Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Discovery of penta-peptides inhibiting activity of formylglycine generating enzyme and its potential antibacterial effect against *Mycobacterium tuberculosis*

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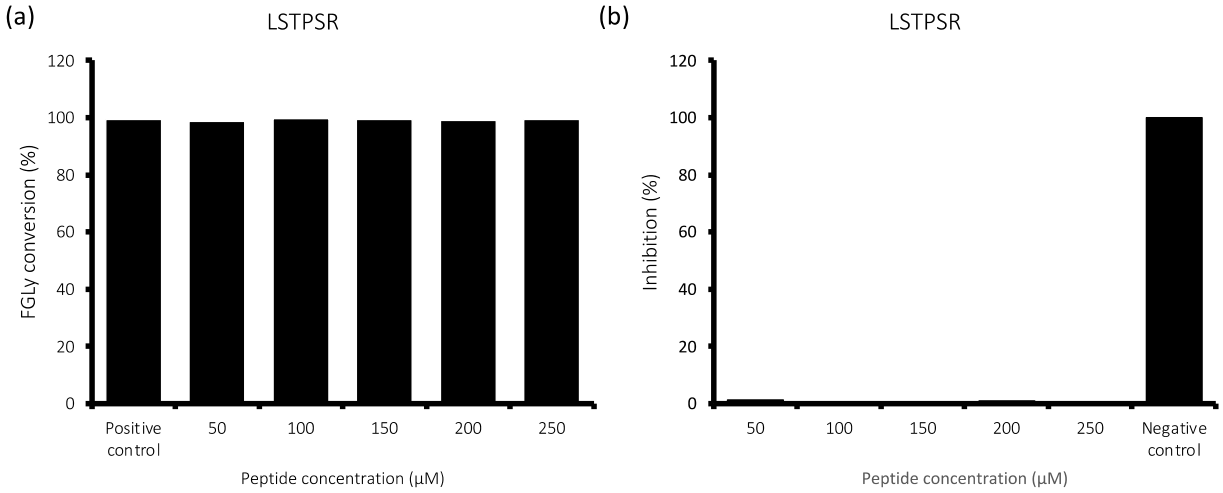


Figure S1. FGE activity inhibition assay upon serial concentration of LSTPSR peptide treatment. Targeted LCMS chromatograms between substrate and fGly product after incubation for 1 hour were used to calculate (a) fGly conversion percentage and (b) activity inhibition percentage.

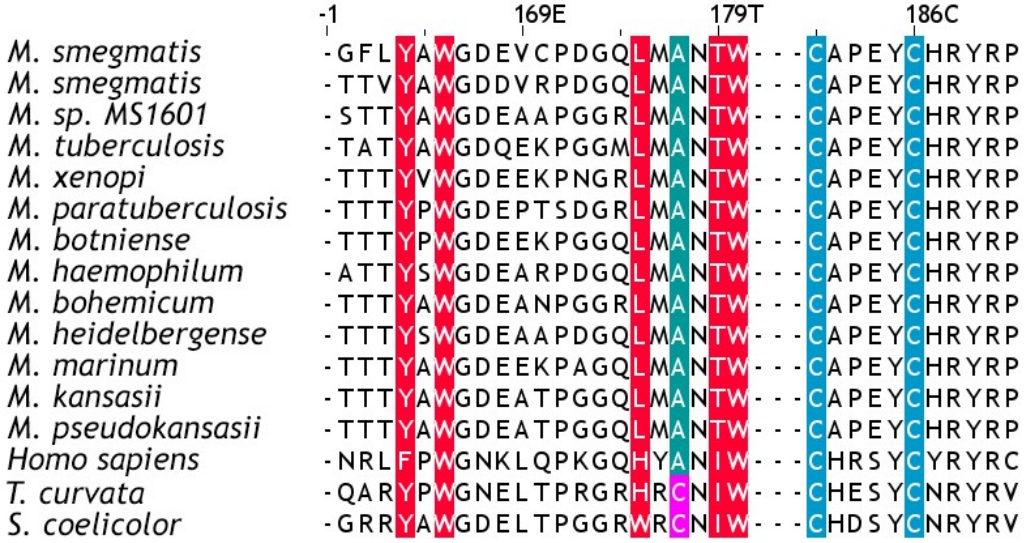
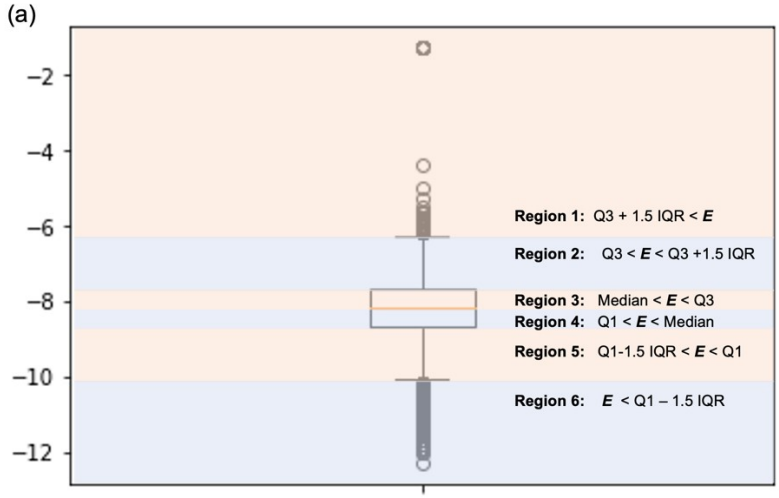


Figure S2. Multiple sequence alignment of FGE from multiple mycobacterium species in comparison with human, T Thermomonospora curvata and Streptomyces coelicolor. Conserved small hydrophobic subdomain containing a buried alanine (pink) which is substituted for cysteine (pink)

(a)



(b)

Region 1	Region 2	Region 3	Region 4	Region 5	Region 6
SMMMC	GWTME	GWTRS	GWTQK	SGWWW	TYWWW
SCGMM	GHGGE	GWTSK	GHGGP	GYWWW	GPWYW
SSCCC	SSCMC				GWWPW
	DGACA				SPWWW
	TPKEK				SWWPW
	TSCKM				

Figure S3. (a) Boxplot of docking energies of penta-peptide ligand (xXXXX: where x: CDEHKLMPQRY, X: any amino acids). (b) Re-sampled and selected peptide belong into the statistical distribution for *in vitro* FGE activity inhibition assay. Inter-Quantile Range (IQR) is distance between upper and lower quantile (IQR = Q3-Q1)

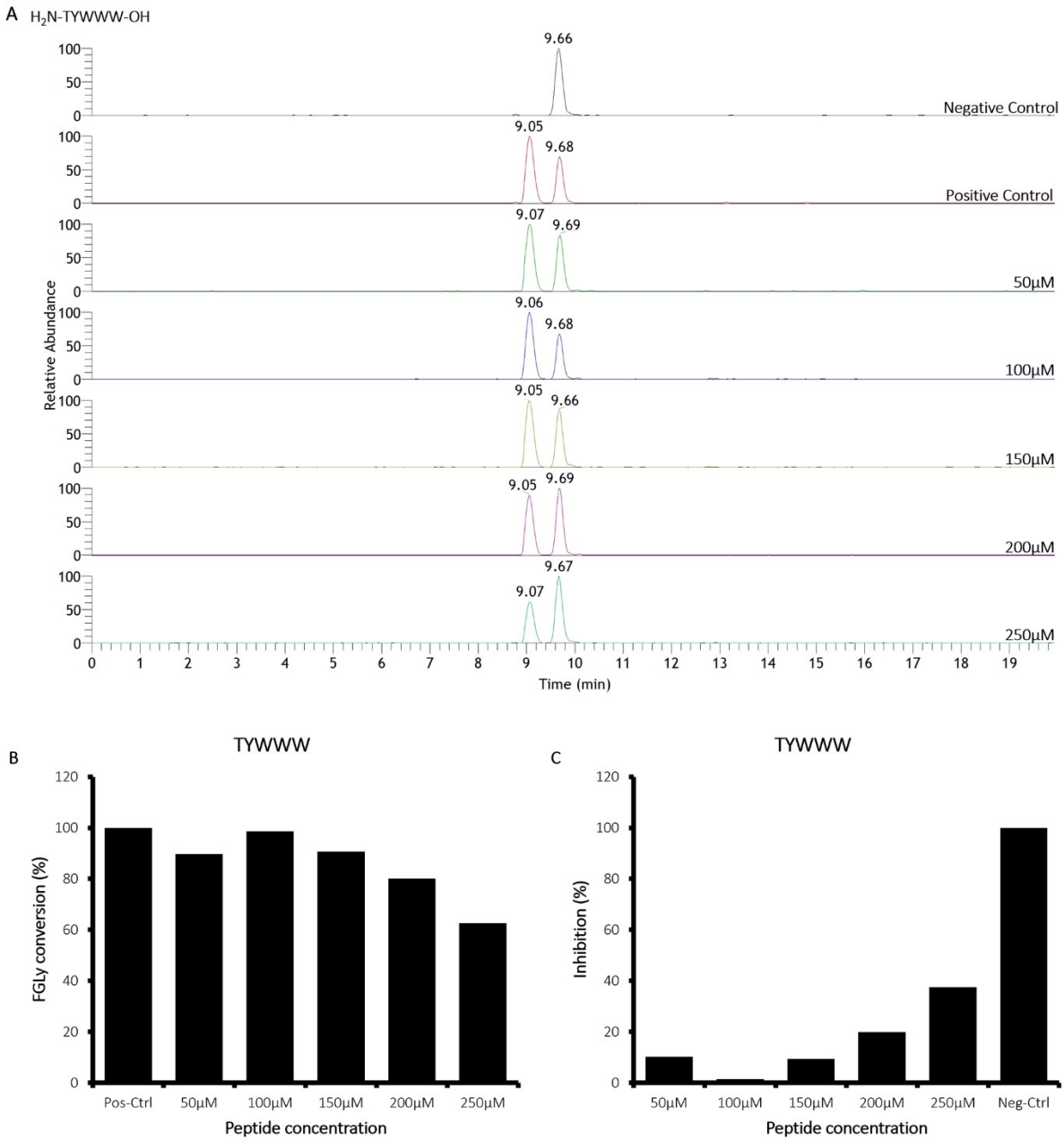


Figure S4. MS-chromatogram profile FGE activity in the presence of various TYWWW concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

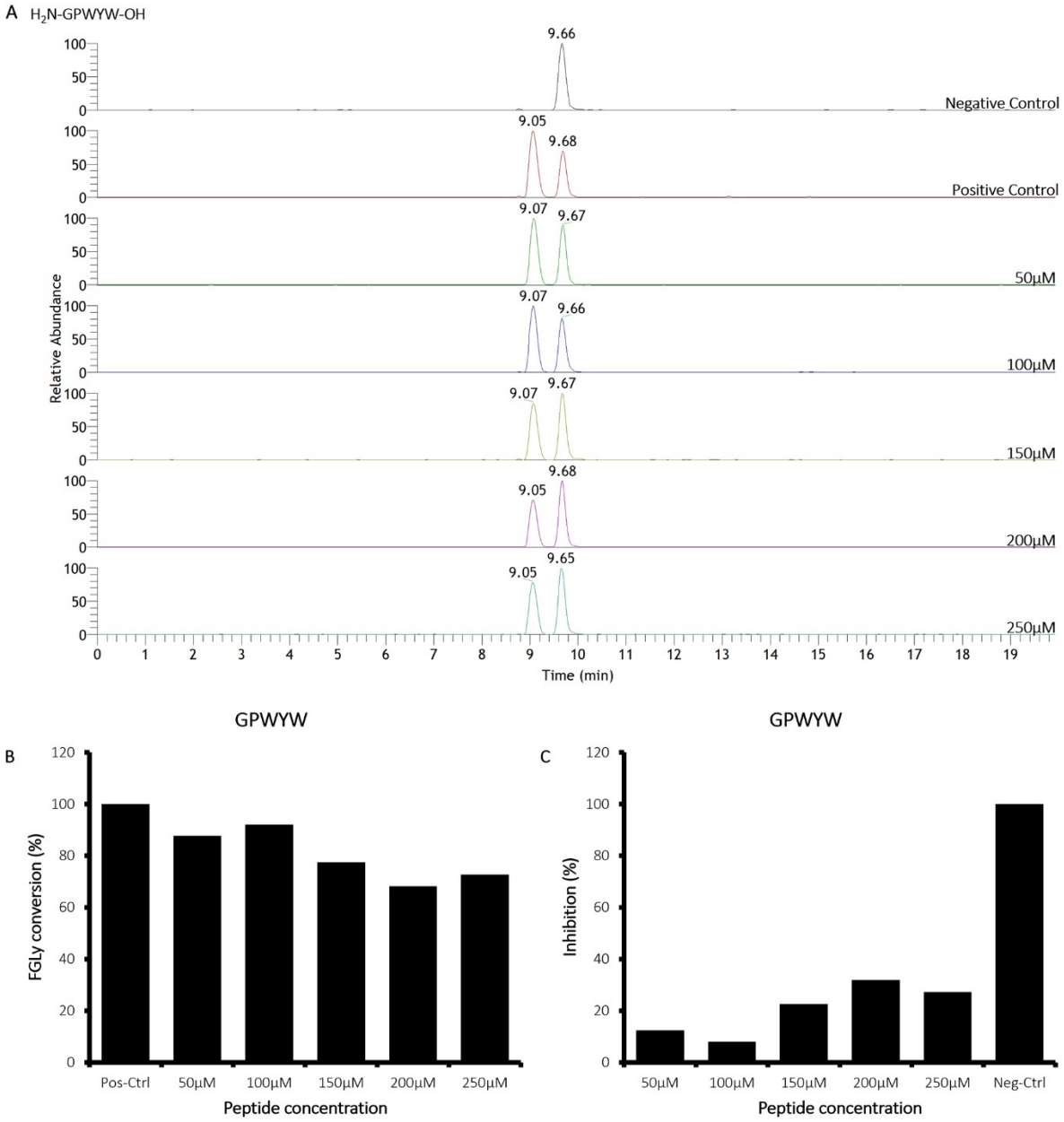


Figure S5. MS-chromatogram profile FGE activity in the presence of various GPWYW concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

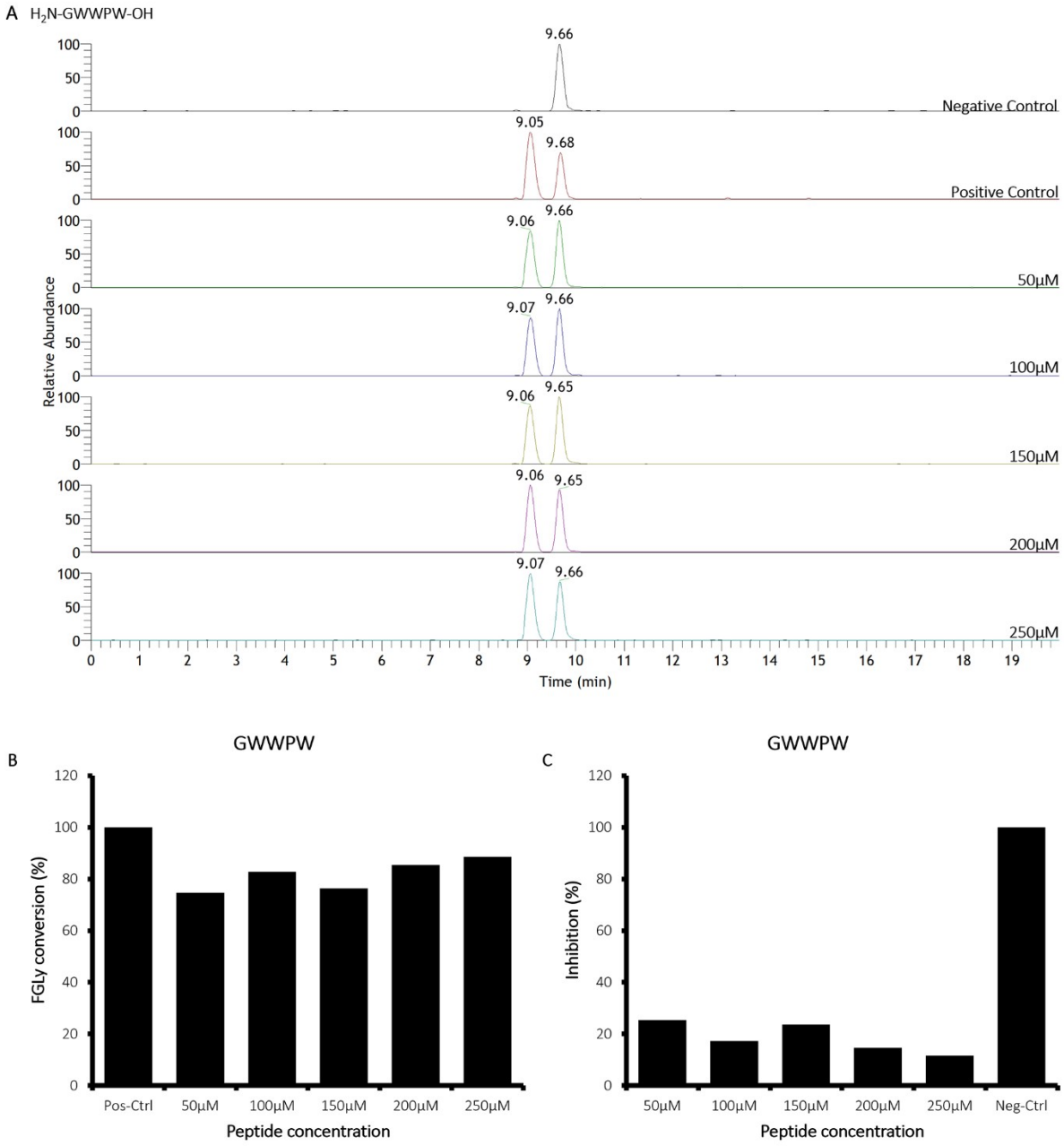


Figure S6. MS-chromatogram profile FGE activity in the presence of various GWWPW concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

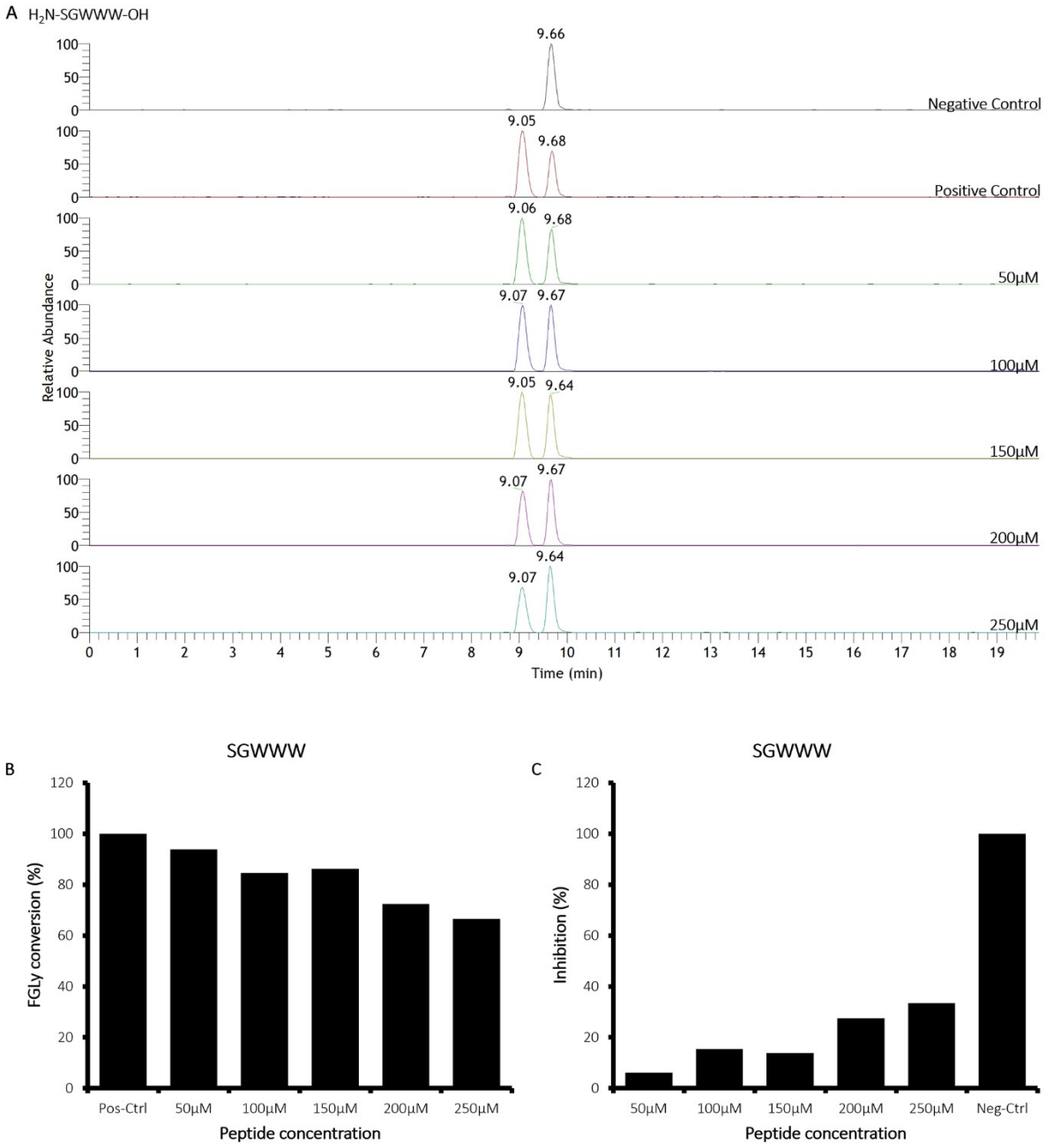


Figure S7. MS-chromatogram profile FGE activity in the presence of various SGWWW concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

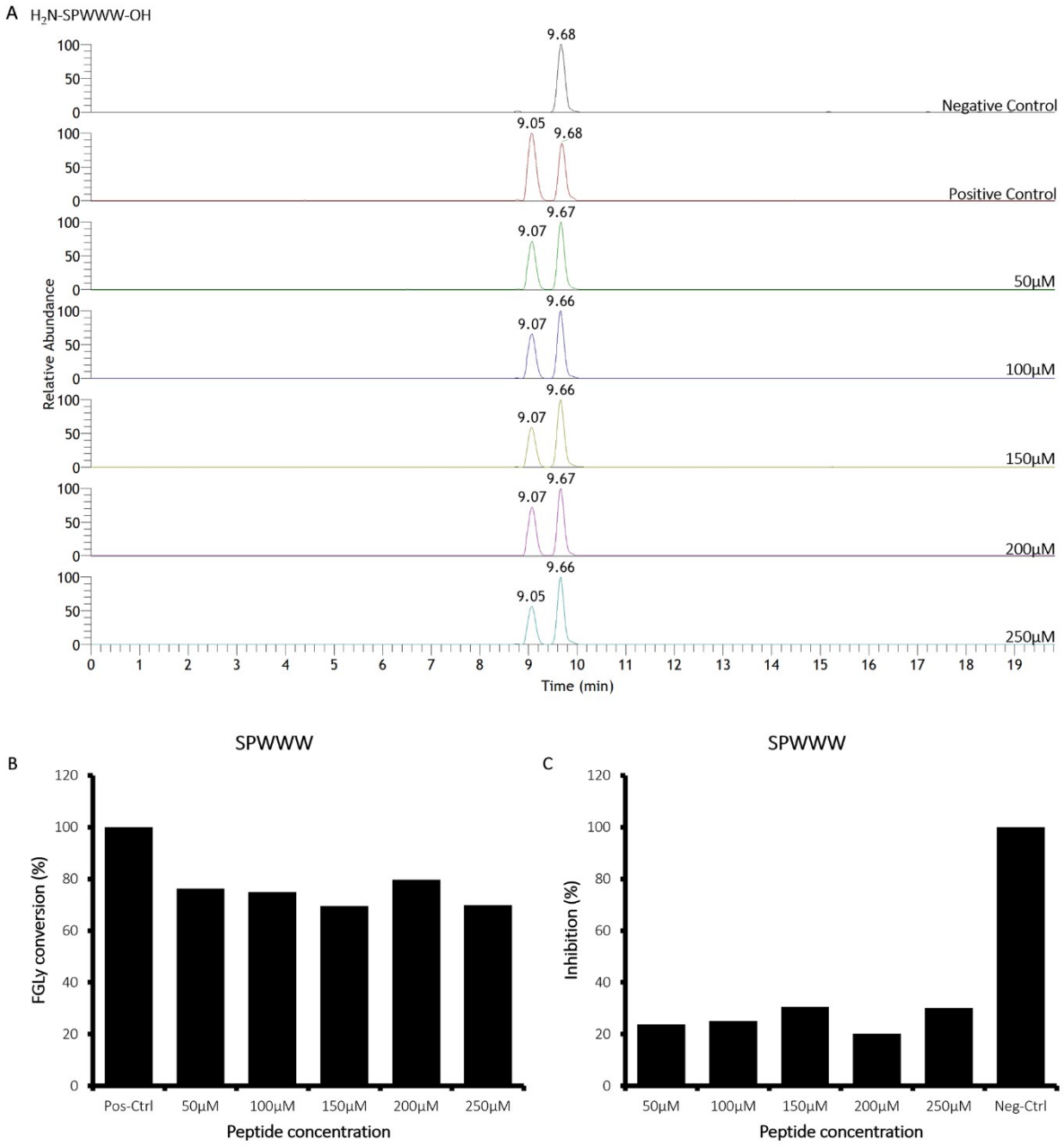


Figure S8. MS-chromatogram profile FGE activity in the presence of various SPWWW concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

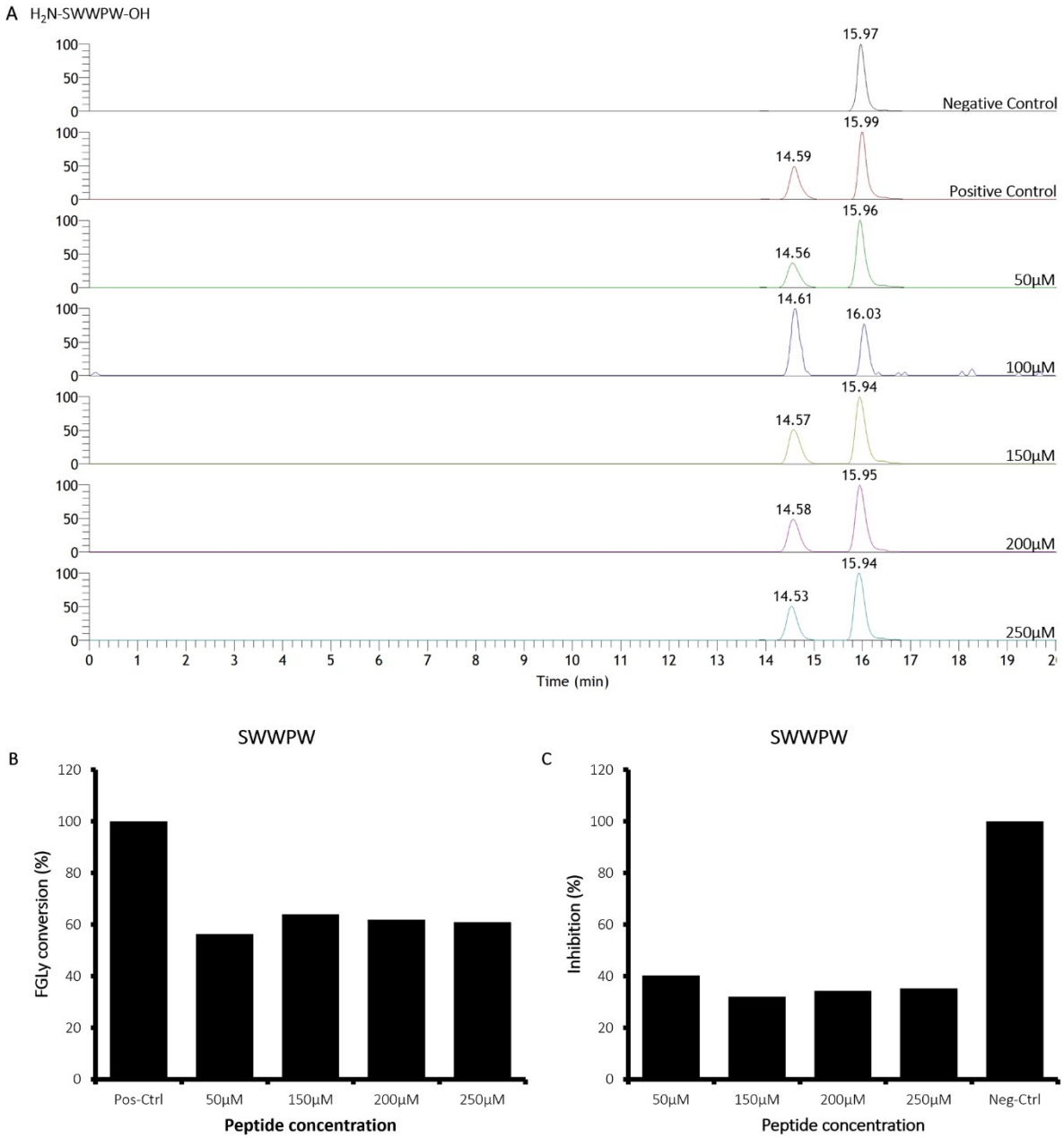


Figure S9. MS-chromatogram profile FGE activity in the presence of various SWWPW concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

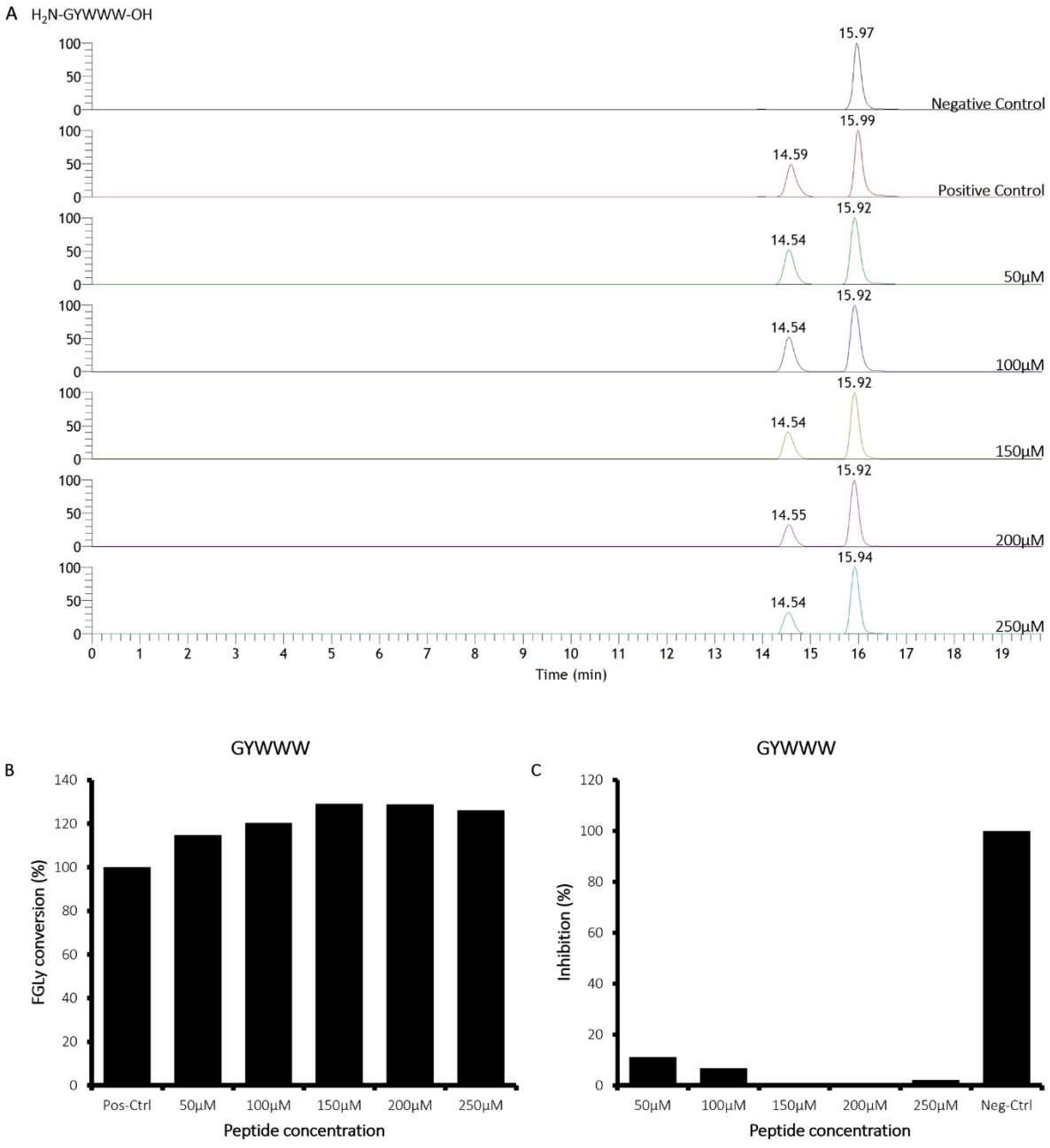


Figure S10. MS-chromatogram profile FGE activity in the presence of various GYWWW concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

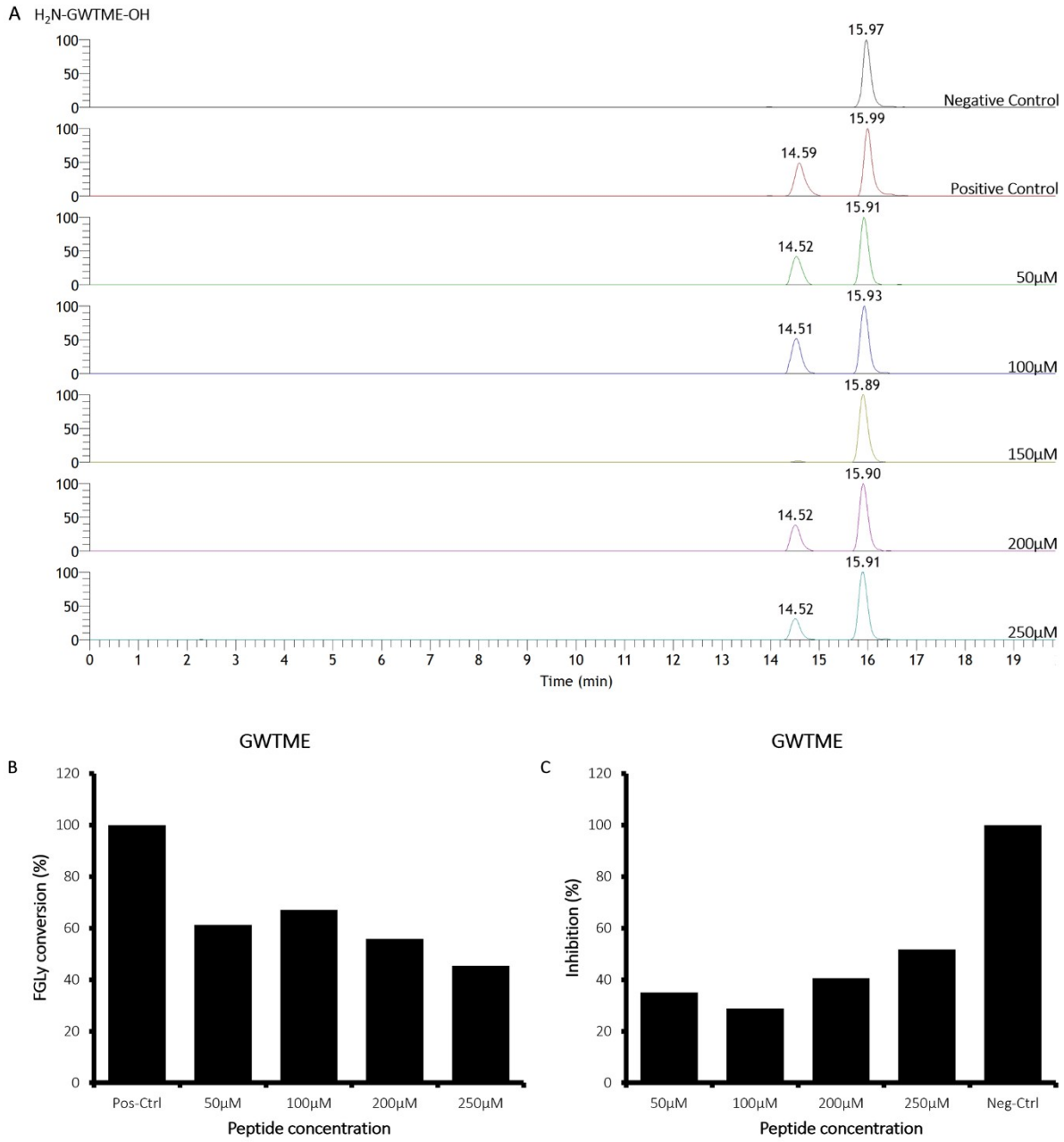


Figure S11. MS-chromatogram profile FGE activity in the presence of various GWTME concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

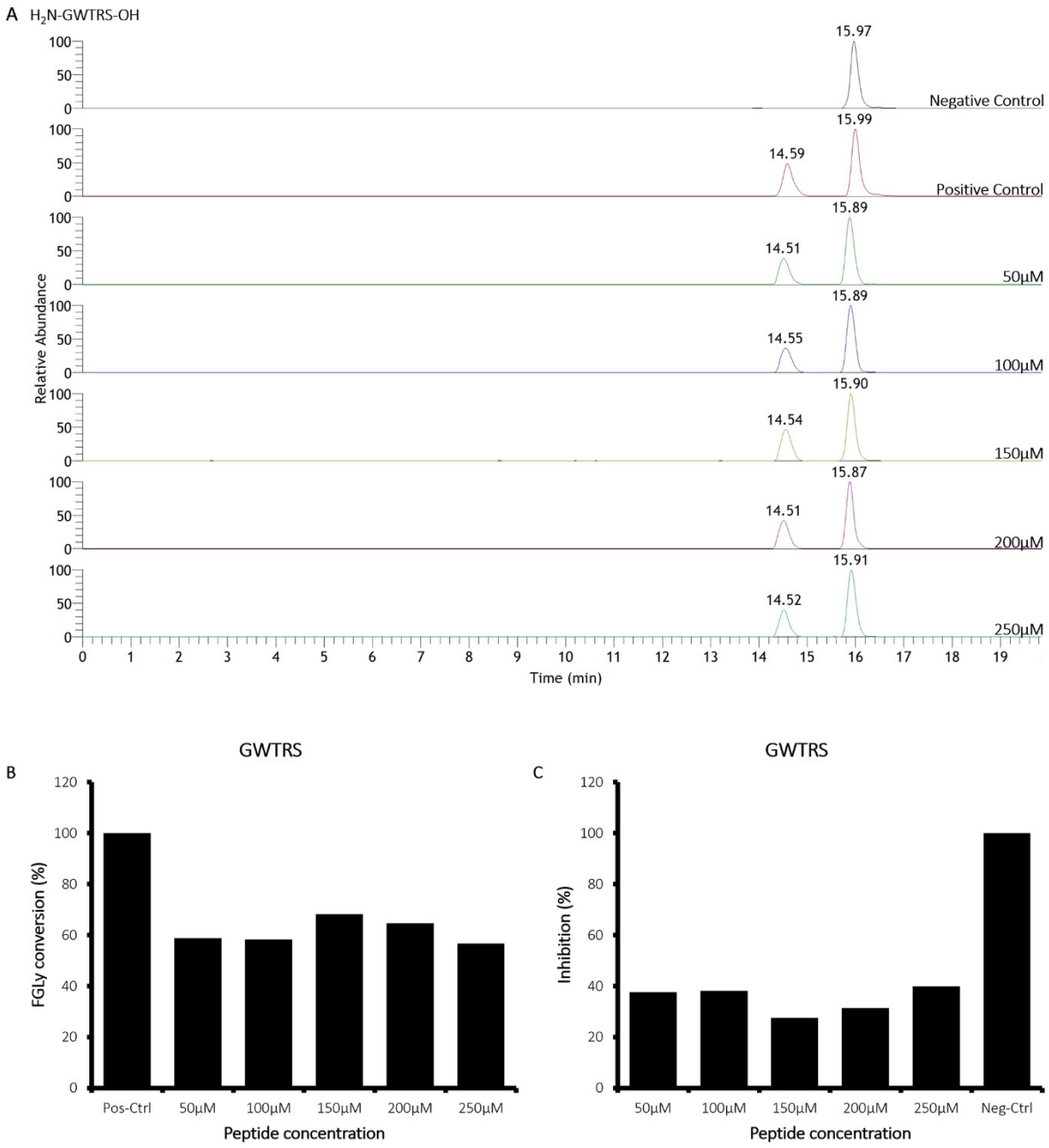


Figure S12. MS-chromatogram profile FGE activity in the presence of various GWTRS concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

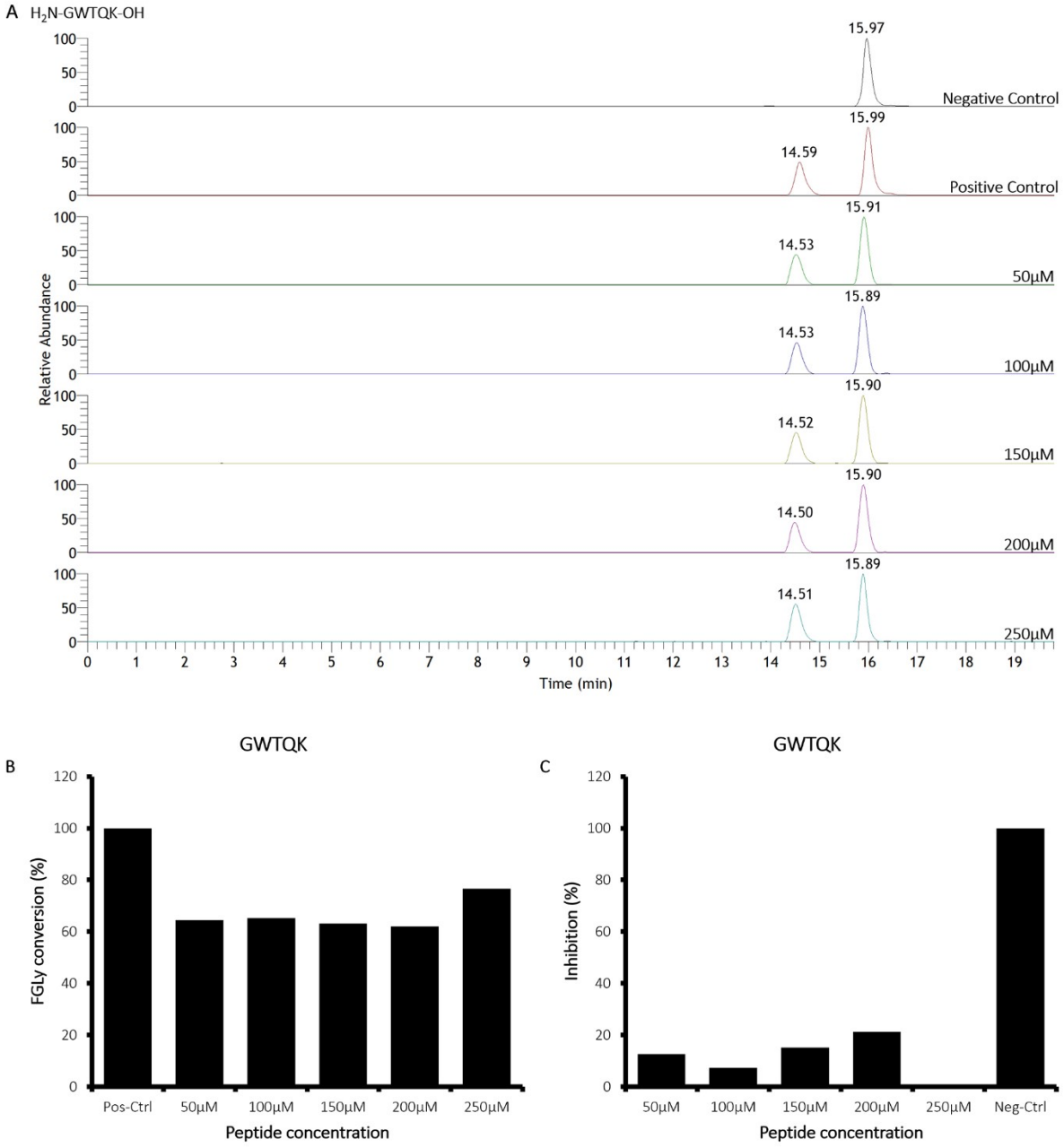


Figure S13. MS-chromatogram profile FGE activity in the presence of various GWTQK concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

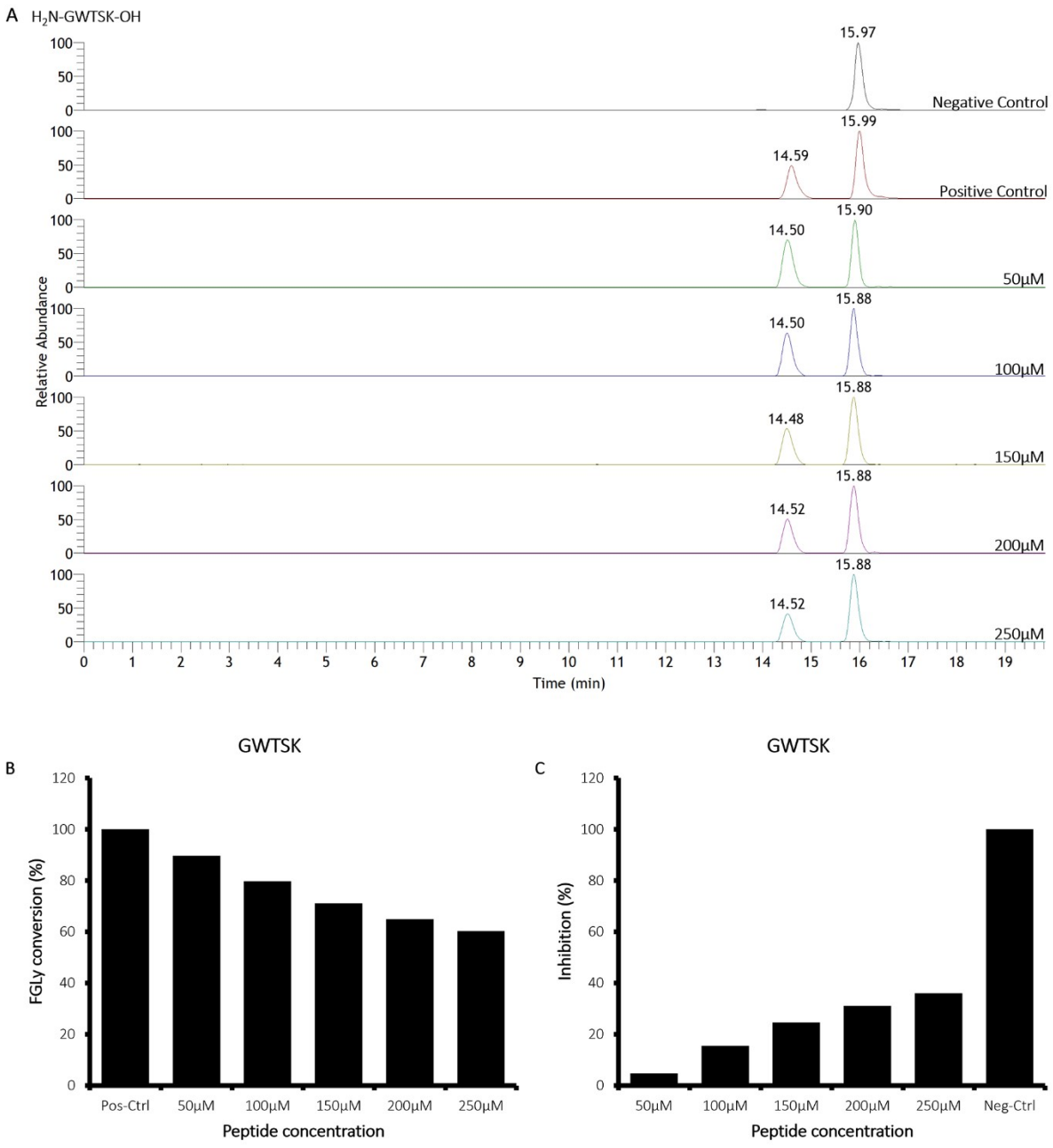


Figure S14. MS-chromatogram profile FGE activity in the presence of various GWTSK concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

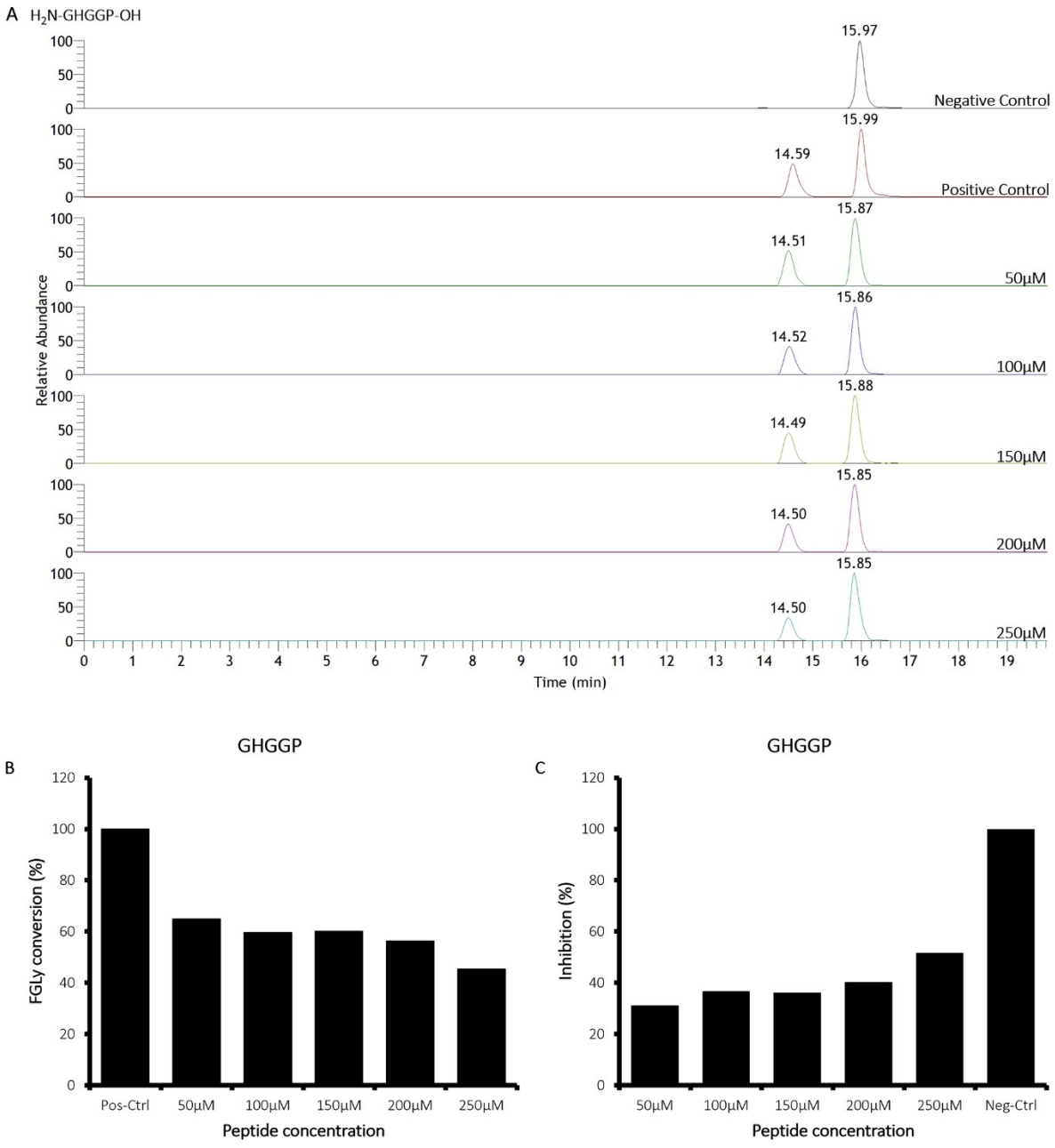


Figure S15. MS-chromatogram profile FGE activity in the presence of various GHGGP concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

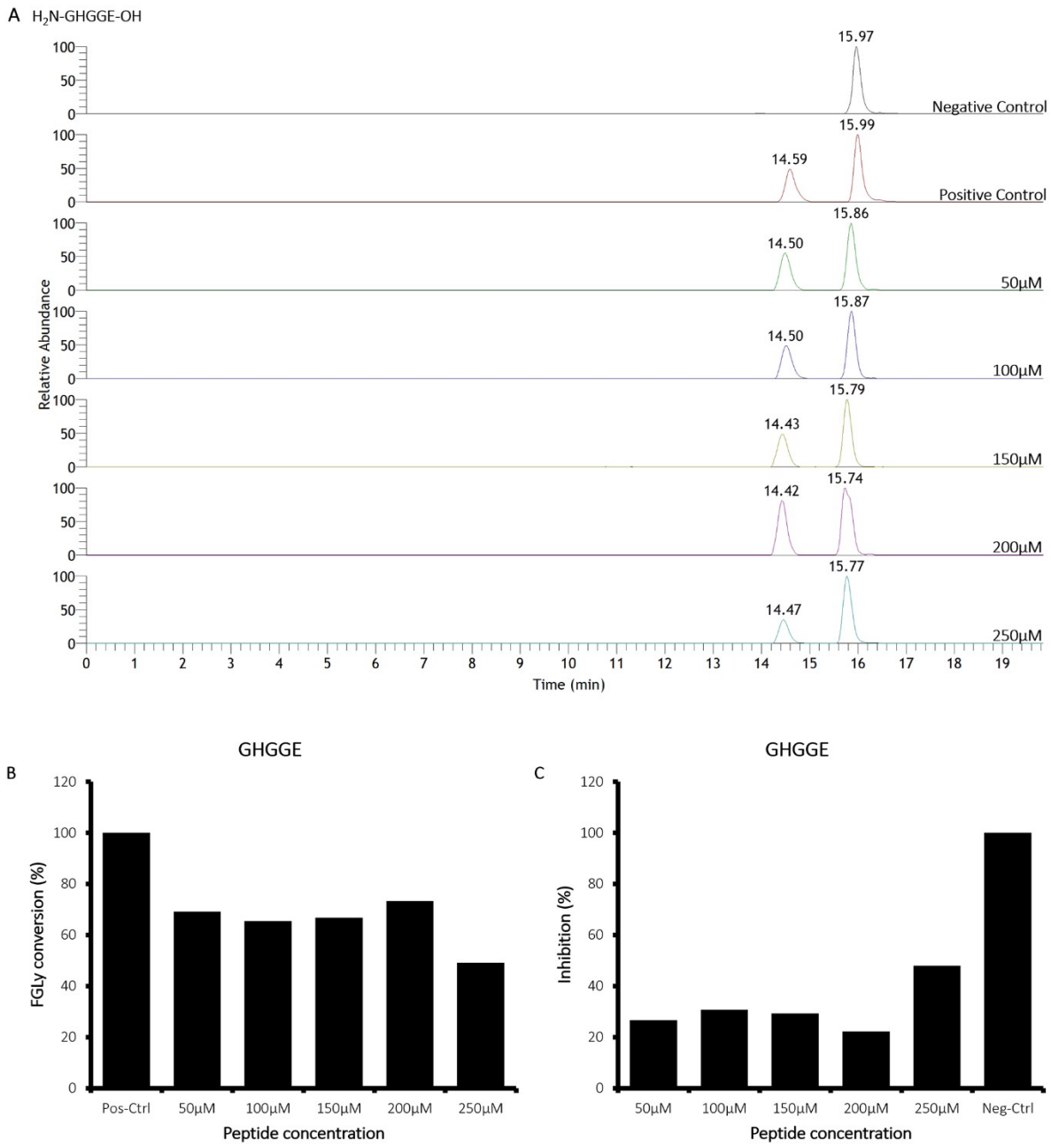


Figure S16. MS-chromatogram profile FGE activity in the presence of various GHGGE concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

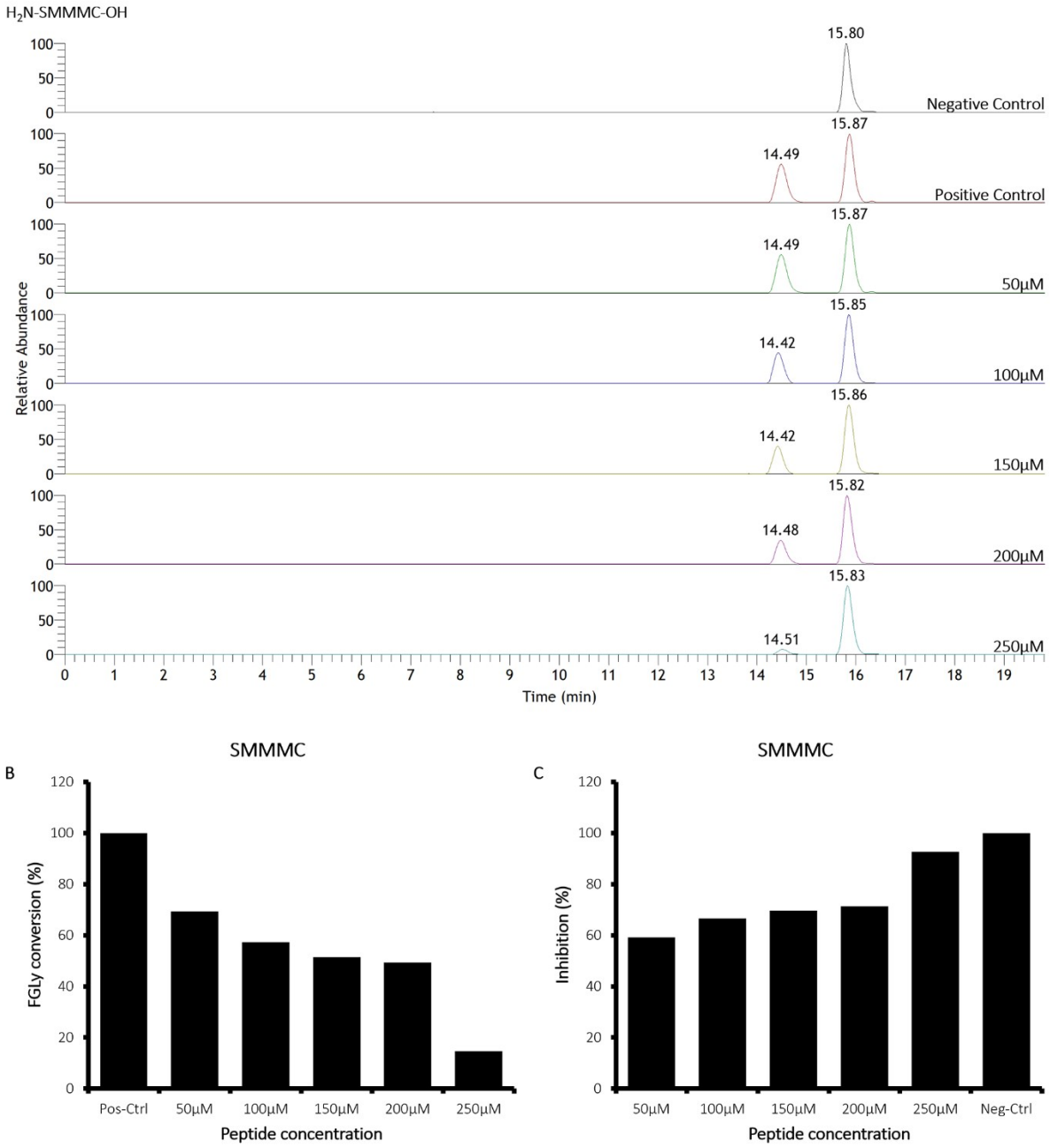


Figure S17.MS-chromatogram profile FGE activity in the presence of various SMMMC concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

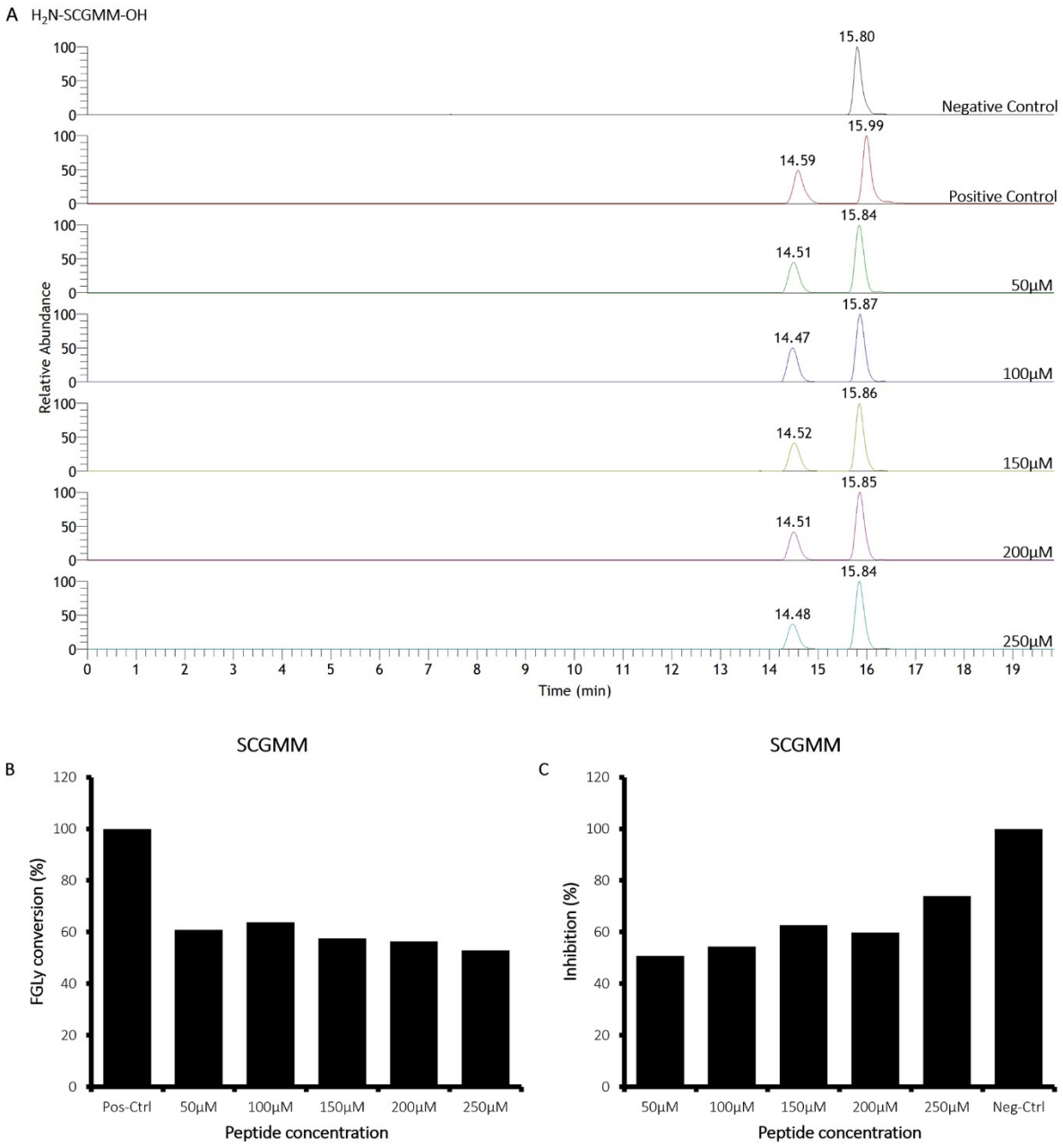


Figure S18. MS-chromatogram profile FGE activity in the presence of various SCGMM concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

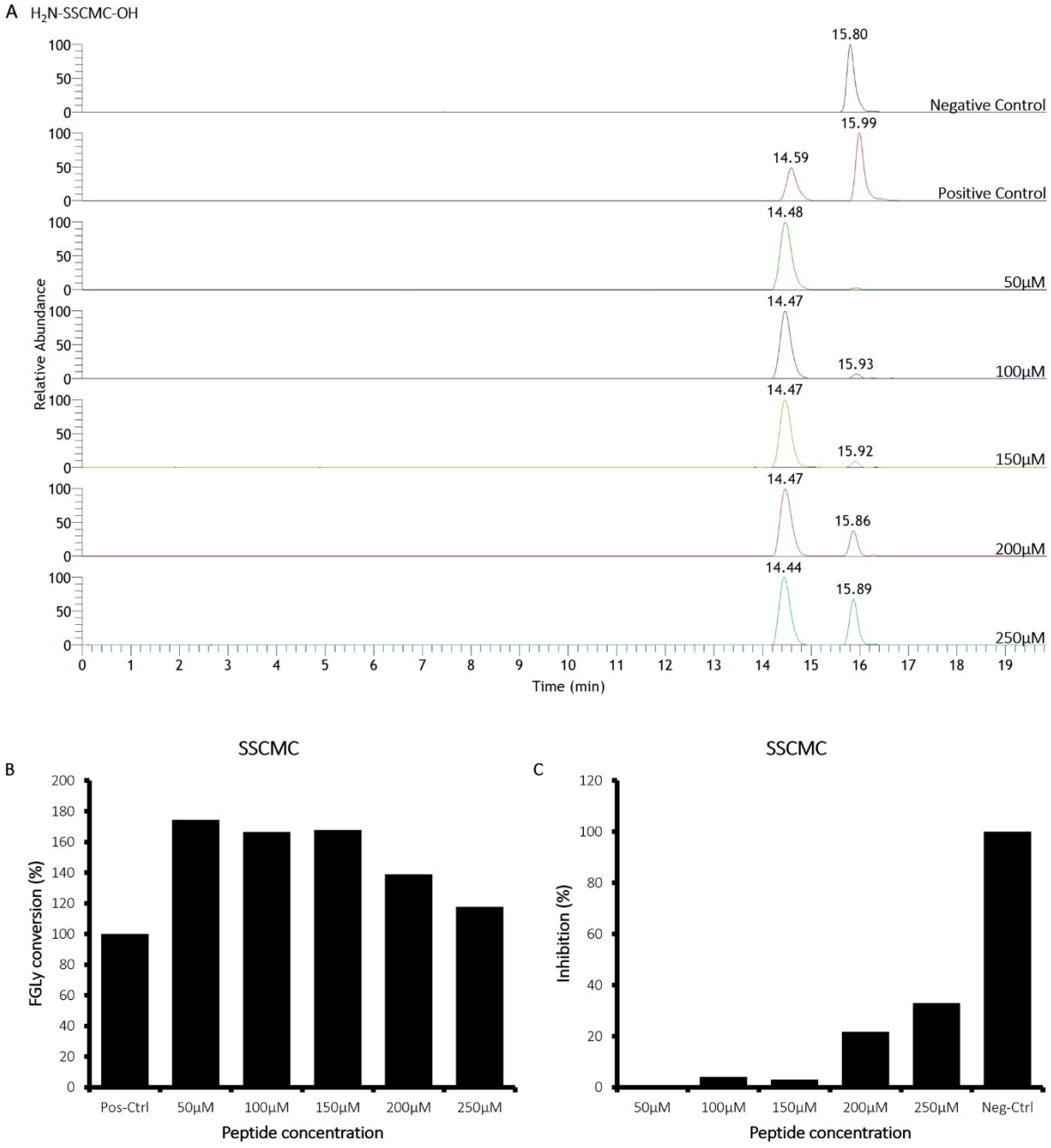


Figure S19.MS-chromatogram profile FGE activity in the presence of various SSCMC concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

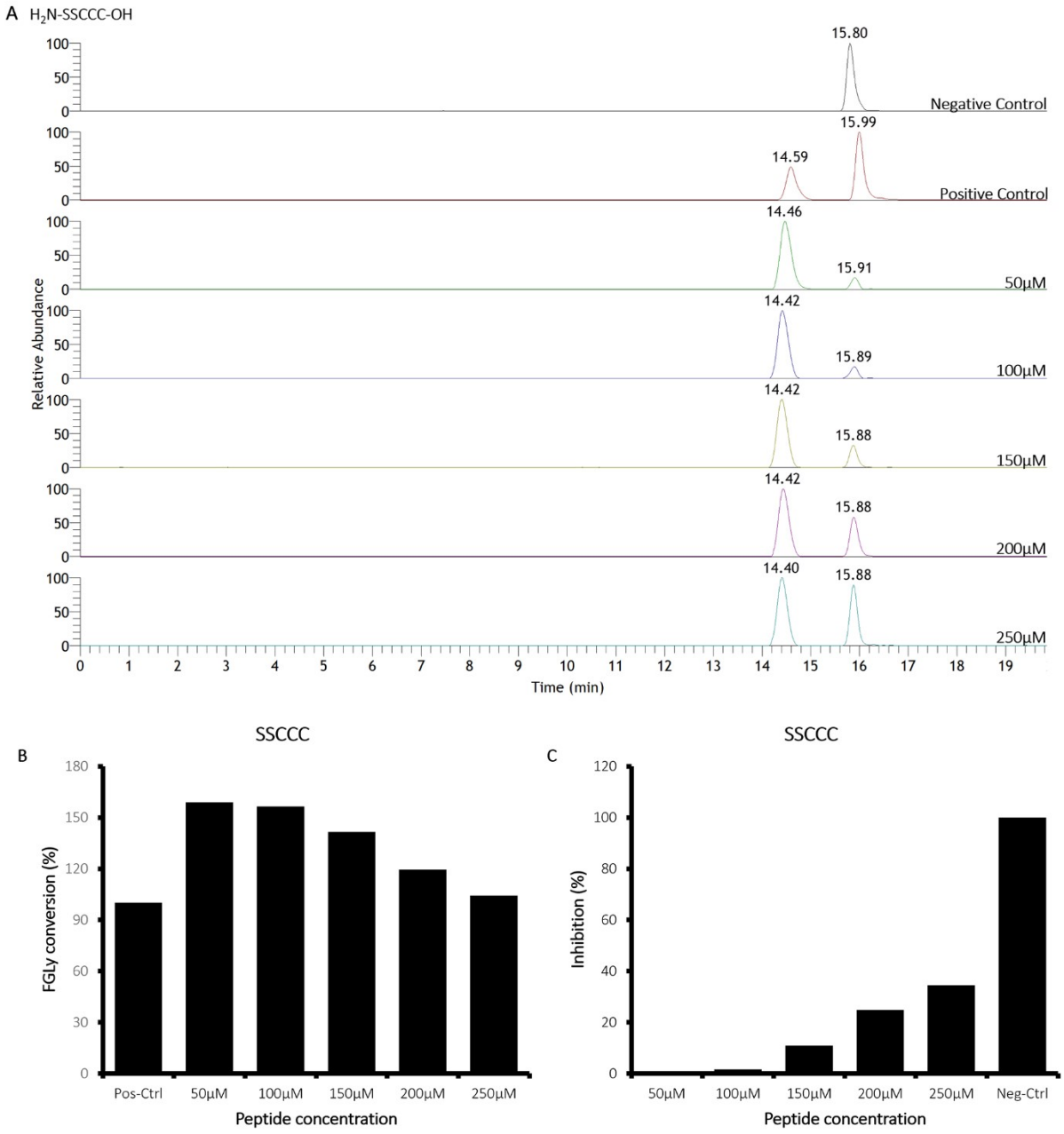


Figure S20. MS-chromatogram profile FGE activity in the presence of various SSCCC concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

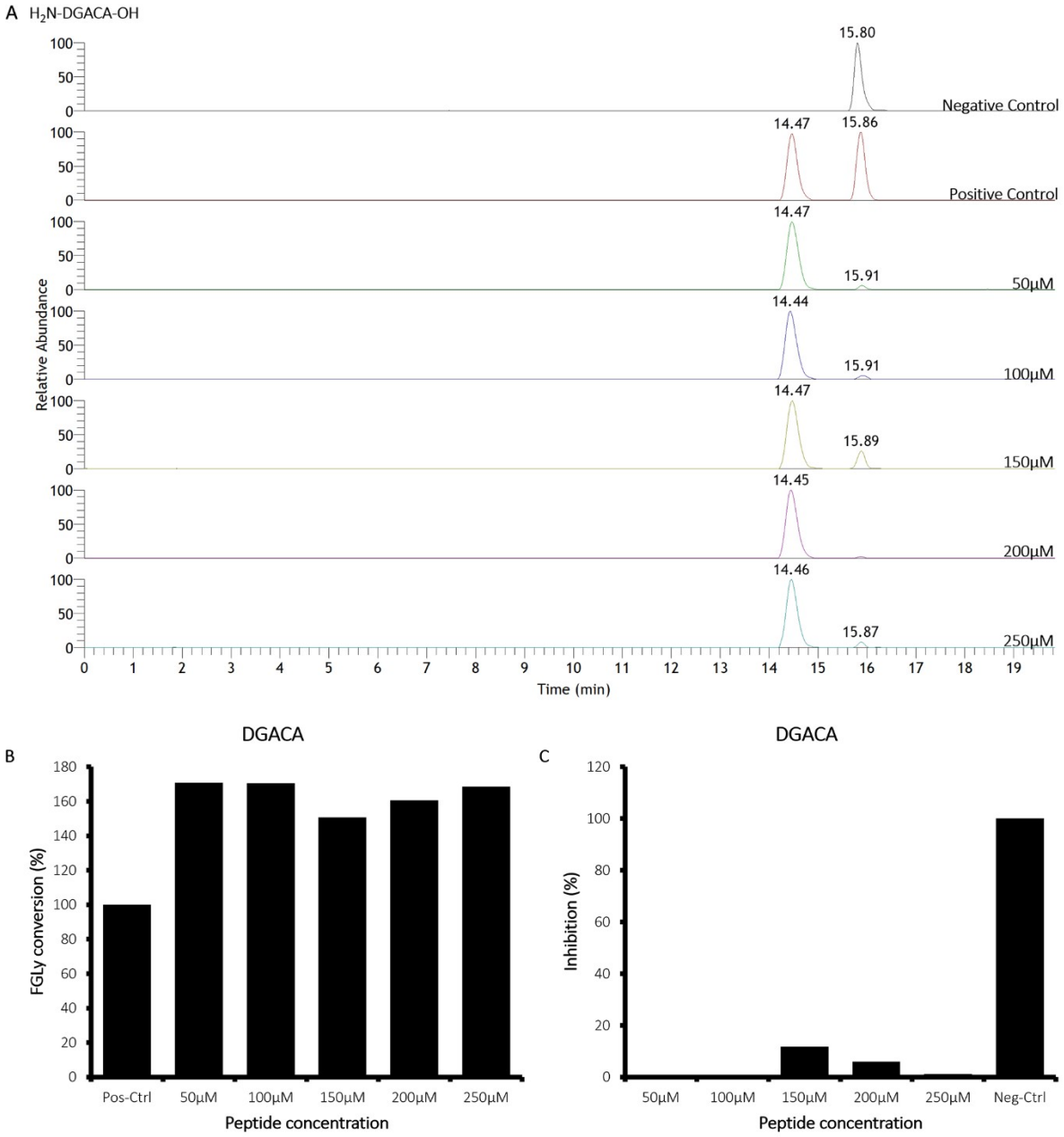


Figure S21. MS-chromatogram profile FGE activity in the presence of various DGACA concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

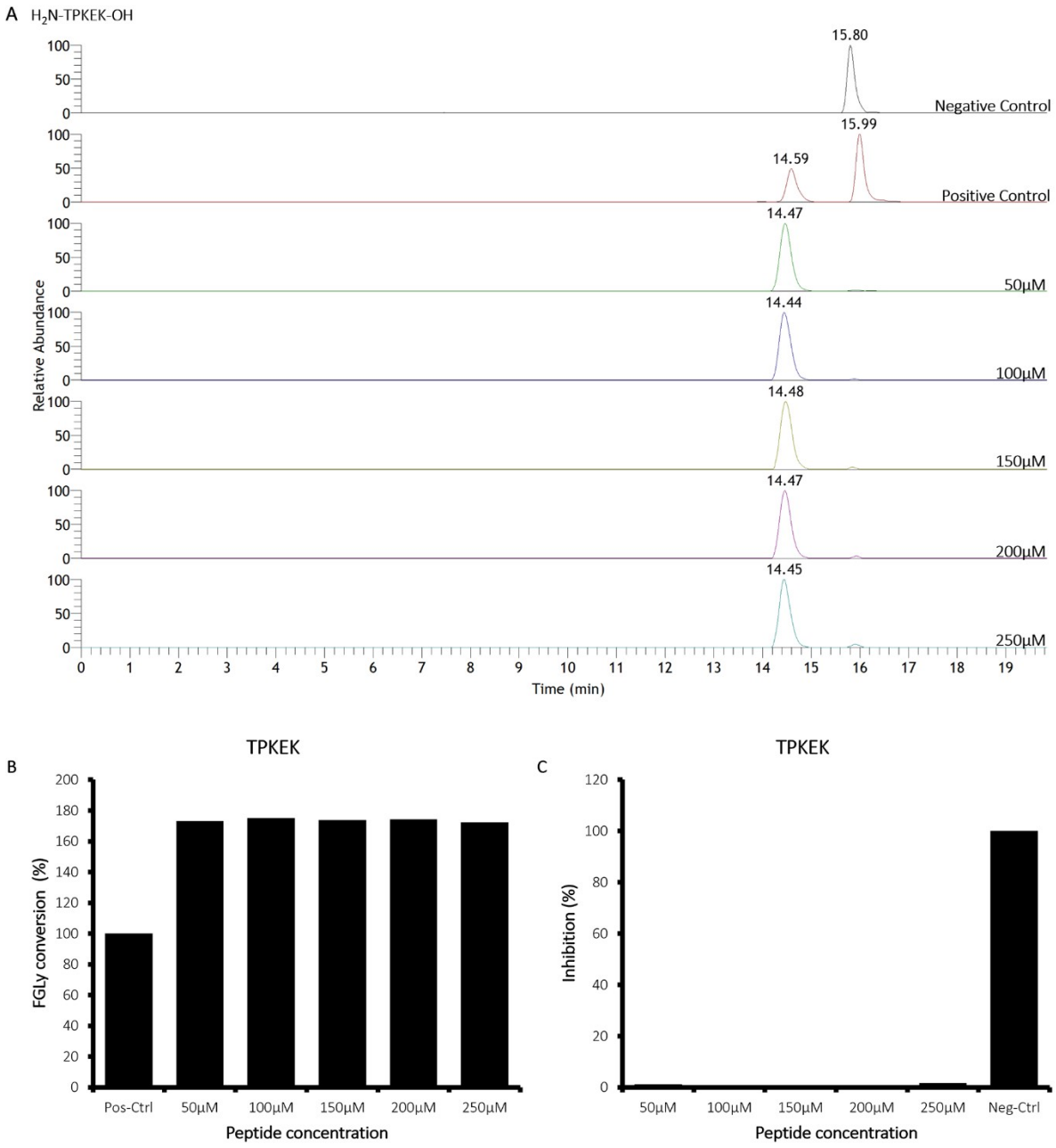


Figure S22. MS-chromatogram profile FGE activity in the presence of various TPKEK concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.

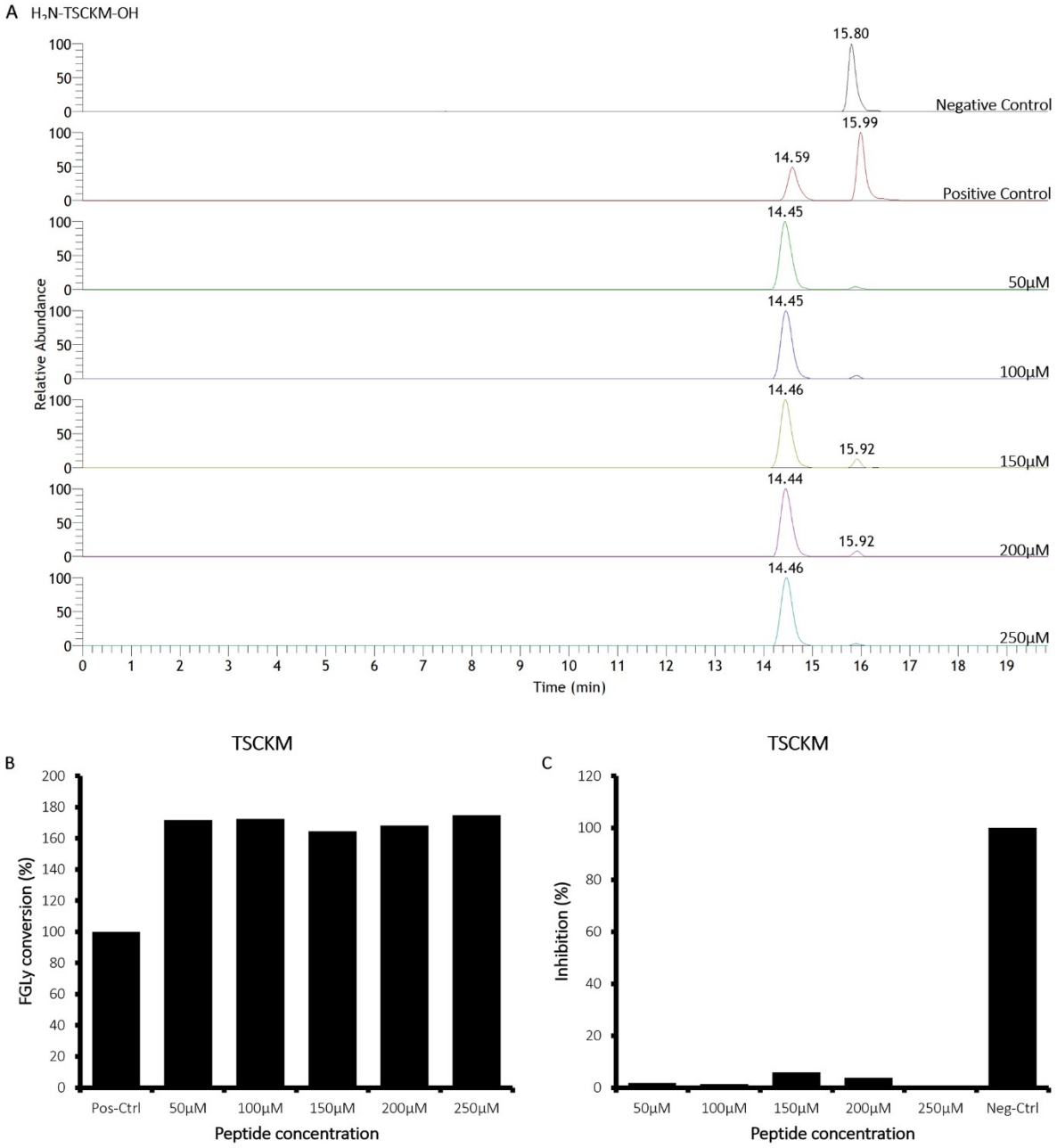


Figure S23. MS-chromatogram profile FGE activity in the presence of various TSCKM concentrations. The peptide inhibitor was neither N-terminal acetylated nor C-terminal amidated and the reaction contained 200µM native enzyme substrate.