

Solid Phase Synthesis of an “Inaccessible” hGH-derived Peptide using a Pseudoproline Monomer and SIT-Protection for Cysteine

Srinivasa Rao Manne,¹ Amit Chakraborty,¹ Karin Rustler,² Thomas Bruckdorfer,² Beatriz G. de la Torre,^{3*} Fernando Albericio^{1,4,5*}

¹ Peptide Science Laboratory, School of Chemistry and Physics, University of KwaZulu-Natal, Westville, Durban 4000, South Africa.

² Iris Biotech GmbH, Adalbert-Zoellner-Str. 1, 95615 Marktredwitz, Germany.

³ KwaZulu-Natal Research Innovation and Sequencing Platform (KRISP), School of Laboratory Medicine and Medical Sciences, College of Health Sciences, University of KwaZulu-Natal, Durban 4041, South Africa.

⁴ Institute for Advanced Chemistry of Catalonia (IQAC-CSIC), 08034 Barcelona, Spain.

⁵ CIBER-BBN, Networking Centre on Bioengineering, Biomaterials and Nanomedicine, and Department of Organic Chemistry, University of Barcelona, 08028 Barcelona, Spain.

Spectral Data

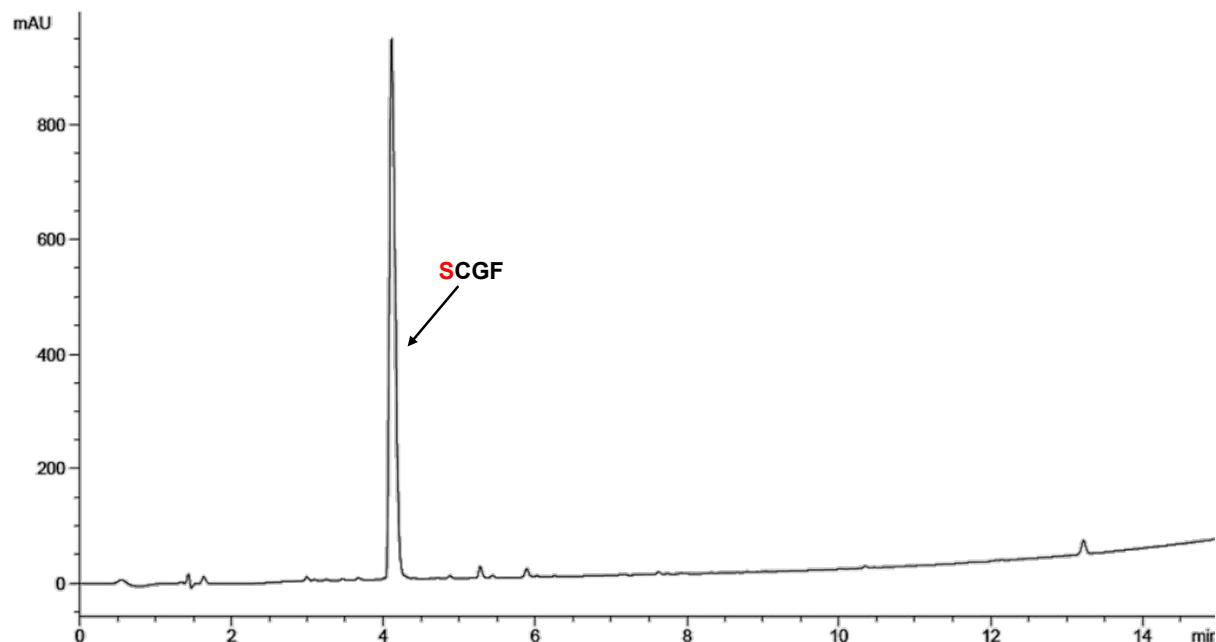


Figure S1. HPLC chromatogram of **H-SCGF-NH₂**, 5-95% B into A

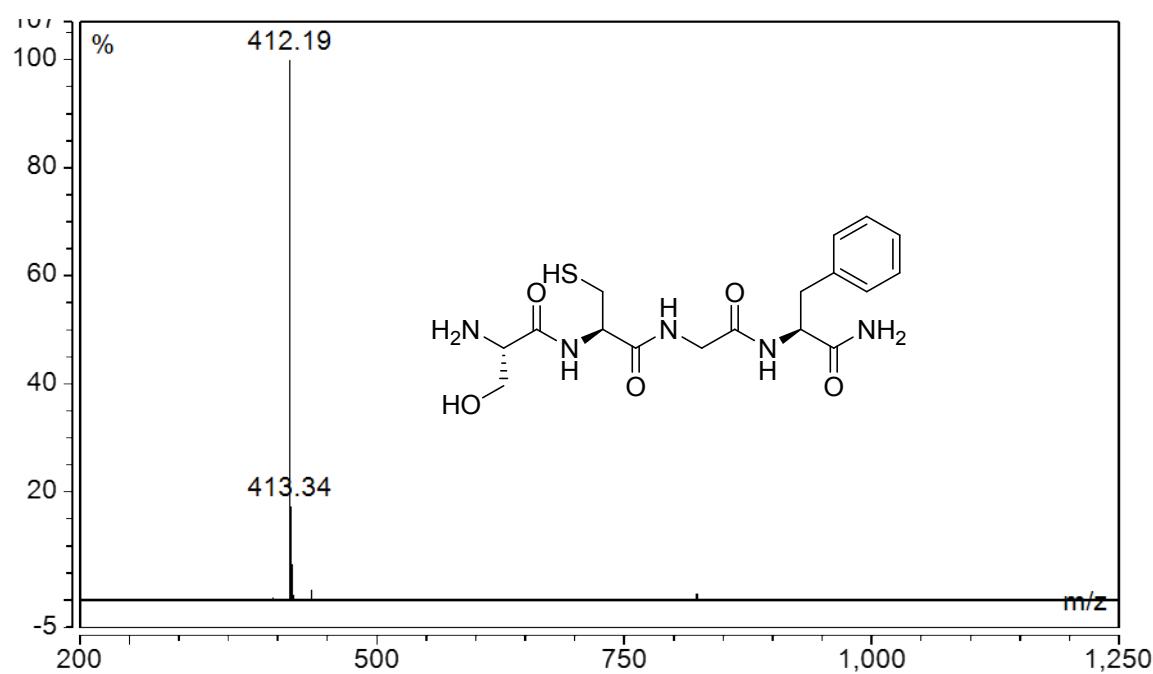


Figure S2. LCMS spectrum of **H-SCGF-NH₂**, Calculated for C₁₇H₂₆N₅O₅S, [M+H]¹⁺ 412.48; Found: [M+H]¹⁺ = 412.19

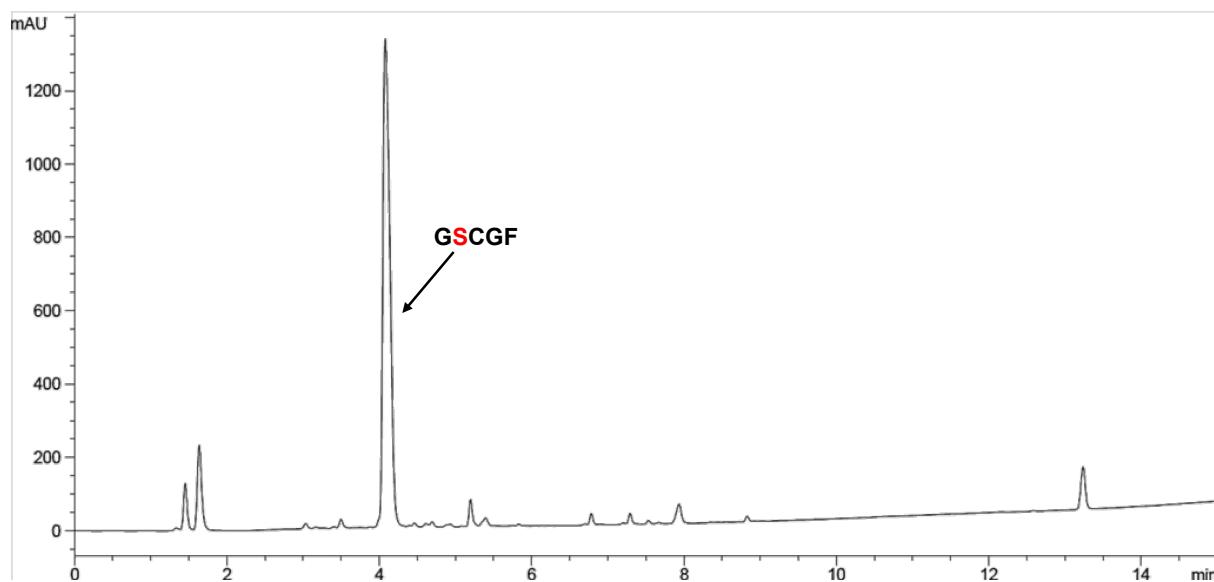


Figure S3. HPLC chromatogram of **H-GSCGF-NH₂**, 5-95% B into A

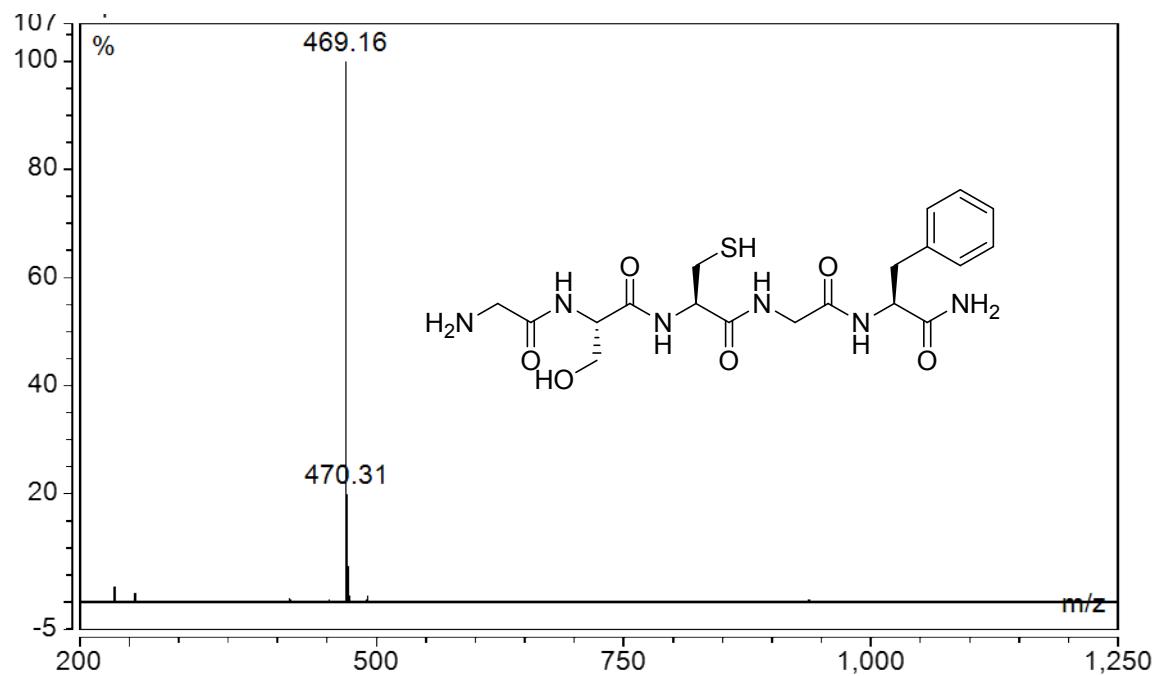


Figure S4. LCMS spectrum of **H-GSCGF-NH₂**, Calculated for C₁₉H₂₉N₆O₆S, [M+H]¹⁺ 469.53; Found: [M+H]¹⁺ = 469.16

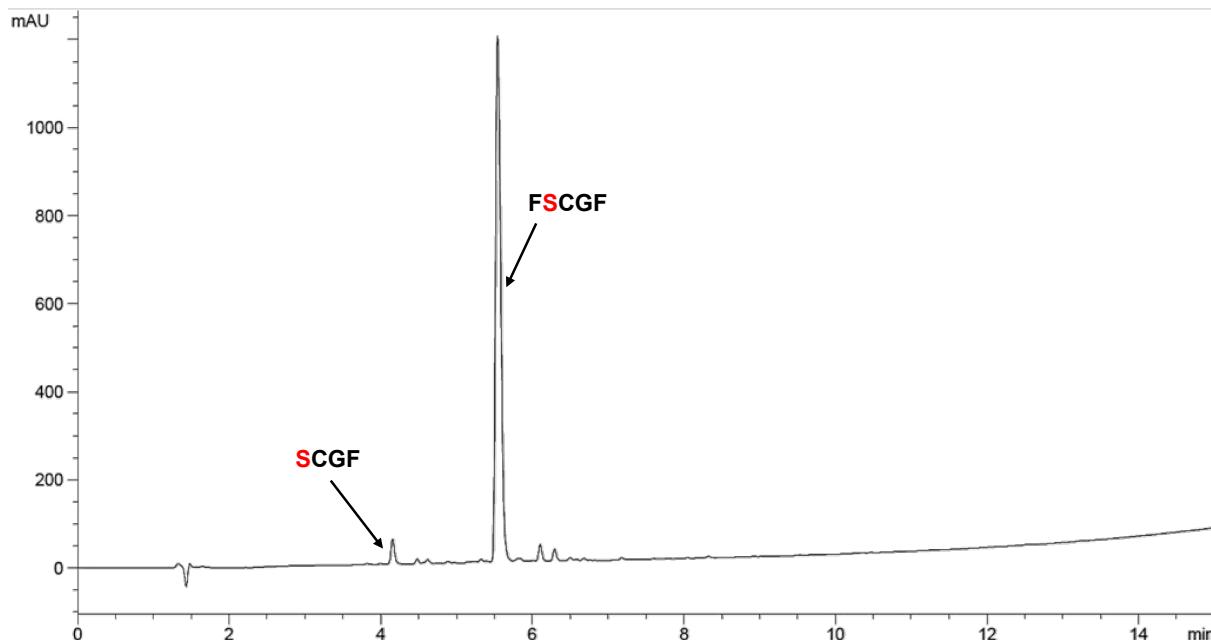


Figure S5. HPLC chromatogram of **H-FSCGF-NH₂**, 5-95% B into A

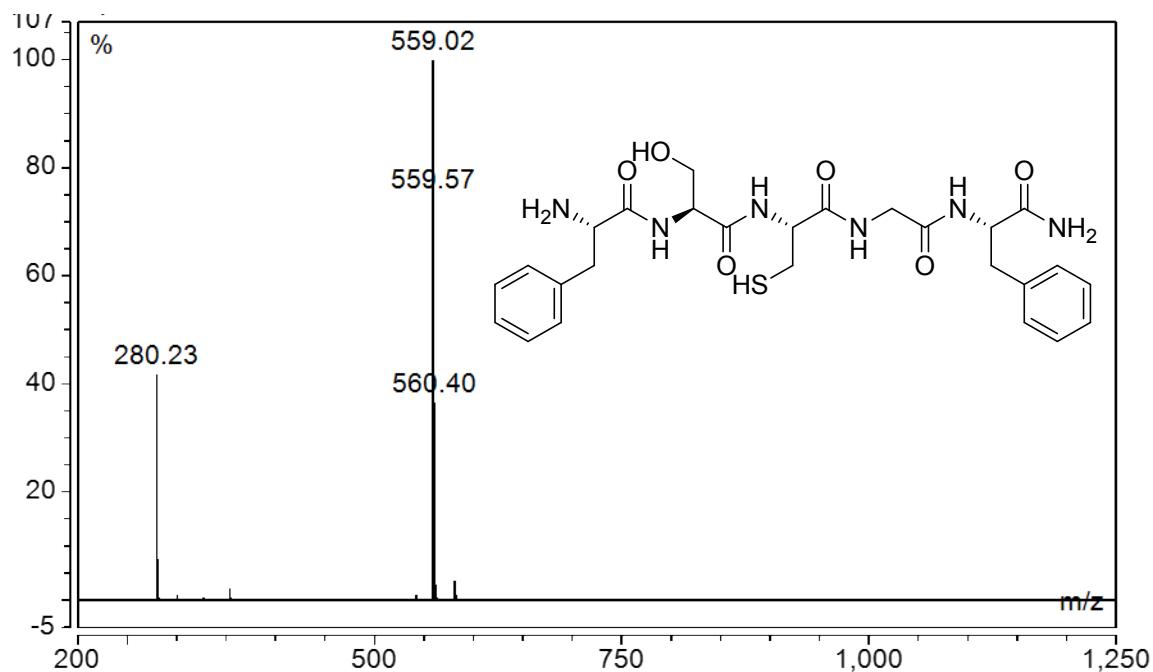


Figure S6. LCMS spectrum of **H-FSCGF-NH₂**, Calculated for $C_{26}H_{35}N_6O_6S$, $[M+H]^{1+}$ 559.65; Found: $[M+H]^{1+}= 559.57$

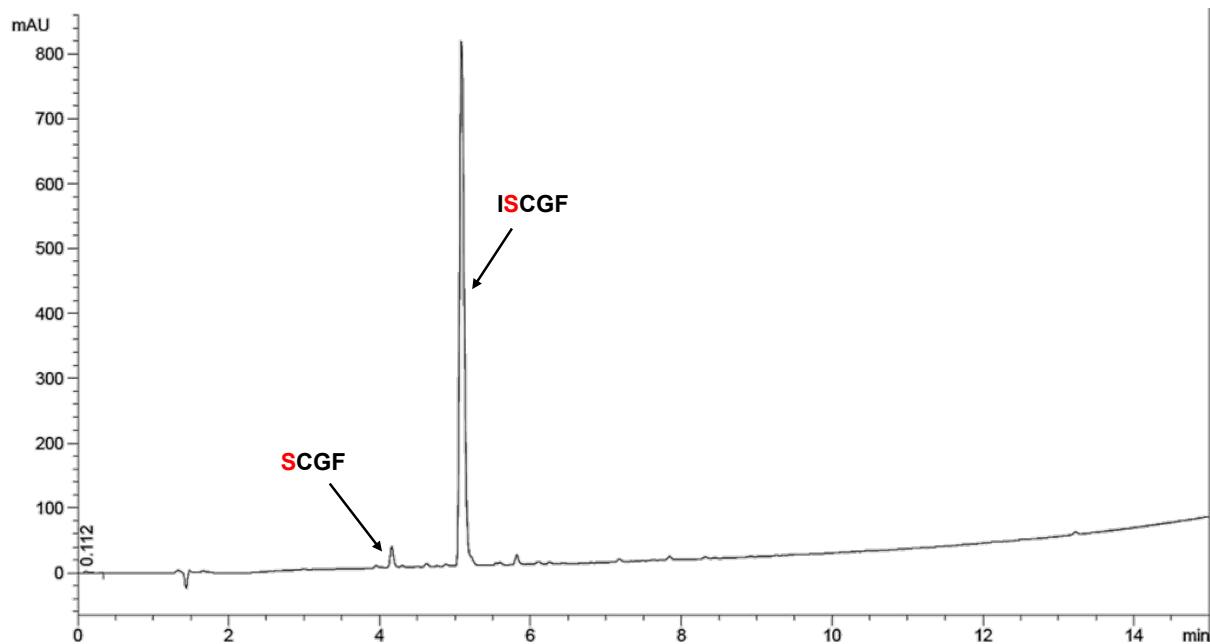


Figure S7. HPLC chromatogram of **H-ISCGF-NH₂**, 5-95% B into A

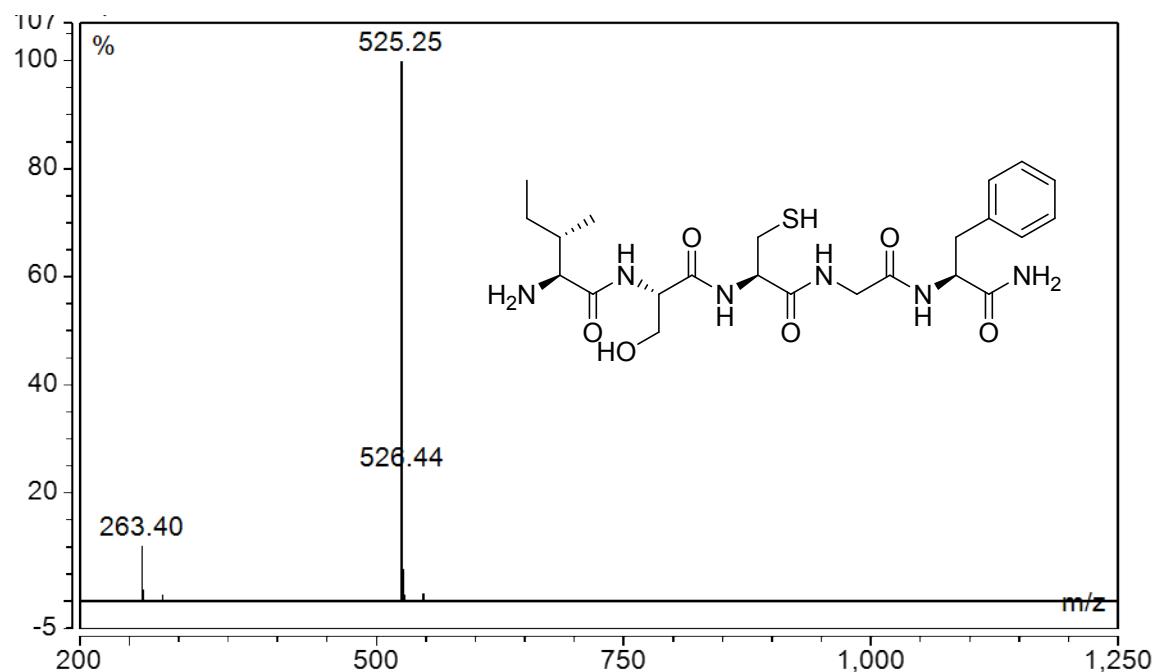


Figure S8. LCMS spectrum of **H-ISCGF-NH₂**, Calculated for C₂₃H₃₇N₆O₆S, [M+H]¹⁺ 525.64; Found: [M+H]¹⁺ = 525.25

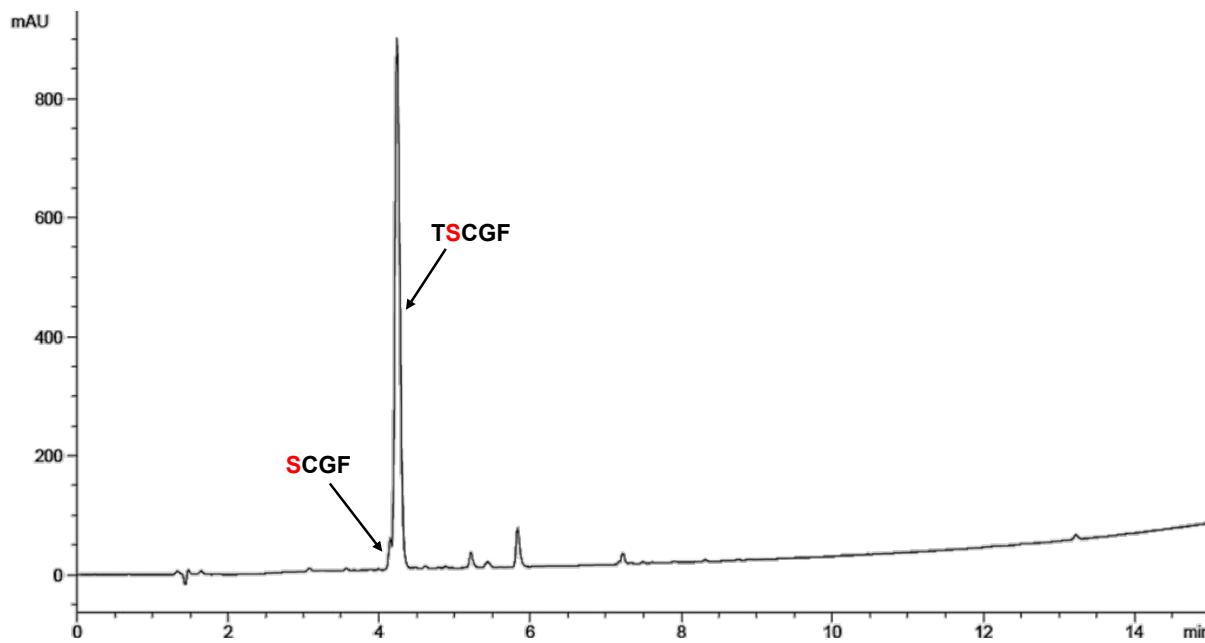


Figure S9. HPLC chromatogram of H-TSCGF-NH₂, 5-95% B into A

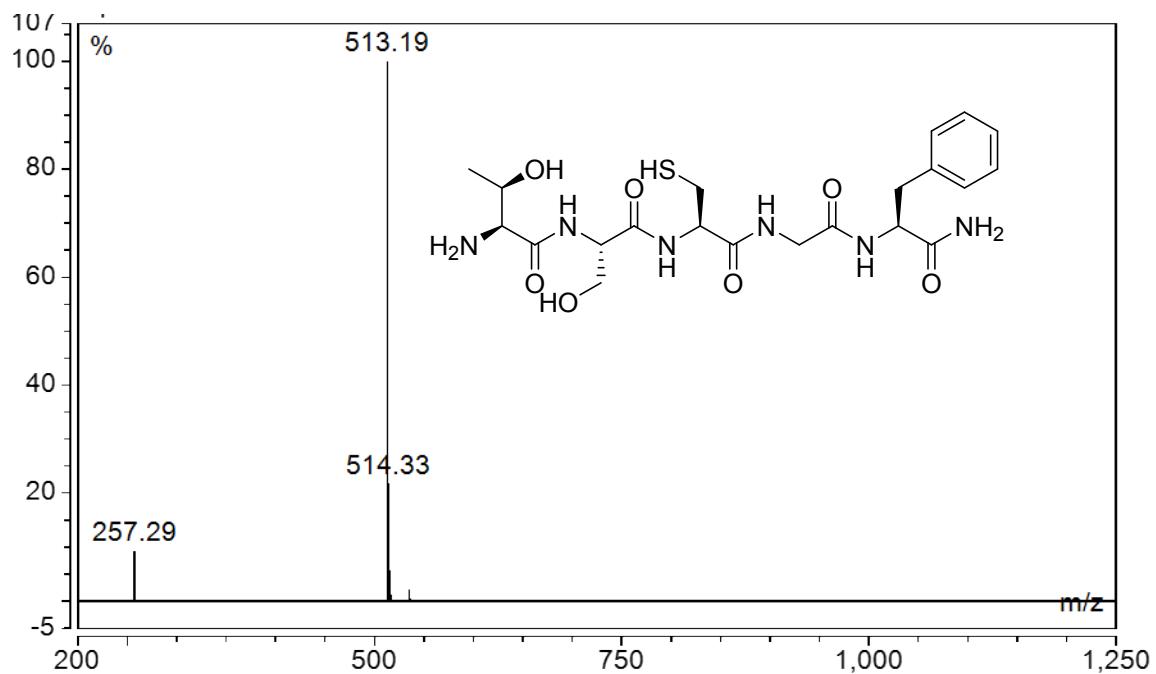


Figure S10. LCMS spectrum of **H-TSCGF-NH₂**, Calculated for C₂₁H₃₃N₆O₇S, [M+H]¹⁺ 513.58; Found: [M+H]¹⁺ = 513.19

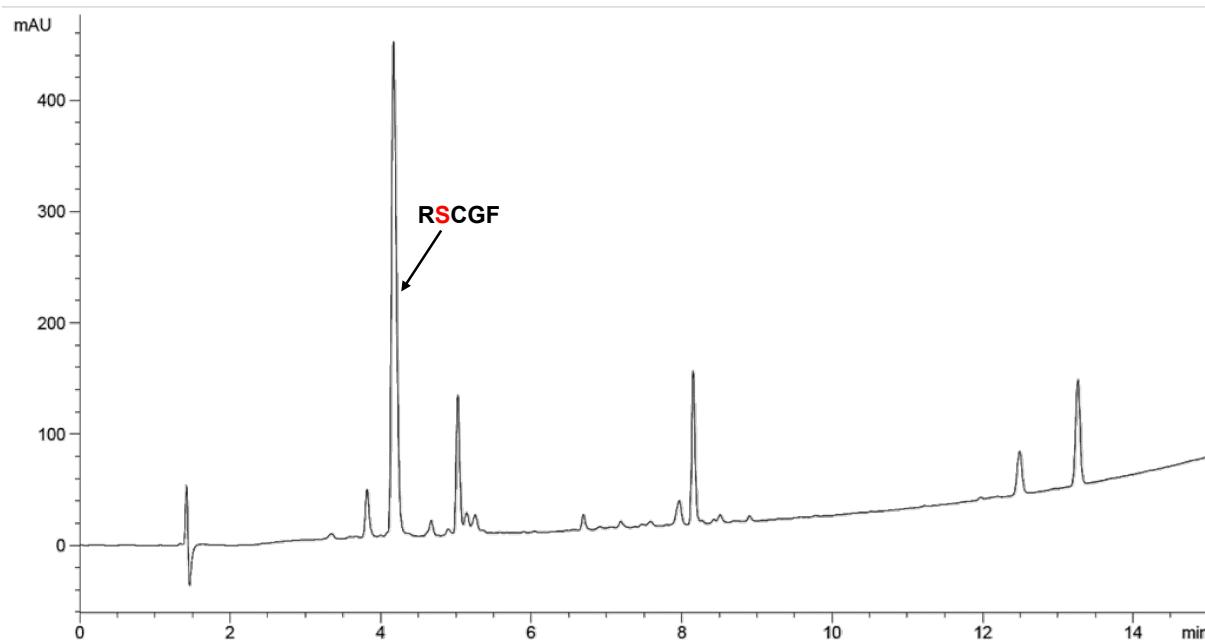


Figure S11. HPLC chromatogram of **H-RSCGF-NH₂**, 5-95% B into A

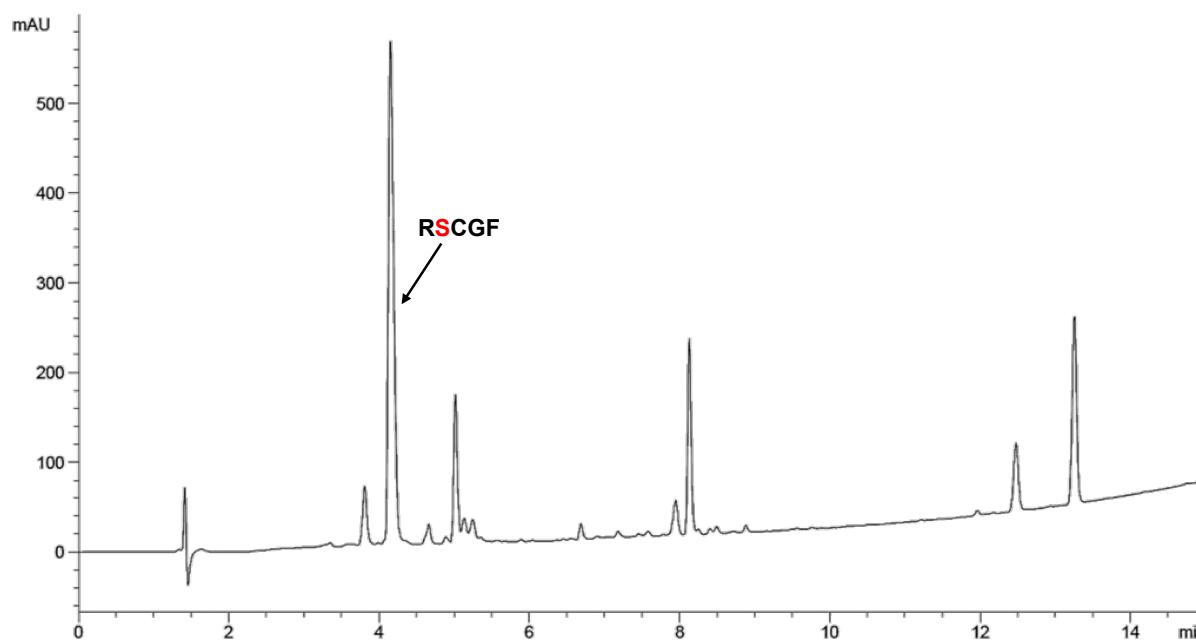


Figure S12. HPLC chromatogram of **H-RSCGF-NH₂**, Insitue-activation, 5-95% B into A

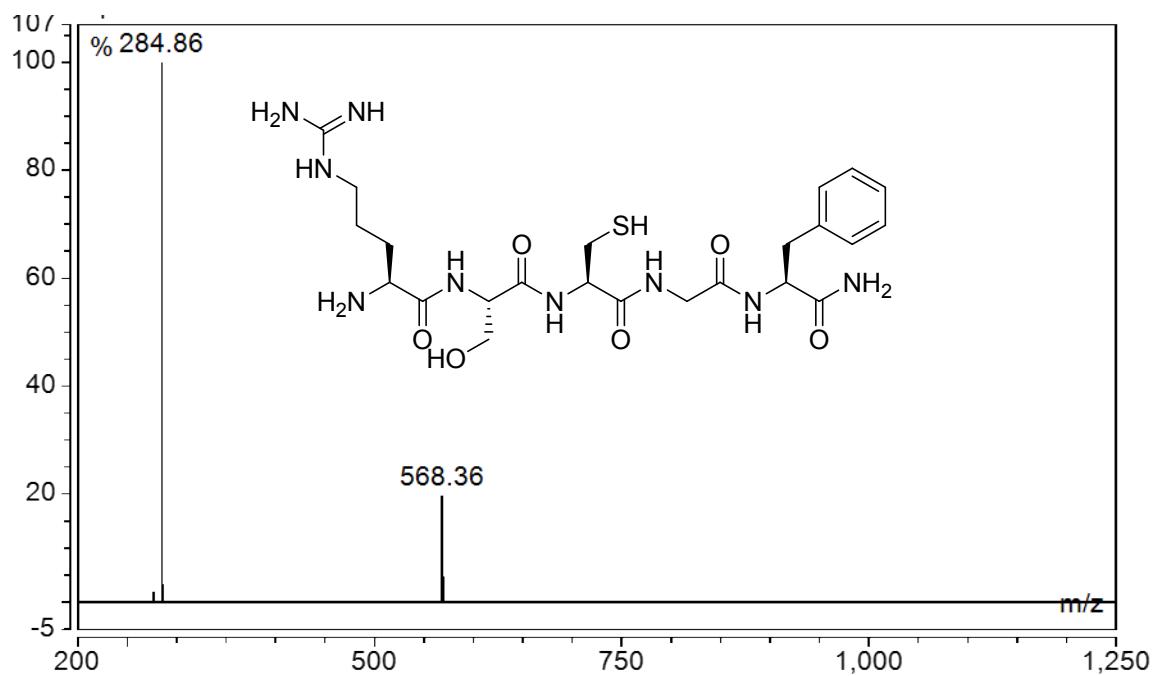


Figure S13. LCMS spectrum of **H-RSCGF-NH₂**, Calculated for C₂₃H₃₈N₉O₆S, [M+H]¹⁺ 568.66; Found: [M+H]¹⁺ = 568.36, [M+2H]²⁺ = 284.86

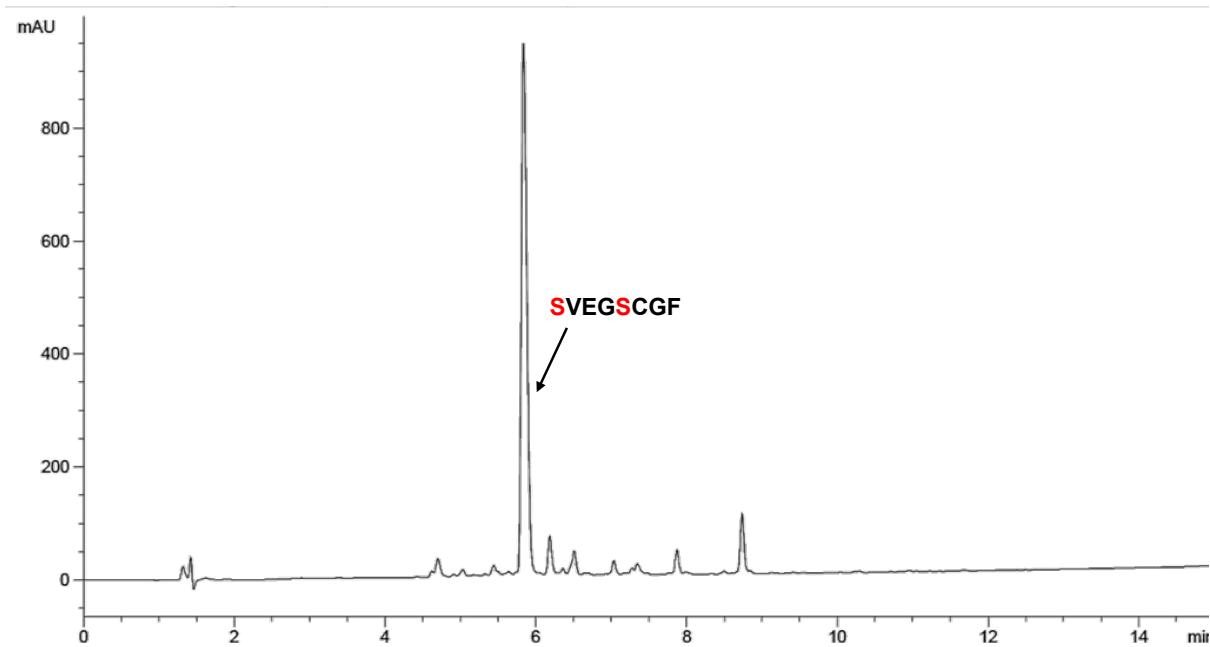


Figure S14. HPLC chromatogram of **H-SVEGSCGF-NH₂**, 5-60% B into A

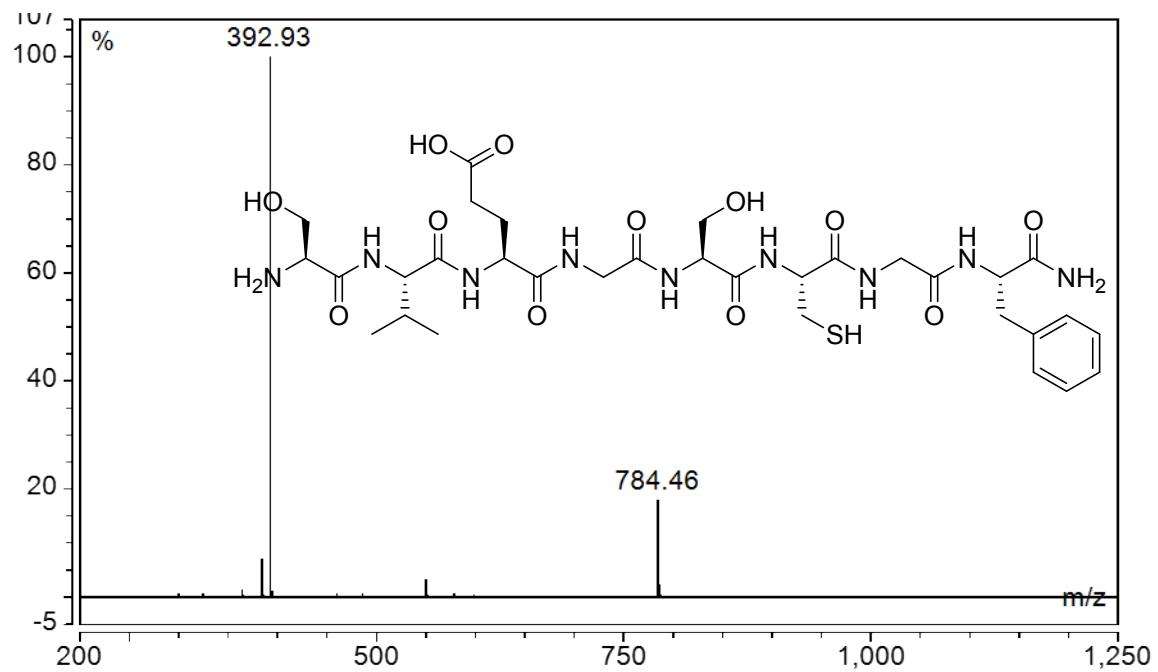


Figure S15. LCMS spectrum of **H-SVEGSCGF-NH₂**, Calculated for C₃₂H₅₀N₉O₁₂S, [M+H]¹⁺ 784.85, Found: [M+H]¹⁺ = 784.46, [M+2H]²⁺ = 392.93

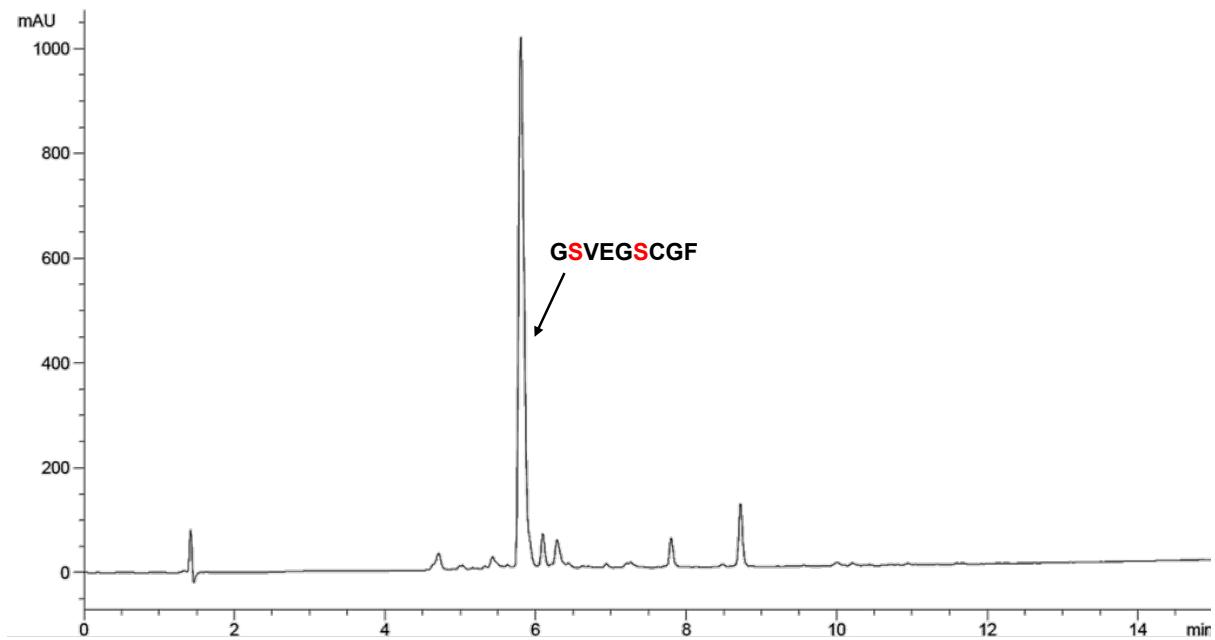


Figure S16. HPLC chromatogram of **H-GSVEGSCGF-NH₂**, 5-60% B into A

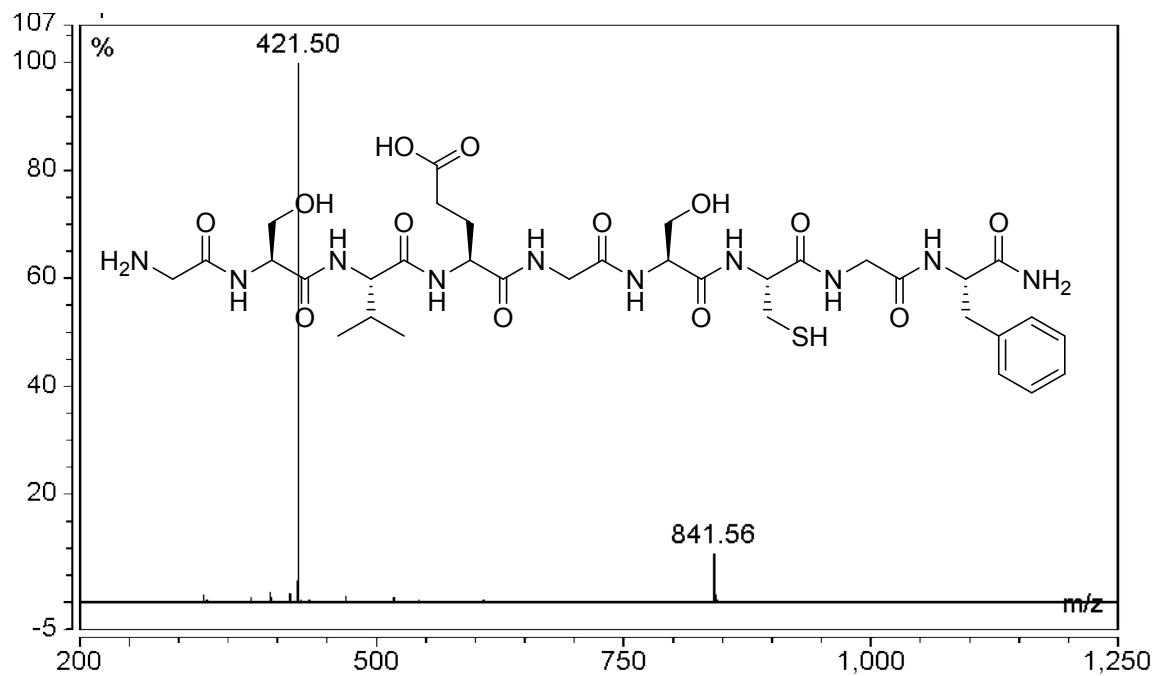


Figure S17. LCMS spectrum of **H-GSVEGSCGF-NH₂**, Calculated for C₃₄H₅₃N₁₀O₁₃S, [M+H]¹⁺ 841.90, Found: [M+H]¹⁺ = 841.56, [M+2H]²⁺ = 421.50

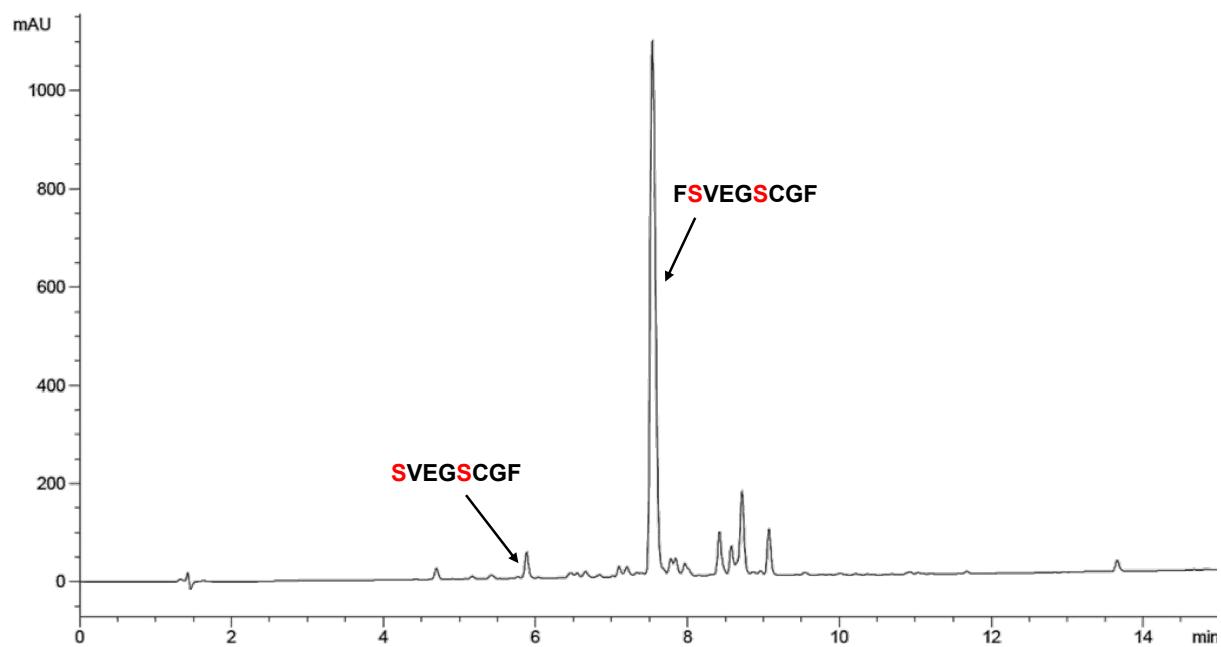


Figure S18. HPLC chromatogram of **H-FSVEGSCGF-NH₂**, 5-60% B into A

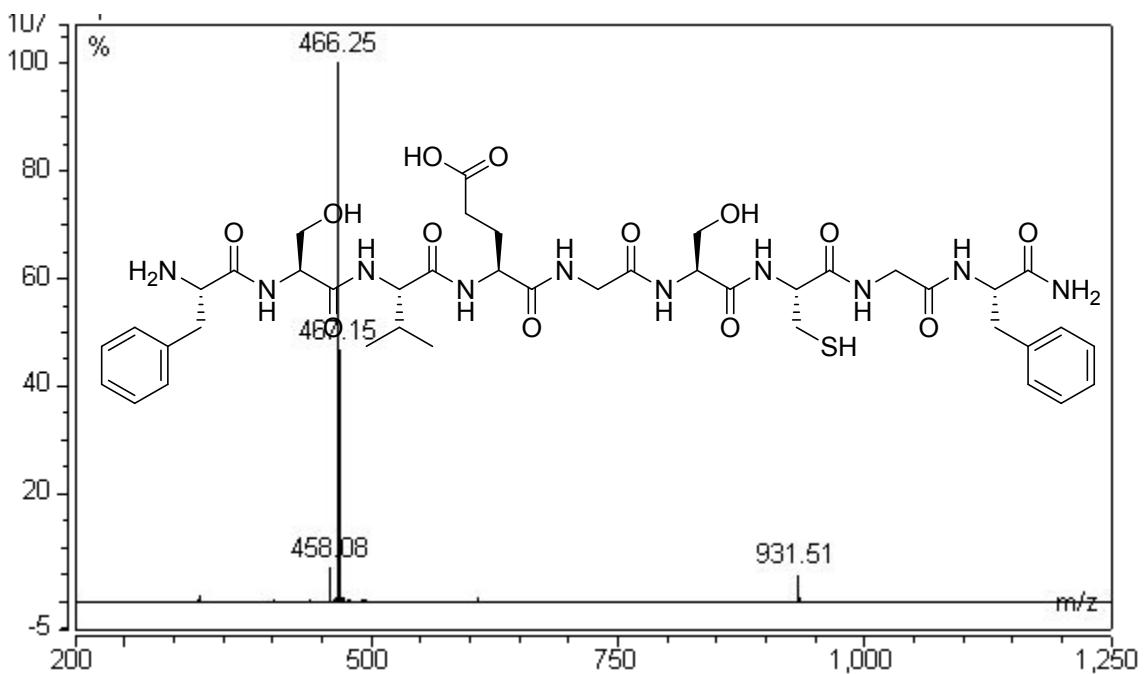


Figure S19. LCMS spectrum of **H-FSVEGS CGF-NH₂** Calculated for C₄₁H₅₉N₁₀O₁₃S
,[M+H]¹⁺ 932.03, Found: [M+H]¹⁺= 931.51, [M+2H]²⁺= 466.25

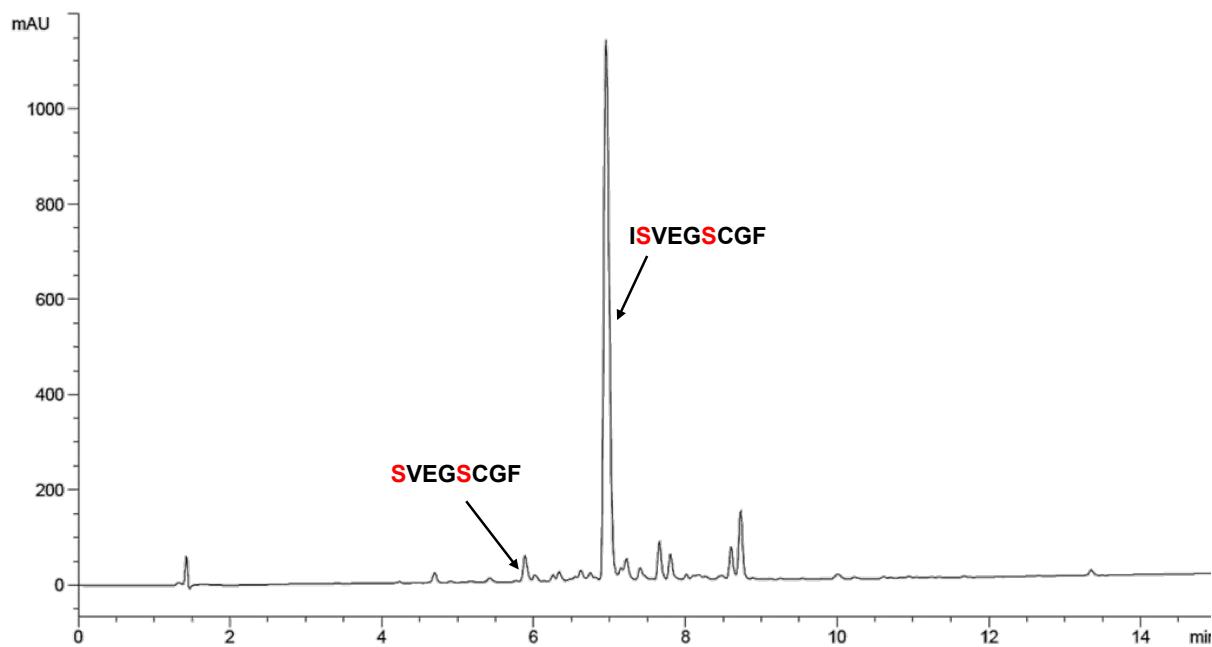


Figure S20. HPLC chromatogram of **H-ISVEGS CGF-NH₂**, 5-60% B into A

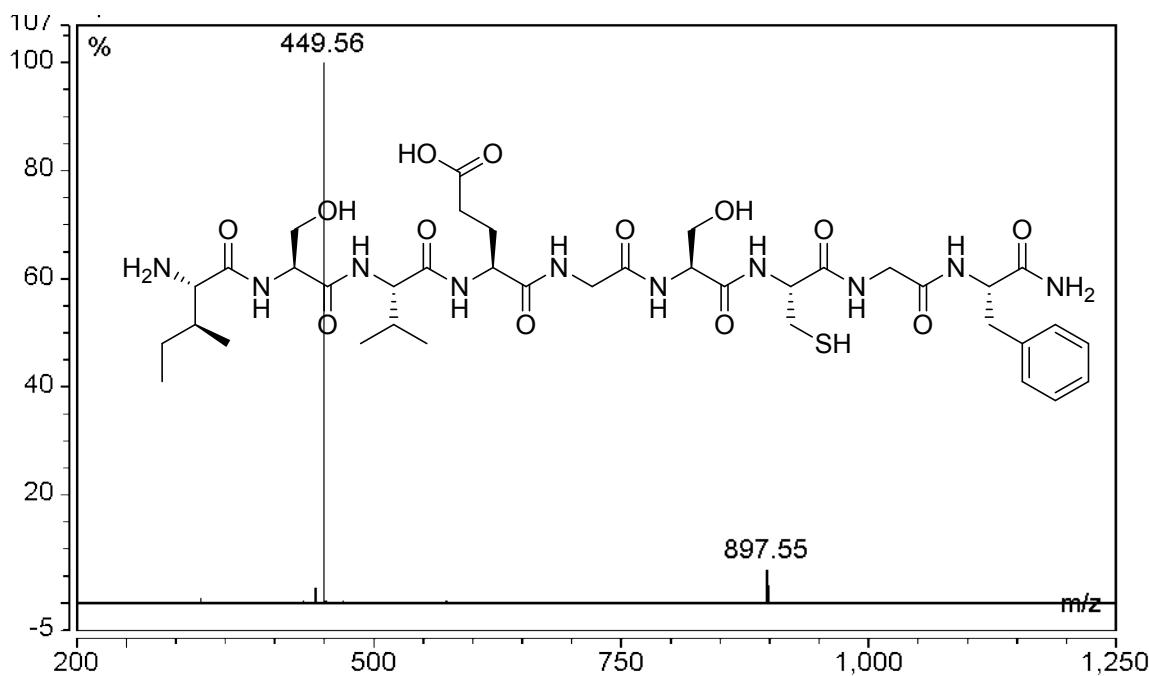


Figure S21. LCMS spectrum of **H-ISVEGS CGF-NH₂**, Calculated for C₃₈H₅₁N₁₀O₁₃S, [M+H]¹⁺ 898.01, Found: [M+H]¹⁺= 897.55, [M+2H]²⁺= 449.56

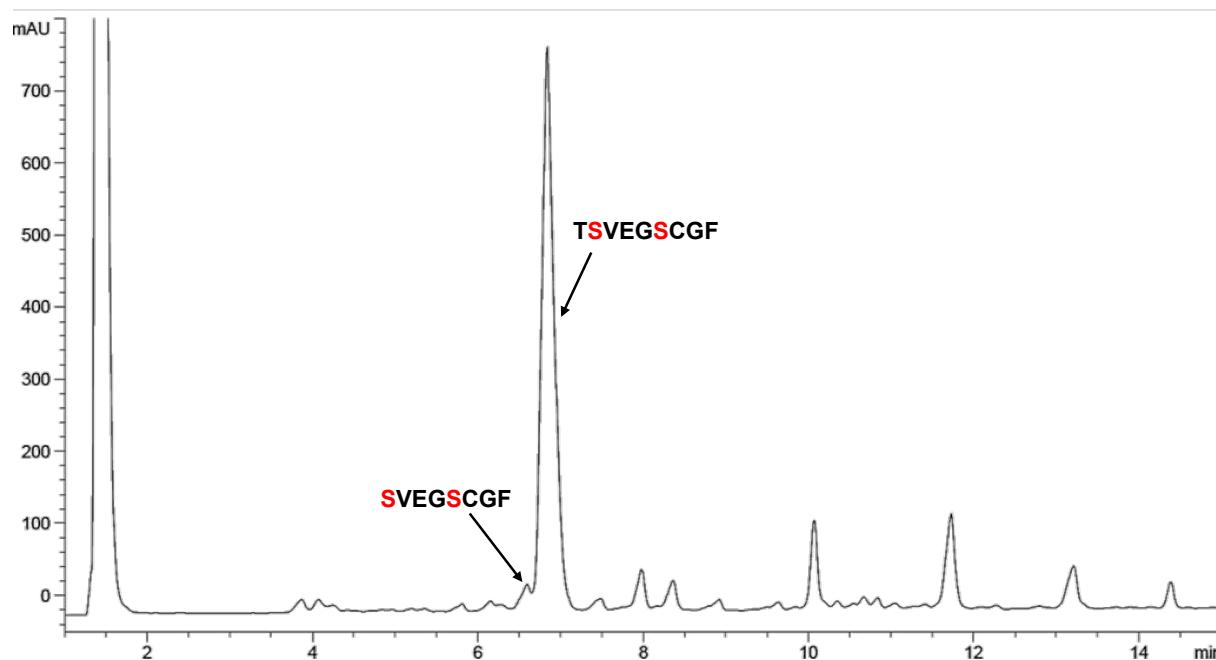


Figure S22. HPLC chromatogram of **H-TSVEGS CGF-NH₂**, 10-30% B into A

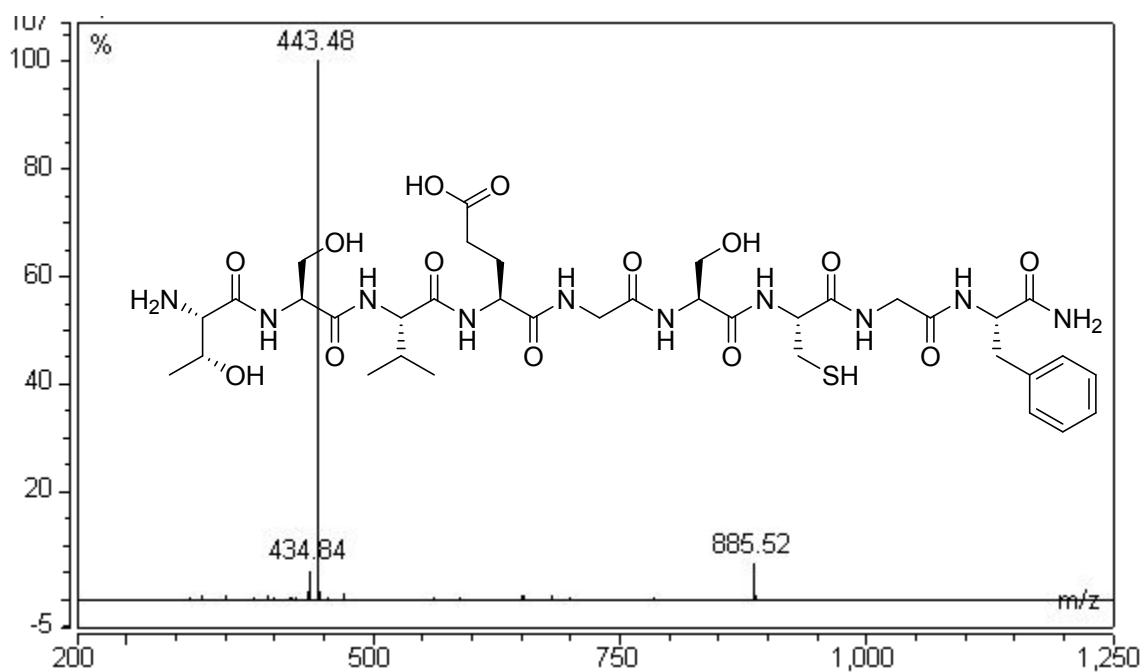


Figure S23. LCMS spectrum of **H-TSVEGS CGF-NH₂**, Calculated for C₃₅H₅₇N₁₀O₁₄S, [M+H]¹⁺ 885.96, Found: [M+H]¹⁺ = 885.52, [M+2H]²⁺ = 443.48

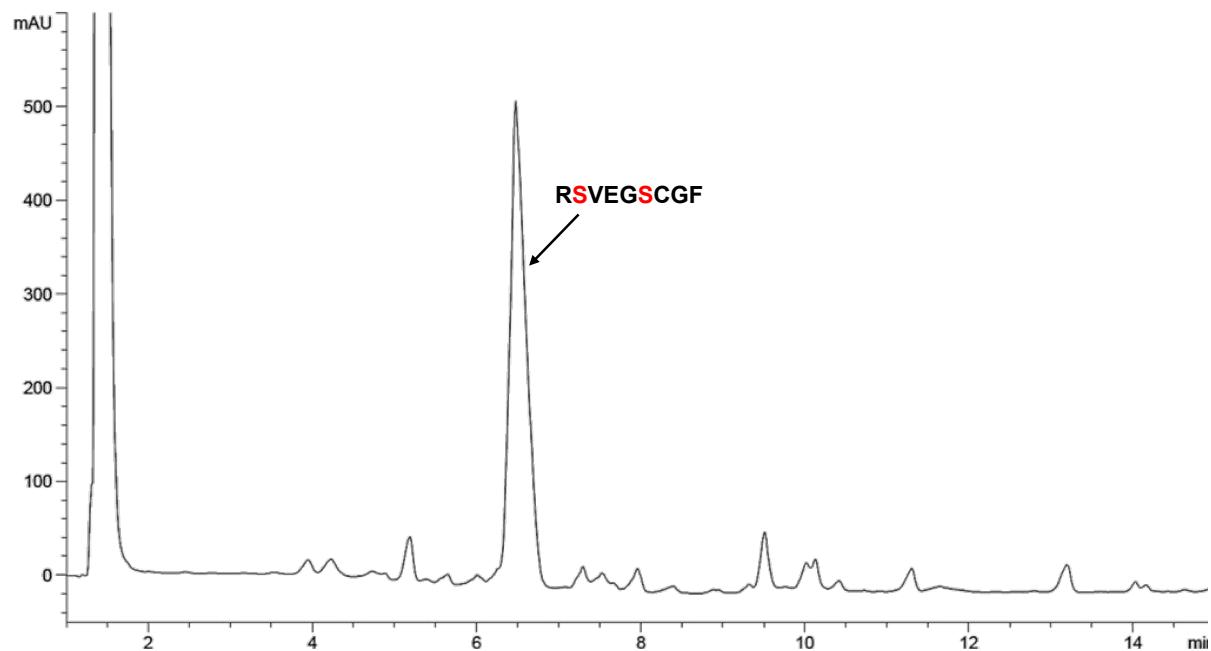


Figure S24. HPLC chromatogram of **H-RSVEGS CGF-NH₂**, 10-30% B into A

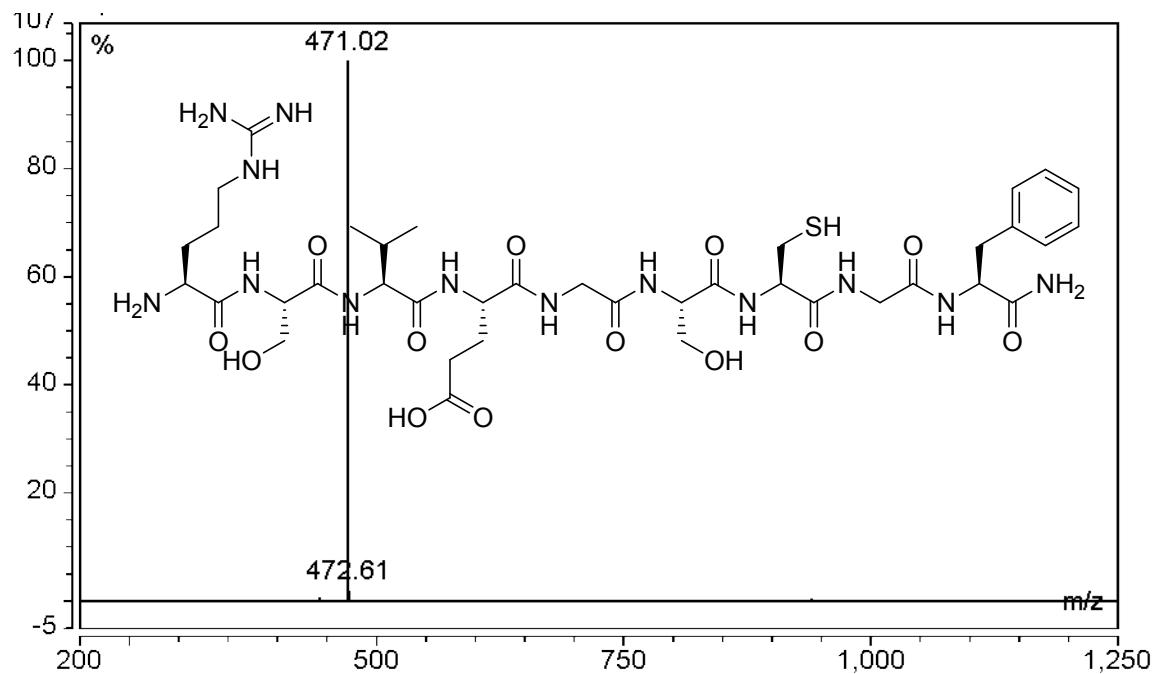


Figure S25. LCMS spectrum of **H-RSVEGSCGF-NH₂**, Calculated for $\text{C}_{41}\text{H}_{59}\text{N}_{10}\text{O}_{13}\text{S}$, $[\text{M}+\text{H}]^{1+}$ 885.96; Found: $[\text{M}+2\text{H}]^{2+}=471,02$

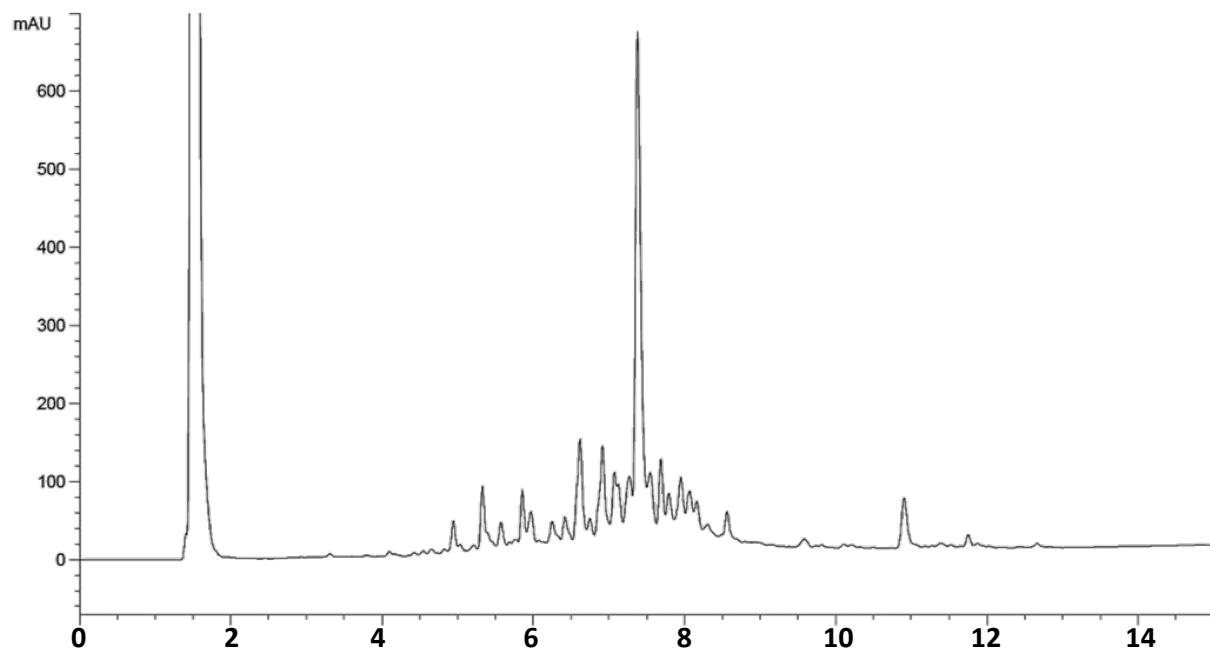


Figure S26. Crude HPLC chromatogram of linear peptide **H-YLRIVQCRSVEGSCGF-NH₂**, 15-60% B into A

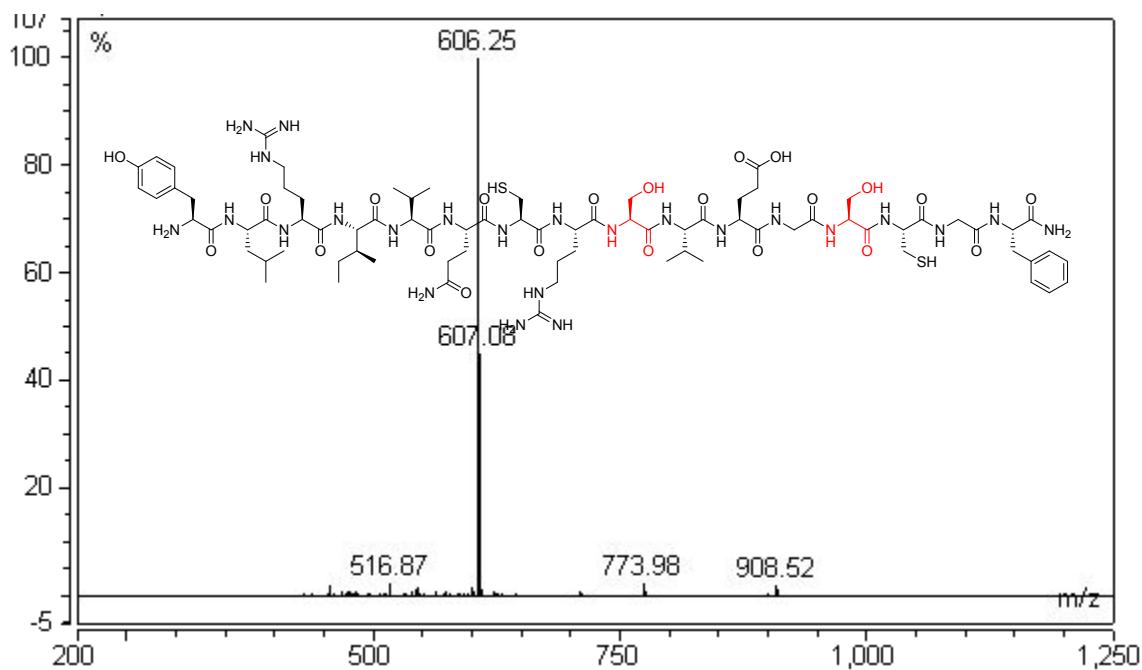


Figure S27. LCMS spectrum of **H-YLRIVQCRSVEGS CGF-NH₂** Calculated for C₇₈H₁₂₇N₂₄O₂₂S₂, [M+H]¹⁺ 1817.12; Found: [M+3H]³⁺ = 606.25

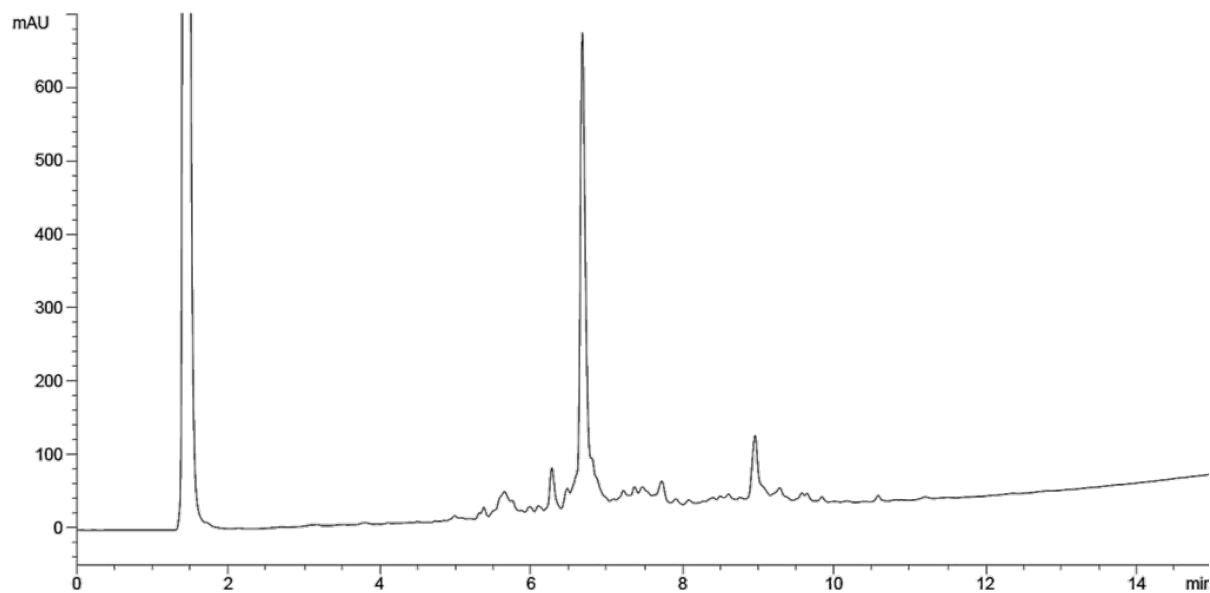


Figure S28. Crude HPLC chromatogram of linear peptide **H-YLRIVQC(SIT)RSVEGS CGF-NH₂**, 15-85% B into A

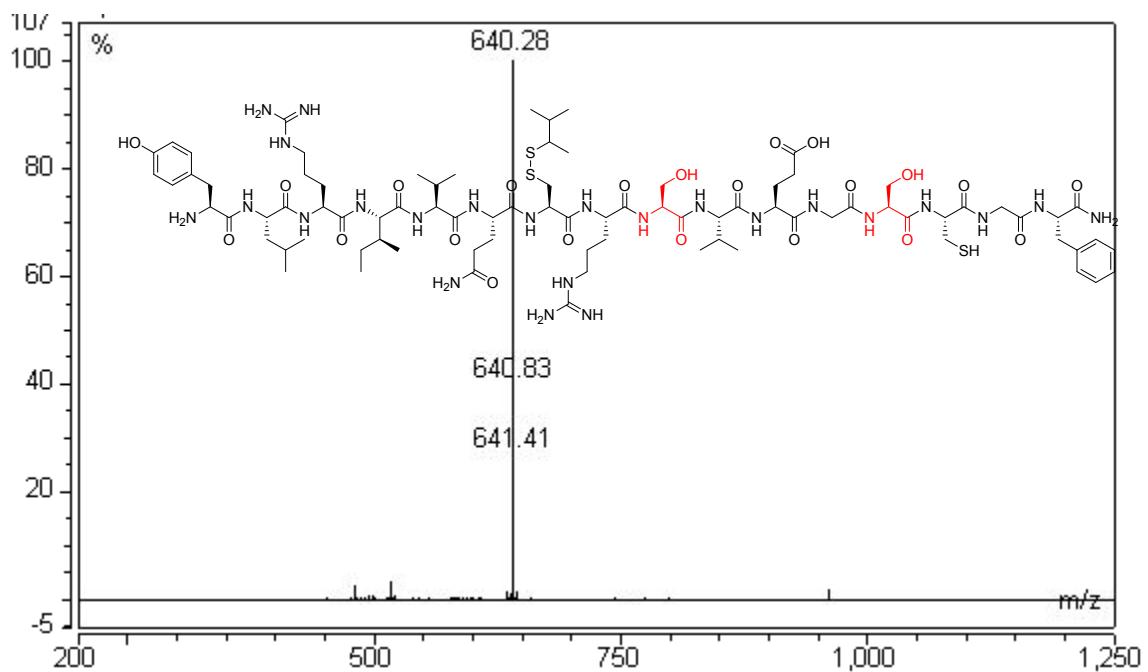


Figure S29. LCMS spectrum of **YLRIIVQC(SIT)RSVEGS CGF-NH₂** Calculated for C₈₃H₁₃₇N₂₄O₂₂S₃, [M+H]¹⁺ 1919.31; Found: [M+3H]³⁺ = 640.28

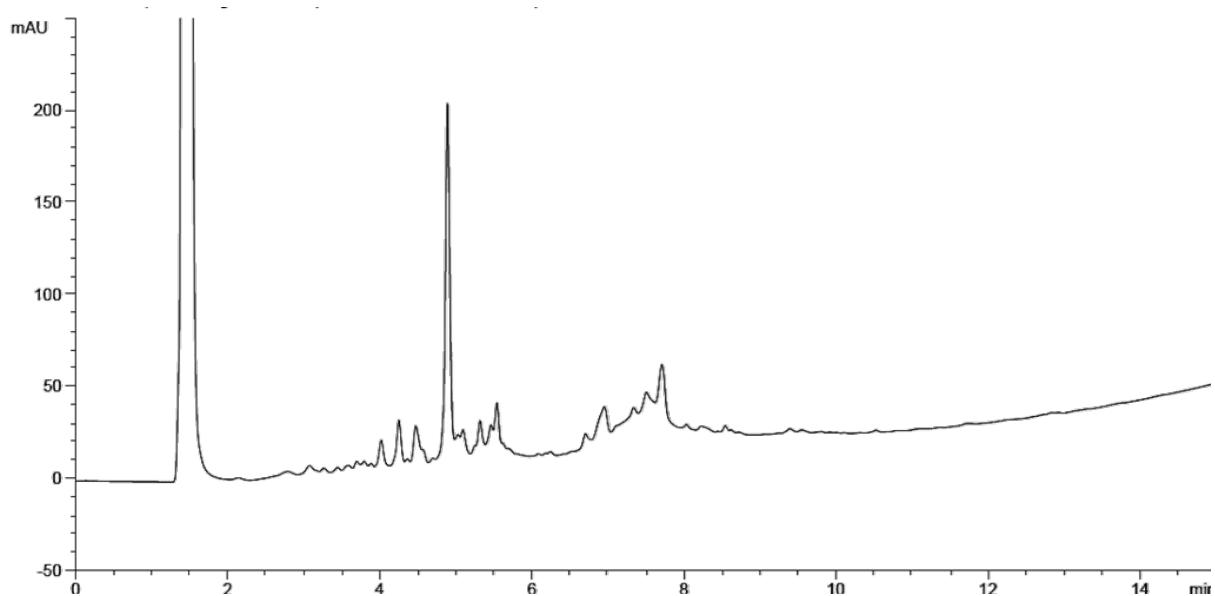


Figure S30. Crude HPLC chromatogram of cyclic peptide **H-YLRIIVQCRSVEGS CGF-NH₂**, 15-85% B into A

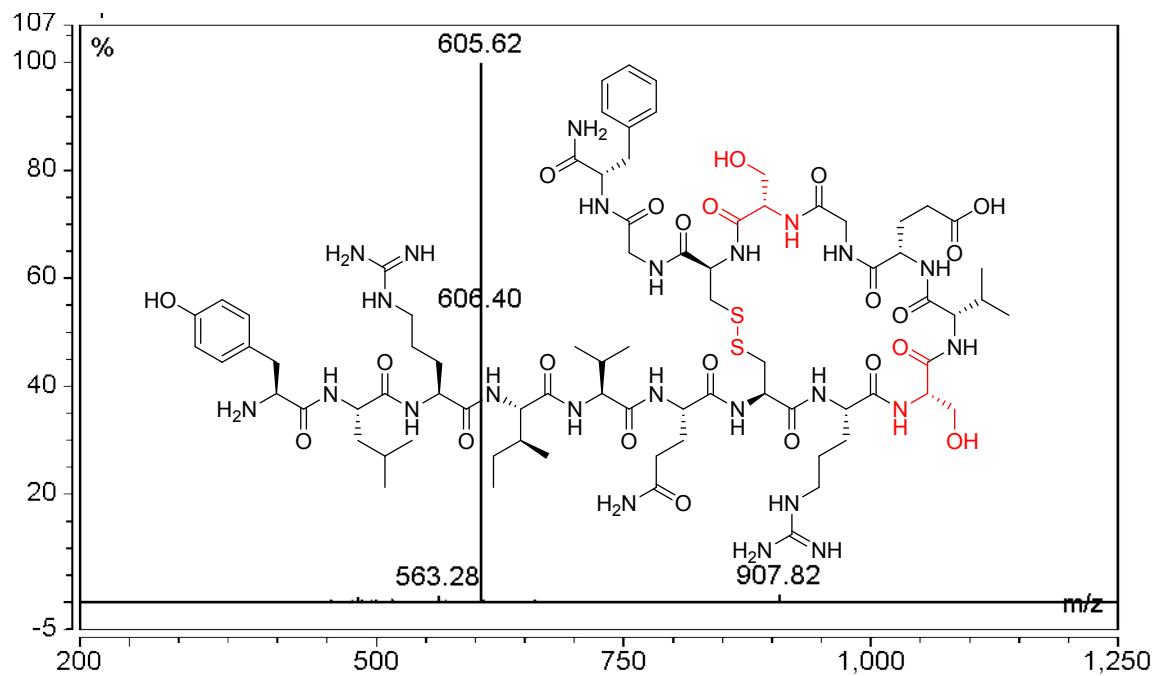


Figure S31. LCMS spectrum of cyclic peptide **H-YLRIVQCRSVEGS CGF-NH₂**,
Calculated for C₇₈H₁₂₅N₂₄O₂₂S₂, [M+H]¹⁺ 1815.10; Found: [M+3H]³⁺ = 605.62