Supporting Information

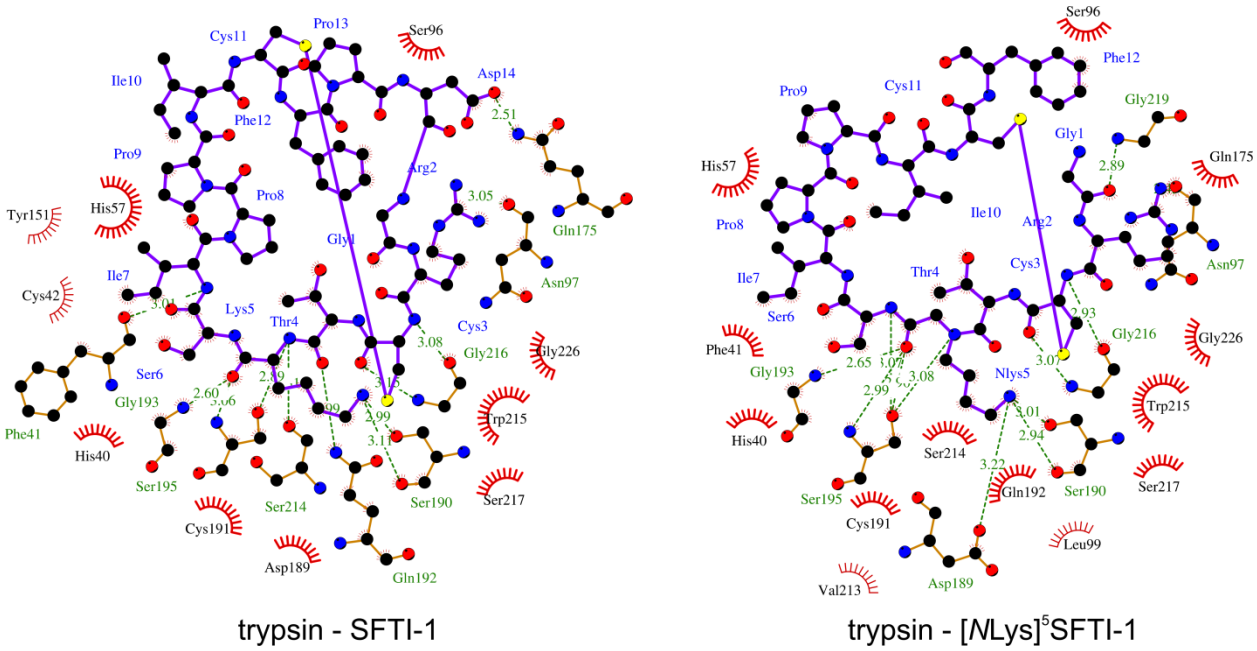

Figure S1.General comparison of trypsin-inhibitor contacts in the native SFTI-1 structure (PDB code 1SFI; Luckett et al., 1999) and in the [*N*Lys]^{5}SFTI-1 complex (this work), generated with the LigPlot+ program (Laskowski & Swindells, 2011).

Table S1. Comparison of side-chain torsion angles χ [°] of the P1 residue in the native SFTI-1 (Luckett et al., 1999) and [*N*Lys]^{5}SFTI-1 structures.

Torsion angle	Lys^5	*N*Lys^5
χ1	-71.4	85.0 [a]
χ2	168.5	-150.8
χ3	-178.5	-177.4
χ4	-176.4	175.4

[a] The χ_1 angle of *N*Lys^5 was measured between the C_α-N-C_β-C_γ atoms.

Table S2. Comparison of key main-chain dihedral angles [°] of residues 4-6 from native SFTI-1 (upper value) (Luckett et al., 1999) and [*N*Lys]^{5}SFTI-1 (bottom).

Residue		φ[°]	ψ[°]
P2	4	-74.0 -89.6	165.6 151.2
P1	5	-104.5 -86.5	32.6 54.5
P1’	6	-88.4 -98.5	174.0 171.1

Laskowski, R. A. & Swindells, M. B. (2011). *J. Chem. Inf. Model.* **51**, 2778-2786.

Luckett, S., Garcia, R. S., Barker, J. J., Konarev, A. V., Shewry, P. R., Clarke, A. R. & Brady, R. L. (1999). *J. Mol. Biol.* **290**, 525-533.