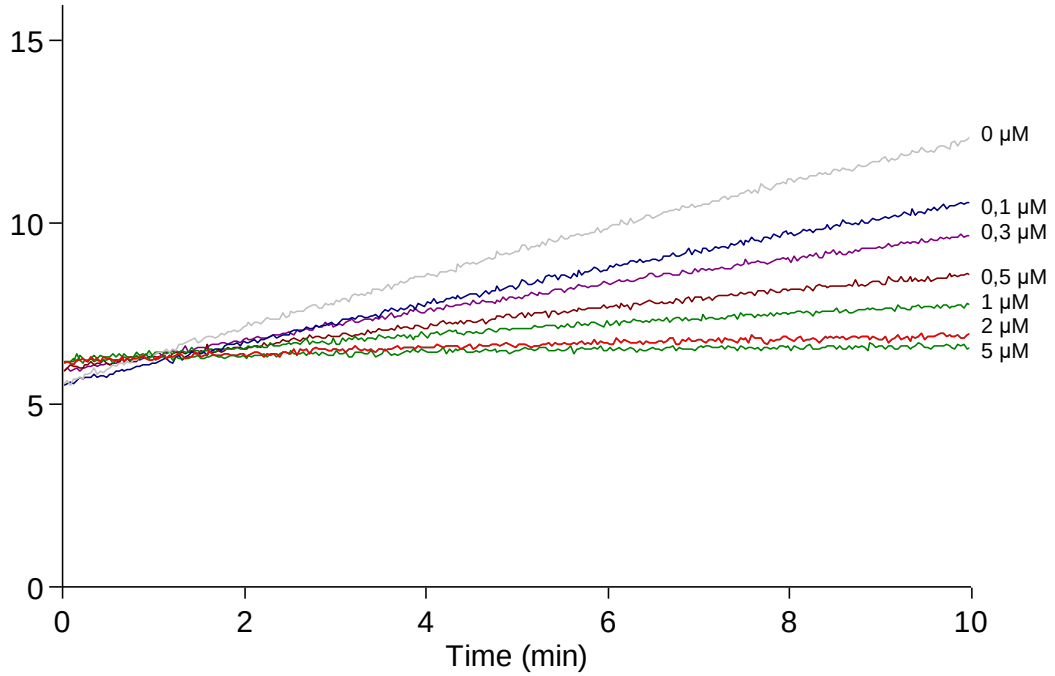


Fig.1a: 10 µg His_6-rhTG2 were preincubated with 0.1-5 µM 1,3-Dimethyl-4,5-diphenyl-2-[(2-oxopropyl)thio]imidazolium, trifluorosulfonic acid salt, containing 10 mM $CaCl_2$. After 5 min at 37°C, remaining activity was measured continuously using Abz-APE(CAD-DNP)QEA-OH as substrate. The substrate carries 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.

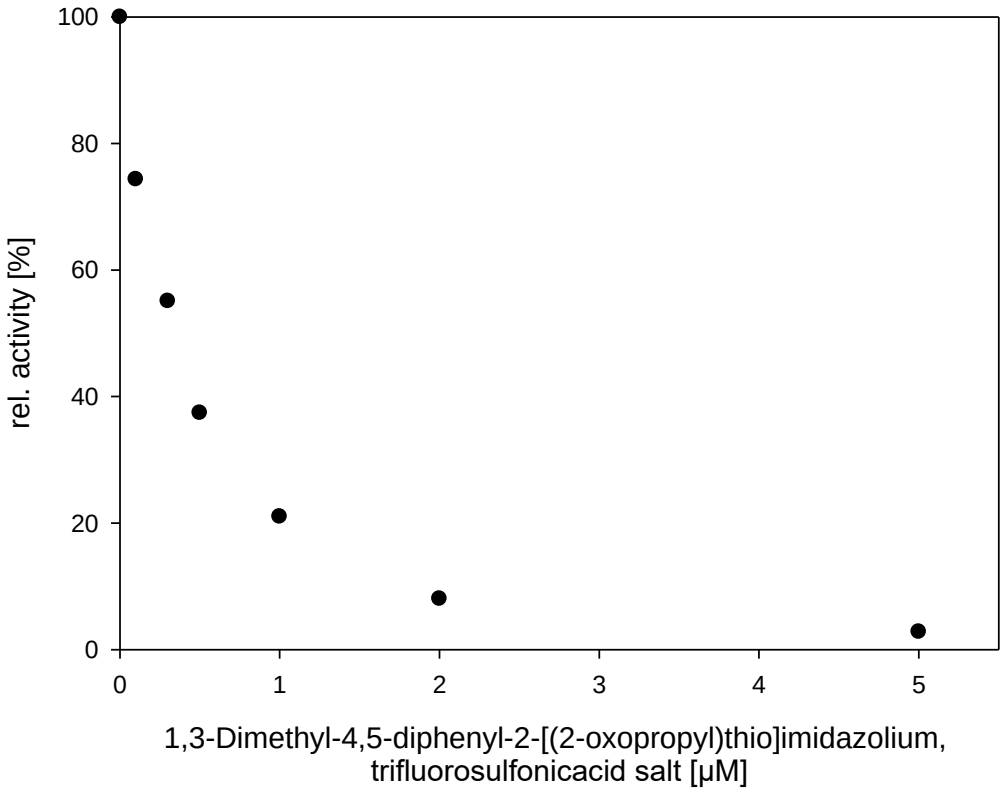


Fig.1b: Transglutaminase activity vs. inhibitor concentration. Illustration results from online-measurements, displayed in Fig.1a. Activity of sample in the absence of inhibitor was taken as 100%, the other values were compared with this value.